Exploring the near-optimal spaces of energy system optimisation models using necessary conditions for better decision making

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School of Engineering
Department of Computer Science and Electrical Engineering
Team of Smart Grids

PhD Thesis

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2019-2023

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Abstract

This thesis delves into the pivotal question:

How can modelisation tools enhance decision-making processes?

In the midst of converging economic, social, and ecological crises, decision-makers are confronted with intricate choices demanding thoughtful deliberation. While tools such as mathematical programming offer a structured framework to rationalise these choices, it is imperative to refine traditional methodologies to reflect the underlying ideologies influencing these decisions. To this aim, this thesis explores the concept of near-optimal space analysis through distinct prisms. Firstly, it introduces an innovative methodology for near-optimal space exploration grounded on necessary conditions. Next, it widens the scope of near-optimal space analysis to encompass multi-objective optimisation. Lastly, it starts a reflection on the influence of model complexity on near-optimal spaces and necessary conditions. Though the proposed methodologies possess universal applicability, they are empirically tested through case studies focused on the energy transition. Notably, the European electricity grid and Belgium's entire energy system were scrutinised to extract actionable insights. Using these methods, we derived valuable decision-making insights on aspects like the minimum capacities of technologies or necessary energy from diverse sources to ensure constrained deviations from objectives such as cost and invested energy. The insights garnered accentuate the pitfalls of exclusively emphasising the optimal solution. They have also led to derive a list of promising research avenues, which encompass harmonised approaches to tackle both parametric and structural uncertainties, the quest for more efficient methods for near-optimal space analysis, and their prospective extension into multi-objective and multi-stage programming.

Résumé

Cette thèse se penche sur une question cruciale :

Comment les outils de modélisation peuvent-ils améliorer les processus de prise de décision?

Au coeur de crises économiques, sociales et écologiques, les décideurs sont confrontés à des choix complexes. Bien que des outils tels que l'optimisation mathématique offrent un cadre structuré pour rationaliser ces choix, il est impératif de perfectionner les méthodologies traditionnelles pour mieux incorporer l'idéologie sous-jacente à ces décisions. Dans cette optique, cette thèse explore l'analyse d'espaces quasi-optimaux au travers de plusieurs prismes. Tout d'abord, elle introduit une méthodologie novatrice pour l'exploration d'espaces quasi-optimaux basée sur le concept de conditions nécessaires. Ensuite, elle élargit la portée de l'analyse des espaces quasi-optimaux pour englober l'optimisation multi-objectif. Enfin, elle initie une réflexion sur l'influence de la complexité du modèle sur les espaces quasi-optimaux et les conditions nécessaires. Bien que les méthodologies proposées possèdent une applicabilité universelle, elles sont testées à travers des études de cas axées sur la transition énergétique. Notamment, le réseau électrique européen et l'ensemble du système énergétique belge ont été examinés pour en extraire des perspectives exploitables. En utilisant ces méthodes, nous avons déterminés des informations utiles à la prise de décision sur des aspects tels que les capacités minimales de technologies ou l'énergie nécessaire provenant de sources diverses pour garantir des écarts contraints par rapport à des objectifs tels que le coût et l'énergie investie. Ces informations ont mis en évidence les pièges d'une focalisation exclusive sur la solution optimale. Elles ont également conduit à définir une liste de pistes de recherche prometteuses, incluant des approches harmonisées pour aborder à la fois les incertitudes paramétriques et structurelles, la recherche de méthodes plus efficaces pour l'analyse d'espaces quasi-optimaux, et leur extension à l'optimisation multi-objectif et multi-étape.

Acknowledgements

During my thesis, my office mate Thibaut and I engaged in a recurring discussion. The subject: the first-person plural pronoun "we" in academic writing. Should it be used when the ideas presented in a paper are primarily our own? While I will not delve into the exhaustive debate surrounding this writing style (ChatGPT can make an excellent summary if you ask it the question), it is worth noting that Thibaut held reservations about its use. At the same time, other researchers in our team strongly advocated for it. Personally, I remained relatively indifferent, though I made an effort to avoid excessive use of the pronoun and occasionally restructured sentences in the passive voice. However, in this thesis, we have chosen to employ "we" to acknowledge the collaborative nature of the work undertaken over the past four and a half years. These collaborations have been professional but primarily human. Therefore, I want to acknowledge all the people I have met along this journey and who made it an unforgettable experience.

In ((very) approximate) order of appearance[1]:

Virginie Petit, forever supporter and first domino. I want to start by thanking my long-time partner and (recent) wife. Since the beginning of the thesis and long before that, she has been bearing with me, putting up with my long work hours (paid against in extended and recurrent massages). However, she is more than just a supporter in this long journey. She is the reason I am writing this thesis. One beautiful day in June 2016, while studying and letting my computer open, she had the brilliant idea of opening my Facebook account and posting the following message: "Pendant la bloque, je débloque." (which could translate something to "During the exams, I decamp"). This was the day before the "Sustainable Energy" exam. One thing led to another: the professor and social network aficionados teaching this class commented on the post ("But Antoine, my exam is not difficult, is it?"), contacted me after the exam and hired me as a research student. This chain of events would partly push me to contact him four years later to start my PhD. Some say "Take your destiny in your own hands." I must thank my wife for taking mine in hers.

[1] not (necessarily) correlated to the importance of the person

Damien Ernst, a unique advisor. Everyone agrees - Damien is one of a kind. And that is what makes him such a special advisor. We have shared some unusual experiences, like the time he hired me through Facebook or when we had a late-night chat about politics and journalism over a few drinks. We should neither forget the photo we took together that got a thousand likes on Facebook and LinkedIn. Not many people can say they have had these experiences with their advisors. Beyond all that, I want to thank Damien for his professional support. While busy with many activities, he always found time to share research ideas and work on articles with me. He trusted me enough to let me manage his energy market class, and for that, I am grateful. Another big thank you goes to Damien for his openness to different ideas. We do not always agree, but he never made me feel less for it. He is always ready to discuss different points of view, even though he sometimes teases me, calling me the “bobo-ecolo-décroissant". Lastly, I need to mention Damien’s positive energy. No matter how long the hours or how challenging the situation is, he keeps his spirits up and always finds something to laugh about. I have learned a lot from Damien over these last four years. I hope he feels the same way about our time together.

Louis Wehenkel, inspiring source of advice. Pr Louis Wehenkel has been a key figure in kick-starting my research career. He was my supervisor during my master’s, but his role went beyond that. I am thankful to Louis for the opportunities he created. He helped me establish the first Erasmus exchange program between Liège and Aalto University in Finland. A year later, he opened up the world of robotics by introducing me to the QUT Center for Robotics. But, what I am most grateful for is his guidance. When I was considering a PhD and when I was lost mid-way through, Louis was my go-to person. His advice was invaluable, helping me navigate the uncertainties and make the right decisions.

Antoine Wehenkel, my first research collaborator. After acknowledging the father, it is only fitting to recognise the son. Antoine may not have been the first person I interacted with during my PhD, but he holds a special place as the first person with whom I ever conducted research. Our paths crossed when we were both working for Damien at the end of our bachelor’s degree, and I had the good fortune to collaborate with him on most of my master’s projects. I want to thank Antoine for that experience and for setting an example with his admirable professionalism (and for giving me the inspiration for the structure of some of these thesis chapters).

Raphaël Fonteneau, the steadfast collaborator. Before wrapping up my shout-outs to pre-PhD collaborators, I must mention Raphaël. As one of the most experienced folks in Damien’s team, he has been around the block a few times and has some stories to tell. From the start of our research adventure, Raphaël was there, offering guidance. Here is a big thanks to him for always being ready with handy advice and sparking thought-provoking discussions.

Théate Thibaut, one of the office's COPAIN. Starting a new job is always filled with expectations. Among them is the hope of being welcomed by your peers, particularly those sharing your office space. I can happily say my experience exceeded my expectations when I met two fantastic office partners, Thibaut and Yves. While Thibaut was a familiar name from our shared engineering studies, we did not know each other well. Over these four years, I have come to know Thibaut as a meticulous worker with a solid work ethic, a collaborative colleague with whom I have worked on various courses, and a friend with whom I have had endless inspired discussions. Our talks spanned from energy and climate to education, research, and countless other intriguing subjects. Yes, these conversations may have borrowed some hours from our workday, but they were worth every minute. Sharing an office with you these past four years has been a true pleasure, Thibaut. I hope our paths intersect again in the future.

Yves Vanaubel, the other office's COPAIN. When I first landed at the university for my PhD, I found myself sharing a desk with a tall, red-headed, bespectacled guy. My first impression of him might not have been the warmest, but as it turned out, he became one of the most entertaining workmates I have had. Yves, you workaholic, your classic “What time do you call this?" and “Leaving already?" became part of our daily routine. Not to mention your affinity for 80s music despite being a 30-something and our impromptu “chair dances" – memories I will cherish. A big thank you for deeming Thibaut and me worthy of an invite to your wedding (even if we ended up with other folks' name tags). Your presence always made the office a brighter place, and when you moved on with the rest of the BLA team after the COVID-induced separation, you left a void that was not easy to fill.

The BLA (or Smash Bross) team. If you have ever wandered around Montefiore's building, specifically on the ground floor near room R137 (better known as my office), you may have heard a raucous mix of cheers, shouts, and occasionally, some choice words not typically associated with a work environment. The culprit? A seemingly innocent game, Super Smash Bros, and a group of enthusiastic, not-so-subtle gamers. This lively crew included not only the occupants of office R137, housing the beloved game console but also the extended family of the BLA team, featuring: **Elodie Burtin**, the sole female warrior of the group; **Jordan Taelman**, whose coffee addiction fueled his gaming prowess; **Thibaut Capuano**, aka the “other" Thibaut; **Quentin Geminne**, the fearless leader and loudest cheerleader; **Michaël Castronovo**, the covert operative from BLA; **Julien Confetti**, the person I hate the most (and Ju, I know it goes both ways); and let us not forget the dedicated interns **Marc-Olivier Metais** and **Maxime Fatoux**. I want to extend a heartfelt thank you to the entire team. Your high-energy gaming sessions transformed countless hours into entertaining ones and honed my skills to reach pro gamer status. Moreover, the vibrant atmosphere you fostered made Montefiore's ground offices a genuinely unique and enjoyable workplace.

David Radu and Mathias Berger, the inseparable duo. Having acknowledged my office comrades, it is time I shift my focus to those I actively collaborated with. I returned to the university in mid-June, diving headfirst into the energy domain – a field I knew little about – and was tasked with a project that required skills I had yet to acquire. I vividly recall my first day back when, after a brief chat with Damien, he ushered me into David's office. That was when I met my future co-author for the first time. David, your patience was commendable as you took the time to explain and re-explain the project you were working on and how I could lend a hand. Soon after, I was introduced to Mathias, the "maths boy" of our team. I am immensely thankful to you both for welcoming me into your dynamic duo. Your guidance eased my transition into research and was instrumental in navigating the initial two years of my thesis. A special mention goes to our memorable trip to Berlin just before the onset of COVID-19 – a journey I wish we could have replicated more often. I remain appreciative of the camaraderie and learning opportunities our time together provided.

We have now to introduce three officers. Three comrades-in-arms who have shared the hard work of establishing our stronghold at the Golden Eagle, who have generated considerable amounts of repetitive jokes quoting a famous French secret agent, who are also fighting the battle against ecological decay, and who stand as formidable forces in work and research, proving themselves to be true warriors in the battlefield of academia.

Jonathan Dumas, the General. When I started my PhD on the ground floor, Jonathan was the neighbour just next door. I remember that our first conversation revolved around energy markets as I sought help to comprehend their intricate dynamics. However, it was not long before Jonathan led me on a journey that would shape the bulk of my PhD experience. I cannot pinpoint the exact catalyst - perhaps our participation in the Sustainability Development program, the eye-opening "Or noir" book recommendation, or my enlistment into The Shifters. Regardless, I found myself on an eco-conscious path that demanded countless hours but bestowed upon me invaluable human experiences. I vividly recall our first day at the Sustainability Development program, crammed in your office with Thibaut, amusing ourselves by stirring up the online chat. Reading Matthieu Auzanneau's work brought a profound revelation - alongside the pressing ecological crisis, a colossal energy crisis was also on the horizon. This understanding fundamentally shifted my perspective. Our initial dinner at your place was another pivotal event. It was the day we watched my first "mensuelle", sparking my involvement in the Education4Climate project. I still hear your enthusiastic response when I suggested, "Oh, Python? I could handle that." With an immediate "Oh yeah, let's go!", the journey began. Not to mention the countless roles you have helped me embrace, such as facilitating the Climate Fresk, the Digital Fresk, and the establishment of the Coconut Shakers. This group was conceived as an embodiment of our lengthy discussions about the potential improvements we could bring to our faculty and the university. Our debates often took place over morning coffee, shared in the quiet of the office before anyone else arrived (including your recurring joke of hiding under your desk whenever I knocked on your door). At other times, we would deliberate into the night, perhaps after a gruelling PhD Trail, Beer Lovers Marathon, or over rum at your place. Your influence also set the stage for a magnificent collaboration with UCLouvain, which resulted in the publication of two articles. In both these works, I had the pleasure of being your co-author. You were the one who introduced me to the wealth of training programs offered by the university, leading me to master the art of presenting my thesis in a mere 180 seconds. Regarding my academic journey, if Virginie was the ignition for my PhD, you were undoubtedly the fuel that propelled me to its completion. You provided unwavering support and advice during a challenging second year when I was unsure if I could persevere. Jonathan, thank you for your boundless energy, for inspiring me to push my limits, and for teaching me never to hesitate to take the plunge. You have been the closest thing to a mentor, and I consider you one of the most valuable friendships I have forged this past year.

François Rigo, the Marshall. The second person in this trio is not made like you and me. A man who can party till dawn and then cycle 150 km at eight in the morning. A fellow who has a closet full of costumes ready to brighten up any gathering. A buddy who always says yes, even when prudence might suggest otherwise. An exceptional researcher who may still be ironing out the wrinkles in his thesis even as I submit mine. This person is none other than the Marshall, better known as François Rigo(lo). François, thank you for all the stolen coffees from your supervisor's stash. Also, for your involvement in the Climate Fresk (giving me the idea to host one at my old secondary school) and your dedication as a fellow member of The Shifters in Liège (the only one sticking with me through the "mensuelles" and accompanying me to a market where nobody came for ten hours). Last but certainly not least, a big thank you for introducing us to the concept of the beer bike, for organising a grand beer pong during the PhD Trail, for making us run our first marathon while drinking beer, and, of course, for hosting memorable parties at your place. These make the special moments that keep us going through a thesis.

Adrien Bolland, the Lieutenant-Colonel (former grenadier-voltigeur). Third in line is the youngest of the trio, but by no means the least courageous: Adrien Bolland. I recall vividly our initial introduction, which took place online. In the throes of the Covid era, I was half-listening to a Fluxys meeting from my grandmother's home. My laptop open on the table, my attention was divided, awaiting a signal for my involvement. Arrived the moment when Damien mentioned a new team member (you guessed it, Adrien) set to present his master's work. From then on, I knew my focus on the meeting was no longer needed. Though this humorous encounter marked our first interaction, it was far from our last. Despite my continued lack of comprehension concerning Adrien's work, we shared countless unforgettable moments. Our bond took a significant leap during our joint participation in CliMACTES and has remained unflinching ever since. While we never found the time to co-author an article (an oversight likely on my part, given Adrien's extensive collaborative writing with nearly everyone in the building), our joint work on the energy market class was rewarding, as he tackled all the dirty math stuff and was the best scarecrow for the students. Whether it is work, breaks, or beers, Adrien's reliable presence is a constant. Adrien, thank you for being the person you are – a genuine, caring friend who never fails to bring a smile to my face each time you (literally) jump through the door to say hi.

The Montefiore Institute is a constant world of change. People come, and people go. When I arrived, a lot of colleagues were already there. I want to express my heartfelt gratitude for their shared moments, advice, and experiences. A big thank you to every individual I have had the chance to share a midday break with, exchange a brief conversation with, or even share a simple morning greeting as we crossed paths in the corridors.

While it is impossible for me to recount every remarkable moment we have shared, I want to tell a few that I hold dear. **Xavier Adriaens** and **Julien Dular**, thank you for the unforgettable after-party at RUDay 2022. Thank you **Gauthier Gain** for setting the mood with your music at every FACSA party. **Vân Anh Huynh-Thu**, thank you for your joyful presence and the unforgettable experiences under Tilff's bridge during two consecutive Beer Lovers Marathons. **Adrien Deliège**, your dedication motivated me to take part in the MT180 competition. Thank you for being that spark of inspiration. **Gilles Chaspierre**, although I initially declined your invitation to present at RUDay 2019, I learned a significant lesson from the experience when I eventually organised it myself. Thank you **Gabriel Digregorio** for joining me on this journey and for your unique blind test ideas. The same goes for **Efthymios Karangelos** for its live animation at this event. **Isabelle Mainz**, thank you for the support in providing the necessary materials for my first-ever Logic class as a PhD student. It did not go unnoticed. **Ioannis Boukas**, thank you for the seamless transition of the energy market class. To **Miguel Manuel de Villena Millan**, the master of servers, thank you for allowing me to harness the power of Zeus. **Daniele Marulli**, thank you for navigating through the FRIA application process with me. **François Van Lishout**, you gave me the opportunity to consistently remind everyone of my small contribution to Montefiore's surveillance system; for that, I thank you. **Laurine Duchesne**, your empathetic listening during difficult times provided the support I will not forget. Finally, thank you **Sébastien Mathieu**, **Romain Mormont**, **Jean-Michel Begon**, **Raphaël Marée**, **Nicolas Vecoven**, **Antonio Sutera**, **Samy Aittahar**, **Michaël Fonder**, **Anaïs Halin**, **Anthony Cioppa**, **Loic Sacré** and **Tom Ewbank** for the moments and discussions we shared.

Pascal Leroy, the Godfather. I first crossed paths with Pascal during my bachelor's under the ritual known as the "baptême". He was one of my godfathers. Then, despite being slightly my senior, his passion for academia had him linger, allowing us to share several classes. Our paths continued to cross when we both decided to join Damien's team for a PhD. And finally, while Thibaut blazed a trail ahead with the writing of his thesis, Pascal, with a kind heart, chose to endure this challenging journey alongside his old "bleu". Pascal, throughout the years, you have always had this radiant, unaltered positivity, and your presence and your sense of humour invariably uplifts the mood. Whether inside or outside the university, our interactions have always been pleasurable. I am grateful to have walked along the same paths as you, and I eagerly anticipate the many crossings our futures might hold.

Inside this old building, there is also a group of unalterable, fixed figures that have haunted the classrooms and the hallways for several years and will for another eternity. They are called professors.

I would first like to extend my gratitude to those professors who shared their lunch breaks with us. This opportunity for casual interaction and dialogue is not a common privilege across all faculties or departments, making it a uniquely enriching aspect of our community. Among the unfailing midday participants is **Gilles Louppe**. I owe a special thanks to the one who might have been my promoter - which would have made my PhD completely different - if I had been less undecided when we called each other in Australia. Gilles, thank you for contributing your positive energy and deep expertise to our department. Please accept my apologies for the numerous times I inadvertently disrupted your discussions with Arnaud when you were tucked away behind his door. Equally consistent in attendance is **Pierre Geurts**. Having previously collaborated with Pierre during my studies, I found it highly rewarding to once again team up with him for the preparation of this year's RUDay. Next in line regarding lunchtime presence is **Bertrand Cornélusse**. While I hold all our professors in high regard, the level of societal engagement can sometimes leave something to be desired. Yet, Bertrand proves to be the exception. Our interactions and your actions make it clear that you are deeply committed to addressing climate and energy challenges. This dedication not only inspires me but also gives me hope for what lies ahead. I also want to express my gratitude for the countless cups of coffee I have "borrowed" from your machine, fuelling numerous discussions and research ideas. Another occasional participant at our midday gatherings is **Quentin Louveaux**. I want to thank him for agreeing to be a part of my thesis committee. Lastly, a heartfelt thanks to **Laurent Mathy**, whose distinctive presence always lends a unique touch to our midday gatherings.

Pierre Sacré, the Experimenter. Among the faculty, a singularly heartfelt thank you goes out to Pierre. Over three adventurous years, assisting you in steering the vessels

that are the Probability and Statistics classes was a unique and enriching experience. I deeply appreciate your entrusting me with this responsibility, particularly your openness and encouragement as I experimented with new teaching methodologies.

Let us conclude this section by acknowledging the mentors of the department. Firstly, **Benoit Vanderheyden**, affectionately known as “le chef". Your drive and enthusiasm were pivotal in organising the RUDay events these past two years. Secondly, **Philippe Vanderbemden**, universally recognised for your exceptional teaching skills and, equally important, for your genuine kindness and warm demeanour. Lastly, **Guy Leduc**, as the department head, you entrusted me with my first teaching assistant role, granting me the chance to delve into the world of academia. To each one of you - Benoit, Philippe, and Guy - I express my deepest gratitude.

Within Montefiore, there resides another unwavering group without whom the institute simply would not function. Known as the PATO, they are the unsung heroes essential to our daily operations.

A special thanks to **Marc Frédéric** for the times he has come to our rescue to fix various IT issues. To **Eric Vangenechten**, I extend my gratitude for accommodating all our unusual and sometimes peculiar requests. **Denis Bourguignon**, our vigilant guardian, keeps the building safe and secure. Last but not least, thank you to **Sophie Cimino**, especially for your central role in the organisation of Research Unit Day. Without her dedication, determination, and incredible efficiency, this recurring event would not be possible.

I embarked on my PhD journey in June 2019, and over the ensuing four-plus years, many new faces have crossed my academic path. They have filled the void left by those who preceded them, constantly rejuvenating the offices with fresh energy and novel perspectives. In the lines that follow, I wish to express my heartfelt thanks to all of these individuals, each of whom has uniquely contributed to making these four years not only productive but incredibly enjoyable. To remain faithful to the timeline, I have tried to list them by order of appearance. (PS: If you find yourself out of place, it is your own fault; you should have kept your LinkedIn profile updated.)

2019

Having begun my journey in June, a few comrades managed to join in during the six months that led us to the close of that year. Among them, some, such as **Sami Ben Mariem**, took advantage of my gap year to bridge the distance with me. Thank you, Sami, for your positive energy and for treating us to that fantastic restaurant after the 24-hour Televie. The same goes for **Vincent Schmitz**. Even though you are not from Montefiore, your good vibes are always appreciated.

A special shout out also to **Kathleen Jacquerie**, who, just like me, took some time to set up base in Montefiore for a PhD thesis. Kathleen, thank you for your dedication in every part of your work, be it research or teaching, for the energy and cohesion you brought to your nascent lab, and for your involvement in numerous projects outside the scope of your research. You are a very inspiring person; I do not doubt that you are destined for remarkable research achievements.

2020

In the bustling battlegrounds of the modern-day office, a legendary rivalry brews with intensity and steams with controversy. A war so decisive it has divided break rooms and polarised water coolers across the land. It is the battle between Coffee and Tea. In this war, I found an ally who knows how to play both sides: Mister **Arnaud Delaunoy**. Arnaud, thanks for all the tea I swiped from your office, always promising to replace it and never doing so. Your continued acceptance of me, despite this downright treachery, deserves a medal or something. I hope I made up for some of it by backing you up during those tough internship times. Besides tea theft, we have had some great chats over that very tea about work and life. I will not soon forget (and neither will Adrien) how you wreaked havoc on our Smash Bros battles with your maddening Zelda gameplay. We also have had some excellent times sharing wine at stationary tables and beers at moving ones. Thank you for all these moments.

Arnaud, while I have many thanks for you, there is one act that broke my heart, for which I simply cannot thank you: your allegiance to the infamous card table at lunch. That is right, the wrong table! And I cannot help but suspect the dark influencer who lured you there: **Renaud Vandeghen**. Renaud, you might be a great colleague, and our chats have always been pleasant, but this lunchtime betrayal is a treachery I cannot overlook. I will remember it every time I see an empty chair at our table and a deck of cards at yours.

The B.

He is a professional
A padawan, then an angel
Always surprised of seeing me
Always tired of making D
Selling his tool around the world
GBOML, you know the words

Of PhD, he owns the game
After the B, his baby's named
With BAV, does some rappin'
To the letters, add some mixin'
OLGMB, ain't no hard feel
Oh Le Goat, Miftari Bardhyl

In a faculty where, according to my recollection of a faculty meeting, less than 20% of the workforce is female, the statistical enigma of having four women join our teams in 2020 stands out. It is an intriguing deviation from the norm that warrants investigation – or at least a celebratory note.

The first of these women is among the early birds who make it to the office before 9 a.m. And until recently, **Amina Benzerga** was also the only woman on our team. These facts alone deserve a tip of the hat. Amina, our midday debates were sometimes heated, and we did not always see eye to eye, but I appreciated our exchanges. I will also cherish the memories from our train journey to Rome, where we took our conversations beyond the confines of our office walls. And let us not forget the many PhD Meetings you graciously hosted – events that always hold a special place in my heart. Speaking of which, a shout-out to **Emeline Maréchal** for co-organising those enlightening gatherings. Your dedication and effort have not gone unnoticed. During that Rome trip, I also enjoyed getting to know **Géraldine Brieven** better. She played tour guide and made sure we did not miss out on the city's best spots. Géraldine, your commitment to education and unique insights on the subject resonate with me. I wish we had found more opportunities to discuss our shared passion. Lastly, I would like to mention **Audrey Lempereur**. While we might not have had as many interactions, I am grateful for that ride back to the university after we visited the "Les Pousses Poussent" community garden. Small gestures often leave lasting impressions.

Wrapping up the newcomers for the year, a nod to our corridor's resident post-doc, **Alireza Bahmanyar**. Thanks for bringing that serene vibe to the hallway. And I will always appreciate the genuine concern you showed when I took that tumble off my bike.

2021

In the Montefiore ecosystem, beyond the age-old coffee versus tea rivalry, three prominent tribes emerge: the energy-optimisers, the machine-learners, and the neuro-electronicers. Interestingly, 2021 saw a surge of PhD candidates in all these tribes.

Amongst the few who still dare to dive head-on into the shrinking realm of energy at Montefiore (being slowly eaten by the machine learners and the small but growing faction of neuro-electronicers), there is **Jocelyn Mbenoun**. Jocelyn, there are a couple of things about you that genuinely stand out. First, it is that ever-present sunny disposition. Every single time I have stepped into your office, I have been greeted with an infectious smile and a warm "hello", often punctuated minutes later by your trademark hearty laugh. Granted, there have been times when its echoes through the walls tickled my nerves, but the positivity always made up for it.

Secondly, your commitment is commendable. You are steering the Fluxys project ship steadfastly, even as many have disembarked. The way you have soldiered on, unfazed, is truly inspiring. Your spirited presence and unwavering dedication have been a beacon over the past two years. Cheers to you!

In the same faction but exiled in the B37, there is a pair who seem like they were fated to find each other: the dynamic duo with a sense of humour so unique it is mostly just them laughing while the rest of us scratch our heads. Yet, oddly enough, I have come to cherish it. They are the guys who dream up the quirkiest challenges, whether downing ten beers before a 3 a.m. bike ride or conquering every major staircase they can find on Strava. Hanging out with them is never a dull moment, whether we are sneaking coffee from Bertrand's stash or grooving to live music in a Porto bar. But the pièce de résistance? Their knack for coming up with the zaniest nicknames. (QueenP is my personal favourite.) **Antonin Colot** or should I say Johnny Cancer, **Thomas Stegen**, the Amerindian, it is only natural for me to thank you by giving you a taste of your own wacky medicine!

Let us jump to the machine-learners starting with the one and only **Yann Claes**. Now, Yann, I promise, when I stroll into your office every morning, it is not just about those keys to infiltrate Damien's office and grab my coffee. No. If it were my sole reason, it would mean I hate you. And, if I genuinely despised you, I would throw the coffee at your face and keep the keys so that I do not have to see it again. This anecdote illustrates the quirky bit about Yann: most folks reading this might assume I have lost my marbles or harbour some deep-seated grudge. But Yann? He would probably nod in agreement, chuckle, and even sprinkle in a few zany anecdotes of his own. And that is why I always know that when I am half asleep arriving at work, coffee is not the only thing that will wake me up, but (Yann, I will let you add mentally what would).

Yann's partner in crime is **Gaspard Lambrechts**. Simply put, Gaspard is like a Swiss Army knife of talent. First off, he is a math wizard. I mean, engaging in marathon math debates with Adrien? That is some next-level stuff. Then there is his impeccable taste in transport. Just like me, he is a Brompton enthusiast. Nothing quite compares to the freedom of zipping around on one of those. Now, let us talk about the music. Hand Gaspard an accordion, and he morphs into a maestro. A few drinks might make most of us warble off-key, but not Gaspard. Nope, he will play a melody with you, tapping your feet in no time. Lastly, the cherry on top: the man is a veritable Sherlock Holmes. Sure, he leans a tad towards the conspiracy theory end of things, but his detective skills? Spot on. Gaspard, thanks for the talents you have brought into our lives over the past four years. Cheers to the genius and zest you infuse into every day!

From the ranks of the machine learners emerges then **François Rozet**. While our interactions have been fewer, it is undeniable that François marches to the beat of his own drum. He might not be the first to grab a beer, but when it comes to being passionate about machine learning, his enthusiasm is unmatched. His GitHub profile tells you everything about his love for coding and diving deep into any subject that piques his interest. François, your zeal and dedication are inspiring, so thank you for your unquenchable enthusiasm!

Straddling the line between machine learning and neuro-electronics, we find **Florent De Geeter**. Anchored firmly between these realms by his two promoters, crossing paths with Florent in a corridor always adds a bright spot to the day. Florent is also, with **Anaëlle de Worm**, part of the most bankable couple in Montefiore. Anaëlle, I want to thank you for your cooperation in the probability class. Similarly, I enjoyed working with **Arthur Fyon**, my student anchor, when I took over that class. To all the students and colleagues who have collaborated with me on course organisation, you have my gratitude. And, speaking of dynamic duos, we cannot forget **Sven Goffin**, who shares office space with Anaëlle. Sven is among the few brave souls who tackle the Sart-Tilman hill on a bike without an electric boost. Our shared moments, whether during the Televie 24 hours or other activities, have always been a blast. Cheers to you, Sven!

Of course, Montefiore is not just divided into the factions we have previously discussed. Tucked away in B37, Captain Laurent Mathy helms a team delving deep into the intricacies of networks. In 2021, they welcomed aboard **Vincent Rosetto**, with whom I had a couple of insightful discussions. Similarly, there is **Morgan Diepart** of Microsys, but perhaps more notably, a stalwart member of the RUday team for two years running. Collaborating with you on organising this event, Morgan has been a great experience.

2022

Embarking in 2022, we were greeted by one of the most promising batches across those four years. And how not to start by celebrating the person with the most communicable laughter of all: **Victor Dachet**. Victor, I will, of course, never forgive you for the coffee you made us miss at Colonster, but it is precisely such quirks that define you. You wear your heart on your sleeve, embracing every emotion that comes your way - from unabashed joy to nerve-wracking stress, from sheer wonder to raw disappointment. Our time together is never dull, whether we are sipping Aperol Spritz in Turin, listening to you doubling over with laughter from that unforgettable kayak tale, or navigating the chaos of penning two papers at once. Victor, to put it simply, you were probably my best friend discovery of 2022. For every memory we have crafted and every moment shared, I am profoundly grateful.

While our journey to Rome was the occasion to sip some cocktails with Victor, it was also memorable for the other bonds it forged. In particular, I was pleasantly surprised, and I think that is a shared feeling among all the team, to discover more about the one and only Italian of the group, **Maurizio Vassallo**. Maurizio, beyond your commendable personality and kind nature, you have a delightful sense of humour and decisiveness that comes forth when needed. Your ability to step up and guide us saved the day on more than one occasion during the trip. Heartfelt thanks for being our unexpected anchor in Rome!

Among the team's anchors, we cannot go forth without mentioning **Guillaume Derval**. Guillaume, I want first to congratulate you for your guts. It takes a certain kind of bravery (or maybe a touch of madness) to join Damien's team for a PhD. But to come around for a post-doc? Now that's next level. Anyhow, you managed to fit in and take an essential role in our big, friendly team (even though you consistently try to leave, applying left and right for more important jobs), bringing your own flavour of fun and a heap of know-how to the mix. Every chat with you is a deep dive into a world of ideas, and it is always a good time. So, cheers to you, Guillaume. I am keeping my fingers crossed that our roads cross again, be it in Liège or under the station in Namur.

Meanwhile, other teams have been growing, including my second favourite team of the batch, the one exiled in B37. I already mentioned the inseparable couple, Antonin and Thomas. To the relief of their promoter, Bertrand, the year 2022 saw two new additions to the team: **Geoffrey Bailey** and **Bastien Ewbank**. Geoffrey, I was honoured to be invited back then to be part of the discussion surrounding your choice of thesis topic. I feel like, since then, you have embraced that subject, a testimonial of it being the discussions you organised to create synergies between the works of our two teams. Thank you for this dedication, and good luck in supporting the two crazies for the coming years. But I guess that to support you, you also have Bastien, who is probably one of the people with the best vibes in the whole of Montefiore, the university, or even Liège? The kind of person who would never trash-talk anyone, even when he has every right to do so. Bastien, I discovered in you a man of many passions and action, from boys scouts to music to your supportive act at the 24h Télevie and RUDay. Thank you for this memorable Decrescendo performance on this party night or your incredible solo at RUDay.

As time passed, getting to know the new folks, especially those on different teams, got trickier. Still, I did not want to let those quick hellos and short chats slip by without giving them the nod they deserve. Every shared moment, no matter how brief, added something special to my journey. So cheers to **Boris Martin**. Thank you for accepting us, the noisy band, late at night into your home. Thank you **Loris Mendolia** and **Antoine Debor** for the chats we had together; they were always pleasant. The same goes for **Loic Champagne**, but I must playfully chide you for dodging the newcomers' presentation at this year's RUDay. You should have instead taken inspiration from **François Cubelier**, who I greatly thank for the funniest visual and auditory joke I ever witnessed in the history of RUDay.

2023

We are coming to the closing year of this long journey. In the eight months between January and my last day at the university in September, there were four significant additions to the team. The first one, and not the least, is my boy **Matthias Pirlet**, the man who knows everyone, the friend who is always in for a drink. We have not even known each other for a year, but it feels like I have always known you. I hope, and I know, that even though we are separated professionally, we will have a lot of moments to share personally. I know also that you will take good care of the baby I have raised over those past years: the energy market class. (Please also take good care of Adrien because, like Pascal, he does not know how to drink.) I hope you will enjoy every moment of your PhD, and I will be there to see its achievement.

As I exited from Montefiore, a new trio was stepping in. Two of them even claimed my old office as their own! Yes, I am talking about you, **Laurie Boveroux** and **Lize Pirenne**. But do not get me wrong, I could not be prouder to pass the torch - or rather, the keys - to you both. It is uplifting to see the team embrace more diversity. I trust you will honour the best office in Montefiore. Work diligently, sneak in some rest on the sofa when necessary, and remember, there is a Nintendo Switch ready to help you unwind. Joined by **Arthur Louette**, a soul as kind as they come, I am confident you will uphold the legacy Thibaut and I leave behind.

The best interns

Before we bid farewell to Montef', I want to acknowledge the work and moments shared with three individuals who were our colleagues for a few months during their internships. A hearty thank you to **Adrien Orban** for his pivotal role in our work on EROI and the memorable times in Louvain-la-Neuve. Appreciation is also due to **Dilan Deniz Demir** from Turkey. You entrusted me with the supervision of your work, and I hope I lived up to those expectations. Lastly, expressing gratitude to **Antoine Larbanois** is essential. You have integrated so seamlessly into our team that it feels like you have always been here. Collaborating with you has been a delight from day one, and I am confident that no matter the journey you embark on, success is assured.

If someone asks you what you do as a PhD student, you will probably answer research and sometimes some teaching. And that is, indeed, mostly what you do inside the walls of Montefiore. However, the world does not end at the wall of B28, and a PhD does not resolve to research and teaching. It is composed of a multitude of experiences which are not just add-ons. Instead, they are essential parts of the PhD experience, making it something truly special. In the coming paragraphs, we honour all the people who have not been mentioned yet and who are the roots of these experiences.

The AIM team

In 2023, I got lucky to meet the AIM team, a group mainly made up of super-talented women (and a few great guys, too - but let us give credit where it is due; the women were the stars here) who put together CIRED, a major conference in power systems. I got pulled into this challenge by the B., and, at first, I was not sure what to expect. Would it be fun or just a whole lot of work? Turns out, it was both. And a big part of that was thanks to **Louisa Kara**, **Céline Dizier**, **Michèle Delville**, **Fréderic Olivier** (I had already known him as an awesome researcher when we worked with Antoine for Damien), **Jérémie Delhaxhe**, and **Didier Basleer**. Together, we dove into the hectic but exciting world of organising a conference. It was tiring, sure, but every day was filled with laughs and good moments that made all the hard work worth it. Each brought something unique to the table, turning what could have been a stressful experience into one I will remember fondly.

Training

During my time here, I have learned a ton — not just from my direct experiences but also from the vast range of training opportunities our university offers. Firstly, hats off to the amazing women who make these training happen, and in particular, **Célia Lejeune**, **Nadine Vandermeulen**, and **Anne Goffin**. Also, a shout-out to my buddy Jonathan, who introduced me to this treasure trove of knowledge, covering various fascinating topics led by inspiring trainers. As my first trainer, a big thanks to **Evelyne Favart** for sharing insights on building a harmonious relationship with my supervisor. It put a lot into perspective for me. Thank you, **Thérèse Dupont**. While your tips on daily thesis writing did not quite stick, I did take away some handy tools from your session. Thanks to **Eric Louard** for teaching us how to spot signs of psychosocial trouble among our peers and create a healthier work environment. Thanks to **Jean-Philippe Demaret** for also improving this environment by providing simple but efficient principles for a better ergonomy. Thanks to **Stéphanie Franck** and **Gaëlle Jeanmart** for opening my eyes to how philosophy can be a formidable tool to think about our citizenship, a subject which is very dear to me. Thank you **Laurence Dessart**. Your LinkedIn tips were gold (I might have overused them just a tad). Thank you **Joseph Fléron**. Who knew an old 50s movie could teach us so much about negotiation? Thanks to **Jean-Yves Girin** for reinforcing our assertiveness and for helping me know myself a bit better. Thanks to **Silvana Cappello** and **Joël Michiels** for these superb lessons on public speaking. You nearly made me want to drop out to pursue an acting career (I better not). A special mention to **Pascal Detroz**. While I did not attend many IFRES training sessions, your guidance on using Eduflow for the probability class was invaluable. Lastly, a huge thank you to everyone I encountered during these training sessions. You all played a significant role in making them such enlightening experiences.

MT180

In my previous list, I unintentionally left out a particular training. This is not just any training — it holds a special place in my heart. Of course, I am referring to MT180 (or “My Thesis in 180 Seconds"). I owe immense gratitude to the phenomenal team that made this journey possible, especially the ever-smilling **Virginie Christophe**, the vibrant **Amaël Verbeure**, and the orchestrator **Martine Vanherck**. I also extend a warm thank you to all my fellow competitors: **Alexandra Tits**, **Chloé Galland**, **Alice Collignon**, **Aurore Gaspard**, **El Yamani Siham**, **Fabien Pille**, **Laurent Prunier**, **Raphaël Peiffer**, **Sacha Pszenica**, **Séverine Renardy**, **Sophie Bekisz**, and **Justin Martin**. Thanks to you all, I journeyed through ancient Greek and German tales, football championships, serious pharmaceutical games, neighbour disputes, frog-infested ponds, confused markets, imaginative takes on Magritte, lecture mazes, salmon races, algorithm vessels, and the intriguing house of a certain Mr Henri. The “avatar" is grateful for all of these discoveries.

Liège Créative and beyond

Speaking well in public is a valuable skill. However, without opportunities to present, it would not be handy. Fortunately, there is a space within the university where ideas converge and academics and industry professionals interact through presentations and beyond. That place is Liège Créative. A heartfelt thank you to **Delphine Buchet**, **Anne Peters**, and **Marie-Eve Noiset** for the beautiful conferences they organise. I am also grateful for their invitations to animate climate and digital fresks with Jonathan and François. Liège Créative has offshoots around the region, like the Hub créatif de Seraing. That is where **Aurore Falla** comes from, and I want to thank her for spearheading the fantastic “Révons Liège 2030" project. There are also visionaries in Arlon. Under the leadership of **Christelle Gillet**, they host numerous enlightening conferences to which I am grateful for having added my contribution.

The Green Office

While the previously mentioned team seeks to broaden the horizons of individuals of all ages, their primary audience primarily comprises professionals. However, there is another group dedicated to transforming the university from within, and whose current primary target is the other half of the equation: the students. This other entity, ruled, once again, by women, is the university's Green Office. Thank you **Cécile Van de Weerdt**, **Sarah Robinet** and **Laura Germain** for all the eco-friendly initiatives and the positive changes you are instigating within our institution. I also want to give a shout-out to the students involved in this endeavour, particularly to the one I am familiar with and the sole (?) male member of the team, **Louis Noel**.

Pot'Ingé and ReD

On the Sart-Tilman campus, we have roads, parking spaces, buildings, classrooms, restaurants, and vast stretches of woods. However, four years ago, a fresh biome sprouted, steadily expanding its reach, rallying more people, and becoming an integral part of the campus's vibrant life. This biome is a vegetable garden, charmingly named Pot'Ingé, born and raised by a reckless team of PhD candidates. A word of caution: while I might inadvertently omit some names from the extensive list of this project's promoters, I extend my gratitude to everyone who made this beautiful adventure pop in the middle of our PhD life. So, let us start with the ones I already mentioned: François, Kathleen, Alexandra, and Sophie; thank you for this too. **Bertrand Bastin**, a special thanks to you for initiating the market gardening course and for your unforgettable dance moves at parties. You made me discover that **Victor Mangeleer** is the best (or the worst ?) classmate. Thank you, **Eva Joskin**, for your strong convictions so eloquently expressed in that outstanding opinion piece. Thanks also to **Romin Tomasetti**, **Chloé Stevenne**, **Gilles Quabron**, **Alexis Feutry**, **Robin Glaude**, **Chloé Beaugendre**, **Solal Thomas**, **Astrid Cantamessa**, **Cyril Geortay**, **Victoria Collignon**, **Laura Balzani**, **Benjamin Delvoye**, and **Laura Müller** for all your involvement, but also for the parties, the discussions, the laughs, for all those moments shared.

