# An introduction to simulation-based inference

AI and the uncertainty challenge in fundamental physics
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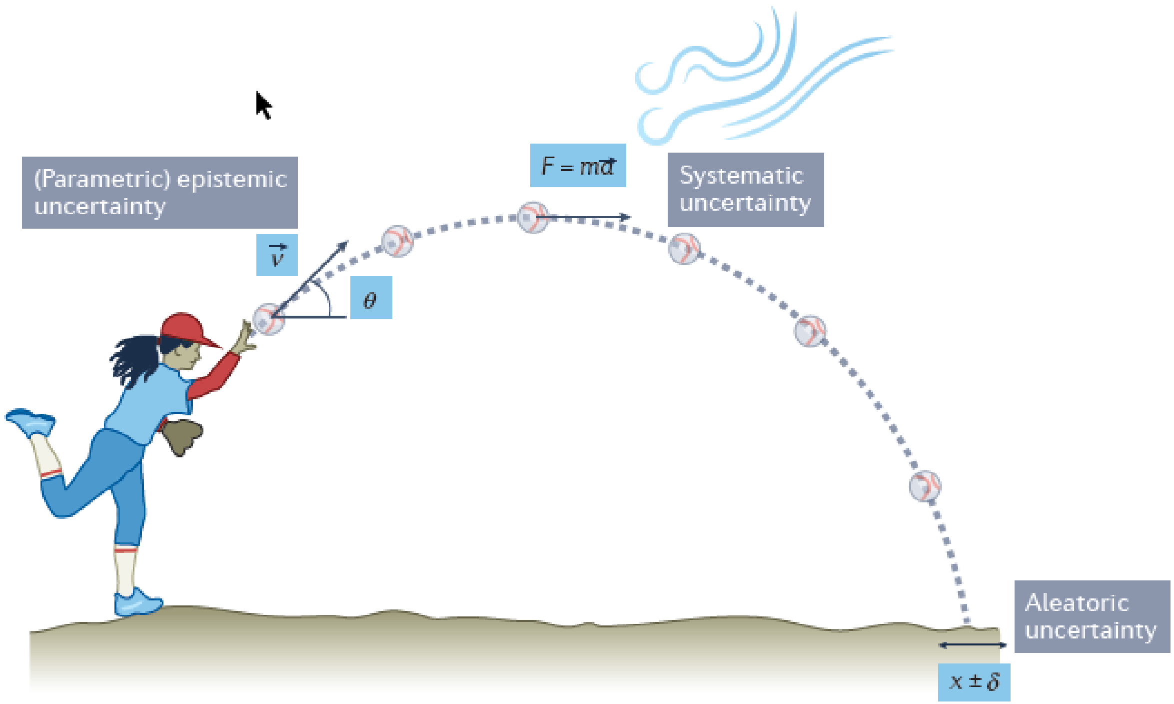

(Parametric) epistemic uncertainty
$\vec{v}$
$\theta$
$F = m\vec{a}$
Systematic uncertainty
Aleatoric uncertainty
$x \pm \delta$

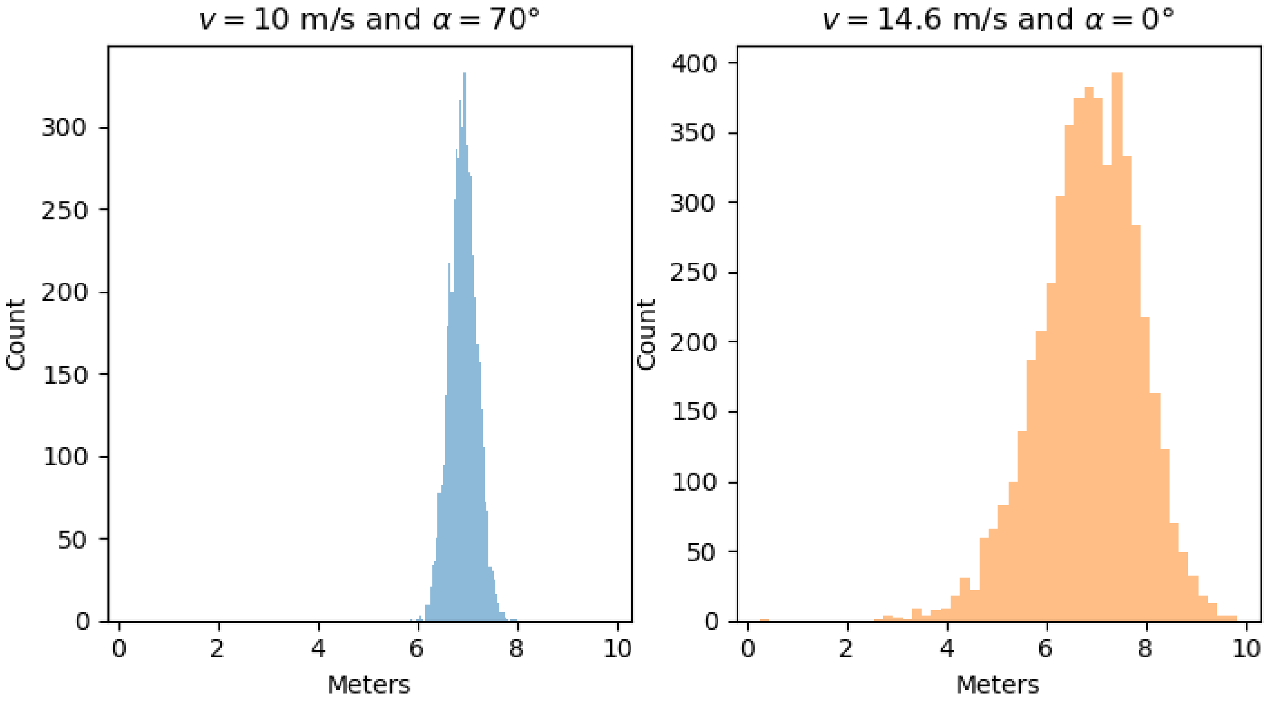
$$v_x = v\cos(\alpha), \quad v_y = v\sin(\alpha),$$

$$\frac{dx}{dt} = v_x, \quad \frac{dy}{dt} = v_y, \frac{dv_y}{dt} = -G.$$

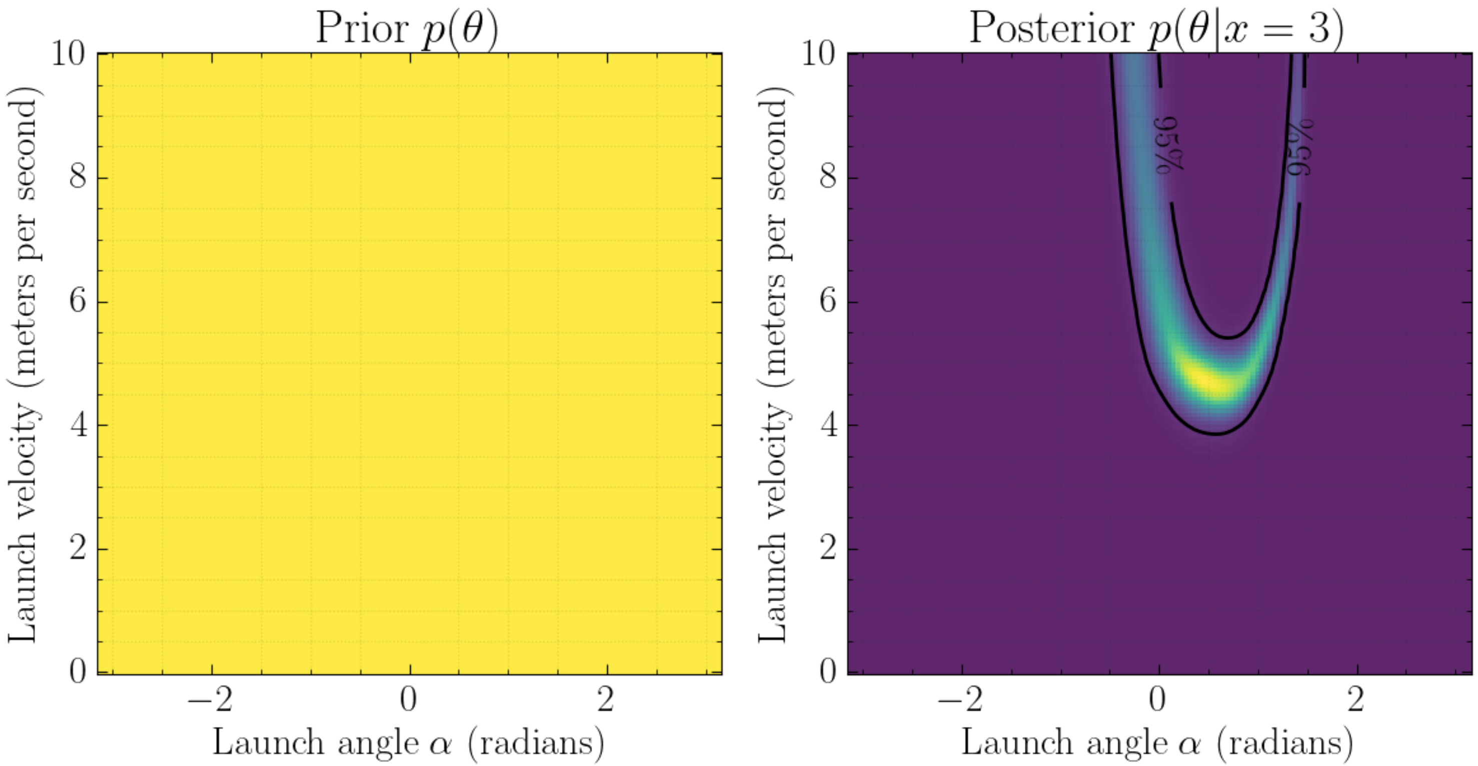
```python
def simulate(v, alpha, dt=0.001):
    v_x = v * np.cos(alpha)  # x velocity m/s
    v_y = v * np.sin(alpha)  # y velocity m/s
    y = 1.1 + 0.3 * random.normal()
    x = 0.0

    while y > 0: # simulate until ball hits floor
        v_y += dt * -G  # acceleration due to gravity
        x += dt * v_x
        y += dt * v_y

    return x + 0.25 * random.normal()
```


$v = 10$ m/s and $\alpha = 70°$
$v = 14.6$ m/s and $\alpha = 0°$
Count
Meters
0
50
100
150
200
250
300
350
400
0
2
4
6
8
10

What parameter values $\theta$ are the most plausible?



