CENTER FOR BIOSYSTEMS AND BIOTECH DATA SCIENCE
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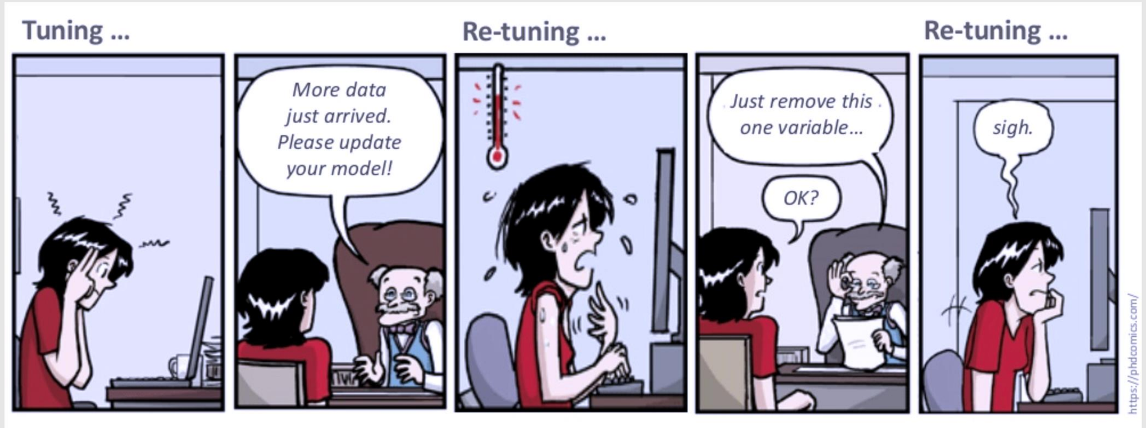
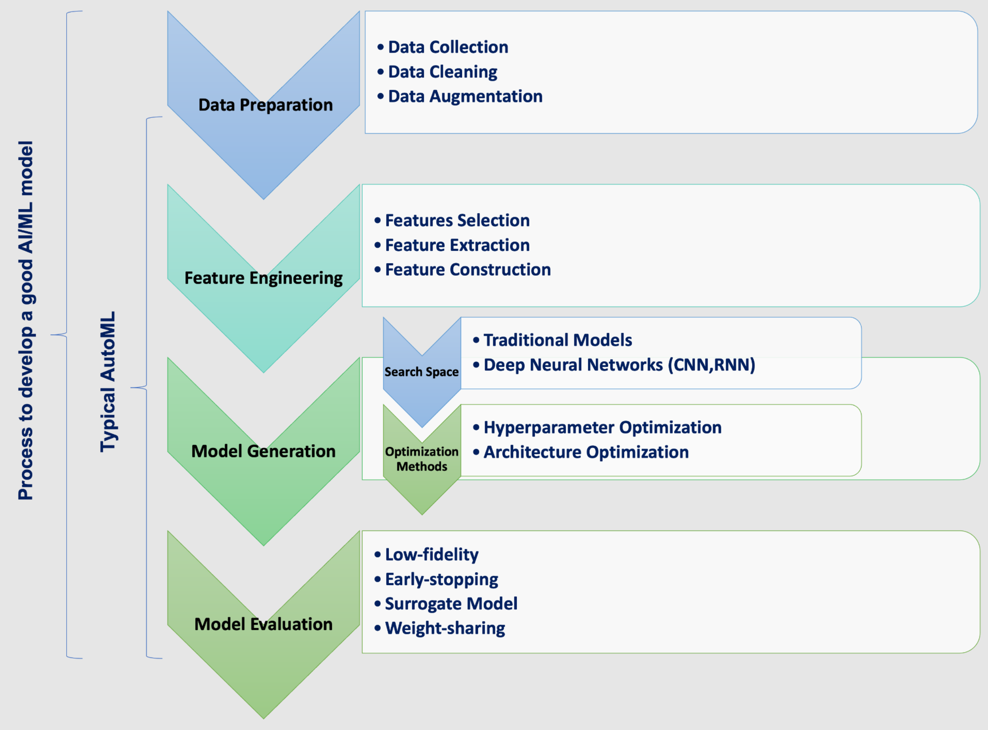
EXPLORING THE POWER OF EVOLUTIONARY COMPUTATION ALGORITHMS IN AUTOML

Automated Machine Learning (AutoML)

Automated Machine Learning (AutoML) has emerged as a promising approach to designing machine learning (ML) pipelines that can select and tune models for a given dataset automatically. Despite its potential benefits, AutoML faces several challenges, including managing large and complex search spaces and finding optimal solutions efficiently. To address these issues, researchers have looked to evolutionary computation (EC) techniques to automatically search for the best ML models and their hyperparameters. These techniques have demonstrated success in achieving good performance across various tasks.