A brief shout-out to those also involved in the Réseaux des Doctorants, which organises fantastic events like the brunch and, notably, the Doc'Trail. Special thanks to three individuals I have not previously mentioned who were, or still are, part of the organising team: **Aline Moreau**, **Maxime Amodei**, and **Caroline Minne**.

Sustainable teachers

Discussing sustainability provides the perfect opportunity to acknowledge several professors and key figures at the university who are effecting change in their unique ways. Beginning with the most distant contributor, hailing from Gembloux, a heartfelt thank you to **Aurore Degré** for pioneering the university's first sustainable development mega class. Thank you to **Felix Scholtes** for championing change within the medicine faculty and extending your influence to the broader university rectorate, and thank you to your rector co-advisor, **Sybille Mertens** as well. Gratitude to **Angélique Léonard** for your passionate advocacy of sustainability concepts and your ability to dispel misconceptions. Thanks **Xavier Fettweis** for your exemplary work on the local impacts of climate change. Similarly, **Sébastien Doutreloup**, your efforts in making climate science accessible to all through your engaging MOOC are commendable. Lastly, a salute to **Patrick Jacquemin**, whose relentless commitment to mobility issues stands as a beacon of positive change within our institution.

Let us step beyond the university's confines and venture into the broader world, or at least Belgium, for now. From collaborations that directly enriched the content of this thesis to volunteer efforts that shaped its philosophy, a host of individuals deserve gratitude for their invaluable contributions and insights.

A great collaboration

In 2021, Jonathan, in collaboration with **Gauthier Limpens** from the Catholic University of Louvain, laid the groundwork for a partnership that flourished over the next two years. Because of their initiative, I was introduced to several brilliant researchers from that university. I had the pleasure of collaborating with **Paolo Thiran** and **Pierre Jacques**. I also enjoyed insightful discussions and the occasional beer with **Martin Colla** and **Xavier Rixhon**. Additionally, professors like **Francesco Contino** and **Hervé Jeanmart** generously shared their time with us. This partnership, which resulted in at least three joint seminars, also brought me closer to researchers from my university, such as **Sylvain Quoilin** and **Thibaut Résimont**. Interacting with these peers was among the most enriching experiences of the past four years, and I extend my heartfelt thanks to everyone involved.

Another collaboration, independent yet equally enriching, stemmed from the energy market class. As the chief assistant, I had the pleasure of collaborating with **Sandra Belboom** from Helmo Gramme to strike the right balance between course content and load. Thank you for your commendable efforts over the past three years.

The Fresks

I have previously mentioned the climate and digital fresks, and among the people listed above, there are numerous facilitators. However, there remain many who have not yet been acknowledged and who truly merit recognition. Some of them, like the brothers **Adrien Corman** and **Gilles Corman**, **Renaud Franssen**, **Alexis Courtejoie**, **Eléonore Dayez** or **Alison Delhasse**, are fellow volunteers. Others, such as **Martin Hüberland** and **Sébastien Morant**, introduced me to new fresks, including the one on circular economy. I would, by the way, like to also express my gratitude to the leading duo of Polygons for the inspirational work they undertake in their enterprise. Lastly, a heartfelt thanks goes out to the educators at HEPL, especially **Jacqueline Somma**, for massively incorporating this outstanding educational tool into their institution.

Les Shifters

I have also devoted significant time and energy to another association, almost as much as I have to my PhD, if not more. I must candidly admit that this group, the Shifters, provided the motivation and drive I needed, especially during times when I questioned the purpose of my work.

Mainly, I must highlight the project, Education4Climate, which consumed countless hours but rewarded me immensely, along with the remarkable team behind it. While I have frequently acknowledged them on social media, I would like to once again extend heartfelt thanks to **Quentin Vantieghem**, **François Collard**, and **Quentin Lancrenon** for steering this project from the outset. I am also grateful to everyone who contributed at various stages. Names like **Noël Schneider**, **Olivier Bailly**, **Noémie Mairesse**, **Mathieu Lecouturier**, **Yohan Courbe**, **Robin De Gernier**, **Aric Wizenberg**, **Axelle Gortz**, **Chantal Winter**, **Hülya Altinok**, **Aymeric Lamant**, **Denis Lebailly**, **Julien Descampe**, and **John De Dryver** come to mind, though there are undoubtedly many I have missed. Special appreciation goes to **Thierry Van de Merckt** for coordinating the ULB field projects with us and to the students who participated, including **Hakim Amri**, **Yanis Triaa**, **Cedric Jansens**, **Yannick-Andre Pambu-Kita-Phambu**, **Elio Sarkis**, **Maxime Couasnard**, **Hamida Takali**, and **Olav de Clerck**. Lastly, a grand thank you to **Camille Tasseroul** for paving the way to introduce the tool in Italy.

I also had the privilege of being part of the Noyau d'Olive, witnessing firsthand the growth and structuring of such an organisation. It was an enlightening experience to connect with extraordinarily inspiring individuals like **Dominique Martin**, **David Grimaldi**, **Thomas Wansart**, **Cécile Levan**, **Grégory Filou**, **Jérémy Pontif**, **Olivier Alsteens**, **Philippe Dejardin**, **Vincent Cordier**, **Amandine Paulet**, **Isabelle Hoberg**, **Perrine Wohlfrom**, **Catherine Lalain**, **Paul Van osselaer**, or**Thomas Legast**.

Lastly, a nod to the team of Shifters in Liège, which includes familiar names such as François and Victor, but also others like **Martin Castin** and **Gil**. I am committed to expanding our network in our vibrant city.

ClimACTES

In 2021, I embarked on a journey that combined two of my passions: education and the environment. This journey was the inaugural edition of ClimACTES, a two-week summer school dedicated to combating climate change through education and the creation of socially responsible enterprises. While my group did not successfully launch a company, the experience was invaluable, and I encountered many remarkable individuals. A heartfelt thanks to the organising committee, particularly **Philippe Gilson**, **Dominique Owieczka**, **Damien Dallemagne**, **Danielle Borsu**,

Isabelle Jonlet, **Jean-Marc Bourdouxhe**, **Josiane Carré**, **Christiane Theunissen**, **Christine Mainguet**, **Anne-Marie Schoenaerts**, and **Stéphanie Brunet**, for turning this event into reality. Special appreciation goes to the education team: **Thibaut Crismer** (a huge shout-out to you for introducing me to the PJWB), **Elise Franssen**, **Nathalie Noël**, **Louis Vinckenbosch**, **Harmonie Lecomte**, **Julie Ghes**, Jonathan, Thibaut, and Adrien. Our brainstorming sessions and discussions were invaluable. Lastly, a big thank you to my fellow participants, including **Juliette Falkenberg**, **Pauline Carbonnelle**, **Arnaud Van Der Cam**, **Michael Horevoets**, **Tatiana Malchair**, **Tania Noël**, **Clara François**, **Loïc Strivay**, **Manon Duchatel**, **Lionel Delchambre**, and **Lino Paoletti**, for making this experience unforgettable.

Youth for Change

Before concluding these acknowledgements, I would like to extend my gratitude to three groups of dynamic young individuals making a significant impact.

Firstly, I express my heartfelt thanks to the enthusiastic individuals I have had the honour to engage with through the activities of the Forum des Jeunes. Whether it was collaborating on your initiatives, presenting E4C, or joining forces at the European Parliament, each moment was truly memorable. I am deeply grateful to **Loïc Perrin**, **Antoine Chavanne**, **Sean Nart**, **Elisabeth Hosszù**, **Emmanouela Tzani**, **Zoé Noël**, **Louise Lebichot**, and **Manon Breda** for these enriching experiences.

I also want to shine a spotlight on the dedicated team at Plas'Kot. Special thanks to **Jennifer Buxant** and **Louis Natalis** for providing us the platform to showcase the work of the Shifters.

Lastly, I am grateful to the passionate team at PJWB. Your acceptance and inclusion, despite me being a bit senior in age, have been deeply inspiring. This experience has not only paved a new direction in my career but has also allowed me to cross paths with many outstanding individuals.

The Jury

Although I have meandered through time in this chapter, it is fitting to conclude this journey by acknowledging those who will officially put an end to it: the jury.

Thank you to its four membres **Pr Francesco Contino**, **Pr Sylvain Quoilin**, **Dr Gauthier Limpens**, **Dr Jonathan Dumas**, its president **Pr Louis Wehenkel** and my promoter **Pr Damien Ernst** for dedicating their time to review my work and provide invaluable feedback both on the manuscript and during my final defence. You are all integral to this significant milestone in my academic journey.

While some may find it extravagant to pen 21 pages of acknowledgements, as I embarked on this chapter, I felt compelled to be thorough. Mentioning just a handful of names or expressing gratitude in broad strokes would not do justice to the myriad of connections I have made. So, I crafted this chapter with a future intention in mind: to revisit it and rekindle memories of the moments I shared with you all.

Given the vast scope of a PhD journey with countless collaborations and discoveries, I endeavoured to mention everyone I have engaged and/or been inspired by within and around the context of this thesis.

For the sake of brevity, however, I have intentionally left out my family and long-standing friends. This does not mean their roles are less significant; quite the opposite. I am immensely grateful to you all for being part of the greater picture, of which this small but fulfilling journey is just part, and for your continual presence in my life.

Such considerations led to the citation of almost 300 distinct names. Still, a couple of you have, without a doubt, been left out of these words. To all those I have encountered during these past four years who remain unnamed, I offer my sincere apologies. I invite you to reach out, allowing me to, over a drink and heartfelt conversation, tell you face to face:

'Thank you'.

Antoine

Contents

Prologue

Synopsis: In a spirited discussion about energy strategies, Anna champions the cause of cost-effectiveness, while Lucas emphasises the importance of energy return on investment. As tensions rise, Eva introduces a groundbreaking approach that could bridge their differences.

Anna: “When we’re talking about which energy sources to choose for the future, we have to prioritise cost. We owe it to our citizens to ensure that energy remains affordable. The lowest cost should be our primary objective."

Lucas: “I hear you, Anna, but it’s not just about cost. We need to think about the energy return on investment. If we’re investing a ton of energy and getting little in return, it’s not sustainable. We should be aiming for the highest energy return, which means the lowest invested energy."

Anna: “But Lucas, if we only focus on energy return, we might end up with solutions that are too expensive."

Eva: “You both have valid points. But what if I told you there’s a way to reconcile both visions? I recently read a fascinating research thesis that might offer a solution."

Lucas: “Go on, Eva. I’m intrigued."

Eva: “The thesis is called ‘Computing the necessary conditions for the transition of our energy systems’. It introduces the concept of ‘necessary conditions’. Think of them as the non-negotiable or minimum requirements to achieve specific objectives. If applied to our case, it could be about finding the least amount of energy from various sources needed to meet both cost and energy return objectives."

Anna: “So, you’re saying that this method allows us to determine the minimum energy required from each source without compromising on cost?"

Lucas: “Or on energy return on investment?"

Eva: “Exactly! By focusing on these necessary conditions, especially when we have multiple objectives like cost and EROI, we can pinpoint the resources we need for a smooth energy transition."

Lucas: “And what else does this thesis tell us about energy systems and their transition ?"

Eva: “I’ll guess you’ll have to read the next pages to find out!"

This is a work of fiction. Names, characters, places and incidents either are products of the author’s imagination or are used fictitiously. Any resemblance to actual events, locales, or persons, living or dead, is entirely coincidental. It was first published on the blog of Pr Damien Ernst. This is a revised version.

1 Introduction

> *Repetition makes us feel secure, and variation makes us feel free.*
>
> — **Robert Hass (1984)**
> (Twentieth-century pleasures: prose on poetry)

The 21st is a century of choice.
Choice in the future we want.

While the window of available options has been shrinking as we delayed action on critical issues like climate change and sustainability, there still exists numerous possibilities and diverse approaches to implementing them. Selecting among these alternatives is a challenging endeavour.

This introduction aims to illuminate the complexities associated with such determinations. Notably, we seek to merge our engineering perspective with a recognition that these decisions are deeply interwoven with human subjectivity and are not merely mechanical determinations. We aim to elucidate these challenges, leading the reader to grasp how this thesis' contributions can significantly inform decision-making processes.

We navigate these challenges and potential solutions through three distinct lenses. In Section 1.1, we adopt a bird's-eye perspective, capturing the breadth of societal choices looming ahead. Section 1.2 then translates these abstract challenges into the precise realm of mathematical programming. Lastly, Section 1.3 delves into the specific application of these concepts within the realm this thesis primarily concerns: energy systems.

1.1 Facing Choices

The myriad existential choices of this century are too vast to be encompassed in a single thesis. Yet, among these, climate, environment, and energy topics increasingly dominate global discussions, news headlines, and our everyday lives. We can distil these pivotal choices into fundamental questions, such as:

- What degree of warming do we aspire to limit and mitigate?
- Should we redirect our efforts from other environmental crises towards tackling climate change?
- Is it sufficient to simply embrace the present abundance and enjoy life, or do we have a moral obligation to take action?
- Should we primarily pursue technological solutions, societal transformations, or a combination of both?
- Should nuclear power be favoured over solar panels and wind turbines in the pursuit of sustainable energy generation?
- Are electric or hybrid cars preferable? What about hydrogen or renewable ethanol trucks? Is there value in embracing a diverse range of options?
- Should an agricultural area be dedicated to producing crops for animal or human consumption? Should we cover it with solar panels to produce energy or with concrete surfaces to install carbon-capture plants? Or, is it more beneficial to return it to its natural state to promote and preserve biodiversity?

Due to varying history, background, knowledge, and sensibilities, the option one favours to answer these questions will differ, and it is natural for these questions to lack definitive answers, as they encompass both rationality and ideology.

Can we rationalise choices ?

By employing scientific tools, we can make diligent efforts to enhance the rationality surrounding these choices: quantifying disparities in impacts between a +1.5°C and +2°C warming scenario, tracking the annual rate of species extinction, calculating carbon and material footprints of technologies or evaluating energy yields from different crop applications.

Nonetheless, despite our capacity to apply rational thinking to these options, our final choices are invariably entwined with our ideological perspectives. This is primarily because the evaluation of these options is intrinsically tied to our ideological views. Furthermore, the ultimate decision among the available options is equally rooted in our ideological standpoints.

Ideology in evaluating options

Supporting this assertion, the primary factor underpinning the ideological foundation behind choices is tied to the inherent uncertainties associated with evaluating available choices.

These uncertainties can be divided into two primary categories. The first type arises due to reliance on random processes. For instance, climate science depends on complex and chaotic natural phenomena, making accurate predictions challenging. The second type of uncertainty is related to the lack of complete knowledge. For example, quantifying the annual rate of species extinction is impossible due to incomplete tracking of Earth's species [MRM04] or obtaining comprehensive information about the production sources of specific materials for technology footprints can be challenging.

While quantifying our choice options, we must factor in these uncertainties. This involves making specific parameter choices and assumptions which are influenced by our subjective perspectives and biases and influence the evaluation of the options. For example, when assessing different electricity production methods, an evaluator might opt for wind profiles favouring wind power plants. Similarly, when comparing technologies, a modeller with a positive outlook on technological advancements may assume an enhanced efficiency for certain technologies when projecting future scenarios.

Therefore, when we are presented with evaluated options to make a choice, it is crucial to remember that they are contingent upon certain influenced decisions.

Ideology in choosing options

Even after uncertainties are incorporated, personal preferences still play a significant role in influencing our choices. Let us take two examples.

We can reasonably determine the differences between a +1.5°C and a +2°C world. Thanks to the extensive work of the IPCC (Intergovernmental Panel on Climate Change), we know that in a +2°C world compared to a +1.5°C world, we can expect more frequent and intense heatwaves, higher sea-level rise leading to increased coastal flooding, and a higher probability of Arctic ice-free summers [Mas+22]. However, individual inclinations towards short-term profit over long-term prosperity may lead some to dismiss the dangers of a +2°C world. Second example: even with knowledge of a substantial number of species facing extinction and the consequential impact on ecosystem services, some governments might decide to make an ecological pause to prioritise immediate action on climate change [GGM23].

These decisions reflect our preferences and the goals we prioritise. For some individuals, the primary objective might be minimising the concentration of carbon dioxide in the atmosphere, while for others, it may be reducing the number of species on the brink of extinction.

Choosing the preferred option

There are instances where preferences will converge and guide us towards identical chosen options – for example, reducing consumption benefits both the climate and biodiversity. However, these preferences can also precipitate divergent outcomes. As an illustration, combating climate change may necessitate the construction of low-carbon power plants wherever feasible, a strategy that might conflict with biodiversity enhancement efforts.

In those instances of conflict, a critical choice must be made regarding which option to favour. This junction is where ideology takes precedence over rationality, with the ultimate decision springing not from a detached, systematic comparison of options but from a nuanced and thoroughly debated dialogue among stakeholders. However, the intensity of this debate may be lessened depending on the strategy employed to reach the final decision.

Continuing with our example, the two extreme options are to either build power plants wherever possible (which, to simplify, would lead to no emissions at the production stage) or to avoid building any power plants at all (resulting in zero direct impact on biodiversity). The first potential strategy is the no-compromise approach, where debates lead to the complete favouring of one option over the other. While decisive, this approach often fosters considerable tension, leaving one party unrewarded and discontented.

A second, more harmonious strategy involves determining trade-offs between the two options to forge a compromise. This might entail reducing the number of power plants to be constructed, thereby partially satisfying both the goal of minimising emissions and preserving biodiversity. Such a middle-ground approach can foster cooperation and mitigate potential discord among stakeholders.

The third strategy: finding common ground using necessary conditions

Unfortunately, such choices are multifaceted and interdependent, impacting various objectives simultaneously. Selecting a specific option to represent a trade-off might, in turn, create tensions with other stakeholders possessing differing preferences. To navigate these complexities, *this thesis proposes a third approach*, which involves not settling on a single, unique option (whether a trade-off or otherwise). Instead, it seeks to compute the commonalities among numerous options deemed 'good enough' for fulfilling the primary objectives while living ground to incorporate the needs of other stakeholders. These commonalities represent the minimum criteria needed to satisfy, to some extent, the primary goals, and this is why we refer to them as 'necessary conditions'.

In the subsequent section, we will delve into some fundamental mathematical content to formalise the concepts outlined in this section. This will set the stage for a specialised exploration of the method's application to the central focus of this thesis: the energy transition. By identifying and leveraging these 'necessary conditions', we aim to craft a more nuanced, inclusive, and practical approach to decision-making that genuinely reflects the diverse nature of the challenges we face.

1.2 Modelling Choices

In the complex landscape of decision-making and problem-solving, several methods are available for modelling choices. These methods range from heuristic techniques, which rely on experience and intuition, to simulation-based methods, such as Monte Carlo, through game theory models to evaluate strategic interactions between decision-makers. Each method has unique strengths and applications, catering to different problems and decision-making scenarios.

In this thesis, the preferred tool is *mathematical programming* (also called mathematical optimisation or simply optimisation).

Mathematical programming is a potent tool among these methods, especially when the goal is to optimise a specific objective subject to constraints. It provides a *formal* and *precise* framework that can represent complex relationships and restrictions, making it suitable for problems where accuracy and optimisation are paramount. Whether maximising profits in a business setting, minimising energy consumption in engineering, or balancing multiple objectives in government planning, mathematical programming offers a *flexible* and *scalable* solution.

Defining Mathematical Programming: Objectives, Variables and Constraints

Although mathematical programming encompasses a range of methodologies, it can be distilled into three primary elements: objectives, variables, and constraints.

In a book by Avriel and Golany [AG96], this field of mathematics is articulated as follows:

"Mathematical programming in its simplest form deals with the problem of maximising a real-valued function, such as the profit resulting from operating a system (or minimising a real-valued function, such as operating cost), subject to constraints, such as capacities or operating conditions, expressed as equations or inequalities."

The central concept in this definition is the optimisation (i.e. maximisation or minimisation) of a specific function. Functions serve as mathematical expressions that encode various *preferences* in the form of real numbers. For example, one function might represent the total power capacity of installed power plants worldwide, while another could quantify the number of species going extinct each year. Generally, we would aim to maximise the first function and minimise the second. In optimisation terminology, the functions we strive to optimise are referred to as *objective functions*, or simply *objectives*, and commonly denoted by the letter f.

An objective function takes one or several unknowns, known as *decision variables*, as input. These variables represent elements in a system with various possible values from which we can choose. In mathematical terms, when a specific value is assigned to each variable, it forms a *solution* to the optimisation problem. This can be equated to a potential *option* we consider in everyday language. For example, in our previous problem, the set of variables could represent the decision to build or not build a power plant at each potential location. A solution would then specify a particular set of sites for construction. In mathematical programming, sets of variables are typically represented as n-dimensional vectors labelled with the symbol $\mathbf{x} = (x_1, \cdots, x_i, \cdots, x_n)$. Each variable can adopt values from specific sets, such as real or natural numbers. When these sets are combined, they form a subset of the n-dimensional space, which Luenberger, Ye, et al. [LY+84] designates as S. The notation $f(\mathbf{x})$ then provides us with the value of the objective function for the given solution $\mathbf{x} \in S$.

The mathematical formalism described above, especially using n-dimensional vectors, offers a decisive advantage: it can represent an expansive array of potential solutions. This is invaluable in real-world scenarios, such as the power plant location example, where numerous configurations must be compared. By representing each of these possibilities, we equip ourselves with a comprehensive view of available options, ensuring no potential solution is overlooked. However, this strength also presents challenges. As the number of variables n grows, the number of potential solutions rises exponentially. Specifically, if each variable can take on v possible values, the total number of solutions becomes v^n. While capturing a vast range of possibilities is beneficial, sifting through this immense solution space can be computationally intensive and time-consuming. In many cases, the number of solutions can be overwhelming, making it difficult to pinpoint the most optimal one. This underscores the delicate balance between ensuring comprehensiveness in solution representation and the practical challenges of processing and evaluating such a vast array of options.

Our definition's third and final component consists of *constraints*, which "limit the selection of decision variable values" as described by Luenberger, Ye, et al. [LY+84]. Constraints serve as the boundaries within the mathematical framework, defining the *feasible region* for the decision variables that we refer to as $\mathcal{X}$. Combinations of variable values within these boundaries are termed *feasible solutions*. For example, a constraint might limit the amount of resources available for building power plants. These constraints capture the real-world limitations and considerations that must be accounted for when seeking to optimise the objective functions. As elaborated in the definition mentioned earlier, constraints are expressed as equations or inequalities in mathematical programming. More formally, these constraints can take the form of inequalities $g_j(\mathbf{x}) \leq 0$ or equalities $h_k(\mathbf{x}) = 0$, where g_j and h_k are real-valued functions of the decision variables x.

Bringing these three components together, we can articulate the general mathematical programming problem in the manner described by Luenberger, Ye, et al. [LY+84]:

$$\begin{aligned} \text{Maximise (or minimise):} \quad & f(\mathbf{x}) \\ \text{Subject to:} \quad & g_j(\mathbf{x}) \leq 0, \; j = 1, 2, \ldots, m \\ & h_k(\mathbf{x}) = 0, \; k = 1, 2, \ldots, p \\ & \mathbf{x} \in S \end{aligned} \tag{1.1}$$

Modelling rationally

Wrapping up our discussion of these three elements, we must touch upon how modelling embeds rationality. Essentially, the embodiment of rationality in modelling comes down to the judicious selection of variables and constraints that aptly mirror the physical phenomena under investigation. It is essential to remember that every model is an abstract representation of the real world (hence the oft-quoted phrase, "All models are wrong, but some are useful"). However, not all models are of equal merit. To make a model that is more in sync with reality and thus more 'rational', it is vital to include relevant variables and impose genuine constraints.

For instance, when modelling water flow in a river, one might select variables such as riverbed slope, water volume, and sediment content. Constraints could include the maximum capacity of the riverbed or even governmental regulations on water usage. Over-simplifying by neglecting sediment interaction could result in incorrect predictions about erosion rates or water flow speed, emphasising the importance of model precision and relevance.

Even if they serve a very different purpose, crafting an accurate representation of objectives is vital for fostering rational decisions. Indeed, while variables and constraints enable us to closely mirror real-world phenomena and restrict what is possible or implausible in the real world, objectives primarily guide our selection among the feasible solutions. Grounding objectives in reality is thus crucial to ensure that the chosen solution aligns with genuine, tangible goals.

Parameters

The last key element in this optimisation model is known as parameters. Parameters are fixed values, for instance, the cost of a technology or the wind potential in a particular area, that help define the objective and constraint functions. Together with the problem's formulation – how we define variables, constraints, and objectives – parameters are pivotal in infusing our models with a sense of real-world rationality.

To illuminate this concept, let us specify the preceding general formulation by exploring the specific case of linear programming. Linear programming is a subfield of mathematical programming in which, according to Bertsimas and Tsitsiklis [BT97], the problem involves "minimising [(or maximising)] a *linear* [...] function subject to *linear* equality and inequality constraints." Highlighting the significance of this method, Luenberger, Ye, et al. [LY+84] aptly remarked: "Linear programming is, without doubt, the most natural mechanism for formulating a vast array of problems with modest effort."

In this context, the objective and constraint functions can be represented as weighted sums of variable components, that is, $\mathbf{w}^T\mathbf{x} = \sum_{i=1}^{n} w_i x_i$, where $w_i \in \mathbb{R}$. Given this structure, a typical linear programming problem can be framed as follows:

$$
\begin{aligned}
\text{Maximise (or minimise):} \quad & \sum_{i=1}^{n} c_i x_i \\
\text{Subject to:} \quad & \sum_{i=1}^{n} u_{ij} x_i \leq 0,\ j = 1, 2, \ldots, m \\
& \sum_{i=1}^{n} v_{ik} x_i = 0,\ k = 1, 2, \ldots, p \\
& x_i \in \mathbb{R},\ i = 1, 2, \ldots, n
\end{aligned}
\tag{1.2}
$$

Although this formulation relates more closely to the general definition proposed in 1.1, linear programming problems are often presented in a standard form, such as:

$$
\begin{aligned}
\text{Minimise:} \quad & \sum_{i=1}^{n} c_i x_i \\
\text{Subject to:} \quad & \sum_{i=1}^{n} a_{i1} x_i = b_1 \\
& \cdots \\
& \sum_{i=1}^{n} a_{im} x_i = b_m \\
& x_i \geq 0,\ i = 1, 2, \ldots, n
\end{aligned}
\tag{1.3}
$$

For a deeper exploration of the equivalence between the general and standard forms of linear programming, readers are encouraged to consult the comprehensive work by Bertsimas and Tsitsiklis [BT97].

The standard form can be further condensed into the following:

$$
\begin{aligned}
\text{Minimise:} \quad & \mathbf{c}^T\mathbf{x} \\
\text{Subject to:} \quad & \mathbf{A}\mathbf{x} = \mathbf{b} \\
& \mathbf{x} \geq 0
\end{aligned}
\tag{1.4}
$$

where $\mathbf{A}$ is an $m \times n$ matrix, b is m-dimensional vector and c a n-dimensional vector. The ensemble of real-valued numbers within these vectors and matrices constitutes what is commonly called *parameters*.

To further clarify these concepts, we delve into an illustrative example below.

Example 1. ***Linear Optimisation Problem: Production Planning for a Manufacturing Company***

Suppose a manufacturing company produces two products, A and B, using two machines, M_1 and M_2. The goal is to determine the optimal production mix of products A and B to maximise profit while considering the constraints of machine capacity. The elements of the optimisation problem are the following:

- ***Objective Function**: Maximise profit, given by the profit contribution per product and the production quantity.*
- ***Decision Variables**: x_A and x_B, representing the quantity of products A and B to be produced.*
- ***Constraints**: Machine hours required for production and machine availability.*

*Next, we define **parameters** that will serve in the linear definition of our constraints and objectives:*

1. *Profit Contribution: The profit per unit for products A and B. For instance, $c_A = 10$ (profit per unit for A) and $c_B = 12$ (profit per unit for B).*
2. *Machine Hours Required: The number of machine hours required to produce one unit of each product on machines M_1 and M_2. Example values could be:*
   - $a_{A1} = 2$ *hours per unit of A on M_1*
   - $a_{A2} = 1$ *hour per unit of A on M_2*
   - $a_{B1} = 1$ *hour per unit of B on M_1*
   - $a_{B2} = 3$ *hours per unit of B on M_2*
3. *Machine Availability: The available machine hours for machines M_1 and M_2. For example, $b_1 = 40$ hours for M_1 and $b_2 = 30$ hours for M_2.*

***Mathematical Formulation**: We can then formulate the linear programming problem as follows:*

$$\begin{aligned} \text{Maximise:} \quad & 10x_A + 12x_B \\ \text{Subject to:} \quad & 2x_A + 1x_B \leq 40 \\ & 1x_A + 3x_B \leq 30 \\ & x_A \geq 0, x_B \geq 0 \end{aligned} \tag{1.5}$$

The solution to this linear optimisation problem will give the optimal production quantity of products A and B that maximises profit while adhering to machine capacity constraints.

Parametric uncertainty

In the preceding sections, we mentioned how uncertainty was prevalent in any choices. In mathematical programming, uncertainty reveals itself primarily in parameters. The technical term for this form of uncertainty is *parametric* (or parameter) *uncertainty* and can generally be divided into two categories: aleatoric and epistemic uncertainty. These two types of uncertainty align with the challenges mentioned in the prior section regarding the inherent biases that can arise when attempting to quantify complex problems. We present them briefly.

Aleatoric uncertainty comes from inherent variability or randomness in a system or process. It represents the unpredictability associated with things like inherent randomness in a physical system or the variability of human behaviour. For example, in a dice roll, the outcome is random, and the uncertainty about what number will come up is aleatoric. This type of uncertainty is typically irreducible because it arises from fundamental randomness in the system.

Epistemic uncertainty comes from a lack of knowledge or information about the process or system. It could be due to incomplete data, lack of understanding of the underlying processes, or errors in model structure. Epistemic uncertainty can often be reduced through further research, more data collection, or improvement in modelling techniques.

To manage parametric uncertainty, practitioners employ a suite of techniques, each catering to different levels of complexity and intricacy. At its simplest, *scenario analysis* evaluates the impacts of several scenarios, affecting the values of some parameters, on the optimisation result. *Sensitivity analysis* investigates how changes in one or multiple input parameters influence the output, identifying critical variables that might sway the results considerably. The *Monte-Carlo* method uses random sampling to estimate the potential outcomes and their probabilities, offering a statistical understanding of the risks involved. Delving into more advanced strategies, *stochastic programming* incorporates known probability densities into the optimisation. *Robust optimisation* aims for solutions that remain viable across a spectrum of uncertain parameter values, emphasising resilience over optimality. *Chance-constrained programming* ensures constraints are met with a specified confidence level, accounting for uncertainty's inherent risks. Lastly, *fuzzy optimisation* navigates ambiguity with fuzzy sets and logic, ideal for decision-making when parameters are vague or imprecise.

While these methods are designed to address and manage uncertainty, they do not claim to eliminate it. The essence of addressing uncertainty is to better understand and account for it, not to eradicate it. The decisions we make – such as choosing specific scenarios, setting the parameter range for sensitivity and robust optimisation, or selecting probability density functions for Monte Carlo and stochastic programming – are pivotal. These choices are critical as they directly impact both the objective function and the constraints and, consequently, the problem's solution – the set of variable values that lead to the optimal objective function value. As elucidated in the previous section, these choices are far from impartial; they often reflect personal preferences and are susceptible to biases. These biases can then propagate through the model, leading to a solution influenced by how uncertainty and individual perspective have been integrated into the problem.

Choosing the best solution

As highlighted in Section 1.1, personal preferences and biases can still influence which solution is optimal, even when there is no uncertainty surrounding the parameters. This highlights the importance of having robust strategies to navigate different options.

In the context of mathematical programming, the 'no compromise' strategy consists of selecting the solution (i.e. a specific set of variable values) that maximises (or minimises) one objective function f (among a series of competing objectives). We typically refer to this methodology as mono-objective optimisation. This approach represents a clear and decisive method but may overlook nuances and potential synergies between objectives.

The second strategy is more complex and flexible, focusing on evaluating and selecting solutions that represent trade-offs between competing objectives, meaning that they are not optimal for any single objective but may offer a more balanced solution overall. In mathematical programming, this strategy can be implemented using multi-objective optimisation techniques to find the best compromises between different objectives. The collection of these compromise solutions is often called the Pareto front or the set of efficient solutions. These represent solutions where no objective can be improved without worsening at least one other objective. The identification and analysis of the Pareto front enable a more nuanced understanding of the trade-offs and potential synergies between different objectives, facilitating more informed and balanced decision-making. For those interested in a deeper exploration of these concepts, more details about multi-objective optimisation techniques and the formalisation of the Pareto front can be found in Appendix A.2.

Multi-objective optimisation addresses some of the constraints of mono-objective optimisation but introduces its limitations. One notable restriction arises from the fact that only a finite number of objectives can be modelled. This limitation is grounded in several realities.

Firstly, while it is possible to consider many objectives, doing so can become increasingly cumbersome and less actionable. Incorporating an extensive set of objectives might complicate the optimisation process and detract from focusing on the most crucial goals. Secondly, modellers do not always know which objectives might be pertinent to their problem. The relevance of objectives can depend on various contextual factors, and it may not always be clear which ones should be prioritised. Finally, some objectives are inherently challenging to model. For instance, quantifying social unrest caused by the construction of new infrastructure is far from an exact science, as it requires the integration of complex human dynamics that resist simple mathematical characterisation.

Structural uncertainty

These constraints on the number and nature of objectives that can be incorporated into a model can be seen as a specific instance of a more comprehensive limitation known as structural or model uncertainty.

Structural uncertainty refers to the uncertainty that arises from choosing a particular model structure or framework to represent a physical system, process, or phenomenon. Unlike parameter uncertainty, which is associated with the specific values of the parameters within a model, structural uncertainty is related to the form and equations of the model itself. Indeed, it is rare for a model to perfectly encapsulate all the intricacies and complexities of the real-world system it represents. Decisions must thus be made regarding the level of detail when modelling different system components, and these choices might diverge between various models, leading to structural differences between them. For example, in modelling the climate system, there might be various ways to represent cloud physics or ocean currents. These choices induce structural uncertainty, meaning there is uncertainty in how well the model reflects the real physical system and how well the conclusions drawn from this model will generalise in the real world.

Selecting a series of objectives to optimise is an integral part of these modelling choices. This decision is not merely a technical task but reflects underlying assumptions and priorities. The choice of objectives to be optimised reveals what is considered important in the representation of the physical system or process and may influence the model's behaviour and results.

Near-optimal spaces

Addressing structural uncertainty presents a real challenge. Yue et al. [Yue+18] observe that even the employment of "larger and more complex models to better represent the world dynamics" fails to eradicate structural uncertainties completely.

According to Pfenninger et al. [PHK14], from this observation, it follows “that interesting solutions are likely not to be the single global optimum."

To put this into context, especially within the realm of mono-objective optimisation: The optimal solution of an optimisation problem, as framed in (1.1), refers to the variable values, $\mathbf{x}^\star$, that adhere to constraints and either maximise or minimise the value of $f(\mathbf{x})$ depending on the problem's aim. It is worth emphasising that multiple such optimal sets of values can exist. For instance, two distinct solutions, $\mathbf{x}^A$ and $\mathbf{x}^B$, might yield identical objective values. The crux of what Yue et al. [Yue+18] and Pfenninger et al. [PHK14] are underscoring is that, given the persistence of structural uncertainty and the inevitable imperfections in our models, the determined $\mathbf{x}^\star$ might not encapsulate the true optimal. As a result, it is prudent to explore alternative solutions. However, if we believe our model to be reasonably accurate, solutions that closely align with the optimum are likely the most pertinent.

This has prompted researchers to devise techniques for exploring near-optimal space – meaning the investigation of solutions whose objective values, though suboptimal, are closely aligned with the optimal objective value. From a mathematical perspective, this equates to exploring solutions derived from the original set of feasible solutions $\mathcal{X}$. In the context of the minimisation of a positive function f, the near-optimal solution space can be defined as:

$$\mathcal{X}^\epsilon = \{\mathbf{x} \in \mathcal{X} | f(\mathbf{x}) \geq (1+\epsilon) f(\mathbf{x}^\star)\} \tag{1.6}$$

This equation illustrates that the epsilon-optimal space (more generally referred to as the near-optimal space) encompasses solutions whose objective values diverge from the optimal objective value by a factor of ϵ. More information on this topic can be found in Appendix A.

One of the cornerstone approaches in this domain is the MGA (Modelling to Generate Alternatives). This is more than a specific methodology; it can be broadly interpreted as “any method used to systematically search the near-optimal solution space for alternative solutions” [Yue+18]. This term was first coined in the 1980s by Brill Jr [Bri79] and applied to land use planning. In recent years, it has regained attention and been applied to different domains, including energy systems, as explained in Section 1.3.

Necessary conditions

MGA encompasses a diverse array of methodologies, each implying distinct decision-making strategies. Many of these strategies leverage MGA techniques to churn out a broad spectrum of alternative solutions, allowing decision-makers a rich pool from which to select. While comprehensive, we postulate that this approach enhances the likelihood of pinpointing a solution that resonates with everyone involved. Nonetheless, a potential pitfall of this approach is the sheer volume of options it might produce, which could inundate and potentially confound decision-makers, potentially paralysing rather than facilitating constructive discourse. Consequently, as we emphasised at the end of Section 1.1, we advocate for another approach: seeking commonalities between these alternative solutions satisfying all stakeholders and then building on this shared foundation.

In the context of mathematical programming, we coin these shared agreements or overlaps as 'necessary conditions'. Think of them as the non-negotiable benchmarks (e.g. a cap on the number of power plants) that must be met to achieve desired outcomes (e.g. capping species extinction over a decade). To delve deeper without becoming overly intricate (comprehensive details are offered in subsequent chapters and Appendix A), we represent conditions as functions of variables, symbolised as ϕ. The particularity of these functions is that they exclusively yield values of 0 or 1. Then, we define a necessary condition as a condition that is valid (i.e. equal to 1) for all near-optimal solutions. Formally, if $\mathcal{X}^\epsilon$ designates an ϵ-optimal space and ϕ characterises a condition, then ϕ is a *necessary condition* for ϵ-optimality if it holds true for every solution within $\mathcal{X}^\epsilon$, i.e.

$$\forall \mathbf{x} \in \mathcal{X}^\epsilon : \phi(\mathbf{x}) = 1 \quad . \tag{1.7}$$

To summarise this section, this thesis positions its focus on near-optimal space exploration. While most methodologies in this sphere focus on identifying alternative solutions, our research diverges by probing the commonalities among these alternatives. This is achieved through techniques tailored to discern necessary conditions. This nuanced perspective aligns seamlessly with our broader goal: to enrich the nuanced human discussions at the heart of decision-making, even in contexts steeped in mathematical rigour.

In the upcoming section, we will delve into the specific scenarios linked to the energy transition where we employed these methodologies and elucidate the particular types of necessary conditions we aimed to uncover.

1.3 Making Choices for the Energy Transition

The energy transition is one of the most pressing challenges of our time, representing a complex interplay between technological innovation, political regulation, social acceptance, and environmental responsibility. As the world grapples with the urgent need to reduce carbon emissions and embrace sustainable energy solutions, the path towards an efficient and resilient energy system is fraught with uncertainty and multidimensional objectives.

Mathematical optimisation is a powerful tool to help us make decisions in this complex area. This thesis uses this tool to address two specific questions about the energy transition in Europe and Belgium. We go beyond the usual limitations of energy system optimisation models by using necessary conditions, providing valuable answers to guide decision-making.

The following sections delve into the complexities of choosing future energy systems, explaining why optimisation models are well-suited for addressing the questions at hand and examining the strengths and weaknesses of Energy System Optimisation Models (ESOMs). Ultimately, we detail the type of necessary conditions we determine to help make relevant choices regarding these questions.

Choosing future energy systems

The energy transition challenge is rooted in complex decisions encompassing a range of technological, political, and social factors. In the context of this thesis, our investigation centres on two pivotal questions:

1. What type of power system is required in Europe to reduce carbon emissions effectively?

2. Which strategies should be implemented to ensure the sustainability of the entire energy system in Belgium?

These probing inquiries, integral to regional and global sustainability, have been the subject of rigorous research in the existing literature [PHK14]. They form the foundational pillars of the case studies examined in the articles that constitute our research.

Using mathematical programming for planning the energy transition

Mathematical programming emerges as an ideal tool to tackle complex questions that pervade various domains, particularly in the context of energy systems.

The primary reason for its suitability lies in a shared characteristic among the two addressed questions: they present a broad spectrum of potential answers stemming from the interplay of two intricate factors.

Firstly, there is a multitude of available technologies that can satisfy the same energy demand. For instance, low-carbon electricity can be generated through various means, such as nuclear power plants, solar panels, wind turbines, or gas plants equipped with carbon capture, utilisation, and storage (CCUS) technologies. This multifaceted landscape extends to whole-energy systems, where cars might be fueled by electricity, hydrogen, or other e-fuels, and houses can be heated using electricity or low-carbon synthetic gas.

Secondly, there are numerous ways in which the different components of the system can be configured and interconnected. For instance, questions arise regarding the number and capacity of wind turbines to deploy, their optimal locations, and the necessary storage backup, among others. When examining the entire energy system, we could be confronted with whether synthetic methane should be produced locally or remotely, utilising CO2 captured on-site or remotely [Dac+23], and whether to use on-site or imported hydrogen.