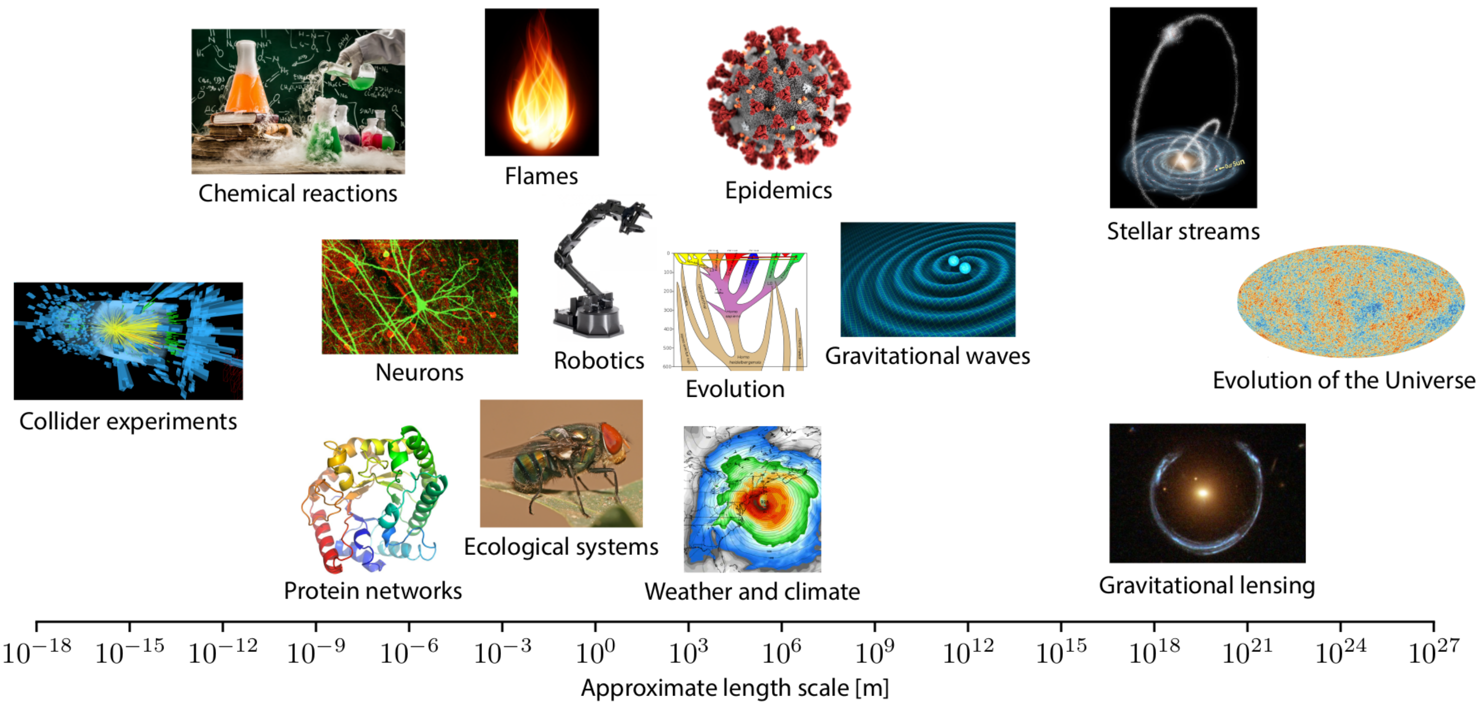
Prior $p(\theta)$
Posterior $p(\theta|x = 3)$
Launch velocity (meters per second)
Launch angle $\alpha$ (radians)
95%
95%

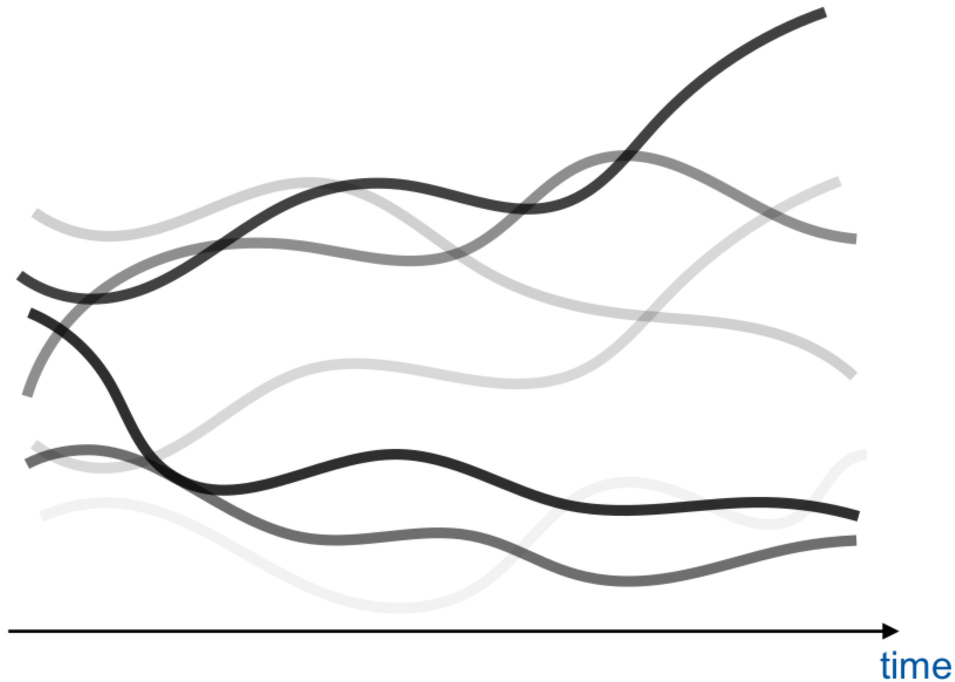
# Outline

1. Simulation-based inference
2. Algorithms
   - Neural ratio estimation
   - Neural posterior estimation
   - Neural score estimation
3. Diagnostics

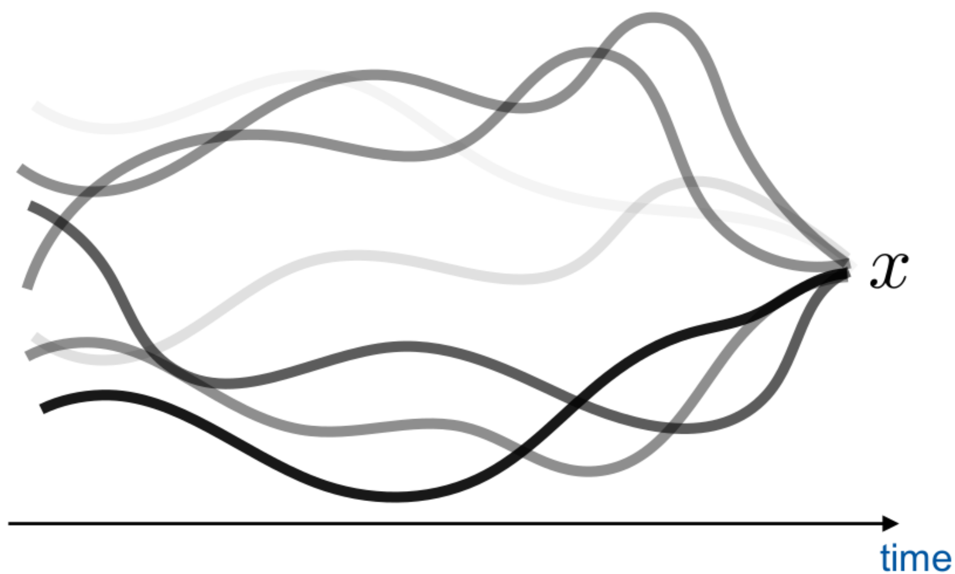
# Simulation-based inference

# Scientific simulators






$$\theta, z, x \sim p(\theta, z, x)$$




$$\theta, z \sim p(\theta, z | x)$$

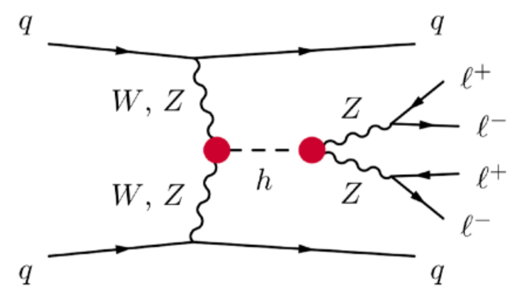
Latent variables

Parameters of interest

Parton-level momenta

Theory parameters

$z_p \longleftarrow \theta$



Latent variables

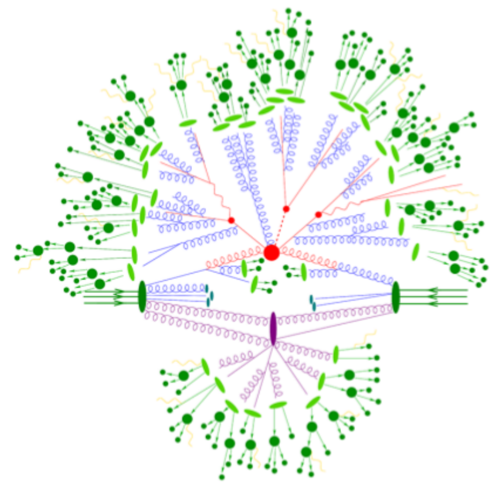
Parameters of interest

Shower splittings

Parton-level momenta

Theory parameters

$$z_s \longleftarrow z_p \longleftarrow \theta$$

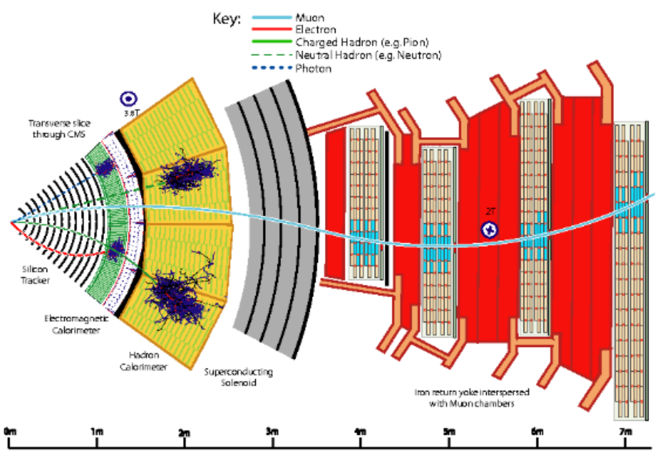


Latent variables

Parameters of interest

| Detector interactions | Shower splittings | Parton-level momenta | Theory parameters |
|---|---|---|---|
| $z_d$ | $z_s$ | $z_p$ | $\theta$ |