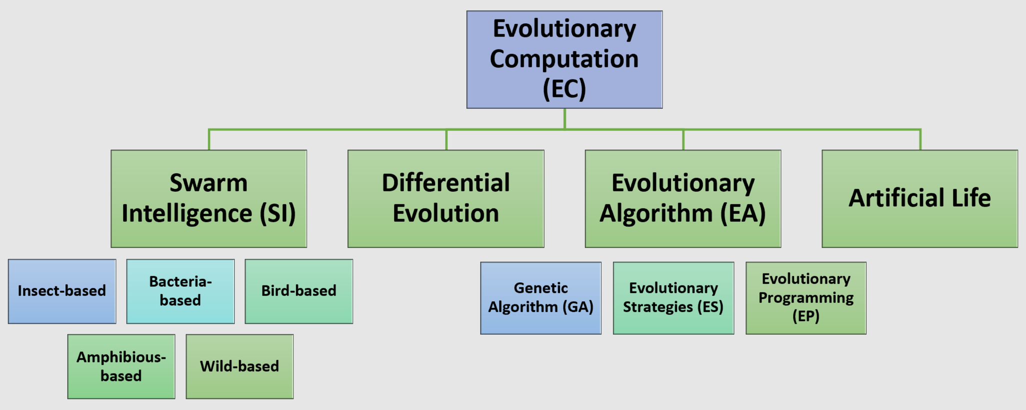


Without AutoML every change in data or features would require lot of manual steps for training and retraining ML models. "Piled Higher and Deeper" by Jorge Cham, PhD Comics.



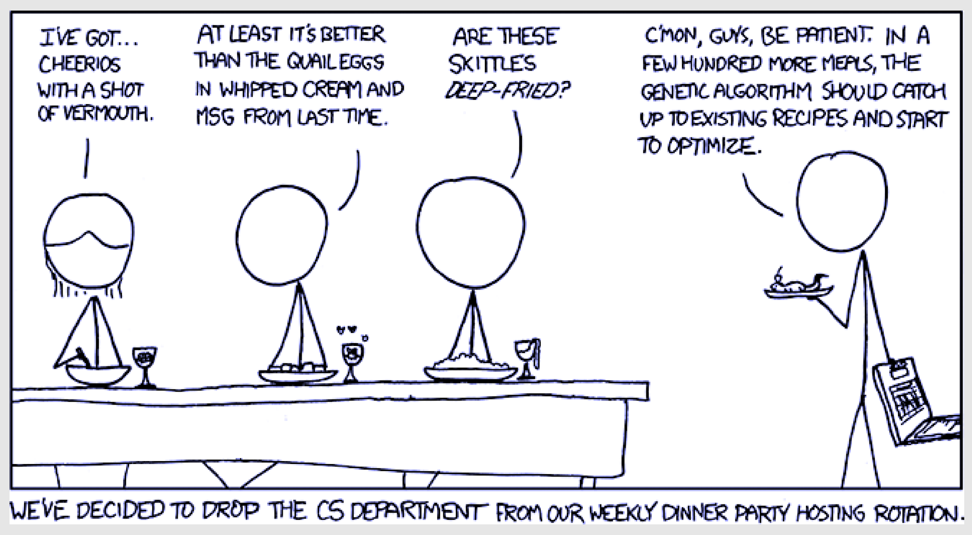
An overview of AutoML pipeline [1,2,3]

Evolutionary Computation (EC) Algorithm



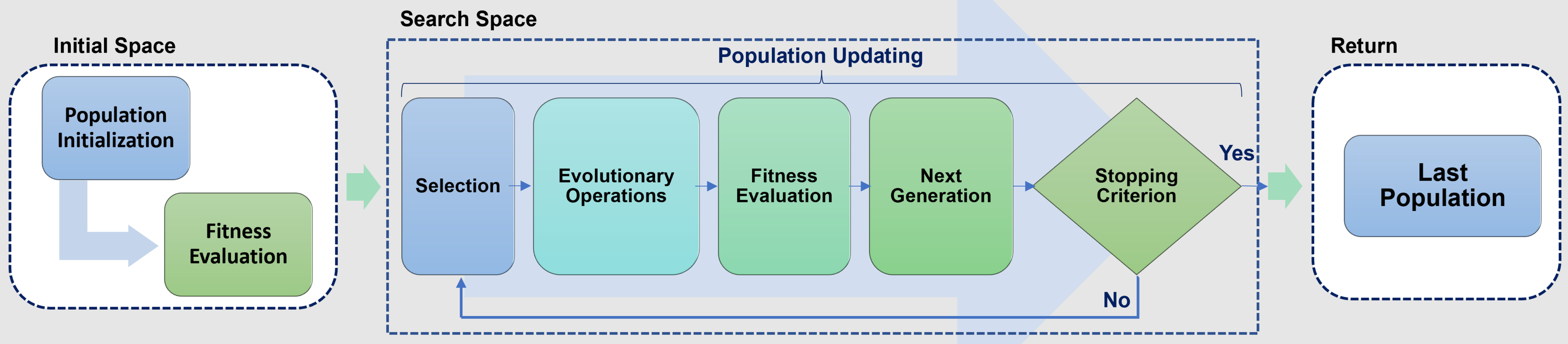
A subset of evolutionary computation (EC) algorithms