From a mathematical perspective, the feasible solution space is vast. Mathematical optimisation is inherently tailored to sift through such expansive realms of possibilities, pinpointing the most suitable choices.

A further rationale for the aptness of mathematical programming is its capability to seamlessly incorporate objectives into the decision-making process. The questions under scrutiny often have multifaceted implications spanning economic, ecological, and social dimensions. Through optimisation, we can systematically traverse the spectrum of potential solutions, aligning them with these diverse objectives to ensure a holistic approach to problem-solving.

Energy System Optimisation Models

The suitability of this tool for addressing energy modelling questions has not only inspired a multitude of researchers to adopt it but has also led to the definition of a distinct category of energy system models within the community, known as Energy System Optimisation Models, or ESOMs [PHK14]. As defined by DeCarolis et al. [DeC+17], by employing optimisation techniques, ESOMs enable us to identify the optimal combination, arrangement, and operation of technologies and resources necessary to achieve a specific objective (e.g. meeting some energy demand at minimum cost) within predetermined technological (e.g. power plant ramping limits) and societal (e.g. limiting greenhouse gas emissions) constraints.

The widespread use of ESOMs in energy modelling is well-founded, as highlighted by a series of strengths identified by DeCarolis et al. [DeC+17]:

1. They provide a consistent accounting framework that clearly defines the techno-economic performance characteristics across all modelled processes, ensuring uniformity and precision.

2. They enable the quick and efficient pursuit of normative goals, even within the most intricate and multifaceted systems.

3. They can illustrate diverse energy futures, aligning with and reflecting the broader objectives of energy and environmental policies.

4. They can encapsulate interactions between different sectors, yielding comprehensive and cross-cutting insights that are often elusive when confined to models targeting specific sectors.

Limitations of ESOMs

However, while these models excel at determining the optimal combination of technologies and resources based on a specific objective, they often fail to address our subjective, personal ideologies and values.

As stated by Pfenninger et al. [PHK14] “energy systems models are neither certain nor value-free; rather, they are situated in an area where both the decision stakes and the system uncertainties are high. They are, therefore, examples of *post-normal science*, which implies seeking a diverse set of opinions, including from non-experts."

Post-normal science [Rav99] recognises the limitations of traditional scientific practices in addressing complex issues where facts are uncertain, and *values are disputed*. In the context of energy systems models, this approach acknowledges that there may be no clear ‘right’ decision and that *ethical and social considerations play a significant role*. Rather than relying solely on conventional scientific inquiry, post-normal science calls for a broader, more inclusive dialogue that integrates diverse preferences, *including those of non-experts*.

These limitations are intimately tied to the inherent structural uncertainty present in ESOMs, as highlighted by Yue et al. [Yue+18]. The sources of this uncertainty are multifaceted and can include, for example, “the default ESOM formulation that ignores the heterogeneity among decision-makers in the energy system, the manner in which non-economic considerations factor into energy purchasing decisions, and the role that politics, social norms, and culture play in shaping public policy."

Employing necessary conditions to accommodate diverse preferences

Using methodologies to incorporate diverse preferences in energy system optimisation is thus indispensable. As mentioned above, multi-objective techniques in mathematical programming can accommodate multiple aims. However, these techniques often fall short in integrating non-economic, ethical and social considerations or preferences from non-experts. This shortcoming is often attributed to the inherent difficulty in quantifying or precisely modelling these factors.

Instead of attempting to encompass all preferences through modelling alone, we propose that embracing the concepts of near-optimal space and necessary conditions offers a more robust solution.

Exploring the near-optimal space can unearth solutions that, although less optimal per the modelled objectives, might align well with unmodelled ones. This potential is precisely why there has been a revival in the use of the MGA methodology in energy system modelling, as evidenced by the works of DeCarolis [DeC11] and DeCarolis et al. [DeC+16]. Such endeavours have invigorated interest in these techniques. For instance, James and Ilkka [JI17] pioneered new exploration algorithms, while Li and Trutnevyte [LT17] merged MGA with Monte-Carlo exploration aiming to reduce parametric uncertainty. Furthermore, the methodology's adaptability and robustness are highlighted by research such as Pedersen et al. [Ped+21], Neumann and Brown [NB21], and Grochowicz et al. [Gro+23], effectively employed MGA in strategising the evolution of energy systems.

Among this framework, the computation of necessary conditions is a methodology that can elucidate factors that guarantee a specific degree of performance for the optimised objectives while providing room for discussions that can integrate unmodeled factors. This strategic approach is at the core of the three articles constituting this thesis's contributions.

In their basic formulation, briefly presented in the previous section, conditions are typically functions with binary outcomes. In our work on energy systems, the focus was directed towards a particular type of condition, which yields distinct insights highly pertinent for energy system optimisation. Specifically, we zeroed in on conditions framed as constrained sums of variables: $\sum_{i=1}^{n} d_i x_i \geq c$, where $d_i \in 0, 1 \; \forall i$. This type of condition holds true if the cumulative variable values of a given solution surpass the real-valued threshold, denoted by $c \in \mathbb{R}$. A necessary condition is then obtained by determining the threshold that validates the condition across all solutions within a designated near-optimal space. This threshold ensures the attainment of a specific suboptimality level linked to this near-optimal space.

To provide context, let us examine a power system expansion scenario. Within this framework, we aim to determine the capacities of specific power plants, such as onshore wind turbines in Europe. As indicated in [DE22], the optimal capacities for these wind turbines might span several hundreds of GW. However, this capacity, while cost-effective, might not meet other objectives.

By computing an appropriate necessary condition, we can discern the least capacity needed for onshore wind turbines to attain a specific near-optimality level (characterised by the sub-optimality coefficient ϵ) in cost while giving leeway to other objectives. This necessary condition, modelled as the constrained sum of unknown wind turbine capacities, corresponds to the condition that is valid for all solutions whose objective value is not lesser than $(1+\epsilon)$ times the optimal objective value. The right-hand side c of this condition corresponds to the minimum capacity needed to be installed to ensure that the cost does not exceed this value. In the case study of Dubois and Ernst [DE22], this minimal value is 0 for a less than $\epsilon = 5$ per cent hike in cost.

In the initial article presented in this thesis, we unearthed similar insights for transmission, offshore wind, photovoltaic, and Li-Ion battery capacities, as referenced in [DE22]. The sequel [Dub+23] pivoted its focus onto resources, identifying the least local and imported resources necessary to optimise both cost and energy return on investment. The concluding paper [DE23] delves into the impacts of spatio-temporal resolution on necessary conditions.

1.4 Roadmap

In this introduction, we have charted the thought process that directed our attention to the formalisation of necessary conditions aimed at enhancing decision-making and their application within the energy transition context.

The rest of this thesis is structured around the three articles that collect the contributions of this thesis. These are in order of publication:

- *Computing necessary conditions for near-optimality in capacity expansion planning problems* [DE22] by Antoine Dubois and Damien Ernst, published at the 2022 Power Systems Computation Conference in Porto.
- *Multi-objective near-optimal necessary conditions for multi-sectoral planning* [Dub+23], by Antoine Dubois, Jonathan Dumas, Paolo Thiran, Gauthier Limpens and Damien Ernst, published in Applied Energy in 2023.

- *Impacts of spatial and temporal resolutions on the near-optimal spaces of energy system optimisation models* [DE23], by Antoine Dubois and Damien Ernst, published at the 2023 Innovative Smart Grid Technologies conference in Grenoble.

In what follows, each chapter is devoted to a specific article. Every chapter adheres to a consistent structure. It begins by pinpointing the central research question that drove the article, followed by an exposition of the idea for tackling this question. The latter part of each chapter presents the published version of the article. This is prefaced by an overview of the article's primary contributions, an account of the division of labour among the authors, and some reading pointers for those who may wish to skip or streamline certain sections.

In a nutshell, **Chapter 2** lays the foundational groundwork by introducing and formalising the concepts of epsilon-optimality and necessary conditions. This is illustrated through a study of power network expansion planning across Europe. **Chapter 3** broadens these concepts to encompass multi-objective optimisation. While the geographic focus narrows to Belgium, the study widens its sectoral lens to account for various energy carriers. Lastly, **Chapter 4** delves into the influence of model complexity on necessary conditions, conducting a detailed spatiotemporal analysis of the European power system reminiscent of the first article's focus.

Then, **Chapter 5** concludes this thesis by briefly revisiting the critical insights gleaned from the three presented papers and highlighting the myriad of research opportunities they unveil.

At the end of this thesis, two appendices have been included for additional understanding. The first, denoted as **Appendix A**, consolidates all the mathematical developments on near-optimal spaces and necessary conditions discussed throughout this thesis, providing readers with a centralised reference. The subsequent **Appendix B** outlines supplementary efforts that, although not directly contributing to the thesis's primary outcomes, played a foundational role in feeding our main research. These efforts led to the development of various software tools and the publication of the following articles:

- *Model Reduction in Capacity Expansion Planning Problems via Renewable Generation Site Selection* [Rad+21] by David Radu, Antoine Dubois, Mathias Berger, and Damien Ernst, presented at the 2021 IEEE Madrid PowerTech.

- *Siting renewable power generation assets with combinatorial optimisation* [Ber+22] by Mathias Berger, David Radu, Antoine Dubois, Hrvoje Pandžić, Yury Dvorkin, Quentin Louveaux, and Damien Ernst, published in Optimization Letters in 2022.

- *Assessing the impact of offshore wind siting strategies on the design of the European power system* [Rad+22] by David Radu, Mathias Berger, Antoine Dubois, Raphaël Fonteneau, Hrvoje Pandžić, Yury Dvorkin, Quentin Louveaux, and Damien Ernst, published in Applied Energy in 2022.

- *The energy return on investment of whole-energy systems: Application to belgium* [Dum+22] by Jonathan Dumas, Antoine Dubois, Paolo Thiran, Pierre Jacques, Francesco Contino, Bertrand Cornélusse, and Gauthier Limpens, published in Biophysical Economics and Sustainability in 2022.

2 Exploring near-optimal spaces

2.1 The Question

How do solutions that deviate slightly from optimality behave?

The question that brought us on the path of near-optimal space exploration appeared as we worked on the task of renewable power plants siting (see Appendix B for more detail on this research). During this research, we devised algorithms to pinpoint the most suitable locations across Europe for placing renewable assets according to different individual criteria. Given a sufficiently granular spatial resolution, this meant discerning optimal positions from potentially thousands of viable spots for hundreds of installations.

While our algorithms yielded singular cost-optimal solutions, they failed to elucidate if other solutions, slightly suboptimal, would suggest similar or divergent site recommendations. If the sets of recommended locations varied significantly for marginally different objective values, then the confidence in the conclusions drawn from the optimal set would be severely undermined. This prompted the following questions: How can we validate the robustness of our recommendations? Is there a way to algorithmically ascertain the consistency of these solutions?

2.2 The Idea

These questions first prompted our interest in 2020. Other people had asked themselves these questions before, and several others have since then, leading to a substantial increase in publications on near-optimal spaces and related techniques within the past three years.

However, we observed that many existing techniques fell short of providing clear insights. As previously noted, many aimed to generate an extensive set of alternative solutions. This approach has two main drawbacks: (i) it can be computationally demanding (with computational effort increasing with the number of alternative solutions sought), and (ii) it may not serve decision-makers effectively by overwhelming them with too many options.

Rather than focusing on generating many solutions, we reframed the problem. We aimed to determine how to derive valuable insights with minimal computational effort. This shift in perspective led us to conceptualise the idea of necessary conditions. These conditions spotlight elements shared across all alternative solutions, offering a streamlined approach and enabling efficient computational techniques for their identification.

2.3 The Paper: *Computing Necessary Conditions for Near-Optimality in Capacity Expansion Planning Problems*

This article was presented at the 22nd Power Systems Computation Conference held in Porto in June 2022.

2.3.1 Paper's contributions

This article marks the start of our exploration into near-optimal spaces and necessary conditions. Its primary contributions can be summarised as:

1. Establishing the mathematical framework for exploring near-optimal spaces.

2. Demonstrating how the necessary condition approach offers valuable insights into power system expansion planning.

2.3.2 Authors' contributions

This paper is a collaborative effort between Professor Ernst and myself. The research idea was initially presented by me, outlining the thought process discussed in Chapter 1. Together, we developed the mathematical formulation of ϵ-optimal spaces and necessary conditions. Additionally, I designed and conducted the experiments for the case study, demonstrating the methodology. The writing of the paper was primarily led by me, with supervision from Professor Ernst.

2.3.3 Reading tips

The material covered in Section III, “Problem Formulation", which introduces the concepts of ϵ-optimality and necessary conditions, and Section IV, “Proposed Method", which outlines the methodology for deriving necessary conditions, has been rephrased and included in Appendix A. Therefore, it may be redundant for readers who have already gone through this appendix. However, Section III can still be valuable for having a rapid understanding of the various concepts discussed in the presentation of the test case in Section V, “Test Case".

Computing Necessary Conditions for Near-Optimality in Capacity Expansion Planning Problems

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***Abstract*—In power systems, large-scale optimisation problems are extensively used to plan for capacity expansion at the supra-national level. However, their cost-optimal solutions are often not exploitable by decision-makers who are preferably looking for features of solutions that can accommodate their different requirements. This paper proposes a generic framework for addressing this problem. It is based on the concept of the epsilon-optimal feasible space of a given optimisation problem and the identification of necessary conditions over this space. This framework has been developed in a generic case, and an approach for solving this problem is subsequently described for a specific case where conditions are constrained sums of variables. The approach is tested on a case study about capacity expansion planning of the European electricity network to determine necessary conditions on the minimal investments in transmission, storage and generation capacity.**

***Index Terms*—Capacity expansion planning, decision-making, epsilon-optimality, necessary conditions, optimisation**

I. Introduction

In the coming decades, the European power system will have to face the challenges related to the integration of massive amounts of renewable energy sources and a high level of electrification of the heating, transport and industrial sectors.

The size and level of integration of the European electricity network (*i.e.*, at the transmission level, thousands of substations and power lines connecting them) entail a level of complexity in planning this transition that requires using detailed optimisation models. The increased sophistication of these models comes with drawbacks. In particular, these models essentially focus on unique cost-based optimal solutions that are too restrictive and do not encompass the different requirements of many stakeholders intervening in the decision process for new investments in capacity.

In our opinion, it is preferable to provide *necessary conditions* in capacity investments that guarantee a constrained suboptimality and provide a common ground over which decision-makers can settle and create solutions that accommodate their needs. For example, we could compute the minimum required investment in transmission lines per country to ensure a maximum deviation of 10% from the optimum. Alternatively, one might be interested in knowing if a particular technology - for example, Li-Ion battery or some renewable energy source (RES) type - is necessary for a cost-efficient energy transition.

In this paper, a framework is presented to derive necessary conditions for ϵ-optimality and applied to a capacity expansion planning problem. In Section II, we discuss the literature related to the optimisation concepts that underlie the framework. The optimisation framework itself is presented in Section III. Section IV specifies this framework to the case of conditions consisting of constrained sums of variables and provides a fully-defined methodology for computing *non-implied necessary conditions* in such a context. This methodology is afterwards illustrated on an expansion planning problem in Section V. Section VI concludes with the description of future research directions. Finally, Appendix A gathers more detailed data on the modelling of the network used in the test case.

II. Literature review

Decision-making based on optimisation results is a complex task. Indeed, this exercise lies at the frontier between human intelligence and machine power whose coupling is challenging [1], sometimes referred to as post-normal science [2]. Decision-making is linked to *deep uncertainties* [3] where, among other topics, the desirability of alternative outcomes corresponding to different policy objectives is subject to disagreement among stakeholders. These uncertainties and disagreements imply that relying on a single cost-based optimum is often not sufficient. Indeed, there is no guarantee that the findings obtained via this optimum will be robust regarding parameter perturbation, nor that they will satisfy conflicting objectives. Moreover, as shown in [4], cost-optimal scenarios are not adequate to approximate real-world problems, such as those encountered in the context of the energy transition. This problem highlights the need for the "role of optimisation model methods to be re-thought in full recognition of these limitations", as suggested in [5]. Those authors advocate optimisation methods that "should be used to generate planning alternatives, facilitate their evaluation and elaboration, provide insights and serve as catalysts for human creativity".

Antoine Dubois is a Research Fellow of the F.R.S.-FNRS, of which he acknowledges the financial support.

We argue that such a *re-thinking* can be achieved by orienting the use of optimisation methods in the search for conditions that are respected across multiple feasible solutions and guarantee a constrained level of suboptimality. The advantage of this approach over unique cost-optimal solutions is to provide decision elements that all stakeholders can agree on and built on using their creativity.

Those solutions can be obtained in a variety of ways. One possibility is the use of multi-objective (or multi-criteria) optimisation [6]. In this field, one searches not for a single solution but a set of *efficient* or *Pareto-optimal* solutions, translating some trade-offs between objectives. A notable drawback with these methods is the general assumption of knowing which objectives are at stake in the problem and being able to model in some form those objectives. Objectives that are a priori unknown (either because of lack of knowledge or unconscious biases) or non-modellable are, thus, left apart.

A technique that circumvents this limitation is what some authors refer to as *"Modeling to Generate Alternatives"* [7]. It consists of exploring solutions located in the inferior or suboptimal region of an optimisation problem [8]. The underlying motivation of this approach is that this region might contain solutions that are better in terms of some unmodelled objectives. Several authors, such as [9], [10], [11], [12] or [13], exploit this technique. However, their main objective is to show the variety of solutions that can be extracted rather than to systematically compute conditions that are respected by those solutions. In this paper, we present a framework that puts the identification of such conditions at the centre of the optimisation process.

Finally, in the domain of multi-objective optimisation, [14] have surveyed advanced data-driven methods for extracting *commonalities* among Pareto-optimal solutions. Our framework aims at providing the ground for developing such techniques in suboptimal spaces.

III. Problem Formulation

Let us consider the following optimisation problem

$$\min_{x \in \mathcal{X}} f(x) \tag{1}$$

with $\mathcal{X}$ being the feasible space and $f : \mathcal{X} \rightarrow \mathbb{R}^+$ the objective function. Let x^* be an optimal solution. We define an ϵ-*optimal space* as follows:

$$\mathcal{X}^\epsilon = \{x \in \mathcal{X} \mid f(x) \leq (1+\epsilon)f(x^*), \epsilon \geq 0\}.$$

The set $\mathcal{X}^\epsilon$, depicted in Figure 1, contains only the feasible solutions with an objective value no greater than $(1+\epsilon)f(x^*)$. We define ϵ as the *suboptimality coefficient* of such a space, *i.e.* specifying by how much the objective values of the solutions in the space deviate at most from the optimal objective value.

Let us define *conditions* as functions $\phi : \mathcal{X} \rightarrow \{0, 1\}$. Our goal is to identify, among a set Φ of conditions, the ones which are true for any solutions in $\mathcal{X}^\epsilon$. These conditions are called

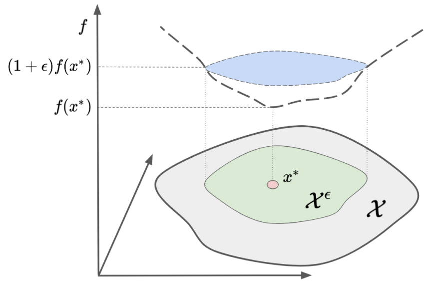


Fig. 1. Three-dimensional representation of an ϵ-optimal space. In the horizontal plane, the space of feasible solutions $\mathcal{X} \subset \mathbb{R}^2$ is depicted while the vertical axis represents the objective function. The red dot is the optimal solution x^* corresponding to the minimal value of the objective function over the feasible space. The blue space coincides with the hyper-plane $f(x) = (1+\epsilon)f(x^*)$ allowing one to determine the ϵ-optimal space $\mathcal{X}^\epsilon$ shown in green.

necessary conditions for ϵ-optimality, where the parameter ϵ allows one to monitor the level of suboptimality of those necessary conditions. Mathematically,

$$\Phi^{\mathcal{X}^\epsilon} = \{\phi \in \Phi \mid \forall x \in \mathcal{X}^\epsilon : \phi(x) = 1\}$$

is the set of necessary conditions for a given feasible space $\mathcal{X}$, sets of conditions Φ and suboptimality coefficient ϵ.

A. Non-implied necessary conditions on sets of parametric conditions

The goal of the methodology presented in this paper is to support decision-makers in their decision process. However, as explained in the next paragraph, even for a single set of conditions, an infinite number of necessary conditions can be derived. Such quantity of information can not be used efficiently to take decisions. In this section, the concept of *non-implied necessary condition* is introduced as a solution to this problem.

Let consider the feasible space $\mathcal{X} = \mathbb{R}$ and and a set of parametric conditions of the type

$$\Phi = \{\phi_c(x) := x \geq c | c \in \mathbb{R}\}.$$

This set contains an infinite number of conditions and can lead to identifying an infinite number of necessary conditions, with which decision-makers might find it cumbersome to deal.

For instance, let $\phi_1(x) := x > 1$ be a necessary condition for ϵ-optimality (*i.e.* $\forall x \in \mathcal{X}^\epsilon : \phi_1(x) = 1$). This automatically *implies* that all ϕ_c where $c < 1$ are necessary conditions. Indeed $\forall x \in \mathcal{X}^\epsilon : x > 1 \Rightarrow x > c$. The only condition that cannot be implied to be a necessary condition from the knowledge of other necessary conditions is the necessary condition ϕ_c with the largest value of c.

This necessary condition is what constitutes a *non-implied necessary condition*. This is a condition that cannot be *implied* to be a necessary condition from the sole knowledge of other conditions that constitute necessary conditions. To minimise the number of necessary conditions that need to be identified and presented to decision-makers, the focus should be placed on the identification of non-implied necessary conditions.

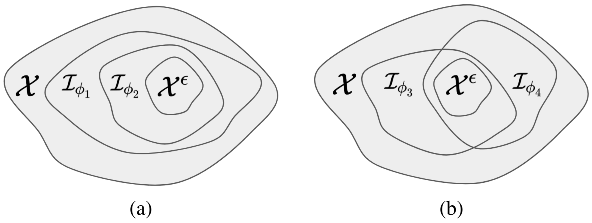


Fig. 2. Graphical illustration of implication using spaces over which conditions are true.

The notion of implication can be formalised by defining the space over which a condition ϕ is true,

$$\mathcal{I}_{\phi} = \{x \in \mathcal{X} \mid \phi(x) = 1\}.$$

A condition ϕ_2 implies ϕ_1 if $\mathcal{I}_{\phi_2} \subset \mathcal{I}_{\phi_1}$, *i.e.* ϕ_1 is true for all $x \in \mathcal{X}$ over which ϕ_2 is true. Considering sets of parametric conditions, $\mathcal{I}_{\phi_2} = \mathcal{I}_{\phi_1}$ happens only if both conditions are equal. Using this notion, conditions can be defined to be necessary conditions if the space over which they are true encloses $\mathcal{X}^{\epsilon}$, and non-implied necessary conditions if this space does not include any of the spaces over which other necessary conditions are true. Mathematically, the set of non-implied necessary conditions for ϵ-optimality is defined as

$$\overline{\Phi}^{\mathcal{X}^{\epsilon}} = \{\phi \in \Phi^{\mathcal{X}^{\epsilon}} \mid \forall \phi' \in \Phi^{\mathcal{X}^{\epsilon}} \setminus \{\phi\} : \mathcal{I}_{\phi'} \not\subset \mathcal{I}_{\phi}\}.$$

Figure 2a provides an illustration of two necessary conditions ϕ_1 and ϕ_2, with ϕ_2 implying ϕ_1. Considering a set of conditions $\Phi = \{\phi_1, \phi_2\}$ containing uniquely ϕ_1 and ϕ_2, the set of necessary conditions is given by $\Phi^{\mathcal{X}^{\epsilon}} = \{\phi_1, \phi_2\}$, and the set of non-implied necessary conditions by $\overline{\Phi}^{\mathcal{X}^{\epsilon}} = \{\phi_2\}$. Figure 2b provides an illustration of two other necessary conditions ϕ_3 and ϕ_4, with no implication. Considering a set of conditions $\Phi = \{\phi_3, \phi_4\}$, then $\overline{\Phi}^{\mathcal{X}^{\epsilon}} = \Phi^{\mathcal{X}^{\epsilon}} = \Phi$.

IV. Proposed Method

In this section, a specific instance of the generic problem specified in Section III is considered. This instance is characterised by conditions consisting of parametric constrained sums of variables. We show how for each value of the parameter defining these sums, a unique non-implied necessary condition can be determined.

Theorem 1. Let $\mathcal{X} \subset \mathbb{R}^n$, $f : \mathcal{X} \to \mathbb{R}^+$ and

$$\Phi_{\mathbf{d}} = \{\phi^c_{\mathbf{d}}(\mathbf{x}) \coloneqq \mathbf{d}^T\mathbf{x} \geq c \mid c \in \mathbb{R}\},$$

where $\mathbf{x} \in \mathcal{X}$, be a set of conditions consisting of constrained sums of variables $\mathbf{d}^T\mathbf{x} = \sum_{i=1}^{n} d_i x_i$ defined by $\mathbf{d} \in \{0,1\}^n$. Let $c^* = \min_{\mathbf{x} \in \mathcal{X}^{\epsilon}} \mathbf{d}^T\mathbf{x}$ then

$$\phi^{c^*}_{\mathbf{d}} \coloneqq \mathbf{d}^T\mathbf{x} \geq c^*$$

is the only element in the set of non-implied necessary conditions $\overline{\Phi}^{\mathcal{X}^{\epsilon}}_{\mathbf{d}}$.

Proof. Let us first show that the set of necessary conditions is equal to

$$\Phi^{\mathcal{X}^{\epsilon}}_{\mathbf{d}} = \{\phi^c_{\mathbf{d}} | c \leq c^*\}.$$

By definition,

$$c^* = \min_{\mathbf{x} \in \mathcal{X}^{\epsilon}} \mathbf{d}^T\mathbf{x}$$

is the smallest value that $\mathbf{d}^T\mathbf{x}$ can take over $\mathcal{X}^{\epsilon}$. This implies that

$$\phi^{c^*}_{\mathbf{d}}(\mathbf{x}) \coloneqq \mathbf{d}^T\mathbf{x} \geq c^*$$

is true for all $\mathbf{x} \in \mathcal{X}^{\epsilon}$. Similarly, if $c < c^*$, we know that

$$\mathbf{d}^T\mathbf{x} \geq c^* > c$$

is true for all $\mathbf{x} \in \mathcal{X}^{\epsilon}$. Thus, all conditions $\phi^c_{\mathbf{d}}$ such that $c \leq c^*$ are necessary conditions. For $c > c^*$ however, at the optimum $\mathbf{x}^*_{\epsilon} = \arg\min_{\mathcal{X}^{\epsilon}} \mathbf{d}^T\mathbf{x}$, we have

$$\mathbf{d}^T\mathbf{x}^*_{\epsilon} = c^* < c$$

which implies that the condition

$$\phi^c_{\mathbf{d}}(\mathbf{x}) \coloneqq \mathbf{d}^T\mathbf{x} > c$$

is not true for all $\mathbf{x}$ in $\mathcal{X}^{\epsilon}$, as $\mathbf{x}^*_{\epsilon} \in \mathcal{X}^{\epsilon}$. Therefore, all conditions $\phi^c_{\mathbf{d}}$ such that $c > c^*$ are not necessary conditions.

Now let us prove

$$\overline{\Phi}^{\mathcal{X}^{\epsilon}}_{\mathbf{d}} = \{\phi^{c^*}_{\mathbf{d}}\}.$$

This means that all $\phi^c_{\mathbf{d}}$ with $c < c^*$ are implied by and do not imply $\phi^{c^*}_{\mathbf{d}}$. This can be shown by proving that, for any $c < c^*$,

$$\mathcal{I}_{\phi^{c^*}_{\mathbf{d}}} \subset \mathcal{I}_{\phi^c_{\mathbf{d}}} \text{ and } \mathcal{I}_{\phi^c_{\mathbf{d}}} \not\subset \mathcal{I}_{\phi^{c^*}_{\mathbf{d}}}.$$

We have $\mathcal{I}_{\phi^{c^*}_{\mathbf{d}}} \subset \mathcal{I}_{\phi^c_{\mathbf{d}}}$ because, as shown before, for any $\mathbf{x}$, if $\phi^{c^*}_{\mathbf{d}}(\mathbf{x})$ is true, $\phi^c_{\mathbf{d}}(\mathbf{x})$ with $c < c^*$ is also true. Moreover, $\mathcal{I}_{\phi^c_{\mathbf{d}}} \not\subset \mathcal{I}_{\phi^{c^*}_{\mathbf{d}}}$. Indeed, the element $\mathbf{x}$ such that

$$\mathbf{d}^T\mathbf{x} = c$$

is an element of $\mathcal{I}_{\phi^c_{\mathbf{d}}}$ but not of $\mathcal{I}_{\phi^{c^*}_{\mathbf{d}}}$.

□

V. Test Case

This methodology will now be applied to a specific test case. The test case is articulated around the problem of capacity expansion planning of the European electricity grid within the objective of the European Union to be carbon-neutral by 2050. Typically, the objective of this problem is to determine capacity investments in transmission, generation and storage assets as well as operation of those assets to satisfy electrical demand while minimising capital and marginal costs.

Decision-makers might be interested in knowing the necessary conditions on the required amount of capacity to be invested in each of those technologies at the European and national levels to ensure that they do not experience more than a well-specified level of cost-suboptimality.

Our methodology will be applied to this problem for computing non-implied necessary conditions for achieving ϵ-optimality on five technologies. More specifically, required minimum investments are first computed for groups of lines at the European, national and individual-line levels. Then, necessary conditions are determined for storage and RES generation, including onshore wind, offshore wind, and utility-scale PV, over the whole network.

In the following section, a short contextualisation of the test case is presented. The test case is then defined following the terms of the methodology presented above. It is followed by a short analysis of the optimal solution of the expansion planning problem before describing necessary conditions.

A. Context

The geographical scope of the expansion planning problem is set to Europe. All countries in the European continent are included, except for Russia, Iceland and some small countries such as Cyprus, Malta and Liechtenstein. In this problem, the network is represented as a grid made up of nodes and lines. When applied at the European level, nodes are generally clustered by country while lines correspond to aggregations of pre-existing or planned transmission lines between these countries. Figure 3a shows the nodes and lines forming the network. In addition, generators and storage devices are attached to each of those nodes. The temporal scope of the problem is set to one full year, corresponding to the year 2050. More details on the modelling of the network can be found in Appendix A.

B. Optimisation problem

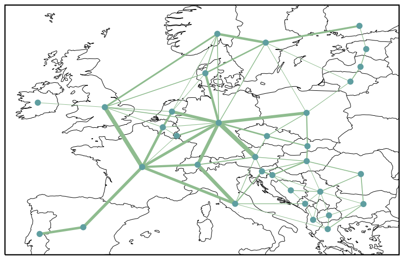
The expansion planning problem is solved using linear optimisation via the open-source tool PyPSA [15]. In this context, the elements composing problem (1) are described briefly below.

Objective function f. The objective of the problem is to minimise the total annual system cost. To be more specific, the objective function f corresponds to the sum of annualised capital fixed costs and variable costs of generation, storage and transmission across the network.

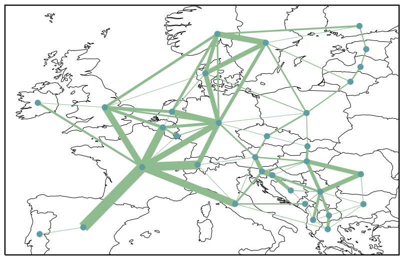
Feasible space $\mathcal{X}$. The feasible space can be modelled as $\mathcal{X} = \{\mathbf{x} \in \mathbb{R}^n | A\mathbf{x} \geq \mathbf{b}, A \in \mathbb{R}^{m \times n}, \mathbf{b} \in \mathbb{R}^m\}$ with $m \in \mathbb{N}$ and $n \in \mathbb{N}_0$. The variables $\mathbf{x}$ correspond to investment (*i.e.* how much capacity must be added where and to what technology) and operational variables (*e.g.* which quantity of energy each generator must produce at each time step). All variables are continuous, as investments are continuous and unit commitment is not modelled. The bounds on those variables are composed via technical and physical constraints modelled as linear constraints. In addition, a constraint imposing a 99% reduction on CO2 emissions compared to 1990 levels is added. This value is set Europe-wise and is not set to 100% to ensure the feasibility of the problem.

Set of conditions Φ. As in Section IV, to compute non-implied necessary conditions corresponding to minimum capacity investments, sets of conditions of form

$$\Phi_{\mathbf{d}} = \{\mathbf{d}^T \mathbf{x}_I \geq c \mid c \in \mathbb{R}\}$$



(a) Initial capacity.



(b) Additional capacity to be cost-optimal.

Fig. 3. European electricity grid representation with the width of lines proportional to capacity in GW.

are used, with $\mathbf{x}_I$ a vector of size $|I|$ that collects the different investment variables and $\mathbf{d} \in \{0,1\}^{|I|}$. Depending on the type of investment variables for which a non-implied necessary condition is desired, it suffices to define an appropriate $\mathbf{d}$, *i.e.* whose elements corresponding to the required variables are set to 1, and others to 0.

Suboptimality coefficient ϵ. As mentioned above, necessary conditions are valid for a given value of the suboptimality coefficient ϵ. In this study, necessary conditions are computed for different values of ϵ - ranging from 0% (*i.e.* optimality) to 20% - to see how minimal capacity investment evolves with the suboptimality coefficient.

Computation of non-implied necessary conditions. As a reminder, the computation consists in the following steps:

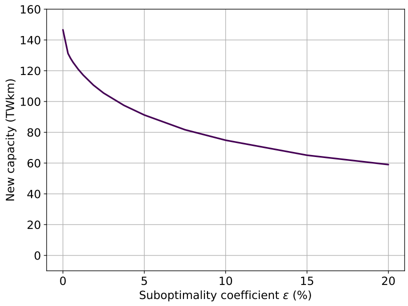
1) Compute an optimal solution $\mathbf{x}^*$ for problem (1).
2) For a given suboptimal coefficient ϵ, compute an ϵ-optimal space $\mathcal{X}^\epsilon$ using this solution.
3) For this ϵ and a value of $\mathbf{d}$, extract a non-implied necessary condition by solving $\min_{\mathbf{x} \in \mathcal{X}^\epsilon} \mathbf{d}^T \mathbf{x}$.
4) Repeat step (2) and (3) to obtain non-implied necessary conditions for different values of ϵ and $\mathbf{d}$.

C. Optimal solution.

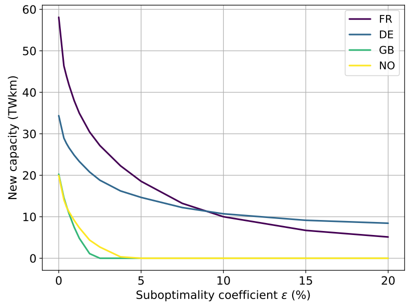
Figure 3 shows the initial topology - with the widths of lines proportional to their capacity in GW - and how much capacity should be added to be optimal (*i.e.* obtained from $\mathbf{x}^*$). Table I lists the optimal capacities for the technologies that are expanded in the problem. Capacities of lines are expressed in TWkm, *i.e.* the power capacity installed over a given distance.

TABLE I
OPTIMAL CAPACITIES.

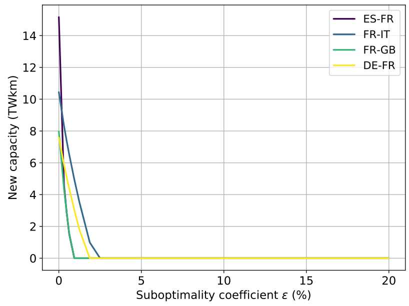
TWkm			GW					
AC	DC	AC+DC	Onshore wind	Offshore wind	Utility PV	CCGT	OCGT	Li-Ion
128	90	218	168	327	367	49	0	249



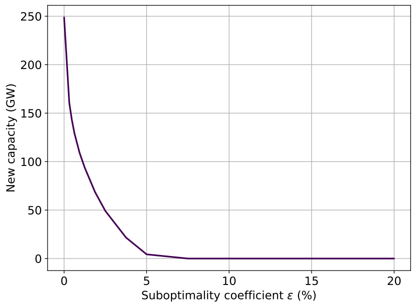
(a) Sum of the capacities of all lines.



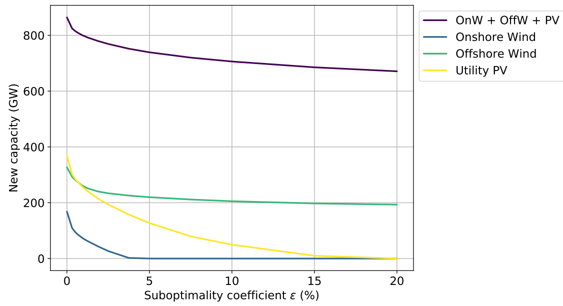
(b) Sum of the capacities of country lines.



(c) Capacity of individual lines.



(d) Sum Li-Ion batteries capacities.



(e) Sum of renewable energy generators capacities (onshore wind, offshore wind, utility PV and sum of the three).

Fig. 4. Non-implied necessary conditions on new capacity for different levels of suboptimality.

For transmission, with the addition of 146 TWkm of lines, the initial 72 TWkm is tripled. Capacity is added to almost all lines, but major investments are made in some countries like Germany and France. In these particular cases, the sums of the optimal capacities of the lines connected to the country are equal to 79 TWkm (from an initial capacity of 21 TWkm) and 57 TWkm (from 23 TWkm).

The capacities of RES, including onshore wind, offshore wind and utility PV, are massive, reaching 862 GW across the three technologies. Gas plants are also deployed though on a smaller scale due to the constraint on CO2 emissions. Finally, a substantial amount of Li-Ion batteries is built all around Europe with the main hub being in Spain where a lot of PV is also deployed. Note that the initial capacity of these technologies (*i.e.*, RES, storage and gas) are null.

From this optimal solution, the ϵ-optimal spaces corresponding to the values of ϵ listed in the previous section are defined and necessary conditions for transmission, Li-Ion storage and RES generation are computed.

D. Necessary conditions on transmission capacity

In this case, the variables of interest correspond to transmission capacity variables, *i.e.* how much capacity - in TWkm - should be added to each line. We minimise capacity in TWkm (*i.e.* the power capacity of the line multiplied by its length) because this value is a good representative of both the physical and economic investments in transmission assets. Necessary conditions are first computed for the sum of capacities of all lines in the network. The analysis is then refined by looking at the sum of capacities of lines connected to a given country and, finally, at the capacities of unique lines.

Whole network. The first non-implied necessary conditions to be ϵ-optimal consist of the required minimum capacity to be added to the whole network. These are obtained by setting to one all values of $\mathbf{d}$ corresponding to transmission capacity investment variables. The other values of $\mathbf{d}$ are set to zero.

Figure 4a shows the values of the required new capacity to sustain a certain ϵ-optimality for different values of ϵ. The required new capacity drops rapidly for small values of ϵ and, for a suboptimality coefficient ϵ of 10%, it has already been divided by a factor two compared to the optimum. However, for larger ϵ, the decrease slows down, and the necessary conditions start reaching a slowly decreasing plateau around 60 TWkm.

National lines. These first results show how much capacity should be added to the initial network to keep costs above a certain ϵ-optimality. National transmission system operators could also be interested in the minimum capacity required to connect their country to the rest of the system. It can be identified by setting all values in $\mathbf{d}$ to zero except for those corresponding to the lines connected to a given country, in which case they are set to one.

Figure 4b focuses on the four countries with the highest added incumbent capacity (in TWkm) in the optimal solution. In decreasing-capacity order, those are France, Germany, Great Britain and Norway. For the two last ones, the necessary additional capacity converges to 0 TWkm for a suboptimality coefficient ϵ of less than 5% even though they had around 20 TWkm of new installed capacity in the optimal solution. France and Germany start from an even higher capacity level in the optimal solution, with 58 and 34 TWkm of added incumbent capacity. When the coefficient ϵ reaches 20%, they still have a non-zero additional capacity, with respectively 5 and 8 TWkm, but the decrease is greater than 90% for France and 75% for Germany.

Individual lines. Necessary conditions can be used to identify critical lines in the network. In this case, only one value in $\mathbf{d}$ is set to 1. Figure 4c shows the value of the necessary conditions for the four lines with the largest capacity increase (in TWkm) in the optimal solution: ES-FR, FR-IT, FR-GB, and DE-FR.

The main conclusion drawn from this graph is that no individually line needs to be necessarily expanded to avoid a suboptimality greater than 2.5%.

E. Necessary conditions on storage capacity

In the model, there is no pre-existing storage capacity and investment can be made at each bus. In the optimal set-up, 249 GW of Li-ion batteries are built and store 98 TWh over the simulated year. However, Figure 4d shows the necessary condition reaches 0 GW for a suboptimality coefficient ϵ as small as 5%.

F. Necessary conditions on RES capacity

Finally, investments in renewable energy sources, including onshore and offshore wind turbines and utility-scale PV panels, are analysed. Four types of necessary conditions are computed: one per technology corresponding to the required minimum in new capacity for that technology and one for the required minimum in the sum of capacities in the three technologies. As for storage, a greenfield approach is used and the new capacity is equal to the total capacity that is installed.

Figure 4e shows that investments in renewable energies are essential as the minimum capacity required to be ϵ-optimal does not drop below 600 GW even as the suboptimality coefficient ϵ rises to 20%. However, this is less clear for each RES technology individually. While the minimum requirement for offshore wind stays consistent with increasing values of the suboptimality coefficient ϵ, the necessary conditions for onshore wind and utility PV converge to 0 GW.