$$z_d \longleftarrow z_s \longleftarrow z_p \longleftarrow \theta$$



Features

Latent variables

Parameters of interest

Observables

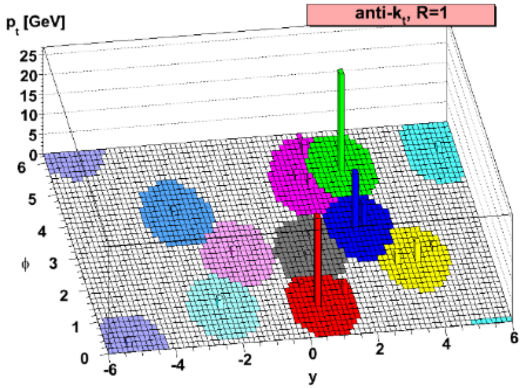
Detector interactions

Shower splittings

Parton-level momenta

Theory parameters

$$x \longleftarrow z_d \longleftarrow z_s \longleftarrow z_p \longleftarrow \theta$$




[Image source: M. Cacciari, G. Salam, G. Soyez 0802.1189]

$$p(x|\theta) = \underbrace{\iiint}_{\text{yikes!}} p(z_p|\theta)p(z_s|z_p)p(z_d|z_s)p(x|z_d)dz_p dz_s dz_d$$

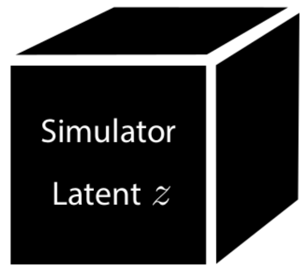
## Bayesian inference

Start with

- a simulator that can generate $N$ samples $x_i \sim p(x_i|\theta_i)$,
- a prior model $p(\theta)$,
- observed data $x_{\text{obs}}$.

Then, estimate the posterior

$$p(\theta|x_{\text{obs}}) = \frac{p(x_{\text{obs}}|\theta)p(\theta)}{p(x_{\text{obs}})}.$$

Parameters $\theta$ → 

→ Observables $x$

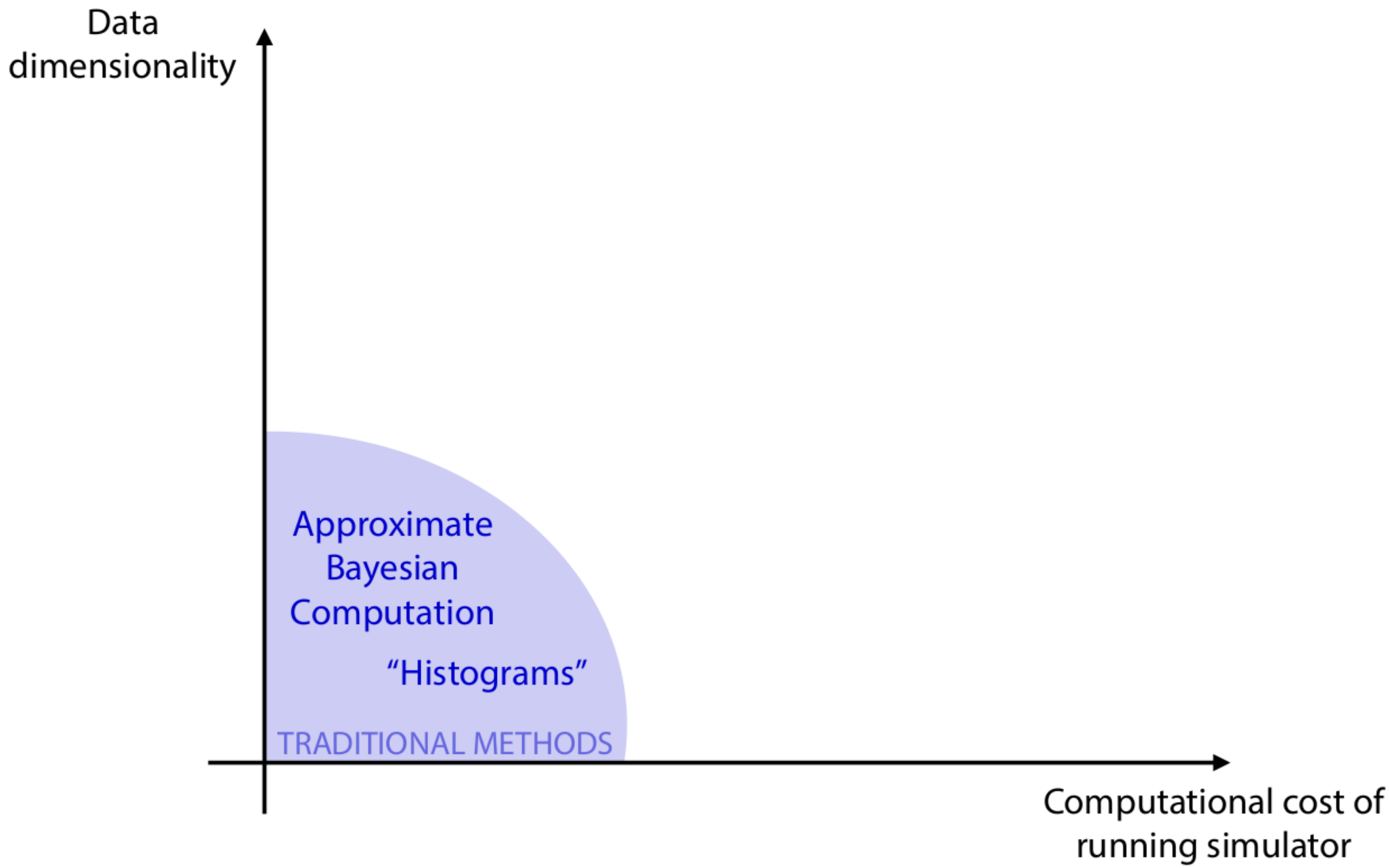
Prediction:

- Well-motivated mechanistic, causal model
- Simulator can generate samples $x \sim p(x|\theta)$

Inference:

- Interactions between low-level components lead to challenging inverse problems
- Likelihood $p(x|\theta) = \int \mathrm{d}z\; p(x, z|\theta)$ is intractable

# Algorithms

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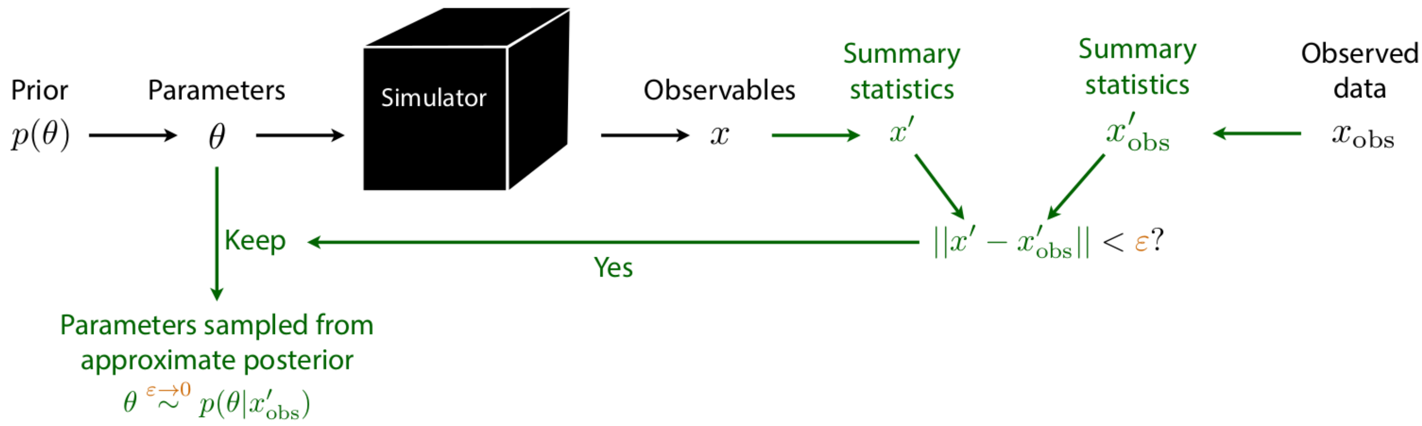
Credits: Cranmer, Brehmer and Louppe, 2020.

# Approximate Bayesian Computation (ABC)




*Issues:*

- How to choose $x'$? $\epsilon$? $|| \cdot ||$?
- No tractable posterior.
- Need to run new simulations for new data or new prior.