Evolutionary Computation (EC) is a sub-field of AI that uses computational models of biological and naturally-inspired processes to solve complex problems. This category of algorithms is population-based and relies on rules of selection and other kinds of operators.



Hyperparameter Optimization (HPO) using EC

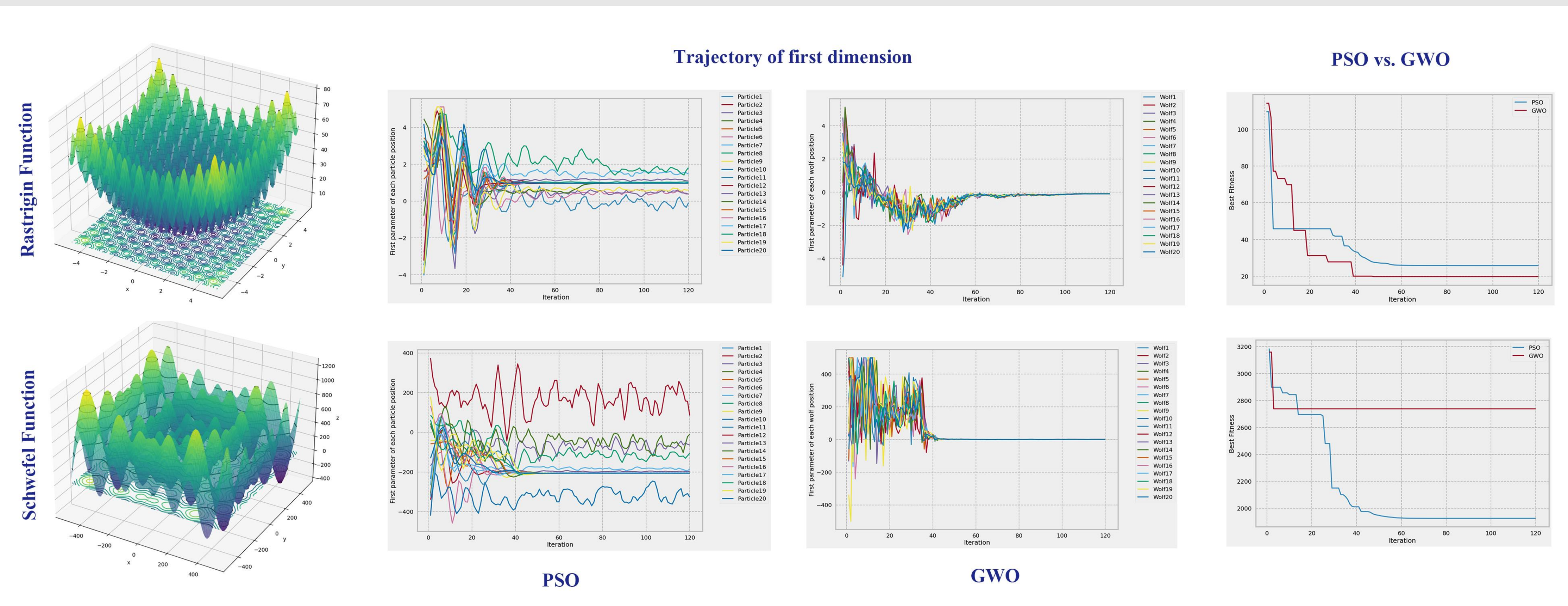
Hyperparameter optimization (HPO) is another vital step in ML pipelines that can significantly affect model performance and requires selecting optimal model parameters to maximize performance.