VI. Conclusion and Future Work

In this paper, a framework offering a change of focus for optimisation model methods was presented and applied for capacity expansion planning. Deviating from cost-optimal focused studies, we advocate for the search of non-implied necessary conditions for ϵ-optimality to inform decision-makers efficiently.

The concepts required to define this search in a generic case were formalised. A methodology was then presented to derive necessary conditions in the specific context where conditions consist of constrained sums. Finally, to illustrate the framework, this methodology was applied to a test case related to capacity expansion planning at the European level, focusing on the minimum investments in transmission, storage and generation required for ϵ-optimality.

This work sets the ground for further developments of the presented framework. First, the framework was specified for a fixed set of parameters that define the shape of the feasible space $\mathcal{X}$ and of the objective function f. Changing the value of the parameters could thus impact $\mathcal{X}$ and f, and in turn, the optimal solution and the ϵ-optimal spaces $\mathcal{X}^{\epsilon}$. As a result, there is no guarantee that necessary conditions found for a fixed set of parameters would remain the same for a different set of parameters. The concept of necessary conditions could thus be extended to overcome this limitation by defining sets of *meta*-necessary conditions valid for different sets of parameters. Determining such necessary conditions and providing guarantees on implications would require more advanced techniques than the one presented in this article.

Second, in this paper, we only presented an algorithmic solution for computing non-implied necessary conditions in the context where conditions consist of constrained sums of variables. It would be interesting to propose algorithmic solutions for other types of conditions.

Third, while we focused on cost-based ϵ-optimality, this concept and the one of necessary conditions can naturally be extended to other objectives.

Finally, it would be interesting to investigate whether other fields than capacity expansion planning could benefit from the framework introduced in this paper.

Appendix

Modelling and optimising the network is done using PyPSA [15] in conjunction with REplan [16].

A. Topology - Buses and Lines

The initial topology of the network is based on the TYNDP18 2027 reference grid developped by ENTSO-E [17]. It consists of bi-directional net transfer capacities (NTC) between countries or regions inside countries. To obtain a one-node-per-country topology, nodes are clustered per country, outgoing lines capacities are summed, and intra-country lines are removed.

Connections are modelled as bi-directional links using a transportation model. The initial capacity of each line is set to the maximum of both NTCs. Lines crossing seas are considered to be HVDC cables, while other lines are represented as HVAC lines. For simulating the N-1 stability constraint, the maximum power flow across any line is set to 70% of its installed capacity (as suggested in [18]).

For keeping the expansion realistic, an upper bound is fixed on the maximum capacity per line. This upper bound is set based on the NTCs of the 'Global Climate Action 2040' scenario of TYNDP2018. However, to provide some slack to the model, this capacity is multiplied by a pre-defined factor of 3. Note that for a multiplication factor equal to 2, around 5% of the load was shed in the optimal solution.

B. Load

The model is solved at a 2-hourly resolution. At each time step, the load must be satisfied or, is shed for a cost of 3k€/MWh. Hourly load series per country are extracted from the Open Power System Data project [19]. The reference year used in this model is 2018.

C. Generation and Storage Technologies

The model contains generation and storage technologies. For each technology, one representative plant is used per node where the pre-existing capacity or capacity expansion potential is not null. As detailed below, some of these technologies are expandable and others are not.

Technologies with expandable capacity. Dispatchable capacity can be deployed in the form of CCGT and OCGT. They are the only technologies that produce CO2 emissions when generating electricity.

Short-term storage can be built as Li-Ion batteries. Those batteries are characterised by two elements: their peak power capacity and the maximum duration during which they can discharge this power. In the test case, this second element is fixed to 4 hours and multiplying by the peak power gives the storage capacity of the battery.

For these three technologies, no initial capacity and no upper limit on the amount of new capacity are considered.

Three types of renewable energy sources are added to the model: onshore wind generators, offshore wind generators and utility-scale PV power plants. The per-country capacity factors profiles are obtained through Renewables.ninja, presented in [20], [21], while expansion potential are computed via GLAES [22]. GLAES is parametrised such that, on a cumulative basis, a maximum of 447 GW can be built for onshore wind, 1077 GW for offshore wind and 1150 GW for PV. No initial capacity is considered. The energy produced by those generators can be curtailed without incurring any supplementary cost.

Technologies with fixed capacity. New investments in nuclear power are not considered. Generators in Belgium and Germany, and those commissioned before 1980, are removed from the model. Using the JRC Open Power Plants database [23], this leads to 94GW of capacity which is in line with the projections made in the 2016 EU Reference Scenario [24].

Hydro-power is modelled through the addition of pre-existing run-of-river generators with a capacity of 34 GW, reservoirs with 105 GW and pumped-hydro storage with 55 GW. Capacities and locations around Europe are extracted from the JRC Hydro-power plants database [25]. For more information on the modelling of input flows, the interested reader can refer to the supplementary material of [26].

D. Input parameters and data

All experiments can be reproduced using the code which is available at [27]. The input data used for generating the results presented in this paper can be retrieved in [28] and is preprocessed using the open-source tool EPIPPy [29]. The repository also contains the output of the PyPSA runs and a document describing the techno-economic parameters used in the model and the sources from which they were determined.

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3 Expanding the exploration to multiple objectives

3.1 The Question

How to expand near-optimal space exploration techniques to multi-objective spaces?

In 2021, our collaborative efforts with the Catholic University of Louvain (UCLouvain) led us to explore the energy return on investment (EROI) concept. Scholars from this institution had already examined the implications of maximising this metric on Belgium's electricity storage requirements [LJ18]. This partnership enabled us to broaden the scope of the study, encompassing entire energy systems and juxtaposing EROI-based analysis with cost-focused evaluations. The output of this joint research was captured in the work by Dumas et al. [Dum+22], which is elaborated upon in Appendix B.

While independent evaluations of both cost and EROI objectives offer valuable insights, the availability of multi-objective techniques presents an opportunity to examine these objectives in tandem. However, as underscored in the introduction, these techniques come with challenges. This collaboration presented an opportunity to determine how to combine multi-objective optimisation techniques and near-optimal space exploration to forge a more insightful and comprehensive approach.

3.2 The Idea

We identified a foundational contribution to advance the techniques of near-optimal space exploration in a multi-objective setting: crafting a clear definition of near-optimal space within the realm of multi-objective optimisation. This refined definition paves the way for deploying any Modelling to Generate Alternative algorithms in multi-objective setups. Using this definition, necessary conditions can be efficiently computed, necessitating only a minor adjustment rooted in the multi-objective near-optimal space to which they align.

3.3 The Paper: *Multi-Objective Near-Optimal Necessary Conditions for Multi-Sectoral Planning*

This paper was published in “Applied Energy", an Elsevier journal, in 2023.

3.3.1 Paper’s contributinos

Using the previous paper as a foundation, this article offers dual contributions:

1. Broadening the near-optimal space concepts to multi-objective optimisation.
2. Demonstrating the application of necessary conditions within a multi-objective framework, emphasising the diverse insights obtainable from this approach.

3.3.2 Authors’ contributions

This paper represents one of the outputs of a collaborative effort between researchers from the University of Liège and UCLouvain. Dr Gauthier Limpens and Dr Jonathan Dumas led this initiative, and several articles were published. Together with Paolo Thiran and I, it was collectively decided to expand upon the methodology presented in [DE22] to incorporate multi-objective optimisation. The decision to include energy investment as a primary objective alongside cost was informed by previous work conducted at UCLouvain, benefiting from the expertise of their researchers in the field. Additionally, UCLouvain significantly contributed by developing EnergyScope TD, a tool created by Dr Limpens and currently maintained, notably by Paolo Thiran. Collaborating closely with Dr Dumas, I then tailored this tool to suit the specific requirements of this paper. Dr Dumas also provided invaluable guidance and support in designing the experiments and structuring the paper. As the lead author, I was responsible for the mathematical formulation, overseeing the experiments, and spearheading the writing process. Professor Ernst provided supervision and offered numerous insightful ideas to refine the mathematical formulation. All co-authors played an active role in the writing and review process, providing regular feedback and suggestions to enhance the quality of the article.

3.3.3 Reading tips

The content of Section 2, “Problem statement", which revisits and extends the concepts introduced in [DE22] to include multi-objective optimisation, has been reformulated and incorporated into Appendix A. As a result, readers who have already studied this appendix may find it redundant. However, this section can still provide valuable insight into understanding the different concepts used in the case study described in Section 3.

Multi-objective near-optimal necessary conditions for multi-sectoral planning

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Abstract

In the energy transition context, restructuring energy systems and making informed decisions on the optimal energy mix and technologies is crucial. Energy system optimisation models (ESOMs) are commonly used for this purpose. However, their focus on cost minimisation limits their usefulness in addressing other factors like environmental sustainability and social equity. Moreover, by searching for only one global optimum, they overlook diverse alternative solutions. This paper aims to overcome these limitations by exploring near-optimal spaces in multi-objective optimisation problems, providing valuable insights for decision-makers. The authors extend the concepts of epsilon-optimality and necessary conditions to multi-objective problems. They apply this methodology to a case study of the Belgian energy transition in 2035 while considering both cost and energy invested as objectives. The results reveal opportunities to reduce dependence on endogenous resources while requiring substantial reliance on exogenous resources. They demonstrate the versatility of potential exogenous resources and provide insights into objective trade-offs. This paper represents a pioneering application of the proposed methodology to a real-world problem, highlighting the added value of near-optimal solutions in multi-objective optimisation. Future work could address limitations, such as approximating the epsilon-optimal space, investigating parametric uncertainty, and extending the approach to other case studies and objectives, enhancing its applicability in energy system planning and decision-making.

Keywords: Energy system modelling; multi-objective optimisation; multi-sectoral planning; near-optimality; necessary condition; suboptimal space

1. Introduction

The undergoing energy transition requires deep restructuring of energy systems in the long term. The objective is to maintain comparable energy services while replacing fossil fuels with sustainable alternatives. Achieving this goal necessitates significant transformations in the supply chain, conversion processes, and utilisation methods. Energy system planning is required to guide this restructuring and determine the appropriate mix of energy sources and technologies to satisfy a community's or region's future energy demand. The goal of this process is to inform decision-makers to allow them to plan an efficient and sustainable transformation of energy systems. Energy system optimisation models (ESOMs) are commonly preferred in energy system planning [1] due to their ability to explore and analyse multiple design solutions. These models utilise optimisation techniques to explore a wide range of possibilities for the energy system, providing answers to technical questions regarding future challenges.

However, the use of ESOMs often limits the quality of insights they provide, thus reducing their usefulness for decision-makers. Typically, these insights are derived from a single cost-optimal solution, whereas decisions are often made based on various indicators. While cost is a crucial indicator for assessing the affordability and viability of an energy system, focusing solely on this objective can overlook other significant factors, such as environmental sustainability and social equity. Additionally, these insights might not meet the needs of stakeholders with differing interests.

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Approaches such as scenario analysis, multi-objective optimisation, and near-optimal space analysis are effective methodologies to surmount the indicated limitation. Scenario analysis enables the indirect integration of objectives by altering the fundamental assumptions underpinning the model. In contrast, multi-objective optimisation directly incorporates these objectives into the model itself. Near-optimal space analysis, the third method, facilitates the inclusion of objectives that can not be modelled in the decision-making process. In the subsequent sections, we delve into the shortcomings of an overly cost-focused approach. Subsequently, we elucidate these three methodologies, their drawbacks, and the potential advantages of merging multi-objective optimisation with near-optimal space analysis.

1.1. The cost as leading indicator - limits and solutions

ESOMs determine the energy system configurations that minimise or maximise a specified objective. Most studies choose the cost as the objective, and the best configuration is the most cost-effective [1]. This choice is historical, as explained by Pfenninger et al. [2]. Indeed, the first ESOMs (from the MARKAL/TIMES [3] and MESSAGE [4] models) were initially designed for cost minimisation. More recent models followed this trend, such as Dispa-SET, which optimises the operation cost [5]. The study of Yue et al. [6] highlights that by default, ESOMs ignore non-economic factors entering into energy investment decisions and how politics, social norms, and culture shape public policies. This claim is also supported by Pfenninger et al. [2], who specifies that energy system models focus heavily on economic and technical aspects. This focus is inadequate for energy system planning as this problem involves multiple stakeholders with different policy objectives, for whom cost-optimal solutions might not be satisfying. For instance, a model might focus on the cost-effectiveness of integrating wind turbines into a power grid, neglecting diverse stakeholder needs. Governments may prioritise economic growth, environmental bodies aim for carbon reduction, and residents might value landscape preservation. Thus, cost-effective solutions like wind turbines may not align with all stakeholders' varying objectives in energy planning. Moreover, several studies have demonstrated that ignoring non-economic factors increases the uncertainty of the models [2, 6]. Fazlollahi et al. [7] also states that, due to uncertainty in some parameters, it is insufficient for energy system sizing to rivet on a unique mono-objective optimal solution. Finally, Trutnevyte [8] shows how cost-optimal scenarios do not adequately represent real-world problems. However, there exist methods for going beyond cost and considering non-economic factors. Some of these methods are presented in the following sections.

1.1.1. Scenario analysis

The first approach to incorporate non-economic factors is scenario analysis. Scenario analysis involves optimising the same model over multiple scenarios with different values for some parameters. Differences between scenarios can result from uncertainties over technological or economic parameters - e.g. future cost of technology. However, they can also stem from political (e.g. nuclear decommissioning) or social considerations (e.g. limitation of onshore wind turbines or transmission lines development). Using scenarios that differ through those considerations allows for studying the effects of non-economic factors. For instance, the study by Fujino et al. [9] compares a fast-growth, technology-oriented scenario to a slow-growth, nature-oriented one. However, as stated in the review of Hughes and Strachan [10], this scenario approach tends to simplify social and political dynamics.

1.1.2. Multi-objective optimisation

A second approach to include non-economic factors is multi-objective optimisation. This approach allows for optimising several objectives simultaneously, highlighting the *trade-offs* that can be obtained. More formally, while different methods exist to apply multi-objective optimisation (e.g. weighted-sum approach, integer cut constraints, ϵ-constraint method, evolutionary algorithm), they exhibit the common goal of obtaining solutions from a Pareto optimal set, also called the *Pareto front*. This Pareto front is composed of *efficient* solutions, i.e. solutions that are at least better than any other solutions in one objective. Thus, it is composed of the set of optimal trade-offs between the studied objectives, i.e. any solution that is not part of the Pareto front is worse in all objectives than at least one solution in the Pareto front. Using multi-objective optimisation, the cost can still be optimised while considering other indicators. For instance, Becerra-López and Golding [11] conducted a study of a Texas power generation system analysing the trade-offs between economic and exergetic costs, i.e. the cumulative exergy - *entropy-free energy* - consumption. They demonstrated how these trade-offs provide insights to the decision-makers by not focusing exclusively on economic cost. Other objectives, such as water consumption, grid dependence on imports or energy system safety, are com-

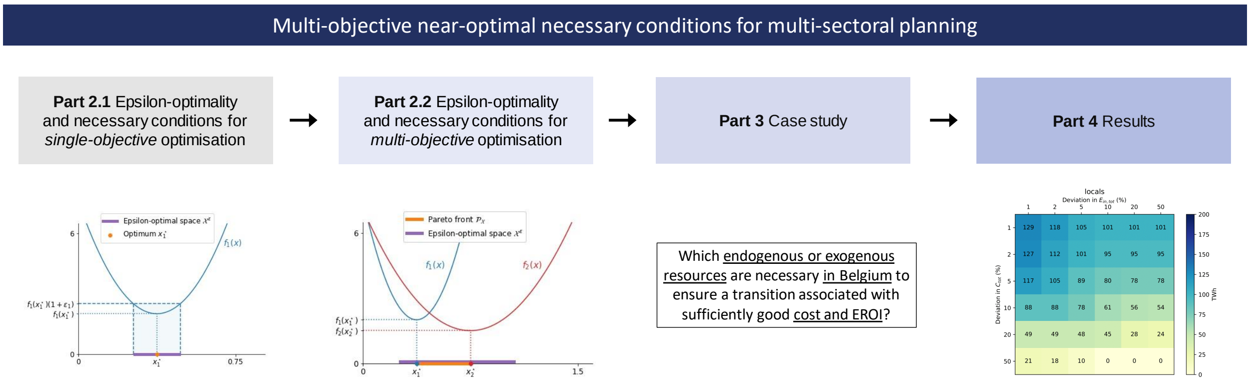


Figure 1: Graphical abstract showing the structure of the paper. The figures are miniatures of figures located further in the document.

pared to cost by Fonseca et al. [12, 13]. They show how much the assessed criteria impact the design and operation of distributed energy systems. A final example of an alternative objective often combined with the cost is the amount of carbon emissions [14].

1.1.3. Near-optimal spaces analysis

A third methodology that allows taking social and political factors into account is the study of near-optimal spaces, also called sub-optimal or epsilon-optimal spaces. The idea is to analyse solutions close to the optimal solution to understand how the use of resources and technologies varies when allowing a slight deviation in the objective function. This paradigm goes further than multi-objective optimisation, as mentioned by DeCarolis [15]. It allows incorporating unmodelled objectives, typical of social factors, as they are unknown or difficult to model. Indeed, the near-optimal region might contain solutions that are worse in terms of the main objective - e.g. the cost of the system - but better in unmodelled objectives such as risk or social acceptance. This concept was introduced in the 1980s by Brill et al. [16]. The authors proposed the first method for exploring those spaces: the Hop-Skip-Jump method. This algorithm was coined as part of a broader exploration methodology that the authors refer to as Modelling to Generate Alternatives (MGA). This methodology was brought back recently and applied to energy system modelling by DeCarolis [15] and DeCarolis et al. [17]. They led to a renewed interest in such methods. Authors such as Price and Keppo [18] developed new exploration algorithms while Li and Trutnevyte [19] combined MGA with Monte-Carlo exploration to minimise parametric uncertainty.

There are several ways of extracting insights from near-optimal spaces. Most researchers exploring near-optimal spaces focus on computing numerous near-optimal solutions from which they derive insights [18, 19, 20, 21]. An alternative approach is to use methods to obtain such insights directly without needing to compute many alternative solutions [22]. The authors of Dubois and Ernst [23] took this approach by introducing the concept of *necessary conditions* for near-optimality, i.e. conditions that are true for every solution in the near-optimal space. For instance, this can provide insights into the required capacity in a given technology to retain a certain level of system cost-effectiveness. More specifically, Dubois and Ernst [23] showed how, for instance, at least 200 GW of new offshore wind need to be installed Europe-wise to stay within 10% of the cost optimum.

1.2. Research gaps, scientific contributions and organisation

The exploration of near-optimal spaces has been used in mono-objective optimisation problems but not, according to the author's best knowledge, in multi-objective optimisation problems. However, these methods could also be valuable in multi-objective optimisation setups. Indeed, while modelling and integrating more objectives, multi-objective optimisation still leaves aside some unmodeled objectives. Analysing solutions in the near-optimal space of multi-objective optimisation problems is a method to address this issue. This paper thus aims to fill this gap by:

1. extending the concepts related to near-optimal spaces to multi-objective optimisation;
2. computing necessary conditions in a multi-objective context to highlight the range of insights that can be derived from them.

The first point is addressed in Section 2 by first introducing the mathematical concepts of near-optimality and necessary conditions in a single-objective framework (see Section 2.1) and then extending them to multi-objective optimisation (see Section 2.2). Section 3 then translates those concepts to a real case study: the multi-sectoral expansion of the Belgian energy system. The results of this case study, including necessary conditions representing the necessary amount of different energy resources, are presented in Section 4 before highlighting the contributions of this paper in Section 5. We can already highlight one of those contributions: the open-source release of the code [24] and the data [25] used to achieve this study. The graphical representation of the organisation of this paper is depicted in Figure 1.

2. Problem statement

In this section, the methodological contribution is described. It is illustrated in a mathematical form to enhance its universality. Indeed, this method could be applied to other problems than ESOM. It will be applied in Section 3 to an ESOM formulation to facilitate understanding of this method.

The first part of this section introduces the concepts of epsilon-optimal space and necessary conditions for single-objective optimisation [23]. The second part extends these concepts to multi-objective optimisation by:

1. generalising the optimisation problem to multiple objectives,
2. presenting generic notions related to multi-objective optimisation, including the image of the feasible space, efficient solutions, and the Pareto front, and
3. explaining the extension of the concepts of epsilon-optimality and necessary conditions to multi-objective optimisation.

2.1. Single-objective optimisation

2.1.1. Optimisation problem and epsilon-optimality

Let $\mathcal{X}$ be a feasible space and $f : \mathcal{X} \to \mathbb{R}_+$ an objective function in the positive reals. The single-objective optimisation problem is

$$\min_{x \in \mathcal{X}} f(x) \quad . \tag{1}$$

Let $x^\star$ denote an optimal solution to this problem that is: $x^\star \in \arg\min_{x \in \mathcal{X}} f(x)$.

Definition 1. *An **ε-optimal space**, with $\epsilon \geq 0$, is defined as follows*

$$\mathcal{X}^\epsilon = \left\{ x \in \mathcal{X} \mid f(x) \leq (1+\epsilon) f(x^\star) \right\} \quad . \tag{2}$$

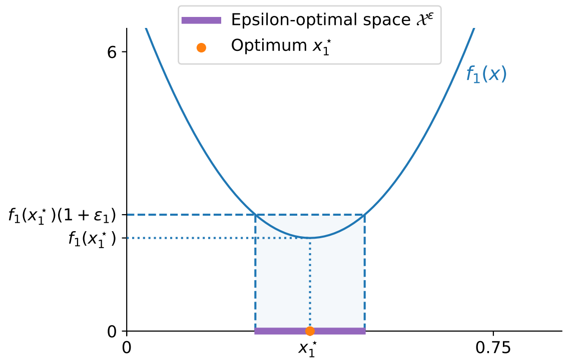


Figure 2: Graphical representation of an ϵ-optimal space of a mono-objective optimisation problem in $\mathcal{X} = \mathbb{R}_+$. The function f_1 that is minimised is shown in blue. Its minimum is located at $x_1^\star$. Using this value and its corresponding objective value $f_1(x_1^*)$ allows to determine an ϵ-optimal space $\mathcal{X}^\epsilon$ with $\epsilon = \epsilon_1$. The values of the different parameters and functions used in this example are described in Appendix A.

Comment: The ϵ-optimal space is the set of the feasible solutions $x \in \mathcal{X}$ with objective value $f(x)$ no greater than $(1+\epsilon) f(x^\star)$. The deviation from the optimal objective value is measured via ϵ, called the *suboptimality coefficient*. Figure 2 illustrates those concepts. A note must be made on the specific case $f(x^\star) = 0$. In this case, $\mathcal{X}^\epsilon$ resumes to $\arg\min_{x \in \mathcal{X}} f(x)$, making the analysis of near-optimal spaces trivial.

2.1.2. Necessary conditions

The concepts of *condition*, *necessary condition*, and *non-implied necessary condition* introduced in this section allow determining features which are common to all solutions in a given ϵ-optimal space. We illustrate each definition using an example.

Definition 2. *A **condition** is a function $\phi : \mathcal{X} \to \{0, 1\}$. A set of conditions is denoted Φ.*

Example: Let the feasible space $\mathcal{X}$ be the set of reals, i.e. $\mathcal{X} = \mathbb{R}$, then, the set of conditions Φ could be the set of conditions of the form $\phi_c(x) := x \geq c$ with $x \in \mathcal{X}$ (thus $x \in \mathbb{R}$) and $c \in \mathbb{R}$.

Definition 3. *A **necessary condition** for ϵ-optimality is a condition which is true for any solutions in $\mathcal{X}^\epsilon$. For a feasible space $\mathcal{X}$, set of conditions Φ and suboptimality coefficient ϵ, $\phi \in \Phi$ is a necessary condition if*

$$\forall x \in \mathcal{X}^\epsilon : \phi(x) = 1 \quad . \tag{3}$$

The set of all necessary conditions for ϵ-optimality in Φ is denoted $\Phi^{\mathcal{X}^\epsilon}$.

Example: Let us consider that the epsilon-optimal space is given by $\mathcal{X}^\epsilon = [0, 1]$. Then, the condition $\phi_0(x) := x \geq 0$ is respected by all $x \in \mathcal{X}^\epsilon$, making ϕ_0 a necessary condition. Moreover, it is straightforward to show that the set of all conditions in Φ which are necessary is $\Phi^{\mathcal{X}^\epsilon} = \{\phi_c \mid c \leq 0\}$. Indeed, any condition $\phi_c(x) := x \geq c$ is true over $\mathcal{X}^\epsilon = [0, 1]$ if $c \leq 0$.

As shown in Dubois and Ernst [23], necessary conditions can provide insights into features common to many near-optimal solutions. However, depending on how conditions are defined, their study also claims the number of necessary conditions can be infinite, which is counterproductive in providing insights. This situation happens, for instance, in our previous example. Indeed, the set $\Phi^{\mathcal{X}^\epsilon} = \{\phi_c \mid c \leq 0\}$ contains an infinite number of necessary conditions. To limit the number of conditions, we introduce the concept of *non-implied necessary conditions*.

Definition 4. *A **non-implied necessary condition** for ϵ-optimality is a necessary condition $\phi \in \Phi^{\mathcal{X}^\epsilon}$ that is not implied by any other necessary condition $\phi' \in \Phi^{\mathcal{X}^\epsilon} \setminus \{\phi\}$, where $\Phi^{\mathcal{X}^\epsilon}$ is the set of necessary conditions for ϵ-optimality. The set of non-implied necessary conditions is denoted $\overline{\Phi}^{\mathcal{X}^\epsilon}$.*

Example: In our example, the only non-implied necessary condition is ϕ_0, *i.e.* $\overline{\Phi}^{\mathcal{X}^\epsilon} = \{\phi_0\}$. The set of necessary conditions is $\Phi^{\mathcal{X}^\epsilon} = \{\phi_c \mid c \leq 0\}$. In this set, ϕ_0 implies all other conditions and is not implied by any of them. Indeed, for any x, knowing that $x \geq 0$ is true implies that $x \geq c$ when $c \leq 0$. Thus, knowing that ϕ_0 is a necessary condition implies that any ϕ_c with $c \leq 0$ is a necessary condition, whatever the ϵ-optimal space. On the opposite, it is not possible to imply that ϕ_0 is a necessary condition from the knowledge of other necessary conditions in the set $\Phi^{\mathcal{X}^\epsilon} = \{\phi_c \mid c \leq 0\}$. This defines ϕ_0 as a *non-implied* necessary condition.

The interested reader can find a more formal definition of implication leading to alternative definitions of non-implied necessary conditions in Appendix B.

2.1.3. Non-implied necessary condition computation

This section presents the detailed computation of a particular type of non-implied necessary condition to provide a practical sense of these concepts. It demonstrates how to compute a non-implied necessary condition from a set of conditions taking the form of constrained sums of variables. In the case studies described in Section 3, this type of condition is used to study the minimum amount of energy that can be driven from different sources.

Let $\mathcal{X} \subset \mathbb{R}^n$ be a feasible space, $f : \mathcal{X} \rightarrow \mathbb{R}_+$ an objective function to minimise over this space, and $\Phi_\mathbf{d}$ a set of conditions defined as follows:

$$\Phi_\mathbf{d} = \left\{\phi^c_\mathbf{d}(\mathbf{x}) = \mathbf{d}^T\mathbf{x} \geq c\right\} \quad , \tag{4}$$

where $\mathbf{x} \in \mathcal{X}$, $\mathbf{d} \in \{0, 1\}^n$ and $c \in \mathbb{R}$. The conditions are constrained sums of variables $\mathbf{d}^T\mathbf{x} = \sum_{i=1}^n d_i x_i$. In this particular case, Dubois and Ernst [23] have proven that $\phi^{c^\star}_\mathbf{d} = \mathbf{d}^T\mathbf{x} \geq c^*$ with $c^* = \min_{\mathbf{x} \in \mathcal{X}^\epsilon} \mathbf{d}^T\mathbf{x}$ is the only non-implied necessary condition that can be derived from $\Phi_\mathbf{d}$. The value c^* represents the minimum value that $\mathbf{d}^T\mathbf{x}$ can take over the set $\mathcal{X}^\epsilon$, that is when allowing a deviation of ϵ from the optimal value $f(\mathbf{x}^\star)$. Algorithm 1 illustrates the computation of this value in three steps.

Algorithm 1: Computation of a non-implied necessary condition - Single-objective case

Data:
- f - objective function,
- $\mathcal{X}$ - feasible space,
- ϵ - suboptimality coefficient,
- $\mathbf{d}$ - binary vector defining the conditions $\mathbf{d}^T\mathbf{x}$

Result: c^*

Steps:
1. Solve $\min_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})$ to obtain $\mathbf{x}^\star$.
2. Build $\mathcal{X}^\epsilon$ by adding the constraint $f(\mathbf{x}) \leq (1 + \epsilon) f(\mathbf{x}^\star)$ to $\mathcal{X}$.
3. Solve $c^* = \min_{\mathbf{x} \in \mathcal{X}^\epsilon} \mathbf{d}^T\mathbf{x}$.

Example: Let us illustrate this algorithm on the travellings salesman problem. This problem aims to find the shortest possible route a salesman can take to visit a set of cities exactly once and return to the starting city. Mathematically, we can model this problem in the following way. Let $G = (V, E)$ be a complete undirected graph, where $V = \{1, 2, ..., n\}$ is the set of cities, and E is the set of edges connecting the cities. Each edge $e = (i, j)$ has a non-negative weight $w(e)$ representing the distance between city i and city j. Let x_{ij} be a binary decision variable equal to 1 if the salesman travels directly from city i to city j in the tour and 0 otherwise. The objective is to minimise the total distance travelled by the salesman, i.e.: $\min \sum_{(i,j) \in E} w_{ij} x_{ij}$. This objective must be met under a series of constraints we will not detail here. Let us assume now that there are two types of routes: paved and gravel. The salesman wants to avoid taking gravel routes while maintaining a path that is not much longer than the optimal path. This new path can be obtained using Algorithm 1. Step 1 consists in solving the original problem. Using the optimal solution of this problem, one can perform step 2 by adding the constraint $f(\mathbf{x}) \leq (1+\epsilon)f(\mathbf{x}^\star)$ to the initial problem. In this constraint, $\mathbf{x}$ is a vector containing all x_{ij}, $f(\mathbf{x}) = \sum_{(i,j)\in E} w_{ij}x_{ij}$, and $\mathbf{x}^\star$ is the optimal solution. The value of ϵ can vary depending on the relative increase in path length the salesman is willing to accept. The third step can then be performed by setting an appropriate $\mathbf{d}$. As the salesman wants to minimise the number of gravel routes travelled, all values of $\mathbf{d}$ corresponding to this type of route are set to 1. The value c^* obtained as the optimal value of this third step gives the minimal number of routes that must be taken to ensure that the total length of the path travelled does not deviate by more than ϵ of the optimal length.

2.2. Multi-objective optimisation

This section extends the concepts presented previously to multi-objective optimisation while introducing notions specific to this type of optimisation problem.

2.2.1. Problem formulation

Let $\mathbf{f} := (f_1, \cdots, f_k, \cdots, f_n)$ be a vector of n objective functions such that $\forall k\ f_k : \mathcal{X} \to \mathbb{R}_+$. We seek to minimise these functions over the feasible space $\mathcal{X}$, which, using the notation of Ehrgott [26], we note:

$$\text{“}\min_{x\in\mathcal{X}}\text{”} \quad \mathbf{f}(x) \quad . \tag{5}$$

Let $\mathcal{Y}$ be the image of $\mathcal{X}$ in the objective space:

$$\mathcal{Y} = \mathbf{f}(\mathcal{X}) = \{y \in \mathbb{R}^n \mid y = \mathbf{f}(x) \text{ for some } x \in \mathcal{X}\} \quad . \tag{6}$$

This space is the image of $\mathcal{X}$ under the objective functions $\mathbf{f}$, and $\mathbf{f}(x) := (f_1(x), \cdots, f_k(x), \cdots, f_n(x))$. Therefore, $\mathcal{Y} \in \mathbb{R}^n_+$ and each of its components y_k are defined by $y_k = f_k(x)$ for some $x \in \mathcal{X}$.

2.2.2. Efficient solutions and Pareto front

A way to highlight compromises between the objectives $(f_1, \cdots, f_k, \cdots, f_n)$ is to compute efficient (or Pareto optimal) solutions. As defined by Ehrgott [26]:

Definition 5. *A feasible solution $\hat{x} \in \mathcal{X}$ is called **efficient** when there is no other $x \in \mathcal{X}$ such that $\forall k\ f_k(x) \leq f_k(\hat{x})$ and $f_i(x) < f_i(\hat{x})$ for some i, that is, no other $x \in \mathcal{X}$ has a smaller or equal value in all objectives $(f_1, \cdots f_k, \cdots, f_n)$ than $\hat{x}$.*

According to Ehrgott [26], multiple denominations exist for the set of efficient points. This paper uses ‘Pareto front’ to indiscriminately name the set of efficient points or their image in the objective space.

Definition 6. *A **Pareto front** $\mathcal{P}_\mathcal{X}$ is the set*

$$\mathcal{P}_\mathcal{X} = \Big\{\hat{x} \in \mathcal{X} \mid \nexists x \in \mathcal{X}, \forall k\ f_k(x) \leq f_k(\hat{x}), \exists i\ f_i(x) < f_i(\hat{x})\Big\}. \tag{7}$$

In the objective space, a Pareto front is defined as:

$$\mathcal{P}_\mathcal{Y} = \Big\{\hat{y} \in \mathcal{Y} \mid \nexists y \in \mathcal{Y}, \forall k\ y_k \leq \hat{y}_k, \exists i\ y_i < \hat{y}_i\Big\} \quad . \tag{8}$$

A Pareto front can be composed of an infinity of points. Thus, it is typical to compute a subset of the efficient solutions which compose it. This set is named *approximated Pareto front*. It is denoted by $\mathcal{P}_{\mathcal{X},m}$ (or equivalently $\mathcal{P}_{\mathcal{Y},m}$) where m is the number of points in the approximation.

Definition 7. *An **approximate Pareto front** $\mathcal{P}_{\mathcal{X},m}$, with $m \in \mathbb{N}$, is a subset of m efficient solutions in the Pareto front $\mathcal{P}_\mathcal{X}$.*

Several techniques exist to obtain those efficient solutions, the two most famous being the ‘*weighted-sum approach*’ and the ‘*ϵ-constraint method*’ [26]. The weighted-sum approach consists of solving:

$$\min_{x\in\mathcal{X}} \sum_{k=1}^{n} \lambda_k f_k(x) \quad \forall k\ \lambda_k > 0 \quad . \tag{9}$$

The ϵ-constraint method resolves in solving:

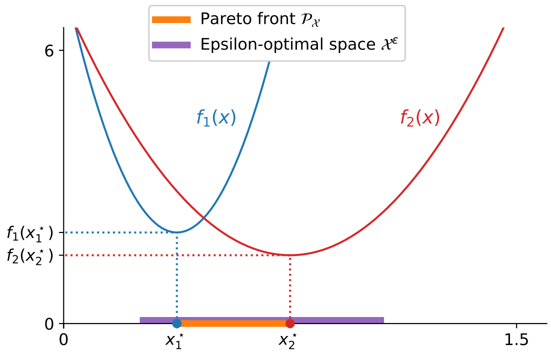
$$\begin{aligned} &\min_{x\in\mathcal{X}}\ f_j(x) \\ &\text{s.t. } f_k(x) \leq \epsilon_k \text{ for } k = 1, \cdots, n \text{ and } k \neq j \quad , \end{aligned} \tag{10}$$

where $\forall k\ \epsilon_k \in \mathbb{R}$.

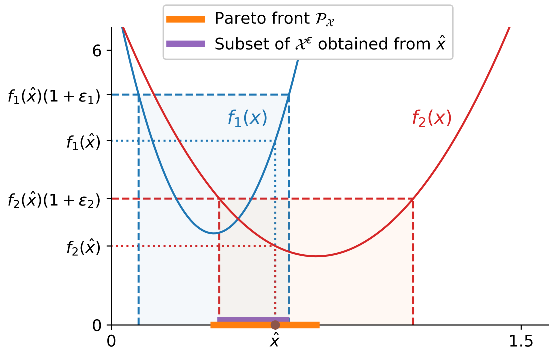
2.2.3. Multi-criteria epsilon-optimal spaces

Starting from a Pareto front $\mathcal{P}_\mathcal{X}$, it is possible to define an $\boldsymbol{\epsilon}$-optimal space, given a *suboptimality coefficients vector* of deviations in each objective: $\boldsymbol{\epsilon} = (\epsilon_1, \cdots, \epsilon_k, \cdots, \epsilon_n) \in \mathbb{R}^n_+$. This space is denoted by $\mathcal{X}^{\boldsymbol{\epsilon}}$ in the decision space and $\mathcal{Y}^{\boldsymbol{\epsilon}}$ in the objective space.

In the mono-objective setup, the ϵ-optimal space is defined as the set of points $x \in \mathcal{X}$ whose objective value $f(x)$ do not deviate by more than an ϵ fraction from the



(a) Full representation of $\mathcal{X}^\epsilon$



(b) Computation of a subset of $\mathcal{X}^\epsilon$ from a single point $\hat{x}$ of the Pareto front $\mathcal{P}_\mathcal{X}$

Figure 3: Graphical representation of an $\boldsymbol{\epsilon}$-optimal space of a multi-objective optimisation problem in $\mathcal{X} = \mathbb{R}_+$. The two functions to be minimised f_1 and f_2 are represented in blue and red, respectively, and their respective minimums are $x_1^\star$ and $x_2^\star$. The Pareto front $\mathcal{P}_\mathcal{X}$ containing all efficient solutions is represented in orange. Figure 3a shows in purple the full $\boldsymbol{\epsilon}$-optimal space $\mathcal{X}^{\boldsymbol{\epsilon}}$ for a suboptimality coefficient vector $\boldsymbol{\epsilon} = (\epsilon_1, \epsilon_2)$. As shown in Equation (12), this space is the union of sub-spaces that can be computed from efficient solutions. Figure 3b shows how one of these subspaces, corresponding to the efficient solution $\hat{x}$, can be computed. From the value $\hat{x}$, the corresponding objective values $f_1(\hat{x})$ and $f_2(\hat{x})$ are obtained. This allows to determine all the solutions in $\mathcal{X}$ whose objective value is smaller than $f_k(\hat{x})(1+\epsilon_k)$ for $k \in 1, 2$. The values of the different parameters and functions used in this example are described in Appendix A.

optimal objective value, i.e. $f(x) \leq (1+\epsilon) f(x^\star)$. In a multi-objective case, there is no optimum but a set of efficient points composing the Pareto front. This leads us to define the $\boldsymbol{\epsilon}$-optimal space as follows:

Definition 8. *In a multi-objective optimisation problem, the **$\boldsymbol{\epsilon}$-optimal space** $\mathcal{X}^{\boldsymbol{\epsilon}}$, with $\boldsymbol{\epsilon} = (\epsilon_1, \cdots, \epsilon_k, \cdots, \epsilon_n) \in \mathbb{R}^n_+$, is the set of points x whose objective values $f_k(x)$ do not deviate by more than an ϵ_k fraction from the objective values $f_k(\hat{x})$ of at least one solution $\hat{x}$ of the Pareto front $\mathcal{P}_\mathcal{X}$ for all k. It is the space*

$$\mathcal{X}^{\boldsymbol{\epsilon}} = \Big\{ x \in \mathcal{X} \,|\, \exists \hat{x} \in \mathcal{P}_\mathcal{X}, \; \forall k \; f_k(x) \leq (1+\epsilon_k) f_k(\hat{x}) \Big\} \quad . \tag{11}$$

Alternatively, this space can be defined as:

$$\mathcal{X}^{\boldsymbol{\epsilon}} = \bigcup_{\hat{x} \in \mathcal{P}_\mathcal{X}} \Big\{ x \in \mathcal{X} \,|\, \forall k \; f_k(x) \leq (1+\epsilon_k) f_k(\hat{x}) \Big\} \quad . \tag{12}$$

Figure 3 depicts a graphical representation of an $\boldsymbol{\epsilon}$-optimal space in a multi-objective framework and how it is built from efficient solutions.

Definition (11) relies on the entire Pareto front. However, practically, only a subset $\mathcal{P}_{\mathcal{X},m}$ of m efficient points of the Pareto front is computed and used to obtain an approximation of the $\boldsymbol{\epsilon}$-optimal space, denoted $\mathcal{X}^{\boldsymbol{\epsilon}}_m$.

Definition 9. *An approximation $\mathcal{X}^{\boldsymbol{\epsilon}}_m$, with $m \in \mathbb{N}$, of an $\boldsymbol{\epsilon}$-optimal space $\mathcal{X}^{\boldsymbol{\epsilon}}$ is the space*

$$\mathcal{X}^{\boldsymbol{\epsilon}}_m = \Big\{ x \in \mathcal{X} \,|\, \exists \hat{x} \in \mathcal{P}_{\mathcal{X},m}, \; \forall k \; f_k(x) \leq (1+\epsilon_k) f_k(\hat{x}) \Big\} \quad . \tag{13}$$

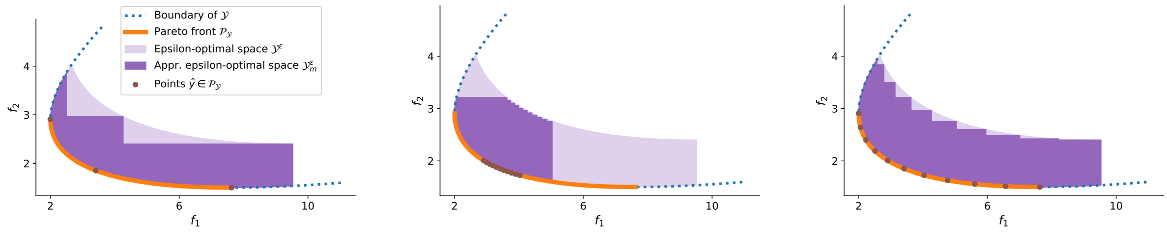
Alternatively, this space can be defined as:

$$\mathcal{X}^{\boldsymbol{\epsilon}}_m = \bigcup_{\hat{x} \in \mathcal{P}_{\mathcal{X},m}} \Big\{ x \in \mathcal{X} \,|\, \forall k \; f_k(x) \leq (1+\epsilon_k) f_k(\hat{x}) \Big\} \quad . \tag{14}$$

The alternative formulation defines $\mathcal{X}^{\boldsymbol{\epsilon}}_m$ as a union of spaces, where each space is the set of points whose objective value in each f_k does not deviate by more than an ϵ_k fraction from the objective values $f_k(\hat{x})$ of one solution $\hat{x}$ in the approximated Pareto front $\mathcal{P}_{\mathcal{X},m}$. Figure 4 shows three examples of approximate $\boldsymbol{\epsilon}$-optimal spaces $\mathcal{X}^{\boldsymbol{\epsilon}}_m$ in the objective space (therefore noted $\mathcal{Y}^{\boldsymbol{\epsilon}}_m$) using three approximated Pareto fronts $\mathcal{P}_{\mathcal{Y},m}$, with different numbers and spread of efficient solutions.