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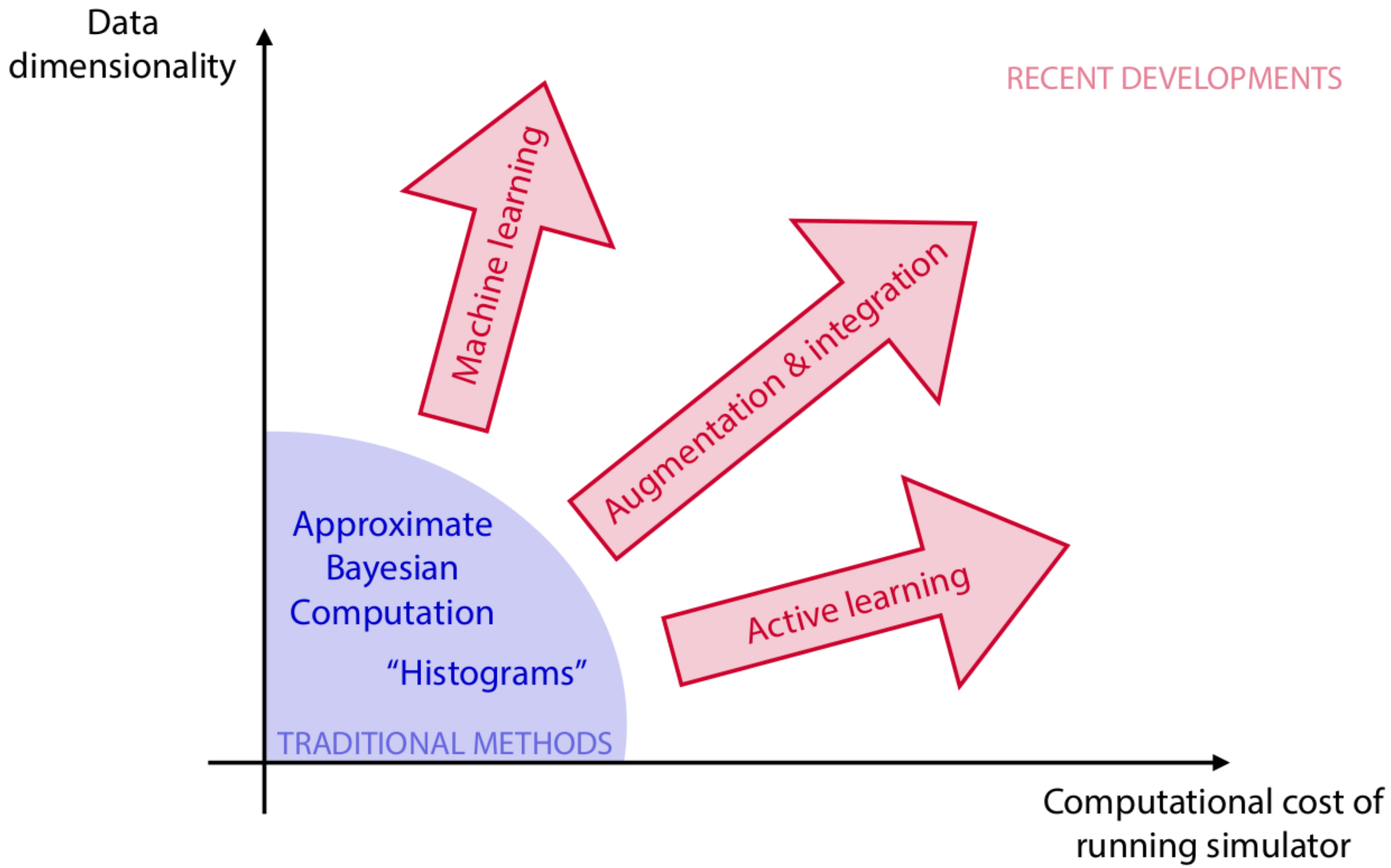
Credits: Johann Brehmer.

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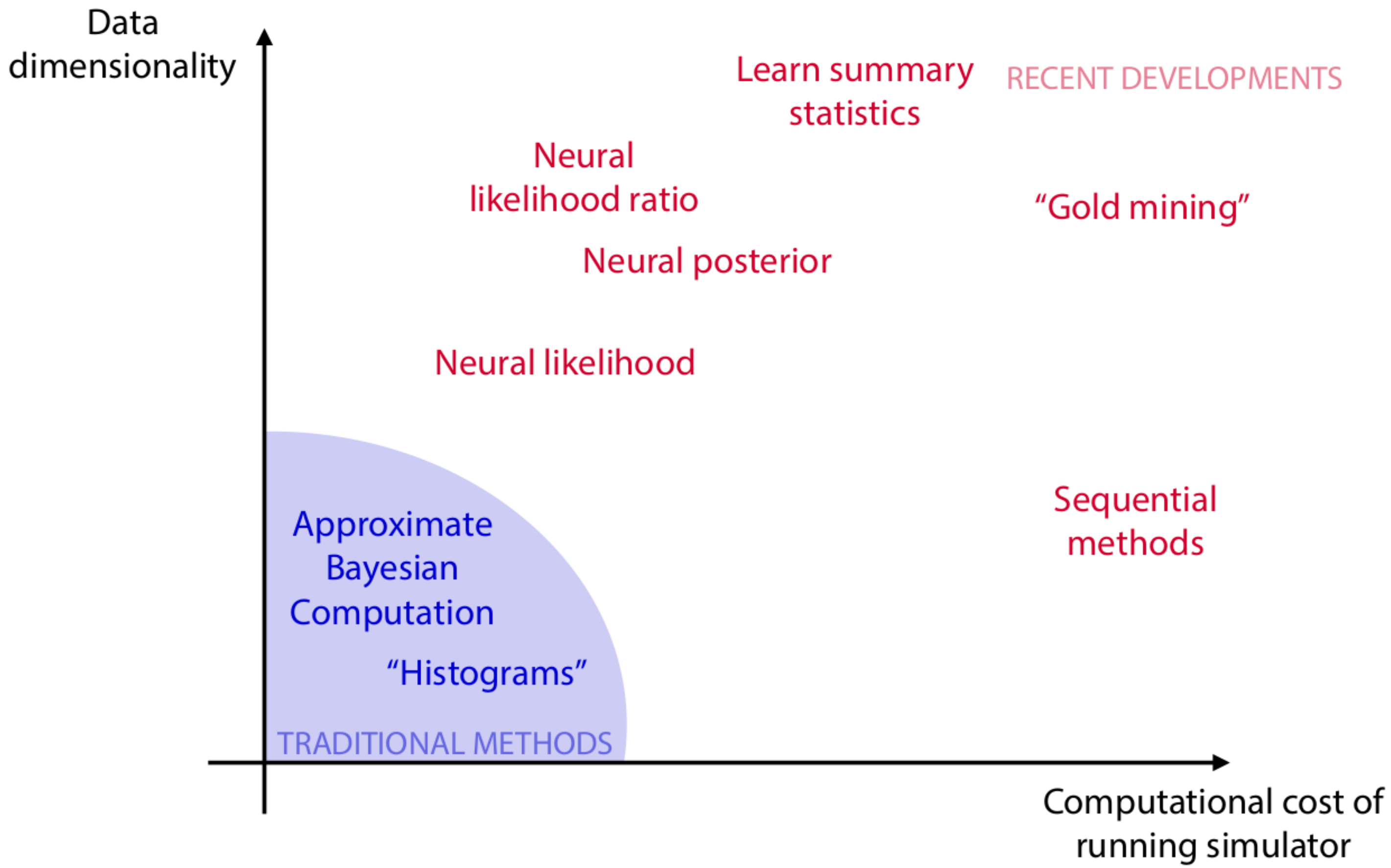
Credits: Cranmer, Brehmer and Louppe, 2020.

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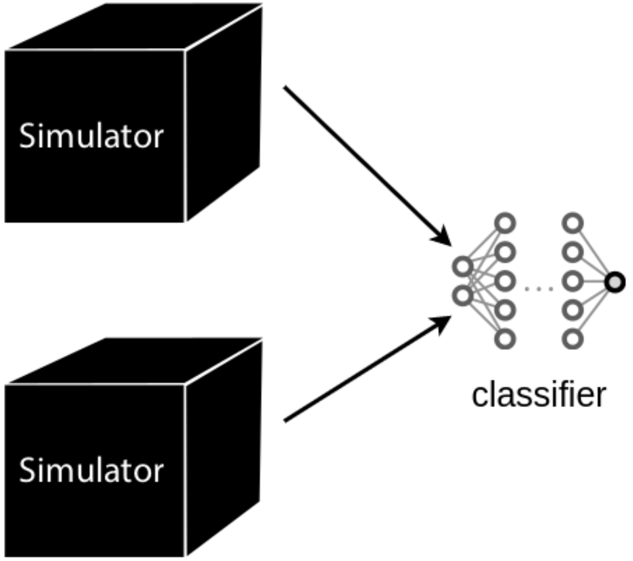
Credits: Cranmer, Brehmer and Louppe, 2020.