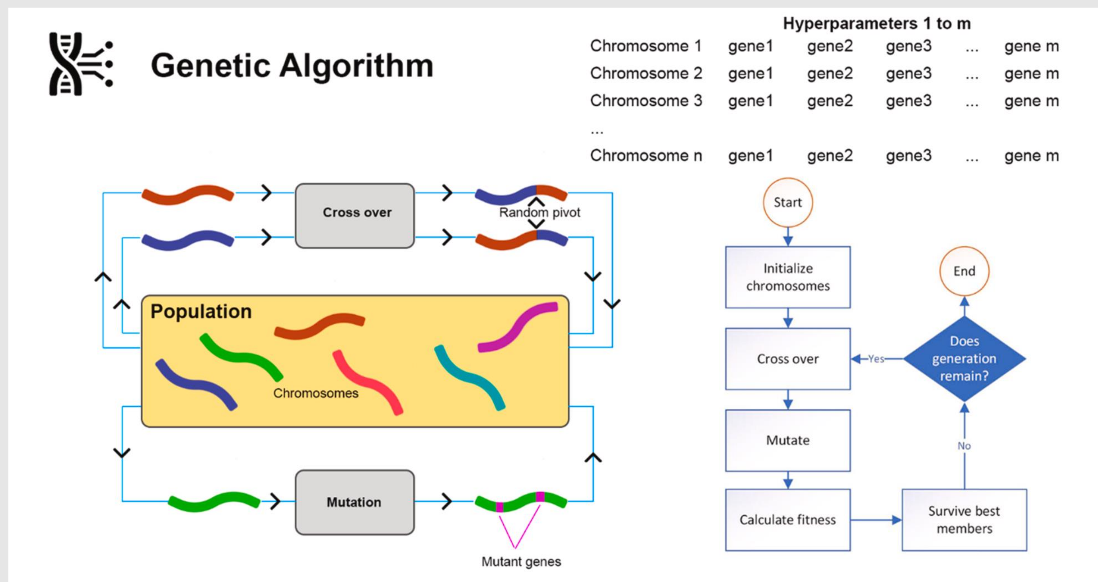


Evolutionary hyperparameter optimization pipeline

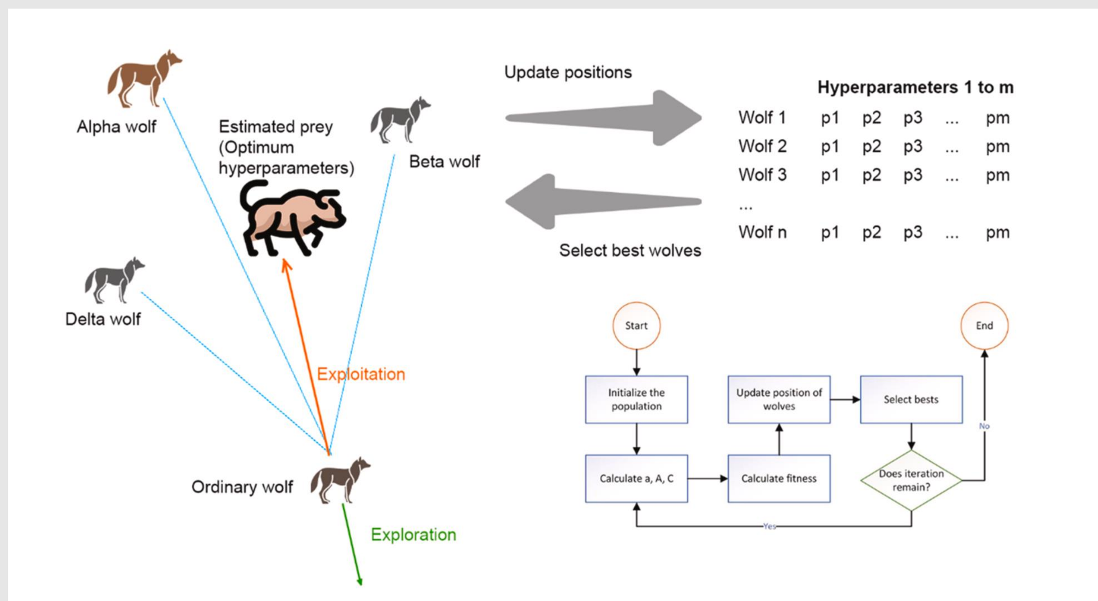
Discussion

I am working on hyperparameter optimization of deep learning models using evolutionary computation algorithms, such as PSO, GWO, GOA, etc. The goal is to find optimal hyperparameters that can improve the performance of the models. Although these algorithms have better performance in comparison to the traditional optimization algorithms, some of these algorithms suffer from center-bias (or zero-bias) problem which has been identified recently [6]. This problem arises when the algorithm tends to converge towards the center of the search space and fail to explore the entire space. As a result, the algorithm may miss potentially good solutions that are located away from the origin. The center-bias problem can lead to local optima and reduce the effectiveness of the SI algorithms in hyperparameter optimization.





GA general working mechanism [5]



Working mechanism of grey wolf optimization (GWO) [5]

Conclusion

My research can show the potential of SI algorithms for hyperparameter optimization. These algorithms can efficiently explore the vast hyperparameter space and find optimal solutions. However, the center-bias problem remains a significant obstacle that needs to be considered.

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