2.2.4. Necessary conditions

In the multi-objective optimisation framework, necessary conditions and non-implied necessary conditions for $\boldsymbol{\epsilon}$-optimality can be defined in the same manner as in the one-dimensional setting (see definitions 3 and 4, respectively). The only difference stems from the replacement of $\mathcal{X}^\epsilon$ by $\mathcal{X}^{\boldsymbol{\epsilon}}$.



(a) Few well-spread points (b) Numerous badly-spread points (c) Numerous well-spread points

Figure 4: Graphical representations in the objective space of approximations $\mathcal{Y}^\epsilon_m$ of an ϵ-optimal space of a multi-objective optimisation problem based on three different approximate Pareto front $\mathcal{P}_{\mathcal{Y},m}$. The axes correspond to the two functions to minimise, i.e. f_1 and f_2. The boundary of the image of the feasible space $\mathcal{Y}$ is represented in blue in the three cases. The part of this boundary corresponding to the entire Pareto front $\mathcal{P}_\mathcal{Y}$ is drawn in orange. The complete ϵ-optimal space $\mathcal{Y}^\epsilon$ corresponding to this Pareto front is coloured in light purple. Each graph corresponds to a different approximate Pareto front $\mathcal{P}_{\mathcal{Y},m}$. These sets of points are represented in brown. From each of these points, part of the approximate ϵ-optimal spaces can be computed, and their union is represented in solid purple. The values of the different parameters and functions used in this example are described in Appendix A.

2.2.5. Non-implied necessary condition computation

The computation of a non-implied necessary condition from conditions of type $\mathbf{d}^T\mathbf{x} \geq c$ presented in Section 2.1.3 is generalised to the multi-criteria case. In the mono-objective case, it was sufficient to minimise the sum $\mathbf{d}^T\mathbf{x}$ over $\mathcal{X}^\epsilon$ to obtain the value c^* corresponding to the non-implied necessary condition $\mathbf{d}^T\mathbf{x} \geq c^*$. However, in a multi-objective setup, we do not have access to $\mathcal{X}^\epsilon$ but to its approximation $\mathcal{X}^\epsilon_m$, which is the union of several subsets, each corresponding to one point in $\mathcal{P}_{\mathcal{X},m}$ (i.e. a subset of the Pareto front). The minimum over this space can thus be obtained by taking the minimum of the minima of $\mathbf{d}^T\mathbf{x}$ over each of these subsets. Even with this approach, $\mathcal{X}^\epsilon_m$ being a subset of $\mathcal{X}^\epsilon$, minimising $\mathbf{d}^T\mathbf{x}$ over it will only provide an upper bound $\tilde{c}$ of the value c^*, i.e. $\tilde{c} \geq c^*$. Algorithm 2 shows how this value can be obtained.

Algorithm 2: Computation of a non-implied necessary condition - Multi-objective case

Data:
$\mathcal{X} \in \mathbb{R}^n$ - feasible space,
$\mathbf{f}$ - objective functions,
m - number of points,
ϵ - vector of suboptimality coefficients,
$\mathbf{d}$ - binary vector defining the conditions $\mathbf{d}^T\mathbf{x}$

Result: $\tilde{c}$

Steps:
1. Draw m points $\hat{\mathbf{x}}^{(1)}, \ldots \hat{\mathbf{x}}^{(i)}, \ldots \hat{\mathbf{x}}^{(m)}$ of the Pareto front using an appropriate method.
2. For all $i \in [1, 2, \ldots, m]$, compute $c^{(i)} = \min \mathbf{d}^T\mathbf{x}$ over the space $\{\mathbf{x} \in \mathcal{X} \mid \forall k\ f_k(\mathbf{x}) \leq (1 + \epsilon_k) f_k(\hat{\mathbf{x}}^{(i)})\}$.
3. Take the minimum $\tilde{c} = \min_{i\in[1,2,\ldots,m]} c^{(i)}$ of these values to find the appropriate condition $\phi_{\tilde{c}}$.

There is no guarantee that the condition $\mathbf{d}^T\mathbf{x} \geq \tilde{c}$ is a (non-implied) necessary condition. Indeed, it could be the case that for a solution $\mathbf{x} \in \mathcal{X}^\epsilon \setminus \mathcal{X}^\epsilon_m$ that $\mathbf{d}^T\mathbf{x} < \tilde{c}$. To make the upper bound $\tilde{c}$ as close as possible to the real minimal value c^*, one must reduce the size of the difference $\mathcal{X}^\epsilon \setminus \mathcal{X}^\epsilon_m$. Minding this gap can be done by improving the number and spread of efficient solutions in the approximated Pareto front. As defined by Alarcon-Rodriguez et al. [27], solutions with a good spread can be seen as having good coverage of the actual Pareto front. The three graphs of Figure 4 show visually how, by increasing the number and the spread of efficient solutions drawn from the Pareto front, the approximated ϵ-optimal space covers a more significant subset of the points of the entire ϵ-optimal space.

Example: Let us continue with the travelling salesman problem introduced in Section 2.1.3. We introduce a new set of non-negative weights $t(e)$ representing the time needed to travel between city i and j. We now have two objectives: the total distance travelled $f(\mathbf{x}) = \sum_{(i,j)\in E} w_{ij}x_{ij}$ and the total time travelled $g(\mathbf{x}) = \sum_{(i,j)\in E} t_{ij}x_{ij}$ to visit all cities. Minimising these two objectives might lead to different solutions. We can use appropriate techniques to determine efficient solutions $\hat{\mathbf{x}}$ from the Pareto front, expressing the trade-offs between these two objectives. If the salesman is still interested in avoiding the gravel routes while maintaining close-to-optimal length and time of travel, we can employ Algorithm 2. For a fixed set of suboptimality coefficients, step 2 implies adding two constraints to the initial problem and minimising $\mathbf{d}^T\mathbf{x}$ for each efficient solution. As in the mono-objective case, the only values of **d** set to 1 are the ones corresponding to gravel routes. Finally, step 3 will give us a value $\tilde{c}$, which expresses an upper bound on the minimum number of gravel routes the salesman needs to take to avoid deviations in time and length larger than ϵ_1 and ϵ_2.

3. Case study

In this section, a case study using an ESOM will illustrate the concepts and methodology presented in the previous section. First, the context of the case study and the question to which it tries to provide an answer are presented. The modelling tool used to implement the methodology is then introduced, and its main features are detailed. Finally, each element introduced in Section 2 is specified to the case study.

3.1. Context

In the European Green Deal [28], the European Commission raised the European Union's ambition to reduce GHG emissions to at least 55% below 1990 levels by 2030. Then by 2050, Europe aims to become the world's first carbon-neutral continent. Europe still relies massively on fossil fuels to satisfy its energy consumption ($\sim$ 75% coming from coal, natural gas and oil according to the International Energy Agency [29]) as well as non-energy usages (e.g. chemical feed-stocks, lubricants and asphalt for road construction [30]). The use of these fuels is the primary source of GHG emissions. Carbon-neutral sources of energy must thus be developed to curb emissions. The possibilities are numerous, and one of the coming decade's main challenges will be deciding which resources to invest in. Several criteria will motivate these choices.

The most common criterion for discriminating between options is cost. Indeed, as highlighted by Pfenninger et al. [2] and DeCarolis [15], most studies use the cost indicator to plan the energy transition. This choice makes sense as the cost of investment, maintenance and operation of the energy system impacts the final consumers' energy bill. Thus, minimising the system cost is a social imperative to allow every citizen access to affordable energy.

A lesser-known indicator, encompassing technical and social challenges, is the system's *energy return on investment* (EROI). When defined system-wise, the EROI is a ratio that measures the usable energy delivered by the system (E_{out}) over the amount of energy required to obtain this energy (E_{in}) [31]. When the amount of energy required to deliver a given energy service increases, the EROI of the system decreases. In some sense, EROI measures the ease with which energy is extracted to transform it into a form that benefits society. There are various manners of defining E_{in} and E_{out}, and incidentally, the EROI of a system. These definitions depend mainly on what parts of the *energy cascade* - as presented in Brockway et al. [32] or Dumas et al. [33] - are considered. This paper considers that invested energy E_{in} encompasses the energy used to build the system infrastructure, 'from the cradle to the grave', and to operate this system. Following the methodology of Dumas et al. [33], E_{out} will correspond to the final energy consumption (FEC) of the system, as defined in the European Commission [34] standard. FEC is the total energy, measured in TWh, consumed by end-users. It encompasses the energy directly used by the consumer and excludes the energy used by the energy sector, e.g. deliveries and transformation.

While cost and EROI can be linked (e.g. the transport of energy resources will increase both the system cost and invested energy), they are not fully correlated and favouring one or the other can lead to different system configurations, as illustrated later in Section 4. Both criteria can be included in the decision process by modelling them as objectives in optimisation problems. These objectives can be optimised individually or co-optimised using multi-criteria optimisation techniques. In this case study, we will show how, using these objectives in the methodology presented in Section 2, the following question can be addressed:

> Which resources are necessary to ensure a transition associated with sufficiently good **cost and EROI**?

Indeed, the answer to this question can be obtained by computing necessary conditions corresponding to the minimum amount of energy that needs to come from these resources.

This question is, however, relatively broad, and for the sake of conciseness, it needs to be specified. On top of decision criteria, considerations such as energy independence (enhanced with the Russian invasion of Ukraine) and social acceptance (e.g. the 'not-in-my-backyard' phenomena) are paramount in planning the energy transition. These considerations will impact the type of resources that will be exploited. Indeed, the first consideration incentivises a push for domestically produced energy, while the latter favours the opposite. The first tends to minimise the amount of exogenous resources in the system, while the latter minimises the amount of energy coming from endogenous resources. To consider these elements, the previous question can be refined to:

Which endogenous or exogenous resources are necessary to ensure a transition associated with sufficiently good cost and EROI?

This study focuses on one of the European countries: Belgium. Belgium made the same commitments for 2030 and 2050 as the European Union [35]. Thus, it faces the challenge of replacing its fossil-based economy with carbon-free solutions while striking the right balance between endogenous and exogenous resources. Belgium's population density exacerbates this challenge. In 2019, Belgium had the second-highest population density in Europe (excluding Malta) with 377 people per km^2, behind the Netherlands (507 people per km^2) [36]. The available land for onshore energy development is thus limited, while offshore production is limited to around 8 GW of wind potential [37]. Other domestic resources such as solar, biomass, waste, or hydro also have limited potential. This situation entails a small local energy potential compared to its demand. The study Limpens et al. [38] evaluates that available local Belgian resources can only cover 42% of the country's primary energy consumption. This situation strongly impacts the type of resources Belgium must rely on.

Therefore, the question that will be addressed in this case study is:

Which endogenous or exogenous resources are necessary **in Belgium** to ensure a transition associated with sufficiently good cost and EROI?

3.2. EnergyScope TD

To answer this question, an appropriate ESOM is needed. The commitments set for 2035 and 2050 cover all sectors of the economy, not just electricity production. To achieve net zero ambitions, carbon-neutral solutions must be implemented for electricity, heat, mobility, and non-energy. These different sectors can be modelled using an open-source whole-energy system model such as EnergyScope TD (ESTD) [39].

ESTD can be categorised as an ESOM. According to Contino et al. [40], ESTD is a *whole-energy* system model, i.e. a model that captures the different energy sectors exhaustively. Moreover, ESTD optimises the energy system with an hourly resolution and has the advantage of having a simple mathematical formulation compared to other models [39]. Using optimisation techniques, it determines the investment decisions and sizing of various technologies (e.g. wind turbines, gas power plants, boilers) as well as the selection of resources (e.g. wind, gas, diesel) required to meet different types of end-use demand (EUD) listed in Appendix C; and the hourly operation of the system. Mathematically, ESTD models the energy system as a linear programming problem. It takes a series of parameters as input and outputs the values of investment and operational variables determined by minimising an objective while respecting a series of constraints. The objective is a linear function; constraints are linear equalities or inequalities.

Parameters and variables can be indexed temporally. The default temporal horizon T is one year with an hourly resolution. To reduce the computational burden of the optimisation, the horizon is clustered by selecting a number of typical days, 12 by default. Thus, time-dependent parameters and variables are indexed by a typical day td and an hour h. The only exception is storage technologies, whose energy levels are computed over all the hours of the year t to allow storage longer than a day up to seasonal. The equivalence between the original hourly-resolution temporal horizon and the typical days is done via a time-indexed set $THTD(t)$ associating each hour t of the year with a corresponding couple $(td, h) = THTD(t)$. This set is essential to understand some of the equations in the rest of this section.

ESTD has been extensively used and validated in the Belgian case [33, 38, 41, 42, 43, 44]. More specifically, in Limpens et al. [38], the authors studied the 2035 Belgian energy system using ESTD and built the corresponding data set. This year is a trade-off between a long-term horizon where policies can still be implemented and a horizon short enough to define the future of society with a group of known technologies. To build on these resources, we will model the Belgian energy system for 2035.

To finish this section, it is essential to note that while the results presented in this paper are valid for Belgium, they could easily be extended to other countries. Indeed, ESTD has already been used to model the energy systems of other countries such as Switzerland [45, 46] and Italy [47]. Moreover, adapting those models to implement the methodology presented in this paper only requires minor modifications, as presented in the following sections.

3.3. Feasible space

In the initial optimisation problem

$$\text{“}\min_{x \in X}\text{”} \quad \mathbf{f}(x) \quad , \tag{15}$$

the first element to define is the feasible space $\mathcal{X}$ over which the optimisation is performed. This study modelled the feasible space using ESTD as a linear programming problem. Therefore, the problem to solve has the following form:

$$\begin{aligned} \text{“}\min_{\mathbf{x}}\text{”} \quad & \mathbf{f}(\mathbf{x}) \\ s.t. \quad & A\mathbf{x} \geq \mathbf{b} \quad , \end{aligned} \tag{16}$$

where $\mathbf{x}$ is the vector of variables of the problem, while A and $\mathbf{b}$ are a matrix and vector of parameters, respectively. More information on the specific variables, parameters and constraints used in ESTD can be found in Limpens et al. [39] and the model's documentation [48].

3.3.1. Constraint on GHG emissions

A constraint that is of particular interest given the context of this case study is the limit on GHG emissions, i.e.

$$GWP_{tot} \leq 35 \text{ [MtCO}_2\text{-eq/y]} \quad . \tag{17}$$

In this section, we briefly describe how this constraint is defined. The total yearly GHG emissions of the system are computed using a life-cycle analysis (LCA) approach. Thus, they include the GHG emissions along the whole life cycle, i.e. 'from the cradle to the grave' of the technologies and resources considered in ESTD. In ESTD, the global warming potential (GWP) expressed in $MtCO_2$-eq./year is used as an indicator to aggregate emissions of different GHG. Then, the yearly emissions of the system, which are denoted GWP_{tot}, are defined as follows:

$$GWP_{tot} = \sum_{j \in TECH} \frac{GWP_{constr}(j)}{lifetime(j)} + \sum_{i \in RES} GWP_{op}(i) \quad , \tag{18}$$

where $TECH$ and RES are the sets of technologies and resources modelled in ESTD. GWP_{constr} represents the GWP for the construction of a technology, while GWP_{op} gives the GWP linked to the operation of a resource. More specifically, $GWP_{constr}(j)$ is the GWP of technology j over its entire lifetime allocated to one year based on the technology lifetime $lifetime(j)$. $GWP_{op}(i)$ is the GWP related to the use of resource i over one year.

The 35 $MtCO_2$-eq/y limit chosen in this case study comes from the following reasoning. According to the International Energy Agency (IEA), Belgium's 1990 territorial GHG emissions were approximately 105 $MtCO_2$-eq [29]. Thus, the targets of the European Green Deal imply reaching 47 $MtCO_2$-eq/y in 2030 and 0 $MtCO_2$-eq/y in 2050[1]. By conducting a linear interpolation between these dates, the 2035 Belgian GHG emissions should reach approximately 35 $MtCO_2$-eq/y. This target is used as a hard constraint for GWP_{tot} in the model: $GWP_{tot} \leq 35$ [$MtCO_2$-eq/y].

3.4. Objectives

The second step in formalising the problem consists in choosing appropriate objectives. As mentioned at the start of this section, our interest lies in solutions with a sufficiently good cost and EROI. This choice implies optimising the system by minimising cost and maximising EROI. To better match the methodology presented in Section 2 where functions are minimised, E_{in} (i.e. the energy invested in the system) will be used as objective instead of EROI (the equivalence is detailed in the following). The following sections define precisely the two objectives used in the case study.

3.4.1. System cost

The first objective is the total annual cost of the system, $f_1 = C_{tot}$, defined as:

$$C_{tot} = \sum_{j \in TECH} (\tau(j) C_{inv}(j) + C_{maint}(j)) + \sum_{i \in RES} C_{op}(i) \quad . \tag{19}$$

The yearly system cost is the sum of $\tau(j)C_{inv}(j)$, the annualised investment cost of each technology with C_{inv} the total investment cost and τ the annualisation factor, $C_{maint}(j)$, the operating and maintenance cost of each technology and $C_{op}(i)$, the operating cost of the resources. This last variable is equal to

$$C_{op}(i) = \sum_{t \in T | \{h,td\} \in THTD(t)} c_{op}(i) \mathbf{F}_t(i,h,td) \quad , \tag{20}$$

where $c_{op}(i)$ is the cost of resource i in [€/MWh] and $\mathbf{F}_t(i,h,td)$ corresponds to the use in [MWh] of resource i at time (h,td). The values of $c_{op}(i)$ for each resource used in the study case are given in Tables 1 and 2. The study of Limpens et al. [39] or the online documentation [48] provides more detail on this indicator.[2]

[1] Practically, the 2050 target is to be climate neutral, meaning the GHG emission can be greater than 0 but must be compensated by carbon capture.

[2] In the mathematical formulation of the model, an additional factor $t_{op}(h,td)$ is added to equation (20), (22), and (26). This parameter is set to 1 in the implementation of the model used in this case study. It is thus removed from equations for clarity.

3.4.2. Energy invested in the system

The second objective f_2 is E_{in}, the energy invested in the system over one year:

$$E_{in} = \sum_{j \in TECH} \frac{E_{constr}(j)}{lifetime(j)} + \sum_{i \in RES} E_{op}(i) \quad , \tag{21}$$

with $E_{constr}(j)$, the energy invested to built technology j, annualised by dividing it by its lifetime, and $E_{op}(i)$ the energy to operate, i.e. produce, and transport resource i over one year. Similarly to the cost indicator, this last variable is equal to

$$E_{op}(i) = \sum_{t \in T | \{h,td\} \in THTD(t)} e_{op}(i) \mathbf{F}_t(i,h,td) \quad , \tag{22}$$

where $e_{op}(i)$ is the energy invested (in [MWh/MWh]) to obtain one MWh of the resource i. The values of $e_{op}(i)$ for each resource used in the study case are given in Tables 1 and 2. More detail is provided by Dumas et al. [33] (in which E_{in} is referred to as $E_{in,tot}$).

Minimising E_{in} would be equivalent to maximising EROI, i.e. E_{out}/E_{in}, if E_{out}, which in our case is the FEC, was constant. It is not the case in ESTD. In this model, only the values for the EUD, presented in Table C.5, are fixed. While EUD measures an energy service, FEC measures the quantity of energy used to deliver this service. FEC is thus always measured in [TWh], while the unit for EUD will depend on the demand. For instance, the EUD for heat will be measured in [TWh] while [Mt-km] will be used for mobility. Using technology-dependent conversion factors, FEC can be converted into EUD and vice-versa. For instance, in ESTD, a FEC of 1 kWh of electricity supplies an EUD of 5.8 passenger-km with a battery-electric car. As the conversion factors depend on the installed technologies, which depend on the optimisation results, FEC is an output of the ESTD model and is not constant. Nonetheless, the constant EUD cannot be employed directly as E_{out} to compute the EROI, as it is an energy service, not an amount of energy. Therefore, the FEC is used to compute E_{out} and, incidentally, the EROI of the system.

3.5. Pareto front

Once all the elements of the initial optimisation problem (5) are set up, one can compute efficient solutions from the Pareto front using one of the methods described in Section 2.2.2. This case study uses a modified version of the ϵ-constraint method. It is applied by minimising E_{in} over the feasible space with the additional constraint $C_{tot} \leq \epsilon(1 + C^{\star}_{tot})$ where $\epsilon \in \mathbb{R}_+$ and $C^{\star}_{tot}$ is the cost-optimal value, i.e. solving

$$\begin{aligned} &\min_{x \in \mathcal{X}} E_{in} \\ &\text{s.t. } C_{tot} \leq (1+\epsilon) C^{\star}_{tot} \end{aligned} \tag{23}$$

This method is a slight modification of the method described in equation (10) where ϵ is a relative rather than absolute value. It has the benefit of defining the constraint proportionally to the optimal value in the associated objective and thus be directly interpretable. For instance, if the optimal cost is 75 B€, one would use ϵ values of 1, 5, and 10% instead of absolute values of 75.75, 78.75 and 82.5 B€. To obtain several points over the Pareto front, the method was repeated for different values of ϵ in $]0, C^{e}_{tot}/C^{\star}_{tot}[$ where C^{e}_{tot} is the value of C_{tot} at the E_{in} optimum and $C^{\star}_{tot}$ is the cost optimum.

3.6. Near-optimal spaces

The efficient solutions are used to define approximate near-optimal spaces $\mathcal{X}^{\boldsymbol{\epsilon}}_m$, with $\boldsymbol{\epsilon} = (\epsilon_{C_{tot}}, \epsilon_{E_{in}})$ following equation (14) of definition 9. They are unions of spaces defined around unique, efficient solutions, $\hat{x} \in \mathcal{P}_{\mathcal{X},m}$. Each space can be easily defined by adding to the original ESTD model the two linear constraints, which are:

$$C_{tot}(x) \leq (1 + \epsilon_{C_{tot}}) C_{tot}(\hat{x}) \quad , \tag{24}$$

$$E_{in}(x) \leq (1 + \epsilon_{E_{in}}) E_{in}(\hat{x}) \quad . \tag{25}$$

3.7. Necessary conditions

The last concept to define is the type of necessary conditions computed in the case study. We are interested in the necessary resources for a transition with a sufficiently low cost and invested energy. We will thus compute the necessary conditions corresponding to the minimum amount of energy that needs to come from a specific individual or group of resources. Mathematically, the set of such conditions would be:

$$\Phi_{\overline{RES}} = \left\{ \sum_{\substack{i \in \overline{RES}, \\ t \in T | \{h,td\} \in THTD(t)}} \mathbf{F}_t(i,h,td) \geq c \right\} \quad , \tag{26}$$

where $\overline{RES} \subseteq RES$ is a set of resources, $\mathbf{F}_t(i,h,td)$ the use of resource i at time (h,td) and $c \in \mathbb{R}_+$. $\overline{RES}$ can contain any resource. However, in the context presented in Section 3.1, we have highlighted a particular interest in two groups of resources: endogenous and exogenous. We will focus primarily on those two sets and give a more detailed description of their resources. In ESTD, endogenous resources (noted RES_{endo}) include wood,

	c_{op} [€/MWh]	e_{op} [MWh/MWh]
Endogenous resources		
Hydro	0	0
Solar	0	0
Waste	23.1	0.0577
Wet biomass	5.76	0.0559
Wind	0	0
Wood	32.8	0.0491
Exogenous resources		
Ammonia	76.0	*0.174
Ammonia (Re.)	81.8	*0.295
Diesel	79.7	0.210
Bio-diesel	120	*0.101
Elec. import	84.3	0.123
Gas	44.3	0.0608
Gas (Re.)	118	*0.147
Gasoline	82.4	0.281
Bio-ethanol	111	*0.101
H2	87.5	0.083
H2 (Re.)	119	*0.134
LFO	60.2	0.204
Methanol	82.0	0.0798
Methanol (Re.)	111	*0.146

Table 1: 2035 values of c_{op}, cost of the resource [€/MWh], and e_{op}, energy invested in obtaining 1 MWh of the resource [MWh/MWh], for each resource. Most values for c_{op} come from [48]. Data for e_{op} relies on Muyldermans and Nève [49], who used the *ecoinvent* database [50]. The values preceded by a '*' are based on the work by Orban [51]. Abbreviations: Renewable (Re.), Electricity (Elec.)

	c^*_{op} [€/MWh]	e^*_{op} [MWh/MWh]
Hydro	53.7	0.0489
Solar	50.0	0.147
Wind	47.0	0.0350

Table 2: Estimated cost c^*_{op} [€/MWh] and estimated energy invested in obtaining 1 MWh of the resource e^*_{op} [MWh/MWh] for hydro, solar and wind. The estimation is done by computing the total cost at the C_{tot} optimum and invested energy at the E_{in} optimum of the technologies that use these resources (i.e. PV for solar, onshore and offshore wind for wind and hydro river for hydro) and then dividing it by the total energy used from these resources at the corresponding optimums, indicated in Table 4.

wet biomass, waste, wind, solar, hydro, and geothermal energy. Exogenous resources (noted RES_{exo}) are the other resources in the model: ammonia, renewable ammonia, imported electricity, methanol, renewable methanol, hydrogen, renewable hydrogen, coal, gas, renewable gas, light fuel oil, gasoline, diesel, biodiesel, and bioethanol. Renewable fuels such as renewable ammonia, methanol, and gas are assumed to be produced from renewable electricity. Tables 1 and 2 list the model's resources and the associated input parameters required to compute the cost and invested energy when employing them.

4. Results

In this section, we provide the answer to the question that was asked at the beginning of Section 3:

> Which endogenous or exogenous resources are necessary in Belgium to ensure a transition associated with sufficiently good cost and EROI?

This answer is obtained by computing necessary conditions corresponding to the minimum amount of energy coming from specific resources required to ensure ϵ-optimality in C_{tot} and E_{in}. However, before diving into the necessary conditions, we first analyse how the system is configured at the two optimums and show the differences between those configurations. Then, by analysing efficient solutions, we determine how this system evolves when trade-offs are made between C_{tot} and E_{in}. Finally, knowing the Pareto front, we compute ϵ-optimal spaces and necessary conditions corresponding to the minimum amount of energy coming from different resources in Belgium. The description of the algorithm used to compute those necessary conditions can be found in Appendix D.

4.1. Analysis of the system configuration at the two optimums

The Belgian energy system is analysed when optimising C_{tot} and E_{in} individually, with a maximum carbon budget GWP_{tot} of 35 $MtCO_2$-eq/y. To set a baseline to which we can compare the necessary conditions computed in the following sections, we analyse the amount of endogenous and exogenous resources used at each optimum. Table 3 shows the value of the two objective functions at the two optimums and Table 4 details which energy sources are used in the system.

	C_{tot} optimum	E_{in} optimum
C_{tot} [B€/y]	**52.8**	56.8
E_{in} [TWh/y]	74.0	**61.0**

Table 3: Values of C_{tot} and E_{in} objectives at the optimums.

Energy [TWh/y]	C_{tot} optimum	E_{in} optimum	Max. potential
Endogenous	**185**	**164**	**185**
Hydro	0.469	0.486	*0.488
Solar	61.5	54.2	*61.6
Waste	17.8	4.12	17.8
Wet Biomass	38.9	38.9	38.9
Wind	42.6	43.0	*43.0
Wood	23.4	23.4	23.4
Exogenous	**202**	**211**	∞
Ammonia (Re.)	65.6	0	∞
Bio-diesel	0	3.14	∞
Elec. import	27.6	27.6	27.6
Gas	28.2	34.5	∞
Gas (Re.)	4.98	48.5	∞
H2 (Re.)	19.4	44.8	∞
Methanol (Re.)	56.4	52.8	∞
Total	**387**	**375**	∞

Table 4: Amount of energy used from each endogenous and exogenous resource at C_{tot} and E_{in} optimums. The last column shows the maximum potential of each resource. The potentials preceded by a '*' are computed from the maximum capacity and capacity factors of the technologies using these resources. The other potentials are directly fixed as parameters.

4.1.1. Results at the cost optimum

The optimal cost $C^{\star}_{tot}$ is eqwholeual to 52.8 B€/y. At this optimum, the total amount of primary energy used in the system is 387 TWh/y, 48% of which comes from endogenous resources and the rest from exogenous resources.

For endogenous resources, the values for wet biomass, waste and wood are equal to their maximum potentials - set as input model parameters. This observation makes sense as the c_{op} of these resources in Table 1 indicate they are among the cheapest. The hydro, solar and wind energy quantities are also very close to their maximum potential. For these resources, the maximum is not set directly on the quantity of energy but on the capacities of the technologies using these resources. For instance, the model can install a maximum of 6 GW of offshore wind turbines and 10 GW of onshore wind turbines, which are the two technologies using wind as a resource. These maximum capacities can then be multiplied by the capacity factors of the corresponding technologies to obtain a maximum energy potential. Moreover, these resources are considered free in terms of cost and invested energy, as shown in Table 1. The cost of using them arises from the technologies to extract them from the environment. Table 2 shows approximated values for c_{op} and e_{op}. They are computed by dividing the cost or energy invested for building and maintaining the technologies using them by the total energy used from these resources - shown in Table 4. These approximated values show that hydro, solar and wind are among the cheapest resources, which explains their extensive use.

The model has no maximum potential for exogenous resources except for imported electricity. This potential is reached as, even though c_{op} is relatively high for imported electricity, it does not require any conversion technology to produce the final electricity demand. Some 65.6 TWh/y of renewable ammonia is used in the system, 55.4 TWh/y of which is used for electricity production and low-temperature heat generation, while the remaining 10.2 TWh/y is used to satisfy non-energy demand. Most renewable methanol is used to produce high-value chemicals, even though 3.6 TWh/y of this resource is used for fuelling boat freight. Finally, gas (renewable or not) is used to produce heat and electricity and fuel buses for public mobility.

4.1.2. Results at the invested energy optimum

The optimal energy invested $E^{\star}_{in}$ amounts to 61 TWh/y. Among the 375 TWh/y of primary energy in the system, 164 TWh/y (44%) come from endogenous resources and 211 TWh/y (56%) from exogenous resources. A series of resources, including wet biomass, wood, wind, hydro and imported electricity, are used at or near their maximum potential. This is not the case for waste and solar. In particular, for solar, e_{op} is about three times higher than any other endogenous resource. This result can be explained by the higher energy needed to build 1 GW of PV combined with a low average capacity factor compared to hydro river plants or wind turbines. Some electricity is produced using natural and renewable gas, while ammonia for non-energy demand is produced from H2 using the Haber-Bosch process. The remaining amount of gas is used to produce heat. Finally, high-value chemicals are produced using renewable methanol, while 3.14 TWh/y of bio-diesel is used for boat freight.

4.1.3. Comparison

Table 3 shows how the two objective functions vary from one optimum to the other. The increase in cost when optimising E_{in} is limited to 7.67%. Invested energy at the C_{tot} optimum is around 74 TWh/y, representing an increase of more than 20% from the E_{in} optimal value.

As shown in Table 4, the total amount of energy needed in the system differs only by 3%, but there are some differences between the two energy mixes. At the C_{tot} optimum, the energy coming from endogenous resources is 21 TWh/y higher, while energy from exogenous resources is 9 TWh/y smaller. At each optimum, the share of endogenous resources in the energy mix (48% and 44%, respectively) is close to the maximum of 42% primary energy coming from endogenous resources computed by Limpens et al. [38]. These values confirm the substantial dependence of Belgium on imported resources to supply its energy consumption.

Looking at individual resources, solar and renewable ammonia, used to produce electricity when optimising C_{tot}, are replaced by fossil and renewable gas at the E_{in} optimum. At this optimum, a percentage of the total 80 TWh/y of gas is used to produce high-temperature heat instead of waste. The additional 35.4 TWh/y of renewable hydrogen is used for three things: ammonia production (which is directly imported when optimising cost), combined heat and electricity production, and public mobility. Finally, while boat freight is fuelled using renewable methanol at the C_{tot} optimum, bio-diesel is preferred at the E_{in} optimum.

4.2. Pareto Front

Figure 5 shows the values of C_{tot} and E_{in} at the efficient solutions obtained using the method described in Section 3.5 for values of ϵ equal to 0.25, 0.5, 1.0, 2.5, 5.0 and 7.5%. The two additional points at the curve extremes correspond to each objective's optimum. The axes are labelled both in terms of the absolute values of the objective functions but also - in parenthesis - in terms of the deviations of these values from the optimal objective value, i.e. $C_{tot}/C^{\star}_{tot} - 1$ and $E_{in}/E^{\star}_{in} - 1$.

This graph shows that E_{in} decreases quite rapidly, saving 10 TWh/y out of 74 TWh/y (~ -14%) when increasing C_{tot} by a relatively small amount of 2.5%. This behaviour can also be interpreted as: choosing the optimal cost implies a considerable addition in invested energy. Inversely, as already mentioned, C_{tot} is still relatively low at the E_{in} optimum, i.e. it only increases by 7.5%.

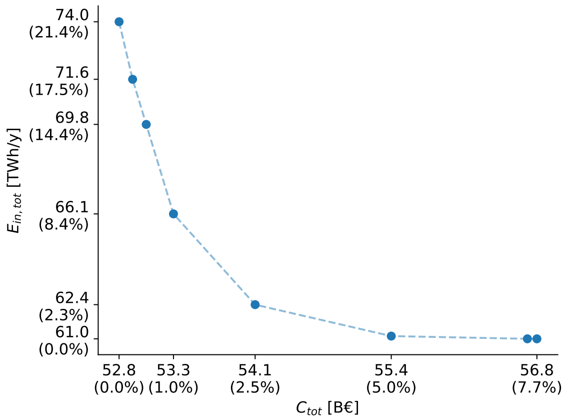


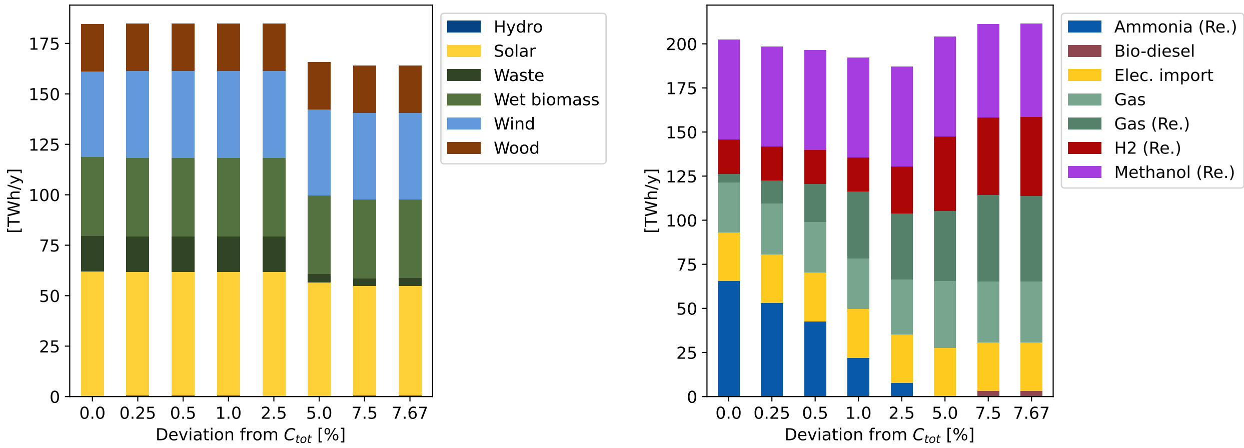
Figure 5: Approximated Pareto front showing trade-offs between C_{tot} and E_{in}. On the axis, the absolute values of C_{tot} and E_{in} are shown and completed, in parenthesis, by the deviations from the optimal objective values in each objective. For instance, for C_{tot}, the value $C_{tot}/C^{\star}_{tot} - 1$ is shown in parenthesis.

Figure 6 shows the amount of endogenous and exogenous resources used at each efficient solution, starting on the left with the cost optimum and moving towards the invested energy optimum on the right. As stated when comparing optimums, there is only a minor change for endogenous resources when going from one optimum to the other. This change, the reduction of solar and waste energy, appears when allowing a 5% deviation in cost.

More change is happening for exogenous resources (Figure 6b). As we increase cost and decrease the invested energy, ammonia is gradually replaced by gas (both natural and renewable). At a 2.5% cost increase, the amount of renewable H2 starts increasing. Ammonia is wholly removed from the system at 5%, while natural gas use reaches its maximum and starts to decline. The same happens for renewable ammonia when reaching a 7.5% cost increase, and some bio-diesel appears. Overall, the change in the total amount of exogenous resources used is non-monotonic. Starting to decrease, it then increases when reaching the 5% threshold, corresponding to the drop in endogenous resources use.

4.3. Necessary conditions

Analysing efficient solutions gives a first appreciation of the variety of system configurations, offering a trade-off between different objectives. However, using the necessary conditions, we can go one step further



(a) Endogenous resources

(b) Exogenous resources

Figure 6: Energy [TWh/y] coming from (a) endogenous and (b) exogenous resources at efficient solutions representing different trade-offs between C_{tot} and E_{in}. The leftmost bars show these values at the C_{tot} optimum, while the rightmost bar shows these values at the E_{in} optimum. The bars in the middle are characterised by their deviation in [%] from the C_{tot} optimum. Abbreviations: Renewable (Re.), Electricity (Elec.).

by providing features respected by all those solutions and some slightly less efficient solutions. We use Algorithm 2 to compute non-implied necessary conditions stemming from different sets of conditions of the type defined by (26) in Section 3.7. The main parameter defining these conditions is $\overline{RES}$, the set of resources over which the constrained sum is computed. The output of this algorithm is a value $\tilde{c}$, which defines a non-implied necessary condition for this set of resources. Practically, this value represents the minimum amount of energy that needs to come from this set of resources to ensure that C_{tot} and E_{in} do not deviate by more than an $\boldsymbol{\epsilon}$ fraction from at least one solution in the Pareto front. We will first compute this $\tilde{c}$ value for conditions defined using the set of endogenous and the set of exogenous resources. We will then look at sets containing one individual resource.

4.3.1. Endogenous vs exogenous resources

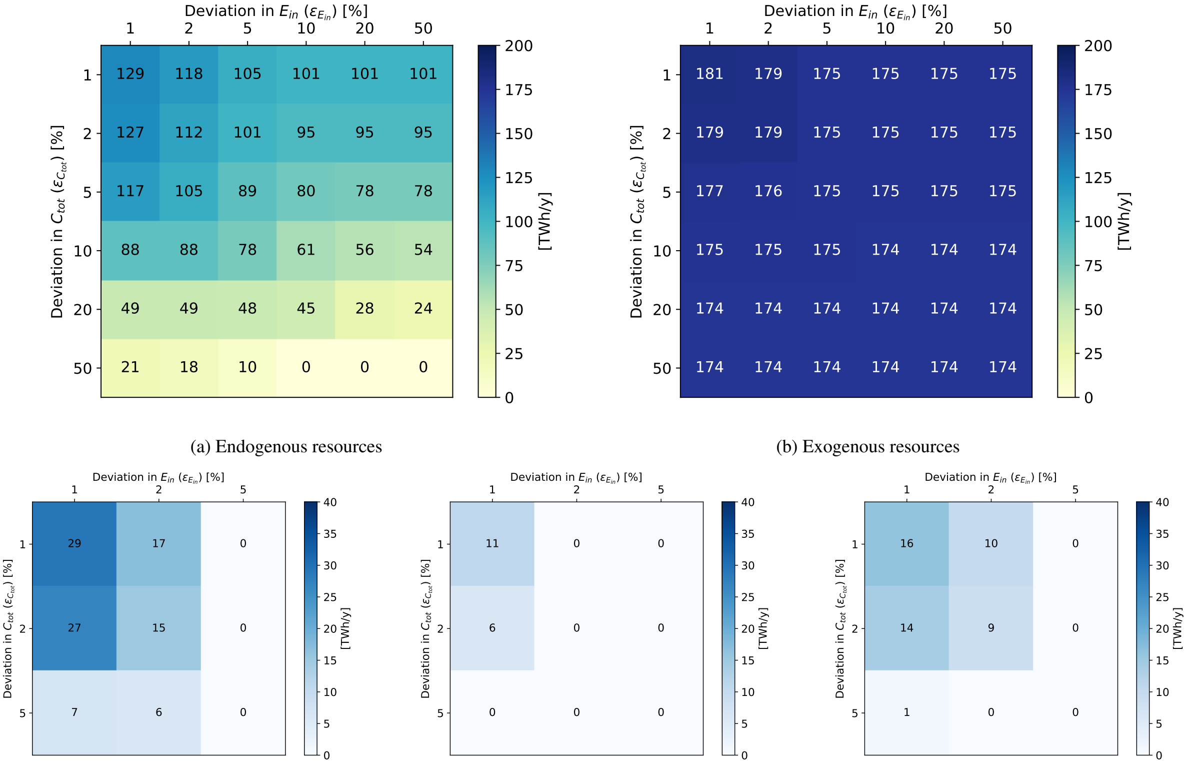
In this first section, we compare the values $\tilde{c}$ of non-implied necessary conditions computed from the sets $\Phi_{RES_{endo}}$ and $\Phi_{RES_{exo}}$. These conditions are computed for different values of deviations $\boldsymbol{\epsilon}$. In this case, the tuples $\boldsymbol{\epsilon} = (\epsilon_{C_{tot}}, \epsilon_{E_{in}})$ corresponds to all the possible combinations of 1, 2, 5, 10, 20, and 50%.