# Neural ratio estimation

The likelihood-to-evidence $r(x|\theta) = \frac{p(x|\theta)}{p(x)} = \frac{p(x,\theta)}{p(x)p(\theta)}$ ratio can be learned, even if neither the likelihood nor the evidence can be evaluated:

$x, \theta \sim p(x, \theta)$

$x, \theta \sim p(x)p(\theta)$




$\hat{r}(x|\theta)$

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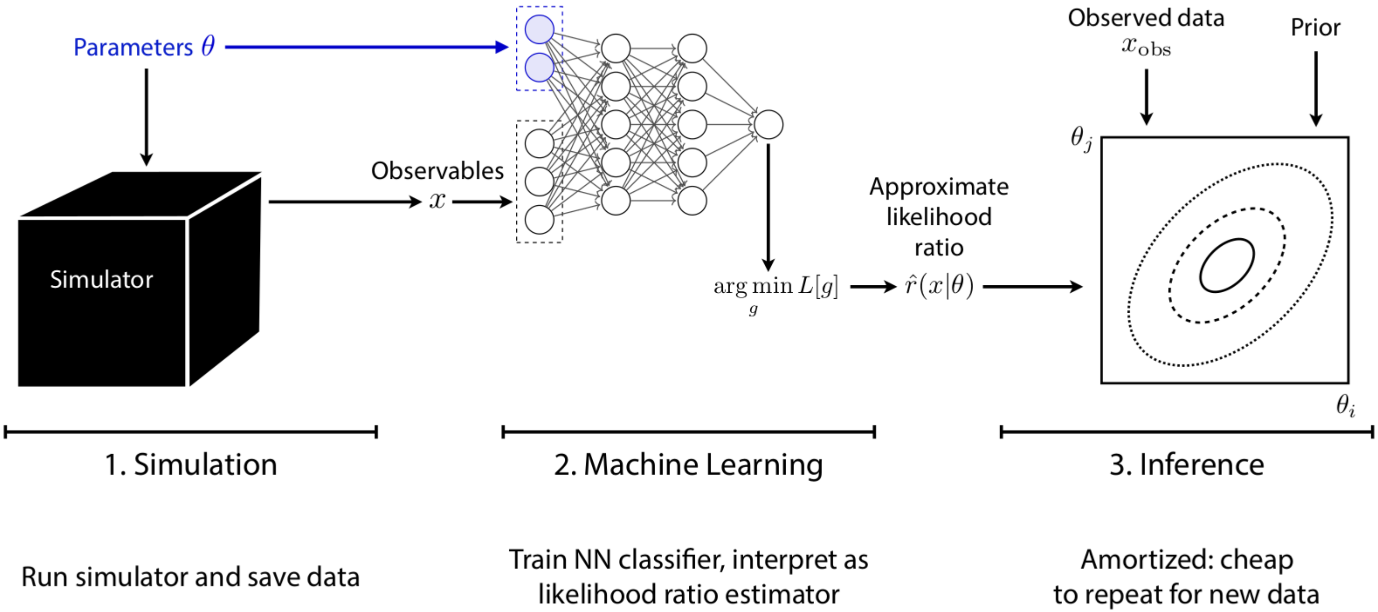
Credits: Cranmer et al, 2015; Hermans et al, 2020.

The solution $d$ found after training approximates the optimal classifier

$$d(x,\theta) \approx d^*(x,\theta) = \frac{p(x,\theta)}{p(x,\theta) + p(x)p(\theta)}.$$

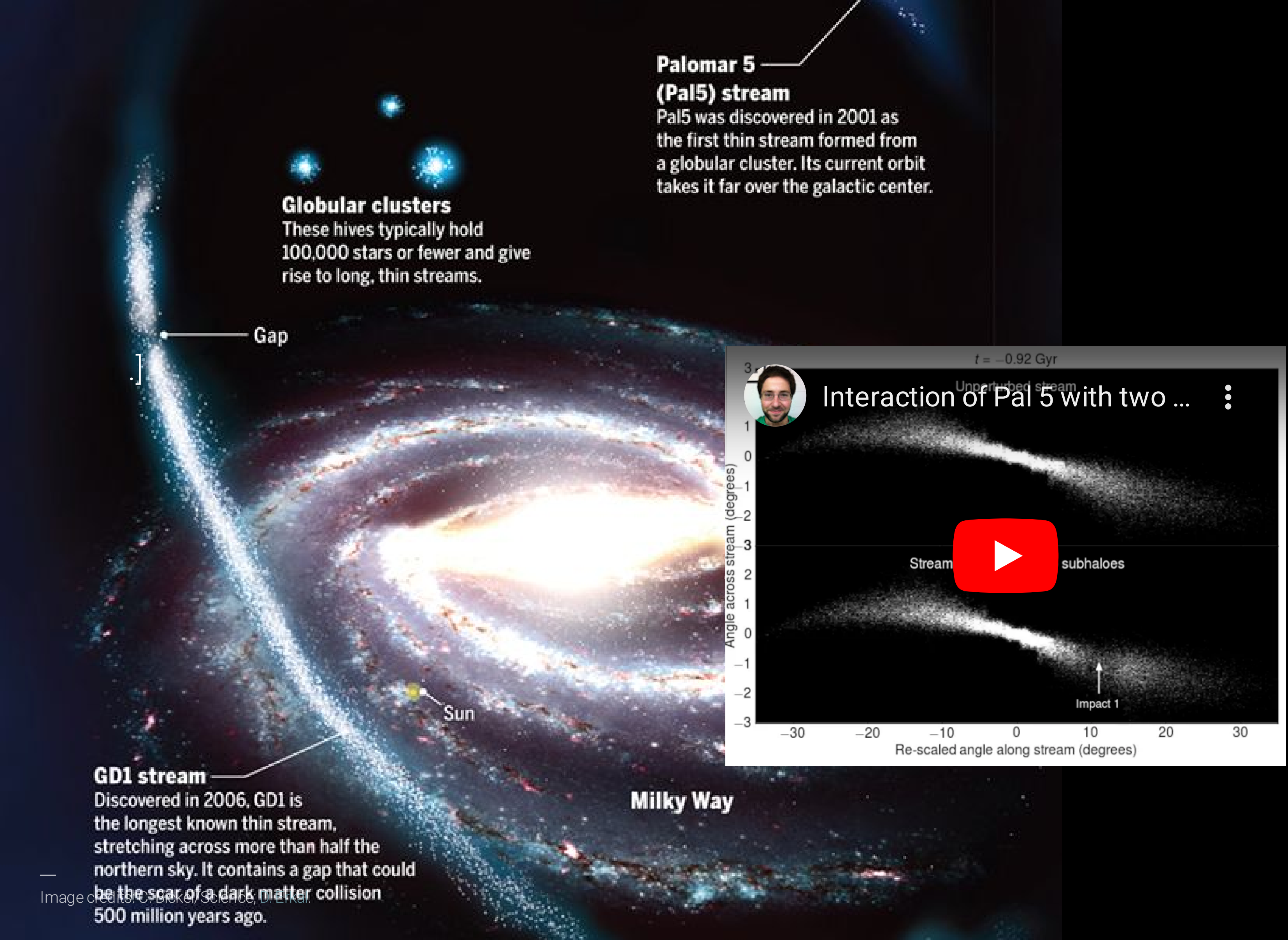
Therefore,

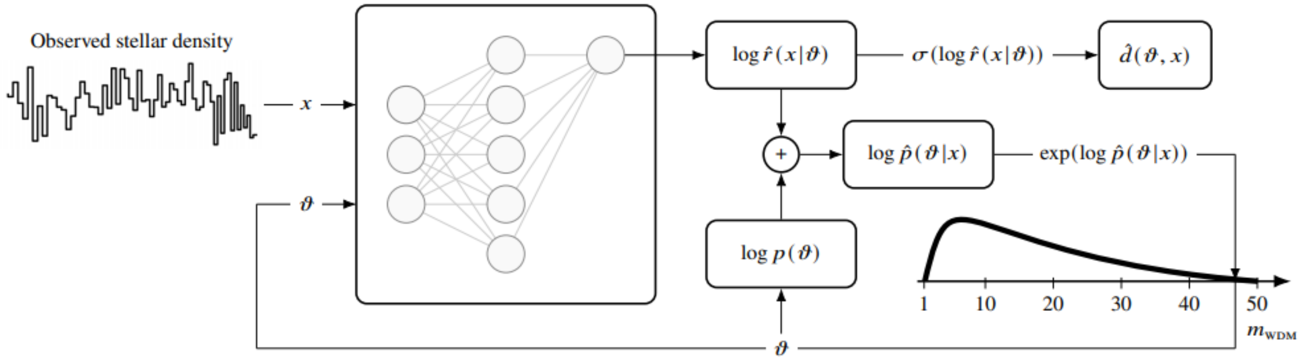
$$r(x|\theta) = \frac{p(x|\theta)}{p(x)} = \frac{p(x,\theta)}{p(x)p(\theta)} \approx \frac{d(x,\theta)}{1 - d(x,\theta)} = \hat{r}(x|\theta).$$