Comparing Figures 7a and 7b shows that the behaviours of the minima in endogenous and exogenous resources are very different. For endogenous resources, the minimum for deviations of 1% in both objectives is already down to 130 TWh/y, representing a 42% and 26% decrease from the C_{tot} and E_{in} optima, respectively. This amount is divided by more than two when the deviation reaches 10% in both objectives, leaving only 60 TWh/y left from endogenous resources. The $\tilde{c}$ value then reaches 0 TWh/y when allowing an increase of 50% in C_{tot}. These results show that energy from endogenous resources can be reduced by a significant amount for reasonably low increases in cost and invested energy.

For exogenous resources, there is little to no decrease in the total energy needed. Starting from 202 and 211 TWh/y at the optimums in cost and energy invested, the minimum amount of this type of energy is still around 174 TWh/y (i.e., -20% and -15% respectively) for deviations of 10%. Most of the decrease is already present for deviations of 1% with an amount of energy of 180 TWh/y, which is only 6 TWh/y less than the energy used at one of the efficient solutions. The $\tilde{c}$ value of non-implied necessary conditions then plateaus at 174 TWh/y. This result shows how, contrarily to endogenous resources, exogenous resources are essential, whatever the cost and energy invested. Indeed, to respect a GWP_{tot} constraint of 35 $MtCO_2$-eq/y, at least 174 TWh/y of energy needs to be imported.

4.3.2. Individual exogenous resources

We have shown that a certain amount of exogenous resources is necessary due to limited endogenous resources. However, the previous results do not show which specific exogenous resource is essential. This analysis can be done by computing necessary conditions for groups of conditions $\Phi_{\{i\}}$ where $i \in RES$ cor-



(a) Endogenous resources

(b) Exogenous resources

(c) Renewable methanol

(d) Gas

(e) Electricity import

Figure 7: Values $\tilde{c}$ of necessary conditions (in [TWh/y]) for conditions of type $\Phi_{\overline{RES}}$. The set of resources $\overline{RES}$ corresponds to endogenous resources RES_{endo} and exogenous resources RES_{exo} for graph (a) and (b), respectively, while for graphs (c), (d) and (e), this set resumes to a single resource: renewable methanol, gas and imported electricity, respectively. The values correspond to the minimum amount of energy that needs to come from these sets of resources to ensure a constrained deviation in C_{tot} and E_{in}. These deviations are defined by the suboptimality coefficients vector $\boldsymbol{\epsilon} = (\epsilon_{C_{tot}}, \epsilon_{E_{in}})$. For (a) and (b), all the combinations of the following percentages are taken as coefficients vectors: 1%, 2%, 5%, 10%, 20%, and 50%. For (c), (d) and (e), they are limited to the combinations of 1%, 2%, and 5%.

responds to a unique resource. We could perform this analysis for all individual resources, but in Figure 6b, the amounts of renewable methanol, gas, and imported electricity are quasi-constant across the Pareto front. Therefore, it is interesting to focus on these resources to see if they are essential or if we can eliminate them by increasing the cost or the invested energy. In this section, we analyse non-implied necessary conditions corresponding to the minimum energy from these three resources.

The $\tilde{c}$ values of non-implied necessary conditions for deviations $\epsilon_{C_{tot}}$ and $\epsilon_{E_{in}}$ of 1, 2 and 5% are shown in Figures 7c, 7d, and 7e. We limit the analysis to deviations of 5% as we can see that we are already equal (or near to) 0 TWh/y for all three resources at this percentage. The amount of energy coming from the resources at the C_{tot} and E_{in} optimums are respectively 56.4 and 52.8 TWh/y for renewable methanol, 28.2 and 34.5 for gas, and 27.6 (at both optima) for imported electricity. The minimum energy from each resource is around 50% lower than at the efficient solutions when allowing deviations of 1% in each objective. For renewable methanol and gas, the amount of necessary energy is more sensitive to deviations in invested energy than to deviations in cost. However, the conclusion is similar for the three resources: for a relatively small increase in cost and invested energy, they can be replaced by other resources.

4.4. Analysis and insights from the results

In response to the initial query of this case study, "Which endogenous or exogenous resources are necessary in Belgium to ensure a transition associated with sufficiently good cost and EROI?" our analysis offers multiple insights. Examination of the optimums for each objective revealed that endogenous resources are instrumental in achieving an attractive cost and EROI. It also highlighted that various exogenous resources could contribute to this outcome. Looking at points along the Pareto front, we then refined this analysis. This next step proved particularly informative for exogenous resources, revealing a spectrum of energy mixes satisfying reasonable cost and EROI trade-offs. Finally, the computation of necessary conditions unveiled an innovative perspective. Despite being maximised at the optimums, endogenous resources could be significantly reduced with relatively minor increases in cost and invested energy. Conversely, while numerous exogenous resource mixes offered a good cost and EROI, the total energy derived from these sources could not fall below a certain threshold. Necessary conditions also corroborated the broad range of exogenous mixes available, indicating that no specific resource is indispensable when accounting for a moderate relaxation of the objectives.

These findings suggest that for Belgium to decarbonise its economy, it must substantially rely on imported resources. This necessitates careful management of factors that can mitigate Belgium's dependence, such as enhancing energy efficiency, increasing land use for renewable energy production, and maintaining positive geopolitical relations with various providers. Fortunately, allowing for acceptable deviations in cost and EROI gives Belgium a wide choice in selecting imported energy sources, offering opportunities for diversification and a more reliable energy system.

While this analysis is specific to Belgium, similar considerations apply to other countries in the European Union, one of the most densely populated regions globally. Therefore, it is crucial to evaluate their dependence on exogenous resources and the potential trade-offs and opportunities.

5. Conclusion

The ongoing energy transition necessitates profound restructuring of energy systems over the long term. Energy system optimisation models (ESOMs) are critical in steering this restructuring and identifying the optimal blend of energy sources and technologies to meet future energy demand. However, focusing solely on cost when using these models limits the value of the insights they can provide decision-makers.

We address this issue by introducing a methodology for exploring the near-optimal spaces of multi-objective problems to answer specific socio-technical questions and applying it to a specific case study.

Building upon the research of Dubois and Ernst [23], we extend the principles of epsilon-optimality and non-implied necessary conditions to multi-objective problems. These concepts are applied to the case of Belgium's whole-energy system in 2035, with an emissions target below 35 $MtCO_2$/y, equating to an approximate 80% reduction compared to 2015 levels [38]. The case study involved identifying the necessary endogenous or exogenous resources to ensure a transition with reasonable cost and EROI. This need is determined by computing non-implied necessary conditions, representing the minimum energy amount derived from various resource sets to ensure a constrained deviation in cost and energy invested. Our research findings suggest that while Belgium could significantly curtail its consumption of endogenous resources, diminishing reliance on exogenous resources presents a complex challenge. Furthermore, our results underscore the versatility of potential exogenous resources.

The current methodology encounters a set of limitations that, if addressed, could enhance the reliability of the results. The primary constraint relates to the approximation of the epsilon-optimal space in multi-objective optimisation problems, which affects the identification of non-implied necessary conditions. Increasing the number of efficient solutions can improve results but amplifies computational time. To mitigate this constraint, future research could examine the influence of the number and distribution of efficient solutions on the findings. Another consideration involves the visual presentation of the results. Specifically, necessary conditions for constrained deviations in two objectives can be effectively displayed on a two-dimensional grid. However, should the objectives exceed two, or if near-optimal space analysis is merged with parametric uncertainty analysis, new innovative techniques will be required to encapsulate the results succinctly.

Potential avenues for future research could contribute to expanding the current methodology. Firstly, the method was developed around the concept of necessary conditions. However, other methodologies were developed to explore near-optimal spaces in a mono-objective setup as presented, for instance, in Price and Keppo [18], Li and Trutnevyte [19], Pedersen et al. [20], Nacken et al. [52]. An interesting research track would be to extend these methodologies in a multi-objective setup. Secondly, the current methodology was developed for fixed feasible spaces and objective functions. Incorporating techniques for addressing parametric uncertainty, such as sensitivity analysis, would enhance the breadth and applicability of the results.

Lastly, extensive research is required to substantiate the utility of the method across varied contexts. Future research could replicate the case study for different nations or regions grappling with resource constraints and challenges of energy dependence. Moreover, while cost and invested energy were the primary objectives in this study, other criteria like land use, water use, or metal resources could be explored. This framework could also be utilised to answer alternative queries about various resources or technologies. Ultimately, this approach could be extended to study near-optimal spaces for various optimisation problems within and beyond the energy systems field.

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Data Availability

Datasets related to this article can be found at https://zenodo.org/record/7665440#.Y_YyltLMIUE, hosted at Zenodo [24].

Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work, the author(s) used ChatGPT in order to improve the formulation of certain sections. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

Appendix A. Numerical values of the epsilon-space examples

The functions depicted in Figures 2, 3, and 4 are

$$f_1(x) = 10 * (2x - 0.75)^2 + 2 \quad \text{and} \tag{A.1}$$
$$f_2(x) = 10 * (x - 0.75)^2 + 1.5 \quad . \tag{A.2}$$

The coordinates of their minimums are $(x_1^*, f_1(x_1^*)) = (0.375, 2)$ and $(x_2^*, f_2(x_2^*)) = (0.75, 1.5)$, respectively.

One-dimensional epsilon-optimal space

In Figure 2, the ϵ-optimal space $\mathcal{X}^\epsilon$ of a one-dimensional optimisation problem was obtained by first computing

$$(1 + \epsilon_1) f_1(x_1^*) = (1 + 0.25) * 2 = 2.5 \tag{A.3}$$

where $\epsilon_1 = 0.25$. Then, the limits of $\mathcal{X}^\epsilon$ can be obtained by computing the inverse image of this value, i.e. the set $\{0.263, 0.487\}$, which leads to $\mathcal{X}^\epsilon = [0.263, 0.487]$.

Two-dimensional epsilon-optimal space

In Figure 3a and 3b, the Pareto front $\mathcal{P}_\mathcal{X}$ is represented in green. This set of points respects definition 6 of a Pareto front. Indeed, each point x in the interval $[x_1^\star, x_2^\star]$ is such that $\nexists \hat{x} \in \mathcal{X}$ where $f_1(\hat{x}) < f_1(x)$ and $f_2(\hat{x}) < f_2(x)$.

In Figure 3b, a subset of the $\boldsymbol{\epsilon}$-optimal space $\mathcal{X}^{\boldsymbol{\epsilon}}$ of a two-dimensional optimisation problem is computed for a suboptimality coefficients vector $\boldsymbol{\epsilon} = (\epsilon_1, \epsilon_2) = (0.25, 0.6)$. This subset is computed from the point $\hat{x} = 0.6$, which is part of $\mathcal{P}_\mathcal{X}$. To obtain the subset of $\mathcal{X}^{\boldsymbol{\epsilon}}$, the images of $\hat{x}$, $f_1(\hat{x}) = 4.025$ and $f_2(\hat{x}) = 1.725$, are computed. Multiplying these values by the corresponding suboptimality coefficients gives

$$(1 + \epsilon_1) f_1(\hat{x}) = (1 + 0.25) * 4.025 = 5.03 \quad \text{and} \tag{A.4}$$
$$(1 + \epsilon_2) f_2(\hat{x}) = (1 + 0.6) * 1.725 = 2.76 \quad . \tag{A.5}$$

The inverse image of these values are $\{0.0997, 0.65\}$ for f_1 and $\{0.395, 1.105\}$ for f_2. The set of points respecting $\forall k \; f_k(x) \leq (1 + \epsilon_k) f_k(\hat{x})$ are then contained in $[0.395, 0.65]$.

To obtain the full $\boldsymbol{\epsilon}$-optimal space depicted in Fig. 3a, one should repeat this process with all points in $\mathcal{P}_\mathcal{X}$. However, in this simple example, one can quickly compute the limits of the entire space by using the two optimums, which are the extreme points of the Pareto front. These limits are obtained by taking the inverse images of

$$(1 + \epsilon_1) f_1(x_1^*) = (1 + 0.25) * 2 = 2.5 \quad \text{and} \tag{A.6}$$
$$(1 + \epsilon_2) f_2(x_2^*) = (1 + 0.6) * 1.5 = 2.4 \quad , \tag{A.7}$$

which gives $\{0.263, 0.487\}$ and $\{0.45, 1.05\}$. The lower and upper bound of $\mathcal{X}^\epsilon$ are then respectively given by the lower and upper bound of those two sets, i.e. $\mathcal{X}^\epsilon = [0.263, 1.05]$.

Approximate Pareto fronts and epsilon-optimal spaces

Figures 4a, 4b, and 4c show approximate $\boldsymbol{\epsilon}$-optimal spaces for three different set of efficient points. These sets are

1. Fig. 4a: [(2.0, 2.91), (3.41, 1.85), (7.62, 1.5)];
2. Fig. 4b: [(2.9, 2.01), (2.99, 1.97), (3.09, 1.94), (3.19, 1.91), (3.3, 1.88), (3.41, 1.85), (3.52, 1.82), (3.64, 1.8), (3.77, 1.77), (3.9, 1.75), (4.03, 1.72)];
3. Fig. 4c: [(2.0, 2.91), (2.06, 2.64), (2.23, 2.40), (2.51, 2.19), (2.9, 2.01), (3.41, 1.85), (4.03, 1.72), (4.76, 1.63), (5.61, 1.56), (6.57, 1.51), (7.62, 1.5)].

Appendix B. Necessary conditions - Advanced definitions

Appendix B.1. Implication

The *implication* between two conditions can be defined mathematically and allow for a more formal definition of non-implied necessary conditions.

Definition 10. *An **implication function** $\psi(\phi_1 \mid \phi_2) \in \{0, 1\}$ is a function that indicates whether condition ϕ_2 implies condition ϕ_1. When $\psi(\phi_1 \mid \phi_2) = 1$, then $\forall x \in \mathcal{X}$, $\phi_2(x) = 1 \implies \phi_1(x) = 1$. When $\psi(\phi_1 \mid \phi_2) = 0$, then $\exists x \in \mathcal{X}$, $\phi_2(x) = 1 \not\Longrightarrow \phi_1(x) = 1$.*

Example: Let us consider conditions $\phi_1(x) := x \geq 1$ and $\phi_2(x) := x \geq 2$ of the example introduced in Section 2.1.2. We have that $\psi(\phi_1 \mid \phi_2) = 1$. Indeed, for all $x \in \mathcal{X}$, if $\phi_2(x) = 1$ this means that $x \geq 2$, that $x \geq 1$ and thus $\phi_1(x) = 1$. Conversely, $\psi(\phi_2 \mid \phi_1) = 0$. Indeed, there exist several $x \in \mathcal{X}$ such that $\phi_1(x) = 1$ and $\phi_2(x) = 0$. For instance, this is the case for $x = 1.5$.

Definition 11. *A **non-implied necessary condition** is a necessary condition $\phi \in \Phi^{\mathcal{X}^\epsilon}$ that is not implied by any other necessary condition. It is a necessary condition $\phi \in \Phi^{\mathcal{X}^\epsilon}$ such that $\forall \phi' \in \Phi^{\mathcal{X}^\epsilon} \setminus \{\phi\} : \psi(\phi \mid \phi') = 0$.*

Example: The condition ϕ_0 respects this definition. Indeed, for any other condition $\phi' \in \Phi^{\mathcal{X}^\epsilon}$, that is any ϕ_c with $c < 0$, we have $\psi(\phi_0 \mid \phi_c) = 0$. The proof is straightforward. For any $c < 0$, $\phi_c(c) = 1$ as $c \geq c$ is true, but $\phi_0(c) = 0$ as $c \geq 0$ is false.

Appendix B.2. Necessary conditions - True spaces

A last way to particularise the definition of (non-implied) necessary conditions is by defining the space over which a condition is true.

Definition 12. *The space $\mathcal{I}_\phi$ is the subset of $\mathcal{X}$ where a condition ϕ is true, that is:*

$$\mathcal{I}_\phi = \left\{ x \in \mathcal{X} \mid \phi(x) = 1 \right\} \quad . \tag{B.1}$$

Example: The spaces $\mathcal{I}_{\phi_c}$ of the conditions $\phi_c(x) := x \geq c$ are the spaces $[c, \infty]$. These spaces might become more complex to determine when considering, for instance, conditions using linear combinations of variables, e.g. $\phi(x) := ax_1 + bx_2 \geq c$ with $x = (x_1, x_2) \in \mathcal{X} = \mathbb{R}^2$.

Definition 13. *A **necessary condition** for ϵ-optimality is a condition ϕ such that $\mathcal{X}_\epsilon \subseteq \mathcal{I}_\phi$.*

Example: For a set of conditions $\Phi = \{\phi_c(x) := x \geq c\}$ with $x \in \mathbb{R}$ and $c \in \mathbb{R}$, and a ϵ-optimal space $\mathcal{X}^\epsilon = [0, 1]$, this definition implies that all conditions ϕ_c with $c \leq 0$ are necessary, which corresponds to same set as definition 3. Indeed, the spaces $\mathcal{I}_{\phi_c} = [c, \infty]$ include the space $[0, 1]$, when $c \leq 0$.

Definition 14. *Let ϕ_1 and ϕ_2 be conditions with $\mathcal{I}_{\phi_1}$ and $\mathcal{I}_{\phi_2}$ the spaces over which they are respectively true, then the **implication function** $\psi(\phi_1 \mid \phi_2)$ is defined as:*

$$\psi(\phi_1 \mid \phi_2) = \mathcal{I}_{\phi_2} \subseteq \mathcal{I}_{\phi_1} \quad . \tag{B.2}$$

This formulation fits definition 10 of an implication function. Indeed, if $\psi(\phi_1 \mid \phi_2) = 1$, then it means $\mathcal{I}_{\phi_2} \subseteq \mathcal{I}_{\phi_1}$, which in turns implies that $\phi_1(x) = 1$ for any $x \in \mathcal{X}$ for which $\phi_2(x) = 1$. Similarly, if $\psi(\phi_1 \mid \phi_2) = 0$, it means that $\mathcal{I}_{\phi_2} \nsubseteq \mathcal{I}_{\phi_1}$, which means $\exists x \in \mathcal{X}$ such that $\phi_1(x) = 0$ when $\phi_2(x) = 1$.

Definition 15. *A **non-implied necessary condition** is a necessary condition $\phi \in \Phi^{\mathcal{X}^\epsilon}$ that is true over a space which does not include any of the spaces over which other necessary conditions are true. It is a necessary condition $\phi \in \Phi^{\mathcal{X}^\epsilon}$ such that $\forall \phi' \in \Phi^{\mathcal{X}^\epsilon} \setminus \{\phi\} : \mathcal{I}_{\phi'} \nsubseteq \mathcal{I}_\phi$.*

Figure B.8 illustrates these concepts, where ϕ_2 implies ϕ_1 as $\mathcal{I}_{\phi_2} \subset \mathcal{I}_{\phi_1}$. They are both necessary conditions because they are true over $\mathcal{X}^\epsilon$. Finally, if no other conditions exist in the set $\Phi = \{\phi_1, \phi_2\}$, then ϕ_2 is a non-implied necessary condition as no other necessary condition implies it.

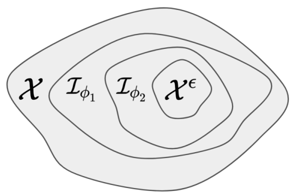

Figure B.8: Graphical illustration of implication using spaces over which conditions are true, adapted from Dubois and Ernst [23]. The four spaces that are represented are the feasible space $\mathcal{X}$, the ϵ-optimal space $\mathcal{X}^\epsilon$, and the spaces $\mathcal{I}_{\phi_1}$ and $\mathcal{I}_{\phi_2}$ where conditions ϕ_1 and ϕ_2 are respectively true. Both these conditions are necessary as $\mathcal{X}^\epsilon \subset \mathcal{I}_{\phi_1}$ and $\mathcal{X}^\epsilon \subset \mathcal{I}_{\phi_2}$. Moreover, ϕ_2 implies ϕ_1 as $\mathcal{I}_{\phi_2} \subset \mathcal{I}_{\phi_1}$.

Appendix C. Types of end-use demand in EnergyScope-TD

Four main types of EUD are considered in the model: electricity, heat, transport, and non-energy demand. Electricity is further divided between lighting

Algorithm 3: Computation of one non-implied necessary condition for a given set of resources and suboptimality coefficients vector. Adaptation of Algorithm 2 to the case study.

Data:
$\mathcal{X} \in \mathbb{R}^n$ - feasible space defined via ESTD,
$\mathbf{f} = (C_{tot}, E_{in})$,
m - number of points,
$\boldsymbol{\epsilon} = (\epsilon_{C_{tot}}, \epsilon_{E_{in}})$,
$\overline{RES}$ - a set of resources

Result: $\tilde{c}$

Steps:

1. Compute the two optimums $C^{\star}_{tot} = \arg\min_{\mathcal{X}} C_{tot}$ $E^{\star}_{in} = \arg\min_{\mathcal{X}} E_{in}$ (and derive C^{e}_{tot} the value of C_{tot} at the E_{in} optimum).
2. Apply method (23) for $m-2$ values of ϵ in $]0, C^{e}_{tot}/C^{\star}_{tot}[$ to obtain points $\hat{\mathbf{x}}^{(2)}, \ldots \hat{\mathbf{x}}^{(j)}, \ldots \hat{\mathbf{x}}^{(m-1)}$ of the Pareto front. Points $\hat{\mathbf{x}}^{(1)}$ and $\hat{\mathbf{x}}^{(m)}$ correspond to the C_{tot} and E_{in} optimums, respectively.
3. For all $j \in [1, 2, \ldots, m]$, compute

$$c^{(j)} = \min \sum_{\substack{i \in \overline{RES},\\ t \in T | \{h,td\} \in THTD(t)}} \mathbf{F}_t(i, h, td) \qquad \text{(D.1)}$$

over the space

$$\{\mathbf{x} \in \mathcal{X} \mid C_{tot}(\mathbf{x}) \leq (1 + \epsilon_{C_{tot}}) C_{tot}(\hat{\mathbf{x}}^{(j)}), \; E_{in}(\mathbf{x}) \leq (1 + \epsilon_{E_{in}}) E_{in}(\hat{\mathbf{x}}^{(j)})\}, \qquad \text{(D.2)}$$

where $C_{tot}(\mathbf{x})$ and $E_{in}(\mathbf{x})$ represent the values of the two objectives at solution $\mathbf{x}$.
4. Take the minimum $\tilde{c} = \min_{j \in [1,2,\ldots,m]} c^{(j)}$ to find the non-implied necessary condition:

$$\phi_{\tilde{c}} = \sum_{\substack{i \in \overline{RES},\\ t \in T | \{h,td\} \in THTD(t)}} \mathbf{F}_t(i, h, td) \geq \tilde{c} \quad , \qquad \text{(D.3)}$$

and other electricity uses. Heat is subdivided into high-temperature heat for industry, low temperature for space heating, and low temperature for hot water. Mobility is composed of public and private passenger mobility and freight demands. Finally, the non-energy demand includes demand for ammonia, methanol, and high-value chemicals (HVCs). Table C.5 lists the values for each EUD type in 2035 based on Limpens [53].

EUD type	Unit	EUD
Electricity (other)	TWhe	62.1
Lighting	TWhe	30.0
Heat high T.	TWh	50.4
Heat low T. (SH)	TWh	118
Heat low T. (HW)	TWh	29.2
Passenger mobility	Mpass.-km	194
Freight	Mt-km	98.0
Non-energy	TWh	53.1

Table C.5: 2035 Belgian end-use demand (EUD) value by type based on Limpens [53]. Abbreviations: temperature (T.), space heating (SP), hot water (HW), passenger (pass.).

Appendix D. Computation of non-implied necessary conditions for the case study

Algorithm 3 is an adapted version of Algorithm 2 allowing to compute a non-implied necessary condition for a fixed set of resources $\overline{RES}$ and suboptimality coefficients vector $\boldsymbol{\epsilon}$.

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4 Explaining how model complexity affects necessary conditions

4.1 The Question

Does system configuration change faster around the optimum when systems are more complex ?

Retrieving the optimal solution to an optimisation problem can be a cumbersome task. Considering this optimum as insufficient and searching for alternative near-optimal solutions makes the problem even more computationally intensive.

Several strategies can be employed to curb the necessity for extensive solution explorations. Primarily, the choice of a specific Modelling to Generate Alternative (MGA) technique can significantly influence efficiency. Generating many solutions with no precise objective can be less productive than targeted efforts, like those employed in computing necessary conditions. Another way to economise computational effort is by limiting the variations in the sub-optimality coefficient, ϵ. For instance, one might opt to use just 1% and 10% as values rather than 1%, 2.5%, 5%, and 10%. Such a strategy, though computationally sparing, might curtail a deeper understanding of how solutions diverge with increasing allowable deviations. This could subsequently reduce the insights available for decision-making.

However, these considerations warrant a caveat. If solutions show minimal alterations upon deviation from the optimum, then a comprehensive exploration of the near-optimal space might be redundant. But how can we determine this trait of the optimum's neighbourhood? It is not evident, but we conjecture that the complexity of a model could serve as an indicator of this trait. For instance, a model with a broader spectrum of technological choices (indicative of higher complexity) might demonstrate a more pronounced solution shift upon small alterations in the objective value, given its increased number of alternatives. Conversely, a model with a more realistic representation of specific technologies (e.g., introducing ramping constraints on generator production) might shrink the near-optimal space. Hence, we endeavoured to probe: Does increased system complexity precipitate a faster or slower shift in configuration near the optimum?

4.2 The Idea

Defining the complexity of a model, especially within the domain of energy modelling, is complex. The intricacy can hinge on multiple factors: the model's sectoral and technological breadth, the granularity with which it portrays the inner mechanics of technologies, or the specific features incorporated to more authentically simulate real-world scenarios. To discern how complexity influences near-optimal spaces, we concentrated on one facet that dictates a model's complexity: its spatiotemporal resolution. This dimension was chosen owing to its quantifiable nature, compared to other features such as the fidelity of representation of a technology. For instance, in a network, the spatial resolution can easily be gauged by tallying the number of nodes, and the temporal resolution pertains to the level of time aggregation, e.g. one hour, one day, or one week.

Next arose the challenge of selecting an appropriate metric to assess how the near-optimal space morphs across models of varying spatiotemporal resolutions. One viable approach might involve calculating the 'volume' of the near-optimal space for each distinct resolution and comparing them across resolutions for fixed sub-optimal coefficients. Yet, computing the volume of a multi-dimensional polyhedron remains intricate. Consequently, we opted for a more straightforward approach based on our previous work by using the variation of necessary conditions over assorted resolutions as our evaluative criterion. Although this may not wholly capture the essence of the near-optimal space's evolution, it embarks on a preliminary pathway to garner insights.

4.3 The Paper: *Impacts of Spatial and Temporal Resolutions on the Near-Optimal Spaces of Energy System Optimisation Models*

This article was accepted for presentation at the IEEE PES Innovative Smart Grid Technologies Europe 2023 conference.

4.3.1 Paper's contributions

The main contributions of this paper are as follows:

1. It pioneers the study of how spatial and temporal resolutions impact the values of necessary conditions for near-optimality.

2. To steer further research in this domain, it furnishes a comprehensive set of observations detailing these impacts.

4.3.2 Authors' contributions

Professor Ernst and myself co-authored this article. I initiated the research idea, conducted the experiments, and took the lead in the writing process. Professor Ernst provided supervision and guidance throughout the entire process.

4.3.3 Reading tips

Although Tables II to IV may appear dense and contain numerous results, the conclusions derived from these findings are straightforward and summarised in Section IV.B as three key observations. Rather than attempting to interpret the tables independently, readers should direct their attention to these concise observations for a clear understanding of the results.

Impacts of spatial and temporal resolutions on the near-optimal spaces of energy system optimisation models

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***Abstract*—Over the past years, the rising penetration of renewable energy in power systems has led to the need for more detailed energy system models. Specifically, spatial and temporal resolutions have become increasingly important, and multiple studies have investigated their impact on the optimal solutions to energy system optimisation problems. However, these studies have yet to be conducted for near-optimal solutions, which can provide valuable insights to decision-makers. This paper aims to initiate this research by examining the effects of spatial and temporal resolutions on the values of necessary conditions for near-optimality. In particular, we investigate how spatiotemporal resolution changes affect minimal capacity investments in the European electricity grid. Our analysis leads to three key observations. Firstly, we show that minimal capacities for near-optimality exhibit similar trends to optimal capacities when each resolution varies. Secondly, the resolutions that result in higher optimal capacities are also the ones where minimal capacities deviate the least from the optimal capacities. Thirdly, as a result of the second observation, spatial or temporal resolution changes have a greater impact on minimal capacities for near-optimality than on optimal capacities. We conclude by suggesting solutions to expand this research track and gain a deeper understanding of the impact of spatiotemporal resolution on near-optimal spaces.**

***Index Terms*—spatiotemporal resolution, near-optimal space, necessary condition, energy system optimisation model, European power grid**

I. Introduction

Energy system optimisation models (ESOMs) are extensively used to plan the transition to low-carbon power systems at local, national and international levels [1]. These models allow for determining the best system investment and operation for optimising an objective, typically cost.

However, researchers have recently highlighted the importance of going beyond classic cost-optimal analysis by studying near-optimal solutions [2]. These solutions, while less cost-efficient, might be better in terms of other objectives - e.g. energy efficiency, ecological concerns, or social factors - which might be challenging to model. Near-optimal solutions analyses have shown how different the system can become when allowing for slight deviations in cost [3]–[6].

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The results of studies using ESOMs are also affected by the complexity with which energy systems are modelled. This complexity depends on the features that are included in the model. Including more numerous and complex features while providing more detailed studies leads to more complex models, which are, in turn, more time-consuming to model and more challenging to solve. One feature that can easily be modified to tune the complexity of a model is its spatiotemporal resolution. This feature has become increasingly important with the increased penetration of new renewable energy technologies, such as photovoltaic (PV) panels and wind turbines in energy systems. Different studies have thus explored the impact of spatial and temporal resolution on the cost-optimal solution of ESOMs [7]–[11]. However, the impact of this form of complexity on near-optimal solutions has yet to be explored. In this paper, we initiate research in this area by analysing how spatial and temporal resolution affects necessary conditions for epsilon-optimality - a concept introduced by [5]. This analysis is done on a case study whose context is the European electricity grid modelled using the open-source ESOM PyPSA.

II. Literature review

An extensive range of ESOMs exhibiting different features exists [1]. Classical features include the models' temporal, geographical and sectoral scopes, the range of modelled technologies, and the complexity with which they are modelled. Some models implement special features such as price-responsive demands, endogenous technological learning, or macroeconomic interactions. The number and sophistication of these features determine the complexity of each model. Among those features, the model's spatiotemporal resolution is paramount. According to [1], setting it appropriately is the second key step in any ESOM application. When modelling energy systems with high renewable energy penetration, a high - typically hourly - resolution is required to represent the system dynamics properly. For system models representing networks, the spatial resolution depends on the number of modelled nodes. For instance, a spatial resolution of one node per country is often used to model transnational power systems. Still, some representations can be much more precise, e.g., a thousand nodes for the European power system represented by PyPSA-Eur [12].

Some studies have shown how the spatiotemporal resolution affects the quality of the system modelling and the analysis it serves. As highlighted in [7], spatial resolution can impact the system's estimated cost. Depending on the grid model, this cost can be over- or underestimated. Another impact mentioned by [7] is the sub-optimal capacity investment in technologies such as wind and solar when using low spatial resolution. Spatial resolution can also impact the curtailment of renewable sources [8]. The impact of temporal resolution is non-negligible, either. Indeed, as mentioned in [9], aggregating this resolution inappropriately can introduce errors in model outputs and the derived insights. For instance, as stated in [10], a simplified resolution implies an under-evaluation of cost. It can also lead to understating the importance of wind generation and energy storage while overstating the value of solar generation. The work of [11] also supports the underinvestment in wind technology.

Overall, improving spatiotemporal resolution leads to better estimating the system's needs. Another way of improving the quality of insights derived from ESOMs is to look beyond cost-optimal solutions. This approach was first proposed in a case unrelated to energy system modelling [13]. It was recently applied to ESOMs by [2] and has since been used by several researchers [3]–[5], [14], [15]. These authors have proposed different approaches for exploring the near-optimal space, i.e., the space of solutions with an objective value close to the optimal objective value. Some propose computing a series of near-optimal solutions and analysing their properties [3], [14], [15]. Others are searching for near-optimal solutions exhibiting specific properties, e.g., those with a minimum capacity in some renewable technology [4], [5]. Authors of [5] translated this second approach through the computation of ϵ-optimal necessary conditions, i.e., conditions which are true for any solution whose cost is, at most, $1+\epsilon$ times more expensive than the cost optimum. More specifically, the methodology consists of computing an ϵ-optimal space $\mathcal{X}^\epsilon$ defined as:

$$\mathcal{X}^\epsilon = \{x \in \mathcal{X} \mid f(x) \leq (1+\epsilon) f(x^\star)\} \; \forall \epsilon \geq 0 \, , \quad (1)$$

where $\mathcal{X}$ is the problem feasible space, $f : \mathcal{X} \to \mathbb{R}_+$ an objective function (e.g., the cost), $x^\star$ an optimal solution, and ϵ the suboptimality coefficient that measures the deviation from the cost-optimal value. This space contains all the solutions whose objective value does not deviate by more than ϵ from the optimal objective value. Necessary conditions for ϵ-optimality can then be computed to derive insights from this space. Those are conditions (i.e. functions $\phi : \mathcal{X} \to \{0, 1\}$) which are true for every element in $\mathcal{X}^\epsilon$. For instance, using conditions corresponding to constrained sums of investment variables, the authors of [5] showed that for a deviation ϵ of 10%, capacity investment in onshore wind, storage, PV, transmission, and offshore wind could be reduced to 0%, 0%, 15%, 50%, and 60% of their optimal capacities, respectively.

These studies were performed with a fixed spatiotemporal resolution and have thus not explored whether increasing it improves the quality of the insights derived from near-optimal solutions. In this paper, we take the first step in filling this gap by exploring how spatial and temporal resolution impacts necessary capacity investments for near-optimality.

III. Case Study

This case study explores the required minimum investments in power transmission, generation, and storage capacities across the European continent to achieve, by 2030, a 99% reduction in greenhouse gas (GHG) emissions compared to 1990 levels while ensuring near-optimality in cost. The goal is to analyse the impact of spatial and temporal resolution on these investments.

To model the European electricity network, the open-source tool PyPSA (Python for Power System Analysis) [16] is used. As described in its online documentation [17], PyPSA allows for "simulating and optimising modern power systems that include features such as conventional generators with unit commitment, variable wind and solar generation, storage units, coupling to other energy sectors, and mixed alternating and direct current networks". It is "designed to scale well with large networks and long time series". This case study uses PyPSA to plan capacity expansion, i.e., determine how much capacity needs to be deployed for each expandable technology at each network node.

PyPSA has been used to model the European network through the PyPSA-Eur project [12]. This model has already been used and validated in a series of studies [5], [18], [19]. In this case study, the default version of the model [20] is used with a few modifications. In addition to onshore and offshore wind, capacities of PV, CCGT (combined cycle gas turbine), OCGT (open cycle gas turbine), transmission, and storage can be extended. The power density of offshore wind is set to 10 MW/km^2 [21] instead of the default 2 MW/km^2. A limit of two times the existing capacity is set on link and line capacities. We consider it a reasonable upper bound on what is possible to build in less than ten years. Finally, nuclear power plants can produce at nominal capacity but have a ramping limit of 10% of nominal capacity per hour, upwards and downwards.

The modelled network contains 6763 lines and 3642 substations [20], and time series for electrical demand and variable renewable generators are available at an hourly resolution. However, the model can be clustered to decrease the number of substations - also referred to as nodes - and, therefore, the number of lines. The temporal resolution can also be reduced by averaging over every n snapshot, where n is a positive integer. This paper studies the following level of clustering: 100, 200, and 400 nodes for spatial resolution and 2, 4 and 6 hours for temporal resolution. The lower limit of a six-hourly resolution was set as decreasing the temporal resolution further led to unreliable storage behaviour.

The cost-optimal network configurations are first computed for all combinations of these resolutions. For each of these optimal configurations, we analyse the sums of new capacities installed for PV panels, wind turbines (i.e., the sum of new capacities of onshore and offshore wind), and transmission (i.e., the sum of new capacities of lines and links) across the European network. Mathematically, we can denote these sums by $\mathbf{d}^T\mathbf{x}_I$ with $\mathbf{x}_I$ a vector of size $|I|$ that collects the different investment variables and $\mathbf{d} \in \{0,1\}^{|I|}$. For instance, the only values equal to 1 in $\mathbf{d}$ could correspond to the investment capacities in wind turbines. The sum would then equal the sum of wind capacities across the network. By changing the values in $\mathbf{d}$, we can obtain investment capacities for different technologies. These sums take different values for each solution to the problem. We denote the value of these sums at the optima by $c^*_{n,h}$ where n and h represent the spatial and temporal resolution of the model, counted respectively in nodes and hours.

Once the optima are computed, the methodology developed in [5] allows determining the minimum new capacity investment needed in PV, wind and transmission to ensure cost ϵ-optimality. To compute the minimum new capacity required in renewable technologies to stay ϵ-optimal, we use conditions of the form $\phi(\mathbf{x}_I) := \mathbf{d}^T\mathbf{x}_I \geq c$ with $c \in \mathbb{R}_+$. If we minimise this sum over $\mathcal{X}^\epsilon$, we obtain a value $c^\epsilon_{n,h}$ equal to the minimal new capacity that needs to be deployed to be ϵ-optimal (see [5] for a proof). These values depend on the model's spatial and temporal resolution and the sub-optimality coefficient. In this case study, we limit our analysis to an ϵ of 10%.

IV. Results

We first analyse the optimal values $c^*_{n,h}$ of new capacities for PV, wind and transmission to see how the system behaves at the optima when changing the resolution. We then analyse how near-optimal solutions are impacted by looking at the minimal new capacities $c^\epsilon_{n,h}$ for these technologies and how these impacts compare to the ones on the optimal capacities.

A. Analysis of optimal solutions

The optimal solutions are computed for time resolutions of 6, 4, and 2 hours and spatial resolutions of 100, 200, and 400 nodes (in order from the least complex system to the most complex). Table I shows the optimal costs for all combinations of resolutions. The values range between 64.4 and 69.8 B€/y, and there is a clear trend: the more complex the network, the higher the cost. Rising investment costs primarily drive the increases. Indeed, increasing the temporal resolution from 6 hours to 2 hours adds between 1 to 2 B€/y in generation capacity investment. This rise is linked to the switch from solar to wind capacity, as shown in Table II. While the added wind capacity is only half that removed for PV, the average wind capital cost is around four times more expensive, explaining the overall rise in investment cost. Improving the temporal resolution decreases the importance of PV because it reveals the mismatch between solar production and demand peaks, making this technology less attractive as it needs to be combined with storage. The increase in storage observed when moving from six to two-hourly resolution confirms this and explains the additional 1.7 to 2.3 B€/y increase in cost. As shown in Table II, transmission investment also increases with the temporal resolution, allowing the absorption of unsmoothed production peaks.

TABLE I: System costs [B€/y] at the optimal solutions for different spatial and temporal resolutions.

	hours $[h]$		
nodes $[n]$	6	4	2
100	64.4	67.4	68.4
200	64.7	67.8	68.7
400	65.9	68.8	69.8

PV and wind capacities increase when using a better spatial resolution. This increase can be explained by the better spatial representation of renewable sources linked to the increased number of nodes in the model. Indeed, in the PyPSa-Eur model, wind and PV capacity can be installed at each node and are associated with a node-specific capacity factor time series. When aggregating nodes to reduce the spatial resolution, the capacity factors of different nodes are averaged, leading to losing some of the better capacity factor signals. This increase in renewable generation again implies greater needs in storage capacity which adds between 1.3 to 1.9 B€/y to the total cost. To finish this analysis, let us note that there is no clear tendency when looking at the evolution of transmission capacity with spatial resolution. Indeed, the capacity rises from 100 to 200 nodes before dropping again when reaching 400 nodes. This behaviour is difficult to analyse as topological changes, impacting the total length of the lines and, thus, their capacities in TWkm, occur when modifying the number of nodes in the network. Thus, in the rest of the paper, the analysis of transmission capacity is limited to its evolution with temporal resolution.

B. Analysis of necessary conditions

This section analyses how temporal and spatial resolutions affect the necessary conditions corresponding to the minimal new capacities in PV, wind and transmission and how these impacts compare to the ones on the optimal new capacities. This analysis is divided into three observations derived the results shown in Tables II to IV.

Observation 1: *Optimal and minimal capacities follow the same trends when modifying spatial and temporal resolutions.*

The values $c^\epsilon_{n,h}$ for $\epsilon = 10\%$ are shown in Table II. The effect of spatiotemporal resolution on these values is similar to its impact on optimal values $c^*_{n,h}$. Firstly, increasing the temporal resolution decreases the minimal PV capacities while increasing wind and transmission capacities. Secondly, an increase in spatial resolution increases PV and wind capacities.

TABLE II: New capacities $c^*_{n,h}$ at the optima, minimum new capacities $c^\epsilon_{n,h}$ with $\epsilon = 10\%$, and ratio $c^\epsilon_{n,h}/c^*_{n,h}$.