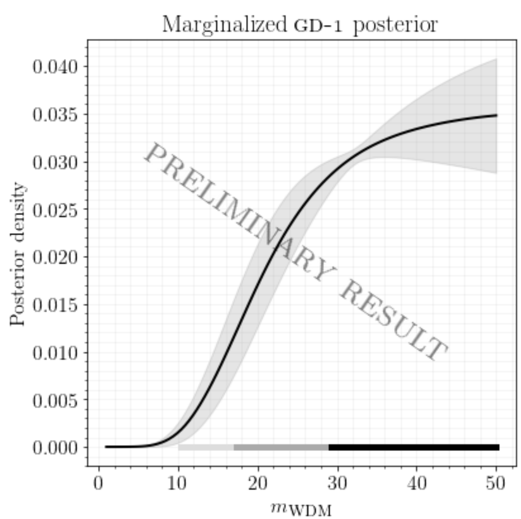


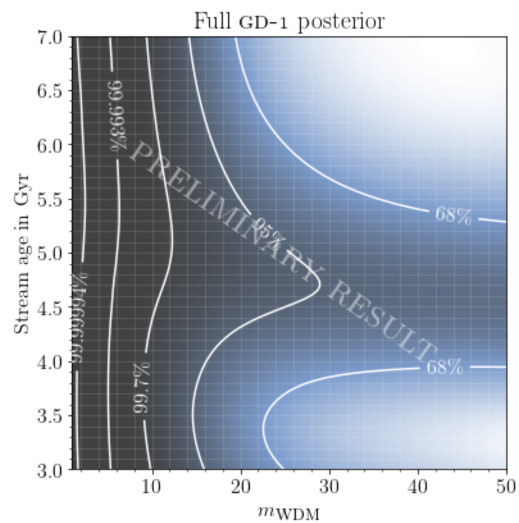

$$p(\theta|x) \approx \hat{r}(x|\theta)p(\theta)$$

# Constraining dark matter with stellar streams



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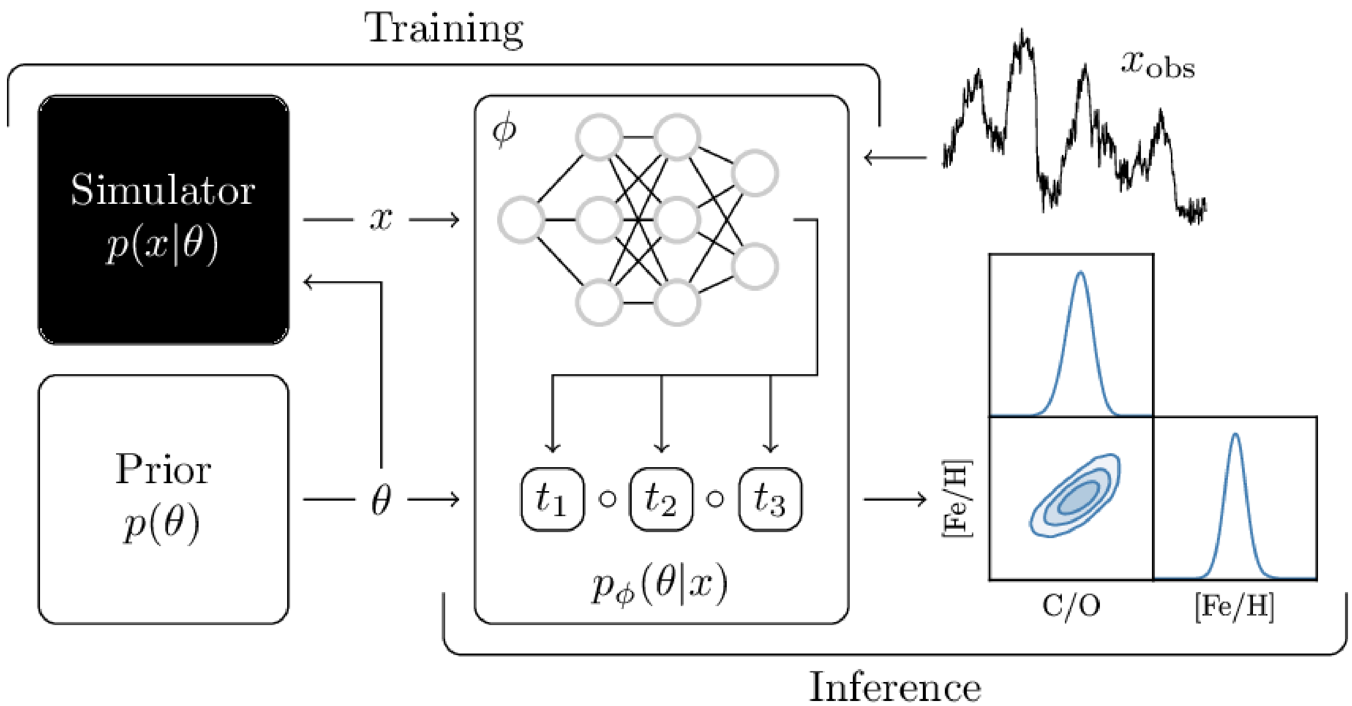
Credits: Hermans et al, 2021.


Preliminary results for GD-1 suggest a **preference for CDM over WDM**.

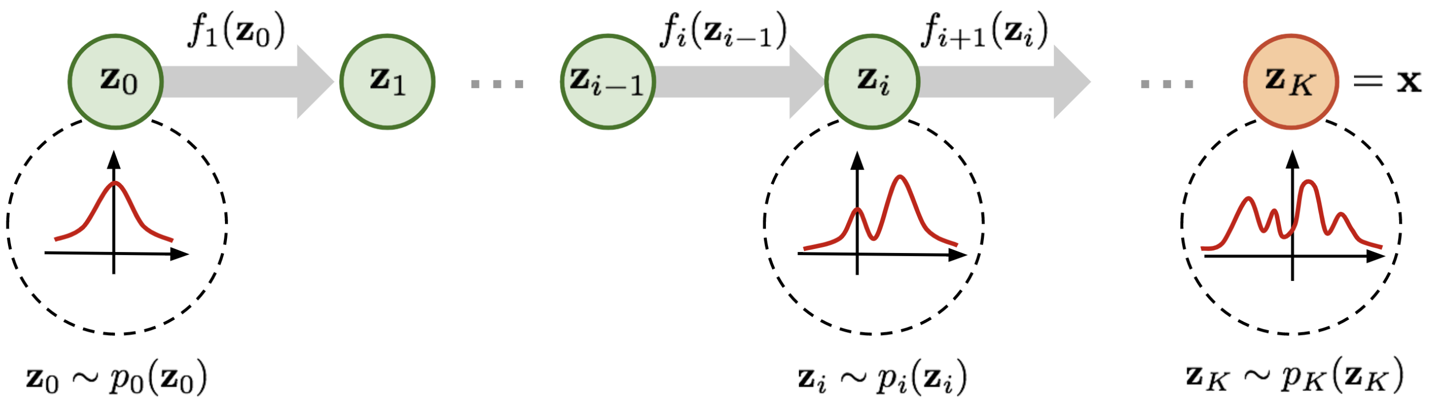
# Neural Posterior Estimation




$$\min_{q_\phi} \mathbb{E}_{p(x)} \left[ \mathrm{KL}(p(\theta|x) || q_\phi(\theta|x)) \right]$$

# Normalizing flows

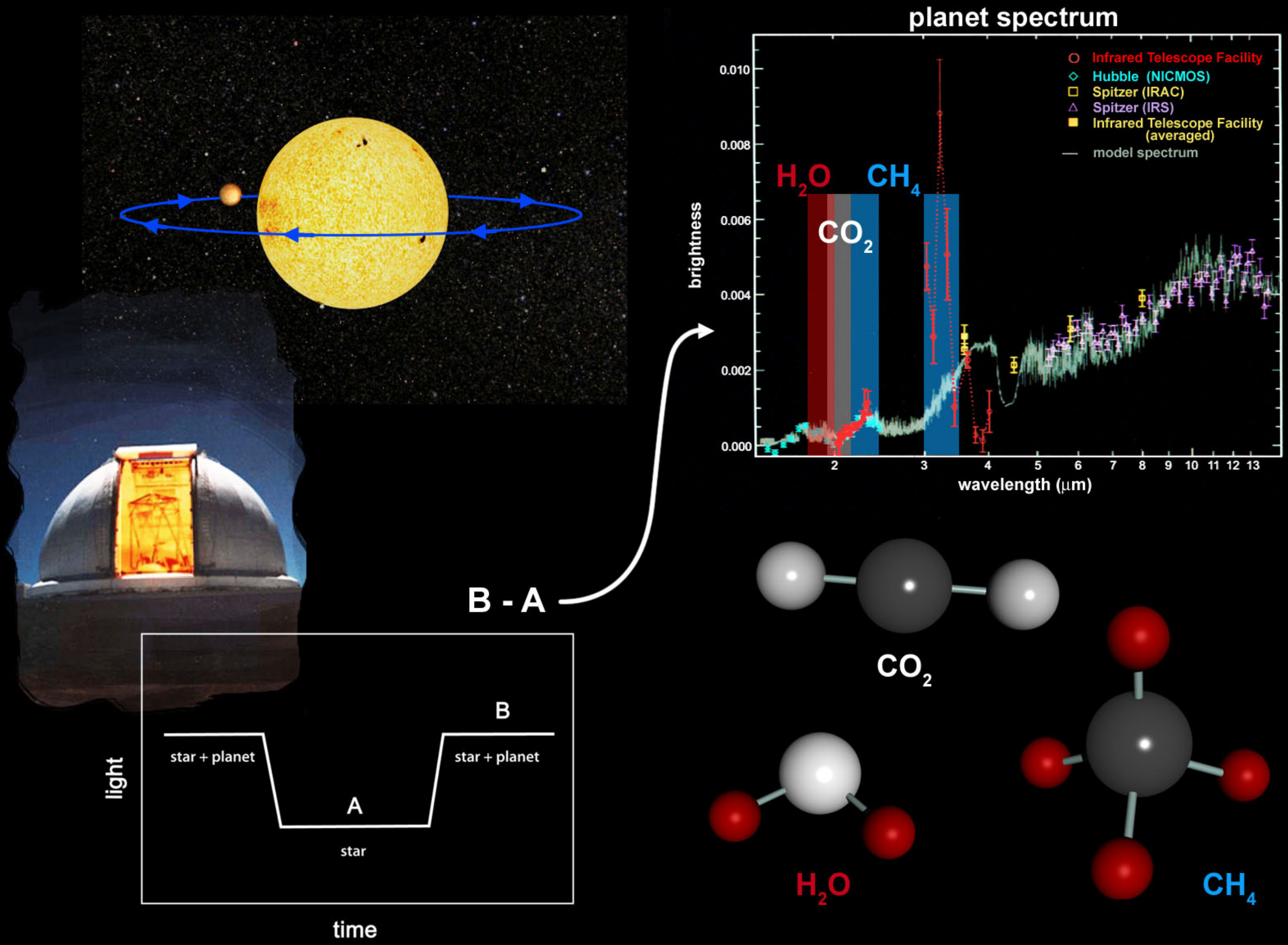
A normalizing flow is a sequence of invertible transformations $f_k$ that map a simple distribution $p_0$ to a more complex distribution $p_K$:

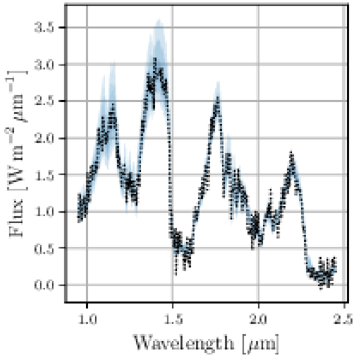


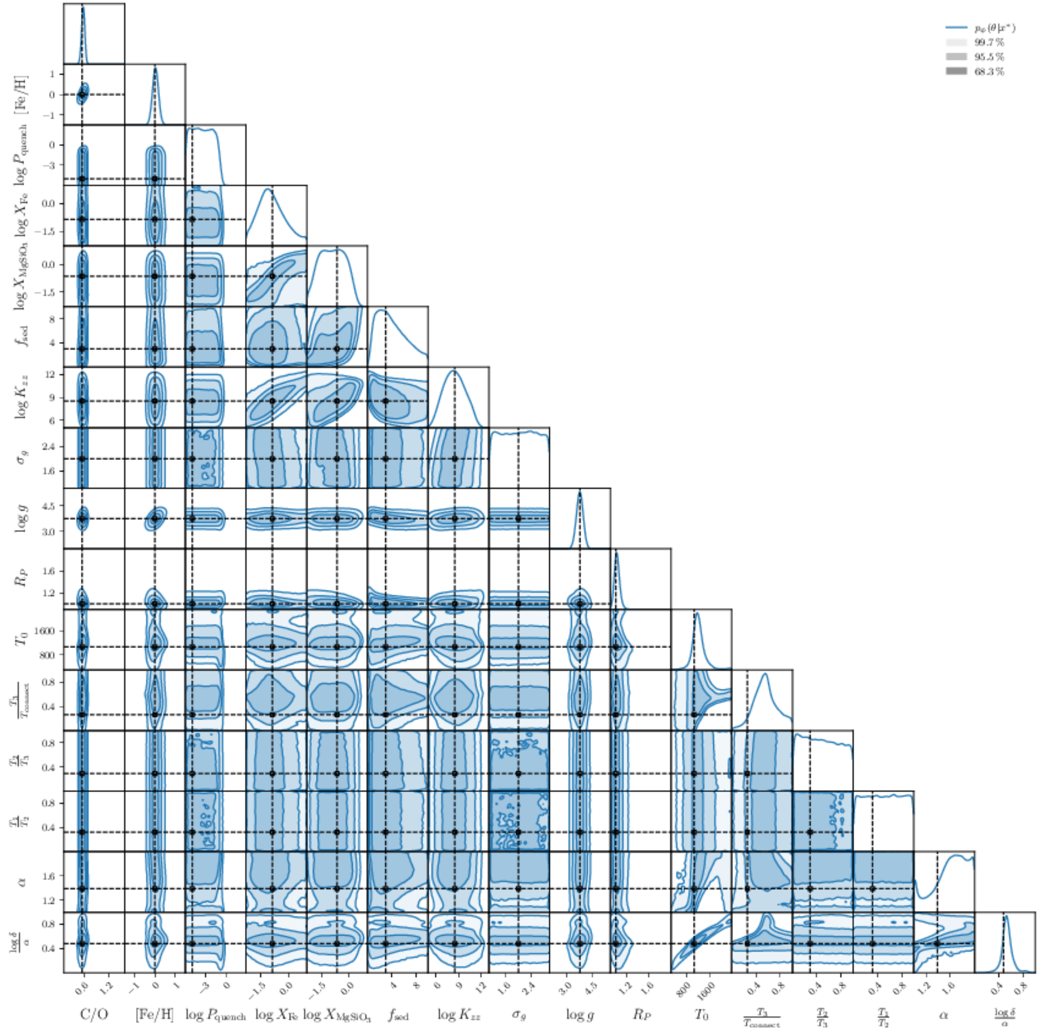

By the change of variables formula, the log-likelihood of a sample $x$ is given by

$$\log p(\mathbf{x}) = \log p(\mathbf{z}_0) - \sum_{k=1}^{K} \log \left|\det J_{f_k}(\mathbf{z}_{k-1})\right| .$$

# Exoplanet atmosphere characterization



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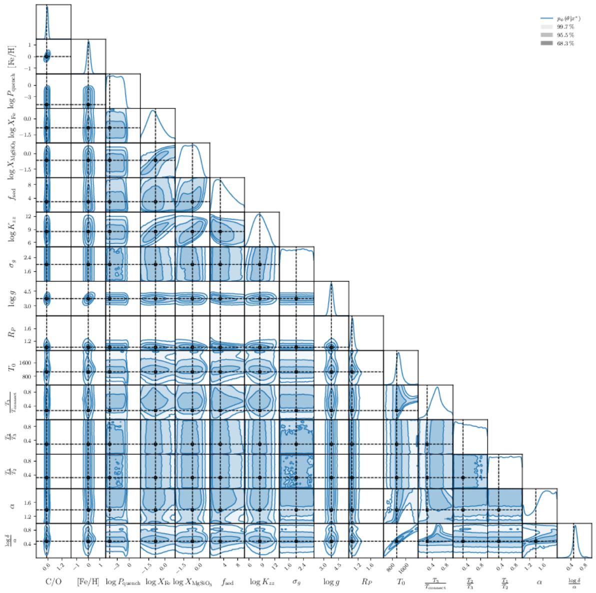
Credits: Vasist et al, 2023.

# Diagnostics

$$\hat{p}(\theta|x) = \text{sbi}(p(x|\theta), p(\theta), x)$$

We must make sure our approximate simulation-based inference algorithms can (at least) actually realize faithful inferences on the (expected) observations.

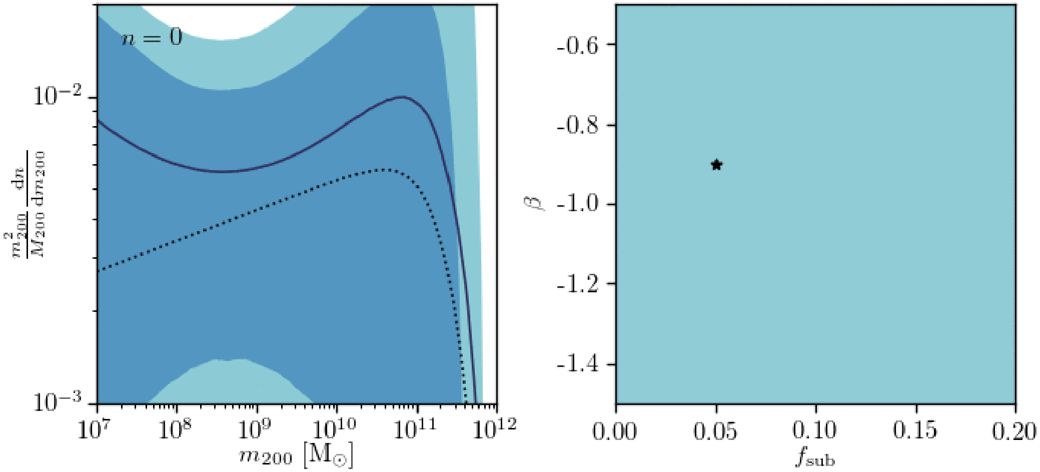


*How certain are you of your uncertainties?*

# Mode convergence

The maximum a posteriori estimate converges towards the nominal value $\theta^*$ for an increasing number of independent and identically distributed observables $x_i \sim p(x|\theta^*)$:

$$\lim_{N\to\infty} \arg\max_\theta p(\theta|\{x_i\}_{i=1}^N)$$
$$= \lim_{N\to\infty} \arg\max_\theta p(\theta) \prod_{x_i} r(x_i|\theta) = \theta^*$$

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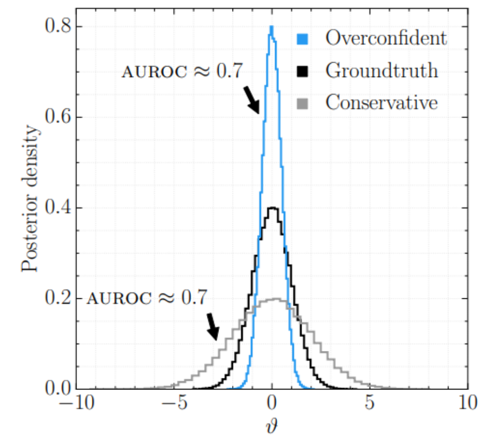
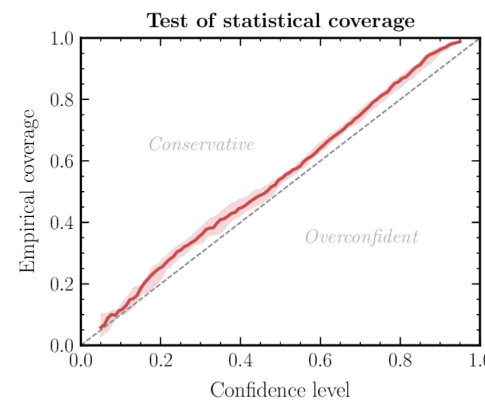
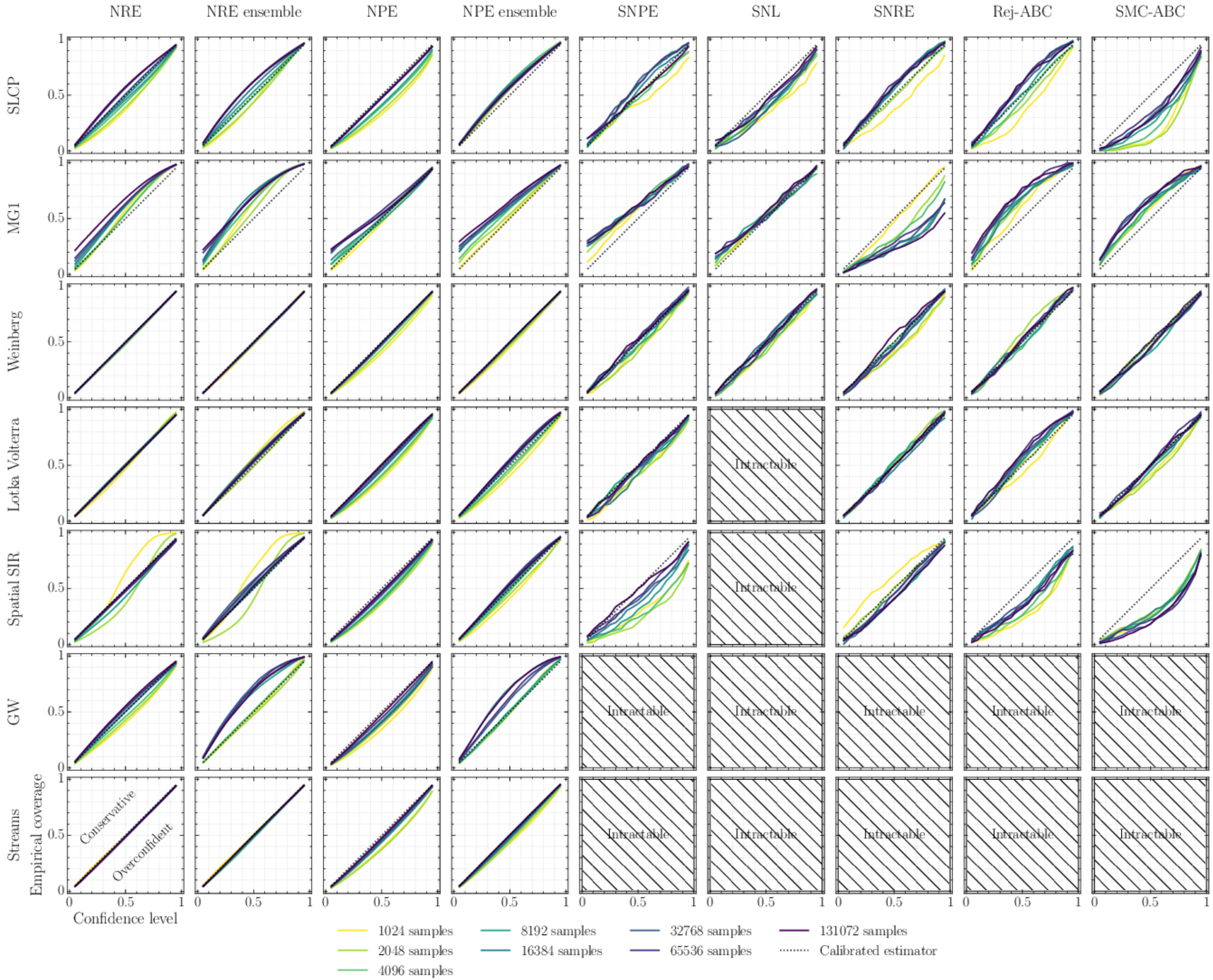
Credits: Brehmer et al, 2019.