		PV				Wind				Transmision			
	$n \backslash h$	6	4	2		6	4	2		6	4	2	
	100	488	399	388		297	342	346		76.0	80.3	81.7	
$c^*_{n,h}$	200	498	410	395	[GW]	312	356	363	[GW]	76.6	81.7	83.6	[TWkm]
	400	513	429	416		324	365	371		70.9	75.5	76.4	
	100	125	85.8	79.8		128	160	163		11.9	14.8	15.2	
$c^\epsilon_{n,h}$	200	130	92.9	85.8	[GW]	146	178	182	[GW]	13.7	16.2	16.7	[TWkm]
	400	144	109	102		157	189	193		11.6	13.9	14.2	
	100	25.6	21.5	20.5		43.0	46.9	47.0		15.7	18.4	18.7	
$c^\epsilon_{n,h}/c^*_{n,h}$	200	26.2	22.6	21.8	[%]	46.8	50.0	50.1	[%]	17.9	19.8	20.0	[%]
	400	28.2	25.5	24.5		48.4	51.7	52.1		16.4	18.4	18.6	

Observation 2: *A resolution leading to a higher optimal capacity than another resolution also leads to a smaller deviation of the minimal capacity from this optimal capacity.*

Table II shows the ratios $c^\epsilon_{n,h}/c^*_{n,h}$ between minimal and optimal new capacities. The first observation is that these ratios vary within narrow ranges. For transmission capacity, the ratios vary between approximately 15% and 20%. This result means that there exist near-optimal solutions costing at most 10% more than the optimal cost and where there is only 15 to 20% of the new transmission capacity installed at the optimum. For PV capacity, these ratios are contained in the range $[20 : 30]\%$; for wind capacity, the range is approximately $[40 : 50]\%$. However, these percentages exhibit structured differences: their variations follow the same trends as optimal capacities. Indeed, the resolutions that lead to higher percentages for each technology have larger optimal capacities. This result can be explained as follows. If the capacity of a technology is larger at the cost optimum for a given resolution, it implies that this technology is more economically valuable at this resolution. When computing the minimum capacity for ϵ-optimality, the model searches for alternative solutions using other technologies for a cost close to the optimum. If the minimised technology is economically advantageous, finding economically attractive alternatives to replace it is challenging, which makes this technology difficult to minimise. Therefore, if a technology is more advantageous at one resolution than another, it has a larger optimal capacity at this resolution and leads to a smaller deviation from this optimum when trying to minimise this technology under a constrained cost deviation. Mathematically, if for resolutions n_a and resolution n_b, we have $c^*_{n_a,h} > c^*_{n_b,h}$ (which, following observation 1, also implies $c^\epsilon_{n_a,h} > c^\epsilon_{n_b,h}$), then observation 2 states that the following inequality is respected:

$$c^\epsilon_{n_a,h}/c^*_{n_a,h} > c^\epsilon_{n_b,h}/c^*_{n_b,h} \quad . \tag{2}$$

This statement is also true if the resolution variation is temporal instead of spatial.

Observation 3: *Modifying the spatial or temporal resolution has more impact on minimal than optimal capacities.*

This statement means that the relative difference between the minimal capacities at two different resolutions is greater than the relative difference between the optimal capacities associated with these same resolutions. Mathematically, let n_1 and n_2 be two different spatial resolutions, with n_1 being the higher of the two (e.g. $n_1 = 400$ and $n_2 = 100$), we have:

$$|c^\epsilon_{n_2,h}/c^\epsilon_{n_1,h} - 1| > |c^*_{n_2,h}/c^*_{n_1,h} - 1| \tag{3}$$

where the first term and second term represent the relative difference between the minimal and optimal capacities, respectively. This result is a consequence of the previous observation and can be proven using (2) where n_a is a resolution with higher optimal and minimal new capacities than n_b. We differentiate between two cases.

Case 1: The higher resolution corresponds to the one with the higher capacity, i.e., $n_1 = n_a$ and $n_2 = n_b$. Ineq. (2) becomes:

$$c^\epsilon_{n_1,h}/c^*_{n_1,h} > c^\epsilon_{n_2,h}/c^*_{n_2,h} \tag{4}$$

$$\Leftrightarrow \quad c^*_{n_2,h}/c^*_{n_1,h} > c^\epsilon_{n_2,h}/c^\epsilon_{n_1,h} \tag{5}$$

$$\Rightarrow \quad |c^*_{n_2,h}/c^*_{n_1,h} - 1| < |c^\epsilon_{n_2,h}/c^\epsilon_{n_1,h} - 1| \tag{6}$$

where (5) $\Rightarrow$ (6) as $c^\epsilon_{n_1,h} > c^\epsilon_{n_2,h}$ and $c^*_{n_1,h} > c^*_{n_2,h}$.

Case 2: The higher resolution corresponds to the one with the lower capacity, i.e., $n_1 = n_b$ and $n_2 = n_a$. Ineq. (2) becomes:

$$c^\epsilon_{n_2,h}/c^*_{n_2,h} > c^\epsilon_{n_1,h}/c^*_{n_1,h} \tag{7}$$

$$\Leftrightarrow \quad c^\epsilon_{n_2,h}/c^\epsilon_{n_1,h} > c^*_{n_2,h}/c^*_{n_1,h} \tag{8}$$

$$\Rightarrow \quad |c^\epsilon_{n_2,h}/c^\epsilon_{n_1,h} - 1| > |c^*_{n_2,h}/c^*_{n_1,h} - 1| \tag{9}$$

where (8) $\Rightarrow$ (9) as $c^\epsilon_{n_1,h} < c^\epsilon_{n_2,h}$ and $c^*_{n_1,h} < c^*_{n_2,h}$.

We obtain the same conclusion, which is also valid if the temporal resolution varies. In our case study, case 1, where the better resolution corresponds to the higher optimal capacity, is valid for wind and transmission capacity for both types of resolutions. It is also valid for PV capacity for spatial resolution, while the variation of PV with temporal resolution corresponds to case 2.

This observation is illustrated by comparing capacities at lower resolutions to those at the case study's best temporal and spatial resolutions, i.e., $h_0 = 2$ and $n_0 = 400$. Table III thus contains the deviations of optimal (or minimal) new capacities at lower temporal resolutions (i.e., $h = 6$ and $h = 4$) from the optimal (or minimal) new capacities at the best temporal resolution $h_0 = 2$, i.e., $|c^*_{n,h}/c^*_{n,h_0} - 1|$ (or $|c^\epsilon_{n,h}/c^\epsilon_{n,h_0} - 1|$). Then, Table IV shows the same type of deviations but from the capacities at the best spatial resolution $n_0 = 400$, i.e., $|c^*_{n,h}/c^*_{n_0,h} - 1|$ and $|c^\epsilon_{n,h}/c^\epsilon_{n_0,h} - 1|$.

TABLE III: Deviations $|c^*_{n,h}/c^*_{n,h_0} - 1|$ of optimal new capacities and deviations $|c^\epsilon_{n,h}/c^\epsilon_{n,h_0} - 1|$, with $\epsilon = 10\%$, of minimal new capacities from best *temporal* resolution $h_0 = 2$. Abbreviation: Transmission (Trans.).

		PV [%]		Wind [%]		Trans. [%]	
	$n\backslash h$	6	4	6	4	6	4
$\|c^*_{n,h}/c^*_{n,h_0} - 1\|$	100	25.7	2.85	13.9	1.07	6.94	1.79
	200	26.3	3.95	14.0	1.74	8.41	2.22
	400	23.4	3.28	12.8	1.73	7.29	1.22
$\|c^\epsilon_{n,h}/c^\epsilon_{n,h_0} - 1\|$	100	56.6	7.60	21.3	1.28	21.8	1.98
	200	51.8	8.20	19.6	1.99	17.7	2.99
	400	41.7	7.22	19.0	2.27	18.3	2.11

By analysing the values of these two tables, the third observation is obvious: deviations are more significant for minimal new capacities for ϵ-optimality than for optimal new capacities.

V. Conclusion

In this paper, we initiate the research on the impact of spatial and temporal resolutions on necessary conditions for near-optimality of energy system optimisation models. This new research track starts with the analysis of the expansion planning of the European power grid and necessary conditions for ϵ-optimality corresponding to the minimal new PV, wind and transmission capacities. The impact of spatial and temporal resolution on these values is explored and compared to the impacts on cost-optimal new capacities for these technologies. Three key observations are derived from this analysis. Firstly, the results show that minimal and optimal capacities exhibit the same behaviour when resolutions are modified. In particular, PV, wind and transmission capacities increase with better spatial resolution, while a higher temporal resolution positively impacts only the capacity for wind and transmission. A second observation is that the resolutions for which more capacity is installed at the optimum correspond to the ones where it is the hardest to minimise this capacity when allowing for a constrained cost deviation. Thirdly, we show that temporal and spatial resolution variations impact minimal capacities more than optimal ones.

This study provides a first insight into the impacts of spatial and temporal resolution on near-optimal solutions. This research track could be continued in the following ways. First, analysing the optimal and near-optimal solutions for higher and lower resolutions might increase the reliability of our three observations. Similarly, necessary conditions for different values of ϵ could be evaluated to see if these observations hold for other levels of near-optimality. Secondly, we chose to study the effect of spatiotemporal resolution on near-optimal space using necessary conditions. However, other methods have been developed to analyse near-optimal solutions. A natural extension of this paper is to study the impact of resolution on the insights obtained with these methods. Finally, we tested the resolutions' impacts on a specific case study using one ESOM. Studies using different models must be performed to understand those impacts holistically.

TABLE IV: Deviations $|c^*_{n,h}/c^*_{n_0,h} - 1|$ of optimal new capacities and deviations $|c^\epsilon_{n,h}/c^\epsilon_{n_0,h} - 1|$, with $\epsilon = 10\%$, of minimal new capacities from best *spatial* resolution $n_0 = 400$.

		PV [%]			Wind [%]		
	$n\backslash h$	6	4	2	6	4	2
$\|c^*_{n,h}/c^*_{n_0,h} - 1\|$	100	4.77	6.97	6.58	8.11	6.31	6.93
	200	2.82	4.46	5.08	3.66	2.39	2.38
$\|c^\epsilon_{n,h}/c^\epsilon_{n_0,h} - 1\|$	100	13.6	21.5	21.8	18.3	15.1	16.0
	200	9.79	15.0	15.8	6.77	5.82	6.10

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5 Conclusion

To encapsulate the findings of this thesis, it is instructive to revisit the numerical insights obtained across our various case studies.

For example, our research in [DE22] revealed the necessity to deploy hundreds of TWkm of transmission lines, along with hundreds of GW of wind turbines and solar panels, to realise cost-optimality while simultaneously achieving 99% reduction in carbon emissions across Europe. However, using necessary conditions, we noted that these infrastructure capacities could be significantly reduced – by factors greater than two in the case of transmission lines and solar panels – with only minor cost deviations – a 10% increase in both cases. This phenomenon was further corroborated in [DE23]. Our comprehensive analysis also suggested consistent, albeit subtle, impacts arise from the spatial and temporal resolutions concerning necessary conditions. Delving further into [Dub+23], our focus shifted from technologies to resources, utilising our methodology to unveil several insightful observations. Notably, by allowing a modest increase of 1% in both cost and energy investment, the reliance on local energy sources can be trimmed by magnitudes of several tens of per cent relative to the optimums. As we increase this deviation, the decline in local energy source utilisation persists. Conversely, imports stabilise, underscoring their vital role in the forthcoming energy transition. Finally, our methodology also revealed that by accommodating cost and energy investment deviations of as little as 5%, each individual resource possesses viable alternative substitutes.

The key message from our findings is thus one of caution. The significant shifts in necessary capacities and resources resulting from small increases in objectives underscore the need for a more nuanced presentation of energy optimisation outcomes. Rather than grandiose claims asserting that specific measures are the pinnacle of certain objectives, it is crucial to emphasise the inherent fragility and conditional nature of these conclusions.

This cautionary note is not exclusive to others; it also applies to the articles presented in this thesis. While the results are intriguing, their standalone value is limited. Their relevance is intrinsically tied to the specific case studies from which they were derived. In areas riddled with complexity and uncertainty, like energy systems, it is essential to approach exact numerical outcomes with caution; even general trends should be treated with discernment. For instance, the insights from [DE23] on the impact of spatiotemporal resolution, though illuminating, are likely bound to their particular case study and should be judiciously applied elsewhere.

This sentiment of caution holds especially true for developing methodologies. The growing popularity of near-optimal space analysis techniques in energy system planning is evident, as reflected by the influx of recent scholarly works on the subject. In just the past two years, there has been a significant uptick in publications in this domain, with notable studies like [CKB22], [Fio+22], [IBD22], [Cha+23], [LPP23], [NB23], [Ped+23], [Pri+23], [ST23], [Sch+23], and [Shi23].

We are certainly encouraged by this growing interest in the field. However, caution is in order: these methodologies are not a cure-all, and there is always room for refinement. In the spirit of advancing knowledge, we offer several avenues for further research. There are numerous ideas we would have loved to explore given more time, and we hope others will take up the mantle in our stead.

Fighting parametric and structural uncertainty in unison

In Section 1.2, we introduced near-optimal space analysis through the prism of structural uncertainty, which we had presented as a complement to parametric uncertainty. To reiterate, we emphasised that even with no uncertainty in parameter values, we can not be sure of the veracity of our results. This observation goes both ways, and addressing structural uncertainty does not absolve us from addressing parametric uncertainty.

It is thus paramount to address parametric and structural uncertainties in tandem. Steps in this direction have already been taken, with pivotal research such as the work by Li and Trutnevyte [LT17], which merges Monte-Carlo simulation with MGA techniques, and the recent study by Neumann and Brown [NB23].

We contend that precious insights can be gleaned only when both forms of uncertainty are concurrently considered. As such, every research endeavour grappling with complex decision-making should adopt this dual approach. Achieving this goal demands a practical shift in optimisation modelling tools. Indeed, they must embed methodologies that combat uncertainty to simplify and generalise their application.

Attention must also be drawn to the significance of multi-model assessments. While methods to address structural uncertainty are available, they are inherently constrained by the model's limitations representing the system under investigation. Distinct models showcase varied characteristics, each adeptly representing specific aspects of the system and overlooking others. Therefore, it is imperative to examine the same issues using diverse tools. One strategy could involve integrating these tools to enhance the precision of outcomes [Cha+23]. Yet, equally significant, if not more so, is the development of comprehensive frameworks that facilitate a seamless comparison of model-derived results [Nik+21].

More, better, faster

The adage “more solutions is better" is not without its caveats. While many solutions broaden the understanding of the system under the loop, it simultaneously demands more computational time, increased computational resources, and, as underscored in the introduction, an additional cognitive effort to process the growing volume of information.

Researchers doing near-optimal space exploration must be meticulous about this challenge. Indeed, the process of solving optimisation problems is already resource and time-intensive. Introducing a plethora of alternative solutions further amplifies these demands, with each added solution proportionally increasing both time and resource requirements. Finally, this challenge becomes even more pronounced when paired with the recommended inclusion of parametric uncertainty.

The first point of attention resides in the methods used to explore near-optimal spaces. Methods such as “Hop, Skip and Jump" [Bri+90], which aim to unearth maximally distinct solutions, rely on iterative processes. The number of iterations can be adjusted, offering a trade-off between computational demand and precision. On the other hand, some approaches pull out all the stops, aiming to identify ‘all’ near-optimal solutions – hence the term Modelling All Alternatives ([Ped+21] and [Ped+23]). To make this viable, they often deploy optimisation tricks to trim down the dimensionality of the near-optimal space.

As we have consistently emphasised throughout this document, many strategies seek alternative solutions without a clear, pre-defined insight. Building a methodology, such as necessary conditions computation, designed to derive specific types of insights effectively counter computational challenges. We thus advocate for the continued development of methodologies in this vein.

Secondly, Chapter 4 provided insight into how complexity might influence near-optimal spaces. Without revisiting the details, the central idea is that identifying markers indicative of the ‘size’ of the near-optimal space could preemptively guide us about the computational resources necessary for achieving a specific precision level. Although the research showcased in [DE23] establishes an initial foundation, further research is warranted to substantiate this hypothesis. Specifically, we believe it is crucial to investigate the influence of complexity on different methods of near-optimal space exploration across various case studies.

Another promising direction is examining the interplay between approaches addressing parametric and structural uncertainties. These sources of uncertainty might seem distinct at a cursory glance, but when viewed within the mathematical programming framework, methods to combat them essentially explore multiple feasible solutions. It is evident for structural uncertainty management, especially near-optimal space analysis, as its primary goal is to analyse a more significant portion of the feasible region around the optimum. For parametric uncertainty, it is a little more complex as managing it can cause two distinct effects on the mathematical representation of the problem.

On the one hand, when tested parameters shape the objective function without altering the feasible region (for instance, during a sensitivity analysis of technology costs), managing parametric uncertainty entails tracing the movement of the optimum across solutions within a fixed feasible region. This is akin to addressing structural uncertainty, indicating a potential overlap in methods that could be harnessed to avoid redundant computations.

On the other hand, if the parameters sway the constraints, such as when altering the operational range of a power plant, the feasible region shifts. Under these conditions, the once fixed feasible region becomes dynamic, revealing solutions that would have been unseen using near-optimal space analysis. It should then make sense to amalgamate the techniques tailored for both uncertainties. However, even in this case, it is paramount to remain vigilant about potential overlaps, as demonstrated by [Gro+23].

As it stands, this conceptual overlap between uncertainties remains relatively uncharted territory. However, tapping into this interplay could pave the way for more computationally efficient strategies to navigate uncertainty.

Multi-objective expansion

Near-optimal space analysis is critical to indirectly incorporate objectives not explicitly modelled into the decision-making framework. Yet, when these objectives can be directly modelled, integrating them via multi-objective techniques becomes a logical choice. Surprisingly, a scant amount of research examines multi-objective optimisation alongside near-optimal space analysis.

A notable exception is the work by [Fio+21] and [Fio+22], which pioneered a method to probe solutions beyond the Pareto front. This emerging intersection of multi-objective optimisation and near-optimal space exploration was also the driving force behind our study, [Dub+23]. Given the inherent complexities of melding these approaches, we earnestly believe that further research in this domain is not just beneficial but essential.

Multi-stage expansion

Incorporating multiple objectives into optimisation for decision-making is pertinent, as is integrating various stages. Indeed, single-stage optimisation – i.e., modelling requirements for a specific, distant future year – provides valuable insights. However, real decision-making relies on practical milestones for achieving this future vision.

A considerable amount of research has ventured into the multi-stage optimisation of energy systems, as evidenced by studies such as [KS10], [Pon+16], [LSC18], and [Vic+20]. Yet, to our best knowledge, it appears that methods to manage structural uncertainty remain under-explored in this context.

Multi-stage optimisation in energy planning typically involves fine-tuning the operation and scale of an energy system across multiple temporal intervals, often spanning years. Within each of these periods, the system's operations are broken down and decided upon (sometimes hourly), while investment choices are made at each interval. Two main paradigms exist. The first one, perfect foresight, assumes that decision-makers have complete and accurate information about all future events and outcomes. In other words, they can 'see' the future perfectly. This is, however, not realistic. The second model, termed 'myopic foresight', is grounded in the idea that decision-makers factor in only the immediate or very near future while charting their course. Although realistic, this model is not without pitfalls. It might not capture the full benefits or costs that would be apparent if a longer time horizon were considered, such as with perfect foresight models.

This leads us to ponder: could near-optimal space analysis, primarily through the lens of necessary conditions, be employed to refine myopic foresight? The underlying rationale here would be to determine, for each time interval, the necessary investment in each sized technology. This approach could help strike a balance – ensuring a constrained deviation from the target objective while offering flexibility in options for ensuing periods. While we are still grappling with the mechanics of melding this with existing multi-stage optimisation techniques – owing to our developing understanding – it is unmistakably clear that this notion has the potential to pioneer transformative research avenues.

Making better choices

To wrap up this conclusion, we would like to expound on the theme of 'multiplicity' that has subtly woven its way through our discussion. As presented in Section 1.3, this thesis' work has set its stage in the realm of the energy transition. Yet, it is essential to underscore that the methodologies developed are not restricted to this domain. Instead, they are universally applicable to intricate decision-making challenges where mathematical programming is the right tool.

Intriguingly, the term MGA (Modelling to Generate Alternatives) was first introduced not in the context of energy but rather in the arena of land use planning [BCH82]. However, given the pressing challenges in the energy sector, the energy community is embracing these techniques, working to expand our comprehension of structural uncertainty management.

Though there is a budding interest in diversifying the application of these tools across other sectors [El +22], there is still vast, untapped potential. Thus, we urge scholars across diverse research domains to delve deeper into this subject, exploring its numerous possibilities.

This assertion underscores a more global recommendation: there exists an imperative to refine our decision-making tools continually. This refinement is two-fold: firstly, enhancing the methods and, secondly, facilitating their assimilation by the decision-makers. Delving into what this second point means from a modelling standpoint, we would like to cite an insightful passage from [DeC11]. This work has been instrumental in guiding the research trajectory presented in this thesis, aptly encapsulating the challenges inherent to the field:

"Analysis aimed at informing decision-makers should involve them from the outset of the project. Modellers should aim for transparency through open-source code and data, well-written documentation, and selective use of ESOM features to avoid unnecessary complications. Reports should focus on communicating robust insights rather than singular projections. Caveats should be communicated, but modellers should avoid vague statements that unintentionally call into question the study findings. Future uncertainty should be adequately addressed."

Though penned with energy modelling as the backdrop, these principles resonate across sectors.

Their adoption becomes all the more urgent when we recognise that choices that will sculpt the future of our next century are being made just as you read the final words of this thesis.

A Mathematical Concepts Summary

This chapter aims to summarise the mathematical concepts presented in [DE22] and [Dub+23]. In Section A.1, the concepts of ϵ-optimal spaces and necessary conditions are introduced for a mono-objective setup. Section A.2 then expands these notions to multi-objective problems.

A.1 Mono-objective

Let us start with a mathematical formulation of the problem. The mathematical problems that we are trying to solve using the following methodologies can be written:

$$\min_{x \in \mathcal{X}} f(x) \quad , \tag{A.1}$$

where

- $\mathcal{X}$ a feasible space,
- x is a feasible solution,
- f an objective function, and
- $f(x)$ the objective value of x.

We set ourselves in a generic setup where the feasible space $\mathcal{X}$ can be of any form. The objective function $f : \mathcal{X} \rightarrow \mathbb{R}_+$, however, is restricted to lie in the positive reals. This restriction is necessary for the methods that will be described in the rest of this section. However, it is often reasonable, particularly in the case of energy systems optimisation problems, where common objectives such as cost, invested energy, quantity of materials, etc., are positive.

A.1.1 Epsilon-optimal spaces

Starting from the optimal solution(s) $x^\star$ of the initial problem, we can define near-optimal spaces, also called suboptimal spaces or inferior regions. We make mention of several spaces because, for the same optimal objective, several near-optimal spaces can be defined depending on the desired suboptimality level. To measure this level of suboptimality and characterise the different near-optimal spaces, we use a *suboptimality coefficient* $\epsilon \geq 0$.

We can define an epsilon-optimal or ϵ-optimal space using the optimal objective and this coefficient.

Definition 1. *Let $\mathcal{X}$ be a feasible space, let $f : \mathcal{X} \to \mathbb{R}_+$ be an objective function and let $\epsilon \geq 0$. Then, if $f(x^\star)$ is the optimal objective value, that is $f(x^\star) = \min_{x \in \mathcal{X}} f(x)$, the* ϵ***-optimal space*** *$\mathcal{X}^\epsilon$ is the space*

$$\mathcal{X}^\epsilon = \Omega(\mathcal{X}, f, \epsilon) = \left\{ x \in \mathcal{X} \mid f(x) \leq (1+\epsilon) f(x^\star) \right\} \quad . \tag{A.2}$$

A solution $x \in \mathcal{X}^\epsilon$ is called an ϵ-optimal solution.

The ϵ-optimal space is the set of the feasible solutions $x \in \mathcal{X}$ with objective value $f(x)$ no greater than $(1+\epsilon)f(x^\star)$. The suboptimality coefficient ϵ specifies by how much the objective values $f(x)$ of the feasible solutions in the near-optimal space deviate at most from the optimal objective value.

In the rest of this work, we will use the notation $\mathcal{X}^\epsilon$ to refer to an ϵ-optimal space, rather than $\Omega(\mathcal{X}, f, \epsilon)$. This notation has the advantage of conciseness but makes abstraction of the influence of f on epsilon-optimal spaces. Let us note that for all the developments made in this thesis, the objective function f is considered constant; therefore, we do not face this problem.

To give a better sense of the notion of epsilon-optimal space to the reader, Figure A.1 and A.2 illustrate those concepts with $\mathcal{X} = \mathbb{R}$ and $\mathcal{X} = \mathbb{R}^2$, respectively.

A note must be made on the specific case $f(x^\star) = 0$. In this case, $\mathcal{X}^\epsilon$ resumes to $\arg\min_{x \in \mathcal{X}} f(x)$, making the analysis of near-optimal spaces trivial.

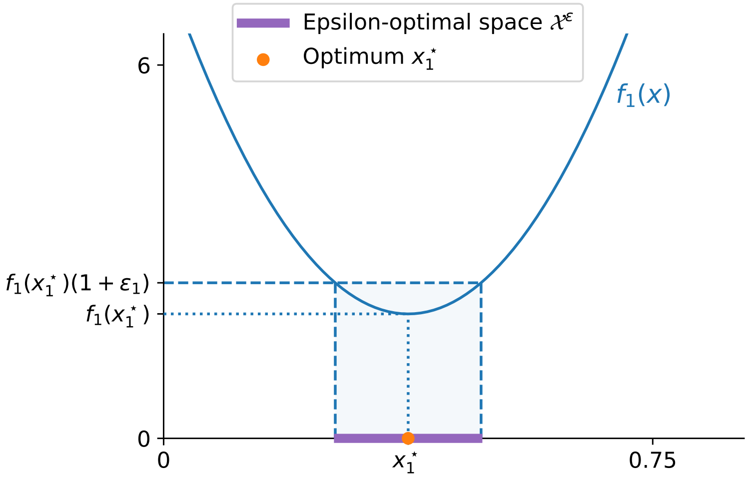


Fig. A.1.: Source [Dub+23]. Graphical representation of an ϵ-optimal space of a mono-objective optimisation problem in $\mathcal{X} = \mathbb{R}_+$. The function f_1 that is minimised is shown in blue. Its minimum is located at $x_1^\star$. Using this value and its corresponding objective value $f_1(x_1^\star)$ allows to easily determine an ϵ-optimal space $\mathcal{X}^\epsilon$ with $\epsilon = \epsilon_1$.

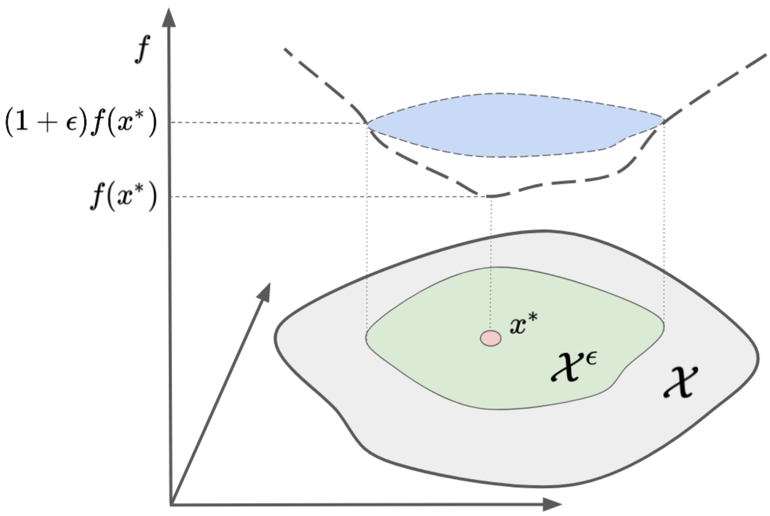


Fig. A.2.: Source [DE22]. Three-dimensional representation of an ϵ-optimal space. In the horizontal plane, the space of feasible solutions $\mathcal{X} \subset \mathbb{R}^2$ is depicted while the vertical axis represents the objective function. The red dot is the optimal solution x^* corresponding to the minimal value of the objective function over the feasible space. The blue space coincides with the hyper-plane $f(x) = (1+\epsilon)f(x^*)$, allowing one to determine the ϵ-optimal space $\mathcal{X}^\epsilon$ shown in green.

A.1.2 Necessary conditions

The concepts of *condition*, *necessary condition*, and *non-implied necessary condition* introduced in this section allow determining features which are common to all solutions in a given ϵ-optimal space. A common example is used to illustrate the definitions.

Definition 2. *Let $\mathcal{X}$ be a feasible space, a* ***condition*** *is a function $\phi : \mathcal{X} \to \{0, 1\}$. A set of conditions is denoted Φ.*

Example: Let the feasible space $\mathcal{X}$ be the set of reals, i.e. $\mathcal{X} = \mathbb{R}$, then, the set of conditions Φ could be the set of conditions of the form $\phi_c(x) := x \geq c$ with $x \in \mathcal{X}$ (thus $x \in \mathbb{R}$) and $c \in \mathbb{R}$.

We search to identify, among a set Φ of conditions, the ones which are true for any solutions in an ϵ-optimal space $\mathcal{X}^\epsilon$. These conditions are called *necessary conditions* for ϵ-optimality.

Definition 3. *Let $\mathcal{X}^\epsilon$ be an ϵ-optimal space and ϕ be a condition, then ϕ is a* ***necessary condition*** *for ϵ-optimality if it is true for any solutions in $\mathcal{X}^\epsilon$, i.e.*

$$\forall x \in \mathcal{X}^\epsilon : \phi(x) = 1 \quad . \tag{A.3}$$

Let Φ be a set of conditions, the set of conditions $\phi \in \Phi$ which are necessary conditions for ϵ-optimality is denoted $\Phi^{\mathcal{X}^\epsilon}$.

Example: Let us consider that the epsilon-optimal space is given by $\mathcal{X}^\epsilon = [0, 1]$. Then, the condition $\phi_0(x) := x \geq 0$ is respected by all $x \in \mathcal{X}^\epsilon$, making ϕ_0 a necessary condition. Moreover, it is straightforward to show that the set of all conditions in Φ which are necessary is $\Phi^{\mathcal{X}^\epsilon} = \{\phi_c \mid c \leq 0\}$. Indeed, any condition $\phi_c(x) := x \geq c$ is true over $\mathcal{X}^\epsilon = [0, 1]$ if $c \leq 0$.

To provide an alternative definition for necessary conditions, we can introduce a new space corresponding to the set of solutions for which a condition is true.

Definition 4. *Let $\mathcal{X}$ be a feasible space and ϕ be a condition, the space $\mathcal{I}_\phi \subseteq \mathcal{X}$ is the space where a condition ϕ is true, that is:*

$$\mathcal{I}_\phi = \Big\{ x \in \mathcal{X} \mid \phi(x) = 1 \Big\} \quad . \tag{A.4}$$

Example: The spaces $\mathcal{I}_{\phi_c}$ of the conditions $\phi_c(x) := x \geq c$ are the spaces $[c, \infty]$. These spaces might become more complex to determine when considering, for instance, conditions using linear combinations of variables, e.g. $\phi(x) := ax_1 + bx_2 \geq c$ with $x = (x_1, x_2) \in \mathcal{X} = \mathbb{R}^2$.

Comparing this space for a given condition to an ϵ-optimal space allows determining if it is necessary.

Definition 5. *Let $\mathcal{X}^\epsilon$ be an ϵ-optimal space, let ϕ be a condition, and let $\mathcal{I}_\phi$ be the space over which this condition is true, then ϕ is a* ***necessary condition*** *for ϵ-optimality if $\mathcal{X}_\epsilon \subseteq \mathcal{I}_\phi$.*

Example: For a set of conditions $\Phi = \{\phi_c(x) := x \geq c\}$ with $x \in \mathbb{R}$ and $c \in \mathbb{R}$, and a ϵ-optimal space $\mathcal{X}^\epsilon = [0, 1]$, this definition implies that all conditions ϕ_c with $c \leq 0$ are necessary, which corresponds to same set as definition 3. Indeed, the spaces $\mathcal{I}_{\phi_c} = [c, \infty]$ include the space $[0, 1]$, when $c \leq 0$.

A.1.3 Non-implied necessary conditions

The goal of necessary conditions is to provide insights into features common to many near-optimal solutions to provide interesting insights to decision-makers. However, depending on how conditions are defined, the number of necessary conditions can be infinite. Dealing with such a quantity of information is not efficient for decision-making. This situation happens, notably, in our previous example. Indeed, the set $\Phi^{\mathcal{X}^\epsilon} = \{\phi_c \mid c \leq 0\}$ contains an infinite number of necessary conditions. To limit the number of conditions, we introduce the concepts of *implication* and *non-implied necessary conditions*.

Informally, a condition ϕ_1 implies a condition ϕ_2 if knowing that $\phi_1(x)$ is true implies that $\phi_2(x)$ is true. Then, if ϕ_1 is a necessary condition and implies ϕ_2, we can infer that ϕ_2 is also necessary, making this information redundant. To provide a more concise set of necessary conditions, we will search for all necessary conditions which are not implied by other necessary conditions.

To make this search more formal, let us define the notion of *implication* mathematically.

Definition 6. *Let $\mathcal{X}$ be a feasible space, $\phi_1 : \mathcal{X} \to \{0,1\}$ and $\phi_2 : \mathcal{X} \to \{0,1\}$ be two conditions, an* ***implication function*** *$\psi(\phi_1 \mid \phi_2) \in \{0,1\}$ is a function that indicates whether condition ϕ_2 implies condition ϕ_1, i.e.*

$$\psi(\phi_1 \mid \phi_2) = \begin{cases} 1 & \text{if} \quad \forall x \in \mathcal{X},\ \phi_2(x) = 1 \implies \phi_1(x) = 1, \\ 0 & \text{if} \quad \exists x \in \mathcal{X},\ \phi_2(x) = 1 \not\Longrightarrow \phi_1(x) = 1. \end{cases} \tag{A.5}$$

Example: Let us consider conditions $\phi_1(x) \coloneqq x \geq 1$ and $\phi_2(x) \coloneqq x \geq 2$. We have that $\psi(\phi_1 \mid \phi_2) = 1$. Indeed, for all $x \in \mathcal{X}$, if $\phi_2(x) = 1$ this means that $x \geq 2$, that $x \geq 1$ and thus $\phi_1(x) = 1$. Conversely, $\psi(\phi_2 \mid \phi_1) = 0$. Indeed, there exist several $x \in \mathcal{X}$ such that $\phi_1(x) = 1$ and $\phi_2(x) = 0$. For instance, this is the case for $x = 1.5$.

The implication function can also be defined using spaces over which conditions are true as defined at Definition 4.

Definition 7. *Let ϕ_1 and ϕ_2 be conditions with $\mathcal{I}_{\phi_1}$ and $\mathcal{I}_{\phi_2}$ the spaces over which they are respectively true, then the* ***implication function*** *$\psi(\phi_1 \mid \phi_2)$ is defined as:*

$$\psi(\phi_1 \mid \phi_2) = \mathcal{I}_{\phi_2} \subseteq \mathcal{I}_{\phi_1} \quad . \tag{A.6}$$

Comment: This formulation fits the previous definition of an implication function. Indeed, if $\psi(\phi_1 \mid \phi_2) = 1$, then it means $\mathcal{I}_{\phi_2} \subseteq \mathcal{I}_{\phi_1}$, which in turns implies that $\phi_1(x) = 1$ for any $x \in \mathcal{X}$ for which $\phi_2(x) = 1$. Similarly, if $\psi(\phi_1 \mid \phi_2) = 0$, it means that $\mathcal{I}_{\phi_2} \not\subseteq \mathcal{I}_{\phi_1}$, which means $\exists x \in \mathcal{X}$ such that $\phi_1(x) = 0$ when $\phi_2(x) = 1$.

Using this definition of implication, we can now differentiate between necessary conditions and *non-implied* necessary conditions.

Definition 8. *Let $\Phi^{\mathcal{X}^\epsilon}$ be a set of necessary conditions for ϵ-optimality, the necessary condition $\phi \in \Phi^{\mathcal{X}^\epsilon}$ is a* ***non-implied necessary condition*** *for ϵ-optimality if it is not implied by any other necessary condition $\phi' \in \Phi^{\mathcal{X}^\epsilon} \setminus \{\phi\}$. The set of non-implied necessary conditions is denoted $\overline{\Phi}^{\mathcal{X}^\epsilon}$.*

Example: In our example with $\Phi = \{\phi_c(x) \coloneqq x \geq c\}$ with $x \in \mathbb{R}$ and $c \in \mathbb{R}$, and $\mathcal{X}^\epsilon = [0,1]$, the only non-implied necessary condition is ϕ_0, *i.e.* $\overline{\Phi}^{\mathcal{X}^\epsilon} = \{\phi_0\}$. Indeed, as shown in the previous section, the set of necessary conditions is $\Phi^{\mathcal{X}^\epsilon} = \{\phi_c \mid c \leq 0\}$. In this set, ϕ_0 implies all other conditions and is not implied by any of them. Indeed, for any x, knowing that $x \geq 0$ is true implies that $x \geq c$ when $c \leq 0$. Thus, knowing that ϕ_0 is a necessary condition implies that any ϕ_c with $c \leq 0$ is a necessary condition, whatever the ϵ-optimal space. On the opposite, it is not possible to imply that ϕ_0 is a necessary condition from the knowledge of other necessary conditions in the set $\Phi^{\mathcal{X}^\epsilon} = \{\phi_c \mid c < 0\}$. This defines ϕ_0 as a *non-implied* necessary condition.

Using Definition 6 of implication, we can refine the previous definition.

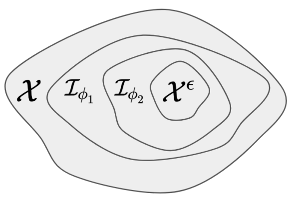
Definition 9. *Let $\Phi^{\mathcal{X}^\epsilon}$ be a set of necessary conditions for ϵ-optimality and let ψ be an implication function, the necessary condition $\phi \in \Phi^{\mathcal{X}^\epsilon}$ is a* ***non-implied necessary condition*** *for ϵ-optimality if $\forall \phi' \in \Phi^{\mathcal{X}^\epsilon} \setminus \{\phi\} : \psi(\phi \mid \phi') = 0$.*

Example: The condition ϕ_0 respects this definition: for any other condition $\phi_c \in \Phi^{\mathcal{X}^\epsilon}$, that is any ϕ_c with $c < 0$, we have $\psi(\phi_0 \mid \phi_c) = 0$. The proof is straightforward: for any $c < 0$, $\phi_c(c) = 1$ as $c \geq c$ is true, but $\phi_0(c) = 0$ as $c \geq 0$ is false.

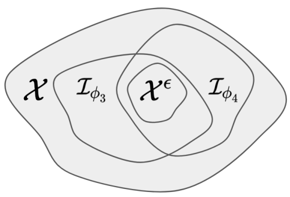
A third version can be written using spaces over which conditions are true.

Definition 10. *Let $\Phi^{\mathcal{X}^\epsilon}$ be a set of necessary conditions for ϵ-optimality, the necessary condition $\phi \in \Phi^{\mathcal{X}^\epsilon}$ is a* ***non-implied necessary condition*** *for ϵ-optimality if is true over a space $\mathcal{I}_\phi$ which does not include any of the spaces $\mathcal{I}'_\phi$ over which other necessary conditions $\phi' \in \Phi^{\mathcal{X}^\epsilon} \setminus \{\phi\}$ are true, i.e. a necessary condition such that $\forall \phi' \in \Phi^{\mathcal{X}^\epsilon} \setminus \{\phi\} : \mathcal{I}_{\phi'} \not\subseteq \mathcal{I}_\phi$.*

Figure A.3 illustrates these concepts. The left part of the figure (A.3a) shows two necessary conditions ϕ_1 and ϕ_2, with ϕ_2 implying ϕ_1. They are necessary conditions because the spaces over which they are respectively true include the ϵ-optimal space. Then, ϕ_2 implies ϕ_1 as $\mathcal{I}_{\phi_2} \subset \mathcal{I}_{\phi_1}$. These two characteristics imply that if we consider the set of conditions $\Phi = \{\phi_1, \phi_2\}$ containing uniquely ϕ_1 and ϕ_2, then the set of necessary conditions is given by $\Phi^{\mathcal{X}^\epsilon} = \{\phi_1, \phi_2\}$, and the set of non-implied necessary conditions by $\overline{\Phi}^{\mathcal{X}^\epsilon} = \{\phi_2\}$. The right part of the figure (A.3b) shows another case with two necessary conditions ϕ_3 and ϕ_4, with no implication. Considering a set of conditions $\Phi = \{\phi_3, \phi_4\}$, then we have two non-implied necessary conditions, i.e. ϕ_3 and ϕ_4, and we have that $\overline{\Phi}^{\mathcal{X}^\epsilon} = \Phi^{\mathcal{X}^\epsilon} = \Phi$.



(a)



(b)

Fig. A.3.: Source [DE22]. Graphical illustration of implication.

Computation of a non-implied necessary condition

This section focuses on a specific type of condition, consisting of a constrained sum of variables to give a practical sense of the concepts presented in the previous sections. First, we prove that there is a unique, non-implied, necessary condition for this kind of condition. Then, we detail how to compute the value characterising this condition.

Theorem 1. *Let $\mathcal{X} \subset \mathbb{R}^n$ be a feasible space, $f : \mathcal{X} \to \mathbb{R}^+$ be an objective function and*

$$\Phi_{\mathbf{d}} = \{\phi_{\mathbf{d}}^c(\mathbf{x}) := \mathbf{d}^T\mathbf{x} \geq c \mid c \in \mathbb{R}\}, \tag{A.7}$$

be a set of conditions consisting of constrained sums of variables $\mathbf{d}^T\mathbf{x} = \sum_{i=1}^n d_i x_i$ where $\mathbf{x} \in \mathcal{X}$ and $\mathbf{d} \in \{0,1\}^n$.

Let $c^* = \min_{\mathbf{x}\in\mathcal{X}^\epsilon} \mathbf{d}^T\mathbf{x}$ then

$$\phi_{\mathbf{d}}^{c^*} := \mathbf{d}^T\mathbf{x} \geq c^* \tag{A.8}$$

is the only element in the set of non-implied necessary conditions $\overline{\Phi}_{\mathbf{d}}^{\mathcal{X}^\epsilon}$.

Proof. Let us first show that the set of necessary conditions is equal to

$$\Phi_{\mathbf{d}}^{\mathcal{X}^\epsilon} = \{\phi_{\mathbf{d}}^c | c \leq c^*\}. \tag{A.9}$$

By definition, $c^* = \min_{\mathbf{x}\in\mathcal{X}^\epsilon} \mathbf{d}^T\mathbf{x}$ is the smallest value that $\mathbf{d}^T\mathbf{x}$ can take over $\mathcal{X}^\epsilon$. This implies that $\phi_{\mathbf{d}}^{c^*}(\mathbf{x}) := \mathbf{d}^T\mathbf{x} \geq c^*$ is true for all $\mathbf{x} \in \mathcal{X}^\epsilon$. Similarly, if $c < c^*$, we know that $\mathbf{d}^T\mathbf{x} \geq c^* > c$ is true for all $\mathbf{x} \in \mathcal{X}^\epsilon$. Thus, all conditions $\phi_{\mathbf{d}}^c$ such that $c \leq c^*$ are necessary conditions.

For $c > c^*$ however, at the optimum $\mathbf{x}_\epsilon^* = \arg\min_{\mathcal{X}^\epsilon} \mathbf{d}^T\mathbf{x}$, we have $\mathbf{d}^T\mathbf{x}_\epsilon^* = c^* < c$. This implies that the condition $\phi_{\mathbf{d}}^c(\mathbf{x}) := \mathbf{d}^T\mathbf{x} > c$ is not true for all $\mathbf{x}$ in $\mathcal{X}^\epsilon$, as $\mathbf{x}_\epsilon^* \in \mathcal{X}^\epsilon$. Therefore, all conditions $\phi_{\mathbf{d}}^c$ such that $c > c^*$ are not necessary conditions.

Now let us prove that the set of non-implied necessary conditions resumes to one element, i.e.

$$\overline{\Phi}_{\mathbf{d}}^{\mathcal{X}^\epsilon} = \{\phi_{\mathbf{d}}^{c^*}\} \quad . \tag{A.10}$$

This means that all $\phi_{\mathbf{d}}^{c}$ with $c < c^*$ are implied by and do not imply $\phi_{\mathbf{d}}^{c^*}$.

This can be shown by proving that, for any $c < c^*$,

$$\mathcal{I}_{\phi_{\mathbf{d}}^{c^*}} \subset \mathcal{I}_{\phi_{\mathbf{d}}^{c}} \text{ and } \mathcal{I}_{\phi_{\mathbf{d}}^{c}} \not\subset \mathcal{I}_{\phi_{\mathbf{d}}^{c^*}} \quad . \tag{A.11}$$

We have $\mathcal{I}_{\phi_{\mathbf{d}}^{c^*}} \subset \mathcal{I}_{\phi_{\mathbf{d}}^{c}}$ because, as shown before, for any $\mathbf{x}$, if $\phi_{\mathbf{d}}^{c^*}(\mathbf{x})$ is true, $\phi_{\mathbf{d}}^{c}(\mathbf{x})$ with $c < c^*$ is also true. Then, $\mathcal{I}_{\phi_{\mathbf{d}}^{c}} \not\subset \mathcal{I}_{\phi_{\mathbf{d}}^{c^*}}$. Indeed, the element $\mathbf{x}$ such that $\mathbf{d}^T\mathbf{x} = c$ is an element of $\mathcal{I}_{\phi_{\mathbf{d}}^{c}}$ but not of $\mathcal{I}_{\phi_{\mathbf{d}}^{c^*}}$.

□

The value c^* represents the minimum value that $\mathbf{d}^T\mathbf{x}$ can take over the set $\mathcal{X}^\epsilon$, that is when allowing a deviation of ϵ from the optimal value $f(\mathbf{x}^\star)$. Algorithm 1 illustrates the computation of this value in three steps.

Algorithm 1: Computation of a non-implied necessary condition - Single-objective case

Data:
f - objective function,
$\mathcal{X}$ - feasible space,
ϵ - suboptimality coefficient,
$\mathbf{d}$ - binary vector defining the conditions $\mathbf{d}^T\mathbf{x}$

Result: c^*

Steps:

1. Solve $\min_{\mathbf{x}\in\mathcal{X}} f(\mathbf{x})$ to obtain $\mathbf{x}^\star$.
2. Build $\mathcal{X}^\epsilon$ by adding to the original problem the constraint $f(\mathbf{x}) \leq (1+\epsilon)f(\mathbf{x}^\star)$.
3. Solve $c^* = \min_{\mathbf{x}\in\mathcal{X}^\epsilon} \mathbf{d}^T\mathbf{x}$.

Example: Let us illustrate this algorithm on the travelling salesman problem. This problem aims to find the shortest possible route that a salesman can take to visit a set of cities exactly once and return to the starting city. Mathematically, we can model this problem in the following way. Let $G = (V, E)$ be a complete undirected graph, where $V = \{1, 2, ..., n\}$ is the set of cities, and E is the set of edges connecting the cities. Each edge $e = (i, j)$ has a non-negative weight $w(e)$ representing the distance between city i and city j. Let x_{ij} be a binary decision variable equal to 1 if the salesman travels directly from city i to city j in the tour and 0 otherwise. The objective is to minimise the total distance travelled by the salesman, i.e.: $\min \sum_{(i,j)\in E} w_{ij}x_{ij}$. This objective must be met under a series of constraints we will not detail here. Let us assume now that there are two types of routes: paved and gravel. The salesman wants to avoid taking gravel routes while maintaining a path that is not much longer than the optimal path. This new path can be obtained using Algorithm 1. Step 1 consists of solving the original problem. Using the optimal solution of this problem, one can perform step 2 by adding to the initial problem the constraint $f(\mathbf{x}) \leq (1+\epsilon)f(\mathbf{x}^\star)$. In this constraint, $\mathbf{x}$ is a vector containing all x_{ij}, $f(\mathbf{x}) = \sum_{(i,j)\in E} w_{ij}x_{ij}$, and $\mathbf{x}^\star$ is the optimal solution. The value of ϵ can vary depending on the relative increase in path length the salesman is willing to accept. The third step can then be performed by setting an appropriate $\mathbf{d}$. As the salesman wants to minimise the number of gravel routes travelled, all values of $\mathbf{d}$ corresponding to this type of route are set to 1. The value c^* obtained as the optimal value of this third step gives the minimal number of routes that must be taken to ensure that the total length of the path travelled does not deviate by more than ϵ of the optimal length.

A.2 Multi-objective

This section extends the concepts presented for mono-objective optimisation to multi-objective optimisation. Using the notation of Ehrgott [Ehr05], our initial problem is:

$$\text{“}\min_{x \in \mathcal{X}}\text{”} \quad \mathbf{f}(x) \quad . \tag{A.12}$$

where:

- $\mathcal{X}$ is a feasible space,
- x is a feasible solution,
- $\mathbf{f} = (f_1, \cdots, f_k, \cdots, f_n)$ is a vector of n objective functions, and
- $\mathbf{f}(x) = (f_1(x), \cdots, f_k(x), \cdots, f_n(x))$ is the vector of objective values of x in each objective.

Similarly to the mono-objective case, we consider objectives whose images lie in the positive reals, i.e. $\forall k \ f_k : \mathcal{X} \to \mathbb{R}_+$. In this formulation, the “$\min$" notation signifies that all functions in the vector $\mathbf{f}$ are to be minimised.

Let us also note that the feasible space is a sub-space of the *decision space* where the variables take their values, whose image is called the objective space, where the objective functions take their values.

In the following sections, we will sometimes refer to $\mathcal{Y}$, the image of the feasible space in the objective space:

Definition 11. *Let $\mathcal{X}$ be a feasible space and let $\mathbf{f} = (f_1, \cdots, f_k, \cdots f_n)$ be a vector of objectives function with $\forall k \ f_k : \mathcal{X} \to \mathbb{R}_+$, then the image of the feasible space is*

$$\mathcal{Y} = \mathbf{f}(\mathcal{X}) = \{\mathbf{y} \in \mathbb{R}^n_+ \mid \mathbf{y} = \mathbf{f}(x) \textit{ for some } x \in \mathcal{X}\} \quad . \tag{A.13}$$

This definition implies $\mathcal{Y} \in \mathbb{R}^n_+$ and $\mathbf{y} = (y_1, \cdots, y_k, \cdots, y_n)$ with $y_k = f_k(x) \geq 0$ for some $x \in \mathcal{X}$.

A.2.1 Efficient solutions and Pareto fronts

One way to highlight compromises between the objectives $f_1, \cdots, f_k, \cdots, f_n$ is to compute efficient or Pareto optimal solutions. Following the definition of Ehrgott [Ehr05]:

Definition 12. *Let $\mathcal{X}$ be a feasible space and $\mathbf{f} = (f_1, \cdots, f_k, \cdots, f_n)$ be a vector of n objectives, a feasible solution $\hat{x} \in \mathcal{X}$ is called **efficient** when there is no other $x \in \mathcal{X}$ such that $\forall k \; f_k(x) \leq f_k(\hat{x})$ and $f_i(x) < f_i(\hat{x})$ for some i, that is, no other $x \in \mathcal{X}$ has a smaller or equal value in all objectives $f_1, \cdots f_k, \cdots, f_n$ than $\hat{x}$.*

According to Ehrgott [Ehr05], multiple denominations exist for the set of efficient points. This thesis uses the term Pareto front to indiscriminately name the set of efficient points or their image in the objective space.

Definition 13. *Let $\mathcal{X}$ be a feasible set and $\mathbf{f} = (f_1, \cdots, f_k, \cdots, f_n)$ be a vector of n objectives, a **Pareto front** $\mathcal{P}_\mathcal{X}$ is the set of all efficient solutions, i.e.*

$$\mathcal{P}_\mathcal{X} = \left\{ \hat{x} \in \mathcal{X} \mid \nexists x \in \mathcal{X}, \forall k \; f_k(x) \leq f_k(\hat{x}), \exists i \; f_i(x) < f_i(\hat{x}) \right\} \quad . \tag{A.14}$$

We note $\mathcal{P}_\mathcal{Y}$ the image of the Pareto front in the objective space.

A Pareto front can be composed of an infinity of points. Thus, it is typical to compute a subset of the efficient solutions which compose it. This set is named *approximated Pareto front*. It is denoted by $\mathcal{P}_{\mathcal{X},m}$ (or equivalently $\mathcal{P}_{\mathcal{Y},m}$) where m is the number of points in the approximation.

Definition 14. *Let $\mathcal{P}_\mathcal{X}$ be a Pareto front and $m \in \mathbb{N}$. Then, an **approximate Pareto front** $\mathcal{P}_{\mathcal{X},m}$ is a subset of m efficient solutions from $\mathcal{P}_\mathcal{X}$.*

Several techniques exist to obtain those efficient solutions, the two most famous being the '*weighted-sum approach*' and the '*ϵ-constraint method*' [Ehr05].

The weighted-sum approach consists of solving:

$$\min_{x \in \mathcal{X}} \sum_{k=1}^{n} \lambda_k f_k(x) \quad \forall k \; \lambda_k > 0 \quad . \tag{A.15}$$

The ϵ-constraint method resolves in solving:

$$\begin{aligned} &\min_{x\in\mathcal{X}} f_j(x) \\ &\text{s.t. } f_k(x) \leq \epsilon_k \text{ for } k = 1, \cdots, n \text{ and } k \neq j \quad , \end{aligned} \tag{A.16}$$

where $\forall k\ \epsilon_k \in \mathbb{R}$.

A.2.2 Epsilon-optimal spaces

Starting from a Pareto front $\mathcal{P}_\mathcal{X}$ and given a *suboptimality coefficients vector* of deviations in each objective: $\boldsymbol{\epsilon} = (\epsilon_1, \cdots, \epsilon_k, \cdots, \epsilon_n) \in \mathbb{R}^n_+$, it is possible to define an $\boldsymbol{\epsilon}$-optimal space. This space is denoted by $\mathcal{X}^\epsilon$ in the decision space and $\mathcal{Y}^\epsilon$ in the objective space.

In the mono-objective setup, the ϵ-optimal space is defined as the set of points $x \in \mathcal{X}$ whose objective value $f(x)$ do not deviate by more than an ϵ fraction from the optimal objective value, i.e. $f(x) \leq (1+\epsilon)f(x^\star)$. In a multi-objective case, there is no optimum but a set of efficient points composing the Pareto front. This leads us to define the $\boldsymbol{\epsilon}$-optimal space as follows:

Definition 15. *Let $\mathcal{X}$ be a feasible space, let $\mathbf{f} = (f_1, \cdots, f_k, \cdots, f_n)$ be a vector of n objectives, and let $\boldsymbol{\epsilon} = (\epsilon_1, \cdots, \epsilon_k, \cdots, \epsilon_n) \in \mathbb{R}^n_+$ be a vector of n suboptimality coefficients, then the **$\boldsymbol{\epsilon}$-optimal space** $\mathcal{X}^\epsilon$ is the set of points x whose objective values $f_k(x)$ do not deviate by more than an ϵ_k fraction from the objective value $f_k(\hat{x})$ of at least one solution $\hat{x}$ of the Pareto front $\mathcal{P}_\mathcal{X}$, for all k.*

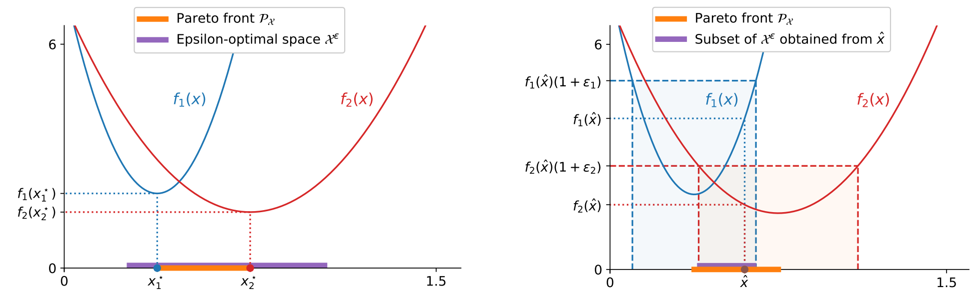
It is the space

$$\mathcal{X}^\epsilon = \left\{ x \in \mathcal{X} \mid \exists \hat{x} \in \mathcal{P}_\mathcal{X}, \forall k\ f_k(x) \leq (1+\epsilon_k) f_k(\hat{x}) \right\} \quad . \tag{A.17}$$

This definition can be interpreted to see the $\boldsymbol{\epsilon}$-optimal space as the union of sub-optimal spaces associated with each point of the Pareto front. An equivalent mathematical definition is, therefore:

$$\mathcal{X}^\epsilon = \bigcup_{\hat{x}\in\mathcal{P}_\mathcal{X}} \left\{ x \in \mathcal{X} \mid \forall k\ f_k(x) \leq (1+\epsilon_k) f_k(\hat{x}) \right\} \quad . \tag{A.18}$$

Figure A.4 depicts a graphical representation of an $\boldsymbol{\epsilon}$-optimal space in a multi-objective framework and how it is built from efficient solutions.



(a) Full representation of $\mathcal{X}^\epsilon$

(b) Computation of a subset of $\mathcal{X}^\epsilon$ from a single point $\hat{x}$ of the Pareto front $\mathcal{P}_\mathcal{X}$

Fig. A.4.: Source [Dub+23]. Graphical representation of an ϵ-optimal space of a multi-objective optimisation problem in $\mathcal{X} = \mathbb{R}_+$. The two functions to be minimised f_1 and f_2 are represented in blue and red, respectively, and their respective minimums are $x_1^\star$ and $x_2^\star$. The Pareto front $\mathcal{P}_\mathcal{X}$, containing all efficient solutions, is represented in orange. Figure A.4a shows in purple the full ϵ-optimal space $\mathcal{X}^\epsilon$ for a suboptimality coefficient vector $\boldsymbol{\epsilon} = (\epsilon_1, \epsilon_2)$. As shown in Equation (A.18), this space is the union of sub-spaces that can be computed from efficient solutions. Figure A.4b shows how one of these subspaces, corresponding to the efficient solution $\hat{x}$, can be computed. From the value $\hat{x}$, the corresponding objective values $f_1(\hat{x})$ and $f_2(\hat{x})$ are obtained. This allows to determine all the solutions in $\mathcal{X}$ whose objective value is smaller than $f_k(\hat{x})(1+\epsilon_k)$ for $k \in 1, 2$.

Definition (A.17) relies on the entire Pareto front. However, practically, only a subset $\mathcal{P}_{\mathcal{X},m}$ of m efficient points of the Pareto front is computed and used to obtain an approximation of the ϵ-optimal space, denoted $\mathcal{X}^\epsilon_m$.

Definition 16. *Let $\mathcal{X}$ be a feasible space, let $\mathbf{f} = (f_1, \cdots, f_k, \cdots, f_n)$ be a vector of n objectives, let $\boldsymbol{\epsilon} = (\epsilon_1, \cdots, \epsilon_k, \cdots, \epsilon_n) \in \mathbb{R}^n_+$ be a vector of n sub-optimality coefficients, and let $\mathcal{P}_{\mathcal{X},m}$ with $m \in \mathbb{N}$ be an approximate Pareto front.*

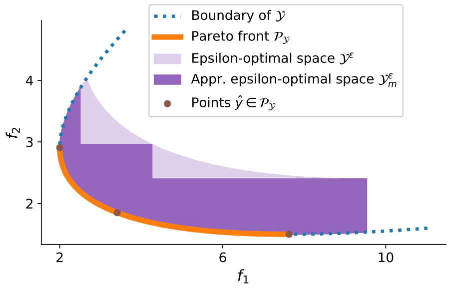
Then, an approximation $\mathcal{X}^\epsilon_m$ of an ϵ-optimal space $\mathcal{X}^\epsilon$ is the space

$$\mathcal{X}^\epsilon_m = \left\{ x \in \mathcal{X} \mid \exists \hat{x} \in \mathcal{P}_{\mathcal{X},m}, \forall k \; f_k(x) \leq (1+\epsilon_k) f_k(\hat{x}) \right\} \quad . \tag{A.19}$$

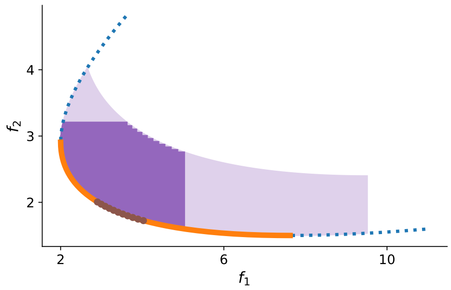
As for Definition 15, we can provide an alternative formulation defining $\mathcal{X}^\epsilon_m$ as a union of spaces, where each space is the set of points whose objective value in each f_k does not deviate by more than an ϵ_k fraction from the objective values $f_k(\hat{x})$ of one solution $\hat{x}$ in the approximated Pareto front $\mathcal{P}_{\mathcal{X},m}$:

$$\mathcal{X}^\epsilon_m = \bigcup_{\hat{x} \in \mathcal{P}_{\mathcal{X},m}} \left\{ x \in \mathcal{X} \mid \forall k \; f_k(x) \leq (1+\epsilon_k) f_k(\hat{x}) \right\} \quad . \tag{A.20}$$

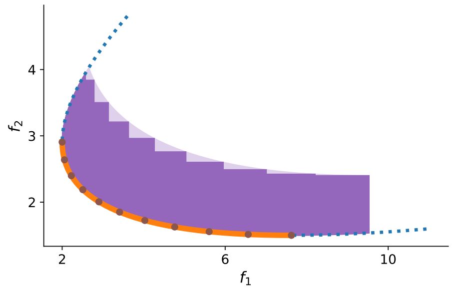
Figure A.5 shows three examples of approximate ϵ-optimal spaces $\mathcal{X}_m^\epsilon$ in the objective space (therefore noted $\mathcal{Y}_m^\epsilon$) using three approximated Pareto fronts $\mathcal{P}_{\mathcal{Y},m}$, with different numbers and spread of efficient solutions.



(a) Few well-spread points



(b) Numerous badly-spread points



(c) Numerous well-spread points

Fig. A.5.: Source [Dub+23]. Graphical representations in the objective space of approximations $\mathcal{Y}_m^\epsilon$ of an ϵ-optimal space of a multi-objective optimisation problem based on three different approximate Pareto front $\mathcal{P}_{\mathcal{Y},m}$. The axes correspond to the two functions to minimise, i.e. f_1 and f_2. The boundary of the image of the feasible space $\mathcal{Y}$ is represented in blue in the three cases. The part of this boundary corresponding to the full Pareto front $\mathcal{P}_{\mathcal{Y}}$ is drawn in orange. The full ϵ-optimal spaces $\mathcal{Y}^\epsilon$ corresponding to this Pareto front is coloured in light purple. Each graph corresponds to a different approximate Pareto front $\mathcal{P}_{\mathcal{Y},m}$. These sets of efficient points are represented in brown. From each of these points, part of the approximate ϵ-optimal spaces can be computed, and their union is represented in solid purple.

A.2.3 Necessary conditions

In the multi-objective optimisation framework, necessary conditions and non-implied necessary conditions for ϵ-optimality can be defined in the same manner as in the one-dimensional setting (see definitions 3 and 8, respectively). The only difference stems from the replacement of $\mathcal{X}^\epsilon$ by $\mathcal{X}^\epsilon$. Nonetheless, we illustrate the computation of a specific type of non-implied necessary condition to illustrate the differences with the one-dimensional case, stemming from the approximation of the epsilon-optimal space.

Computation of a non-implied necessary condition

The computation of a non-implied necessary condition from conditions of type $\mathbf{d}^T\mathbf{x} \geq c$ presented in Section A.1.3 is generalised to the multi-criteria case. In the mono-objective case, it was sufficient to minimise the sum $\mathbf{d}^T\mathbf{x}$ over $\mathcal{X}^\epsilon$ to obtain the value c^* corresponding to the non-implied necessary condition $\mathbf{d}^T\mathbf{x} \geq c^*$. However, in a multi-objective setup, we do not have access to $\mathcal{X}^\epsilon$ but to its approximation $\mathcal{X}^{\boldsymbol{\epsilon}}_m$, which is the union of several subsets, each corresponding to one point in $\mathcal{P}_{\mathcal{X},m}$ (i.e. a subset of the Pareto front). The minimum over this space can thus be obtained by taking the minimum of the minima of $\mathbf{d}^T\mathbf{x}$ over each of these subsets. Even with this approach, $\mathcal{X}^{\boldsymbol{\epsilon}}_m$ being a subset of $\mathcal{X}^{\boldsymbol{\epsilon}}$, minimising $\mathbf{d}^T\mathbf{x}$ over it will only provide an upper bound $\tilde{c}$ of the value c^*, i.e. $\tilde{c} \geq c^*$.

Algorithm 2 shows how this value can be obtained.

Algorithm 2: Computation of a non-implied necessary condition - Multi-objective case

---

Data:

$\mathcal{X} \in \mathbb{R}^n$ - feasible space,
$\mathbf{f}$ - objective functions,
m - number of points,
$\boldsymbol{\epsilon}$ - vector of suboptimality coefficients,
$\mathbf{d}$ - binary vector defining the conditions $\mathbf{d}^T\mathbf{x}$

Result: $\tilde{c}$

Steps:

1. Draw m points $\hat{\mathbf{x}}^{(1)}, \dots \hat{\mathbf{x}}^{(i)}, \dots \hat{\mathbf{x}}^{(m)}$ of the Pareto front using an appropriate method.
2. For all $i \in [1, 2, \dots, m]$, compute $c^{(i)} = \min \mathbf{d}^T\mathbf{x}$ over the space $\{\mathbf{x} \in \mathcal{X} \mid \forall k \ f_k(\mathbf{x}) \leq (1 + \epsilon_k) f_k(\hat{\mathbf{x}}^{(i)})\}$.
3. Take the minimum $\tilde{c} = \min_{i \in [1,2,\dots,m]} c^{(i)}$ of these values to find the appropriate condition $\phi_{\tilde{c}}$.

There is no guarantee that the condition $\mathbf{d}^T\mathbf{x} \geq \tilde{c}$ is a (non-implied) necessary condition. Indeed, it could be the case that for a solution $\mathbf{x} \in \mathcal{X}^{\boldsymbol{\epsilon}} \setminus \mathcal{X}^{\boldsymbol{\epsilon}}_m$ that $\mathbf{d}^T\mathbf{x} < \tilde{c}$. To make the upper bound $\tilde{c}$ as close as possible to the real minimal value c^*, one must reduce the size of the difference $\mathcal{X}^{\boldsymbol{\epsilon}} \setminus \mathcal{X}^{\boldsymbol{\epsilon}}_m$. This can be done by improving the number and spread of efficient solutions in the approximated Pareto front. As defined by Alarcon-Rodriguez et al. [AAG10], solutions with a good spread can be seen as having good coverage of the actual Pareto front. The three graphs of Figure A.5 show visually how, by increasing the number and the spread of efficient solutions drawn from the Pareto front, the approximated ϵ-optimal space covers a more significant subset of the points of the entire ϵ-optimal space.

Example: Let us continue with the travelling salesman problem introduced in Section A.1.3. We introduce a new set of non-negative weights $t(e)$ representing the time needed to travel between city i and j. We now have two objectives: the total distance travelled $f(\mathbf{x}) = \sum_{(i,j)\in E} w_{ij}x_{ij}$ and the total time travelled $g(\mathbf{x}) = \sum_{(i,j)\in E} t_{ij}x_{ij}$ to visit all cities. Minimising these two objectives might not lead to the same solutions. Using appropriate techniques, we can determine efficient solutions $\hat{\mathbf{x}}$ from the Pareto front, expressing the trade-offs between these two objectives. If the salesman is still interested in avoiding the gravel routes while maintaining close-to-optimal length and time of travel, we can employ Algorithm 2. For a fixed set of suboptimality coefficients, step 2 implies adding two constraints to the initial problem and minimising $\mathbf{d}^T\mathbf{x}$ for each efficient solution. As in the mono-objective case, the only values of $\mathbf{d}$ set to 1 are the ones corresponding to gravel routes. Finally, step 3 will give us a value $\tilde{c}$, which expresses an upper bound on the minimum number of gravel routes that the salesman needs to take to avoid deviations in time and length larger than ϵ_1 and ϵ_2.

B Complementary Work

This thesis is nested within the realm of the energy transition. Aside from our contributions regarding near-optimal spaces, we also delved into several complementary research queries. These explorations set the stage for the questions we pursued and enriched the answers we formulated.

This section intends to offer a concise overview of these parallel research endeavours. The output of this work can be categorised into two primary forms: research articles and open-source software. The research papers cover two topics, renewable plan siting and energy return on investment, which are briefly presented in the following sections of this chapter. We then close this chapter by briefly describing our software contributions.

B.1 Sizing, siting and complementarity

All research articles presented in this thesis share a foundational theme: capacity expansion planning. Capacity expansion planning refers to determining the optimal locations and capacities for deploying various assets within a given energy system. In the context of this thesis, our geographical scope encompassed Europe or Belgium, and the assets involved ranged from power generation, transmission, and storage technologies to e-fuel production or transport. This process is also commonly referred to as 'sizing' in the context of energy systems planning.

For any low-carbon energy system heavily reliant on renewable energy, the generation assets encompass intermittent sources such as solar and wind energy. Precise spatial and temporal resolutions are required to accurately model the dynamics of systems dependent on variable energy sources. This level of precision involves identifying the specific locations for each production centre, commonly called 'siting'.

Various methodologies exist for siting renewable plants, aiming to make the most of the diverse signals and resources available across large geographical areas. In the context of Dr David-Constantin Radu's thesis titled "Siting Strategies for Variable Renewable Generation Assets in Capacity Expansion Planning Frameworks" [Rad21], we actively contributed to the development of three articles that explore innovative siting techniques. The central theme of these methods revolves around the concept of complementarity, which seeks to harness the benefits of diverse resources across extensive geographical scopes.

In the following sections, we present the concept of siting and provide a concise overview of three articles that utilised complementarity as a tool for siting.

B.1.1 Siting or where to build wind turbines

Historically, determining where to install wind power plants followed a simple maxim: erect them where the wind is strongest. The default strategy was to situate wind assets in regions with consistent, robust wind resources – sites with superior average capacity factors that promised maximum electricity generation [Ber+20]. However, wind turbine siting can be optimised based on diverse criteria beyond wind intensity.

For instance, Wu et al. [Wu+17] proposed siting wind generators in parts of Africa to minimise peak hourly residual demand over a year. Similarly, studies by Short and Diakov [SD12] and W. Zappa and M. van den Broek [WM18] designed programs for residual demand minimisation over specific periods. Pereira et al. [Per+14] targeted wind farm placements to curtail residual demand variance, while Becker and Thrän [BT18] centred on wind power placement in Germany with a focus on site correlation and the weight of existing installations. A novel approach discussed in [Ber+20] and featured in subsequent research, including ours, focuses on siting that maximises the complementarity of production profiles across sites.

This complementarity revolves around the synchronous relationship between renewable energy production at different sites given their spatiotemporal traits. It is about how varying production patterns across locations can offset each other. For example, when considering wind energy, the wind might be gusting strongly in the plains of Northern Europe during the afternoon while being relatively calm on the Mediterranean coast – yet picking up speed there by night. Similarly, for solar energy, sunlight might be peaking on Spain's southern coast by mid-morning. At the same time, Northern Germany could only experience strong sunlight by early afternoon due to differences in latitude and typical cloud coverage patterns. Strategic siting based on these complementary profiles can help achieve a steady and dependable renewable energy output.

A challenge with these innovative siting methodologies is their computational complexity, particularly for expansive geographical scopes and extended periods. In an ideal setting, every potential site would be represented in a large-scale capacity expansion, each having unique capacity factors. This approach, however, translates to millions of constraints, rendering it untenable to optimise even over a year. Simplifications are then in order – like aggregating production time series or determining wind production capacities for broader areas rather than specific sites. Yet, as we coarsen temporal or spatial resolutions, the precision in estimating required installations and associated costs wanes. Indeed, accurate estimation of capacities and costs in renewable energy systems relies heavily on detailed modelling of renewable energy assets [PHK14]. For instance, in a study led in the USA, using 356 profiles for wind and 134 profiles for solar instead of one single profile per state (i.e. 48 profiles per resource) led to capacity differences exceeding 32 GW, equivalent to 10% of the total installed capacity for solar PV [KC16]. Similarly, in a recent assessment of the European power system, Frysztacki et al. [Fry+21] found that modelling renewables with 1024 profiles resulted in 10.5% lower system costs compared to more simplified setups using only 37 profiles (one per country) per renewable resource.

To ensure results with meaningful precision, we are inherently bound to the original complexity, prompting a need for alternate solutions. This context frames the underlying goal of the three articles presented in the forthcoming section: crafting innovative siting methods grounded in complementarity while enhancing the efficiency of such approaches.

B.1.2 Siting using complementarity

The first of these three articles, “Siting Renewable Power Generation Assets with Combinatorial Optimisation" [Ber+22], elaborates different strategies for sitting renewable power generation assets. In particular, it presents a combinatorial optimisation model that minimises simultaneous low electricity production events from chosen sites, using spatiotemporal complementarity. The model and associated algorithms – such as greedy, local search, and relaxation-based heuristics – are benchmarked against a state-of-the-art mixed-integer programming solver using a realistic case study of onshore wind power plant siting in Europe. The study concludes that the model can efficiently identify optimal deployment patterns, with several heuristics consistently outperforming the solver at a lower computational cost. However, it also found that onshore wind power plants are unlikely to consistently meet a constant share of electricity demand even with optimised siting. Lastly, the model proves robust in cross-validation analysis, leveraging historical data to predict performance on unseen climatological data, except in extreme edge cases. Future research directions include a closer algorithmic analysis and the introduction of economic considerations into siting decisions.

This first paper showed how to select renewable sites to meet some demand but ignored the electricity transmission constraints. These transmission constraints can be considered by using an appropriate capacity expansion model (CEP). However, solving these problems with many renewable energy generation sources is computationally heavy, as the number of variables and constraints increases linearly with the number of sites available. In the article “Model Reduction in Capacity Expansion Planning Problems via Renewable Generation Site Selection" [Rad+21], we propose a two-stage method to mitigate the computational complexity of capacity expansion planning problems while maintaining an accurate representation of variable renewable energy sources (RES). The first stage involves a screening process to identify and discard less significant RES sites, reducing the spatial dimension of the problem. The second stage utilises the selected sites to determine the optimal configuration of the power system in a CEP problem. The method, tested on an EU case study, shows the ability to identify over 90% of optimal sites while decreasing peak memory consumption and computation time by up to 41% and 46%, respectively. Future work may focus on refining the parameters used in the first-stage screening routine and integrating the proposed heuristic into a more structured form, such as a Benders-like decomposition framework.

We used this two-stage method in a third paper called “Assessing the impact of offshore wind siting strategies on the design of the European power system" [Rad+22] to assess how different offshore wind siting strategies can influence the design and economics of the European power system. The study compared two siting schemes at the first stage: one that maximises aggregate power output and another that maximises spatiotemporal complementarity. Two variations of these schemes were also explored, wherein the number of sites was determined country-by-country. Findings indicate that the complementarity-based siting criterion can lead to system designs that are up to 5% cheaper than those relying on the power output-based scheme, assuming no constraints related to country-based deployment targets. However, when such constraints are enforced, the power output-based scheme is consistently 2% cheaper than the complementarity-based strategy. This paper contributes to understanding offshore wind power plants’ potential role in the European power system. It provides crucial insights into how plant siting strategies can impact system design and economics. The study’s findings can guide policymakers and stakeholders in decision-making concerning renewable energy infrastructure development. For future research, we suggest integrating the siting of other RES technologies into the two-stage method, enhancing network modelling, evaluating the impact of unit commitment costs and constraints on system designs for different siting schemes, and representing the effect of short-term RES uncertainty in dispatch decisions.

These articles present innovative approaches to siting. However, working on them also awoke the authors to a limitation of capacity expansion planning models: an emphasis on optimal solutions, often overlooking near-optimal alternatives. This constrained viewpoint is especially problematic when making granular decisions, like choosing hundreds of sites out of thousands, where varied configurations might yield similarly valuable results. To address this challenge, we were inspired to delve into the realm of near-optimal space exploration, which became the main thread of this thesis.

B.2 Energy return on investment

In the energy system optimisation realm, most research focuses on cost as the defining objective. Consequently, the optimal configuration offers the highest cost-effectiveness [DeC+17]. Undoubtedly, cost is paramount in evaluating an energy system's economic feasibility and sustainability. However, anchoring solely on this factor might sidestep other critical dimensions like environmental sustainability and social equity. An alternative, albeit lesser-known metric, encapsulating technical and societal challenges, is the system's *energy return on investment* (EROI).

At a systems level, EROI manifests as a ratio that gauges the amount of usable energy delivered by the system (E_{out}) against the energy used to obtain that energy (E_{in}) [DGJ21]. Consequently, a rise in the energy required to render a specific energy service inversely affects the system's EROI. In essence, EROI sheds light on the efficiency of deriving energy to metamorphose it into a societal benefit. EROI is interesting to study in parallel to cost because, while certain elements can influence both – like transportation of energy resources surging the system cost and invested energy - they are not strictly tied, and prioritising one might yield divergent system configurations.

Our exploration of EROI was propelled by an alliance with scholars from the Catholic University of Louvain (UCLouvain). Their previous endeavours in this domain, such as in works like [LJ18], served as the foundation for two new papers. The inaugural paper is summarised at the end of this section, while the second one has already been described in Chapter 3. This collaborative endeavour was primordial in determining the precise definition of EROI deployed in both research articles. Indeed, given the numerous approaches to quantify E_{in} and E_{out}, and by extension, the resulting EROI for a system, establishing a clear and consistent definition becomes imperative. Such clarity ensures that the findings and conclusions drawn from the case studies presented in these works are both relevant and unambiguous. In parallel, Adrien Orban's master's research [Orb22], conceived in the same collaborative backdrop, delivered a refined version of the energy investment prerequisites for various energy sources, significantly enriching the capacity expansion planning discussed in both papers.

The methodology presented in this work was leveraged, as detailed in [Dum+22], to analyse a comprehensive energy system using EROI as the objective, contrasting it with results from a cost-optimised system. While the 2035 Belgian energy system served as the primary case for evaluation, this innovative approach is versatile and can be adapted to different scales, from national to international contexts. Moreover, this research advanced further by undertaking a global sensitivity analysis to discern key parameters influencing EROI uncertainty, utilising the polynomial chaos expansion technique.

Beyond the techno-economic findings, it is noteworthy to highlight a significant societal conclusion from the paper, which aligns with the decision-making focus of this thesis. The declining EROI raises concerns about meeting climate goals without socio-economic implications, particularly for fossil-fuel-dependent nations like Belgium. This decline suggests that countries might face challenges maintaining current lifestyles while achieving carbon neutrality. Our research underscores the need for policymakers and scholars to re-evaluate energy and economic models, mainly as most models are premised on constant or growing demand. A reduced EROI means fewer services, prompting inquiries about which sectors should be prioritised. This research emphasises the need for a deeper understanding of whole-energy systems using the EROI metric. It calls for more research into renewable fuels, especially regarding their cost, availability, and energy investment.

B.3 Tools for expansion planning

Several tools were developed to evaluate complementarity and facilitate renewable asset siting and capacity expansion planning at the European scale. This development was a substantial part of the first two years of this thesis. In addition, we contributed to the modelling tool EnergyScope TD and its Python version as part of our collaboration with the Catholic University of Louvain. This section provides an overview of these tools and their use in this thesis.

B.3.1 EPIPPy

In the preceding papers and [DE22; DE23], we performed siting and capacity expansion planning at the European scale. The first step to achieve this is to access appropriate data and establish an efficient data pipeline. To address this need, we developed a Python library called EPIPPy (Expansion Planning Input Preprocessing in Python), which is available on GitHub [DRa].

EPIPPy offers a range of functions and scripts for preprocessing various data sources, including generation data (such as hydro capacities and flows, existing and potential capacities, and capacity factors), geographical data (such as country and sub-region shapes), population data, green-house gases emissions, yearly and hourly load, technological parameters such as cost, and network topologies. The library simplifies the preprocessing of these data sources, providing a convenient tool for subsequent analysis.

B.3.2 resite

For the studies [Rad+21; Rad+22; Ber+22], we developed the *resite* library [DRc] to support the development and modification of siting algorithms while maintaining a consistent processing pipeline.

The *resite* library consists of a pipeline with two main steps. In the first step, the territory (e.g., Europe) is divided into sub-regions and sites corresponding to the epicentres of these regions are defined. The sub-regions can either correspond to predefined administrative regions (e.g. countries, NUTS - Nomenclature of territorial units for statistics) or be created using a Voronoi partition. The region's shape, geographical position of the epicentre and data retrieved using EPIPPy allow associating with each site, power generation time series, existing and potential capacities for different technologies, and the load to be satisfied at this site.

The second step involves the siting process, which entails selecting a subset of sites that meet a predefined criterion. For example, the criterion could be selecting the n sites that result in maximum production over a given period. *resite* allows the integration of siting algorithms written in various optimisation modelling languages, such as pyomo, docplex, gurobipy, and Julia. The pipeline can be easily configured to switch between different languages and adapt to specific requirements.

B.3.3 REplan

Capacity expansion planning is a well-studied problem, and various tools exist in Python and other languages to support its analysis. PyPSA (Python for Power System Analysis) [BHS18] is a widely used library. While PyPSA enables the modelling of linear capacity expansion planning problems, it lacks an automated pipeline for modelling large networks like the European network. To address this limitation, the

PyPSA-Eur project, initiated by Hoersch et al. [Hoe+18], "provides an open model dataset of the European energy system at the transmission network level".

In this thesis, we extensively used PyPSA and the PyPSA-Eur dataset for developing and testing ideas (notably in [DE22] and [DE23]). However, to assess the impact of siting techniques on capacity expansion planning results and enhance flexibility, we developed the REplan library [DRb]. REplan is built on PyPSA and draws inspiration from the PyPSA-Eur project. It offers tools that simplify the setup and simulation of grid expansion planning while facilitating the integration of output from siting algorithms. In addition to providing flexibility, one of the goals of the development of REplan was its possible expansion to a more extensive scope than Europe.

B.3.4 EnergyScope TD

In the studies presented in [DE22] and [DE23], the focus was predominantly on power systems. However, we ventured beyond this and broadened the sectoral scope of our research to multi-carrier energy systems in [Dub+23].

To achieve this broader perspective, we sought a comprehensive whole-energy system modelling tool that could represent various energy sectors. We selected EnergyScope TD (ESTD) for this purpose. ESTD provides the capability to model and optimise a system, integrating many technologies (e.g., wind turbines, gas power plants, boilers) and a range of resources (e.g., wind, gas, diesel) to cater to diverse end-use demands.

Dr Gauthier Limpens is credited for developing this tool during his PhD research, as documented in [Lim21]. The tool's mathematical foundation and data processing interface were initially constructed in GAMS. However, as we employed ESTD for our case studies, we recognised the need for more versatility and developed a Python-based version for data processing. Although this did not replace the primary GAMS version, it facilitated the replication of our experiments and sparked subsequent explorations in the same direction.

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Colophon

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