## Coverage diagnostic

- For $x, \theta \sim p(x, \theta)$, compute the $1-\alpha$ credible interval based on $\hat{p}(\theta|x)$.
- If the fraction of samples for which $\theta$ is contained within the interval is larger than the nominal coverage probability $1-\alpha$, then the approximate posterior $\hat{p}(\theta|x)$ has coverage.



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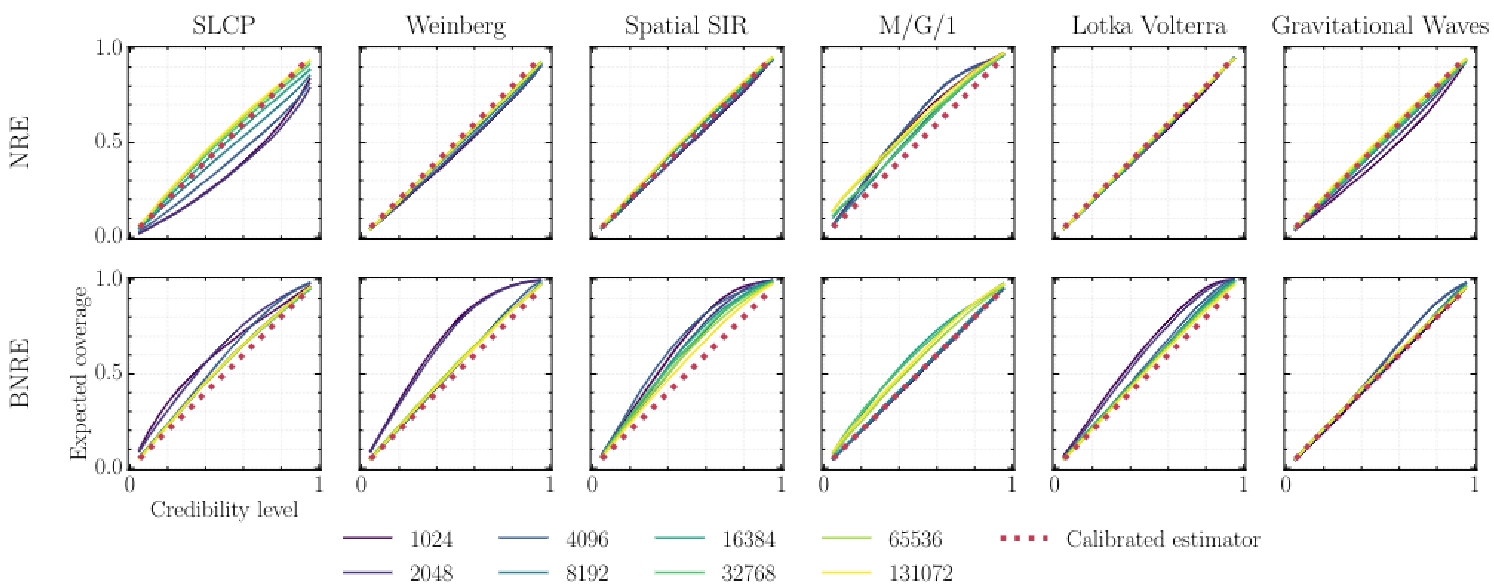
Credits: Hermans et al, 2021.

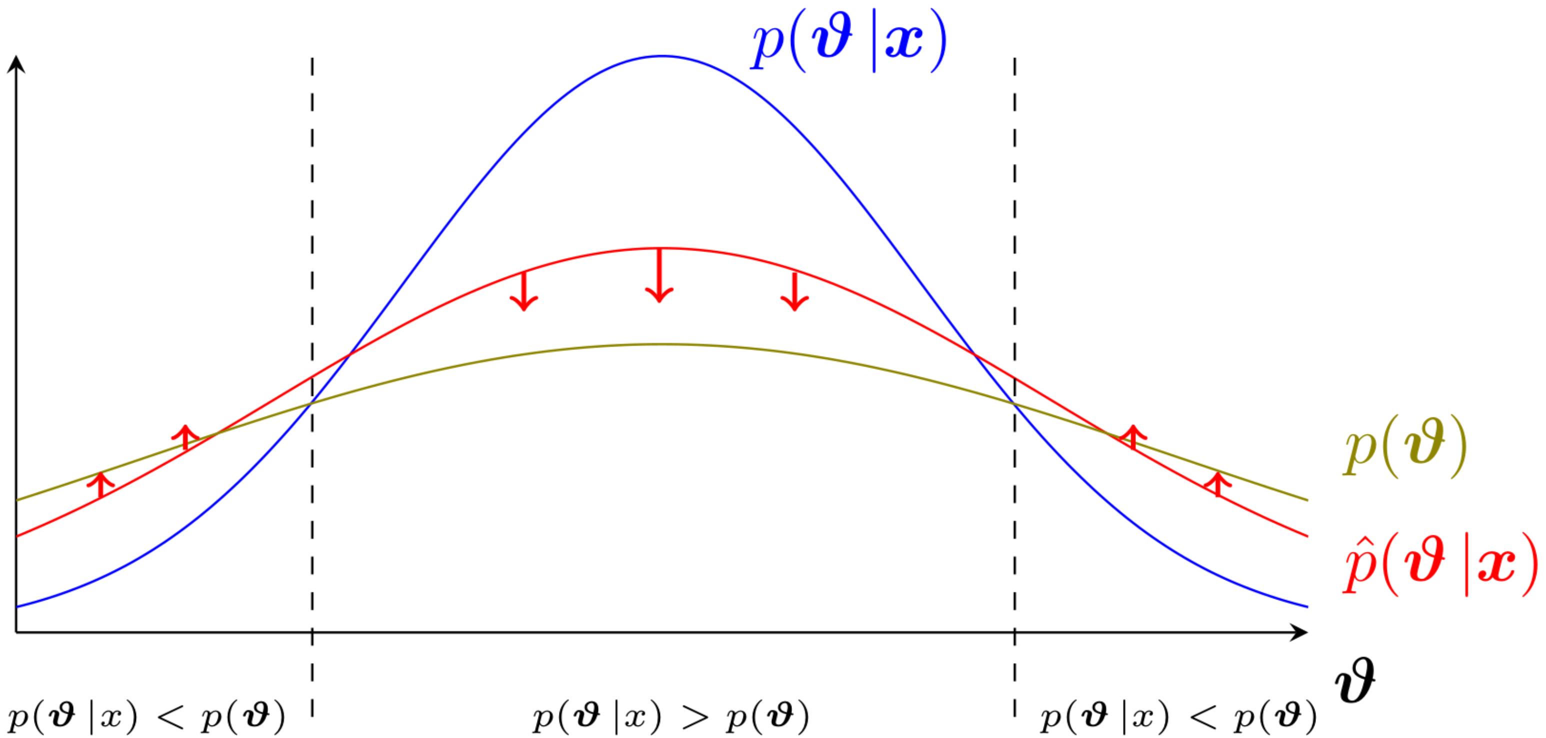
What if diagnostics fail?

# Balanced NRE

Enforce neural ratio estimation to be **conservative** by using binary classifiers $\hat{d}$ that are balanced, i.e. such that

$$\mathbb{E}_{p(\theta,x)}\left[\hat{d}(\theta,x)\right] = \mathbb{E}_{p(\theta)p(x)}\left[1 - \hat{d}(\theta,x)\right].$$



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Credits: Delaunoy et al, 2022.

# Summary

Advances in deep learning have enabled new approaches to statistical inference.

This is major evolution in the statistical capabilities for science, as it enables the analysis of complex models and data without simplifying assumptions.

Inference remains approximate and requires careful validation.

Obstacles remain to be overcome, such as the curse of dimensionality and the need for large amounts of data.

The end.