An introduction to simulation-based inference

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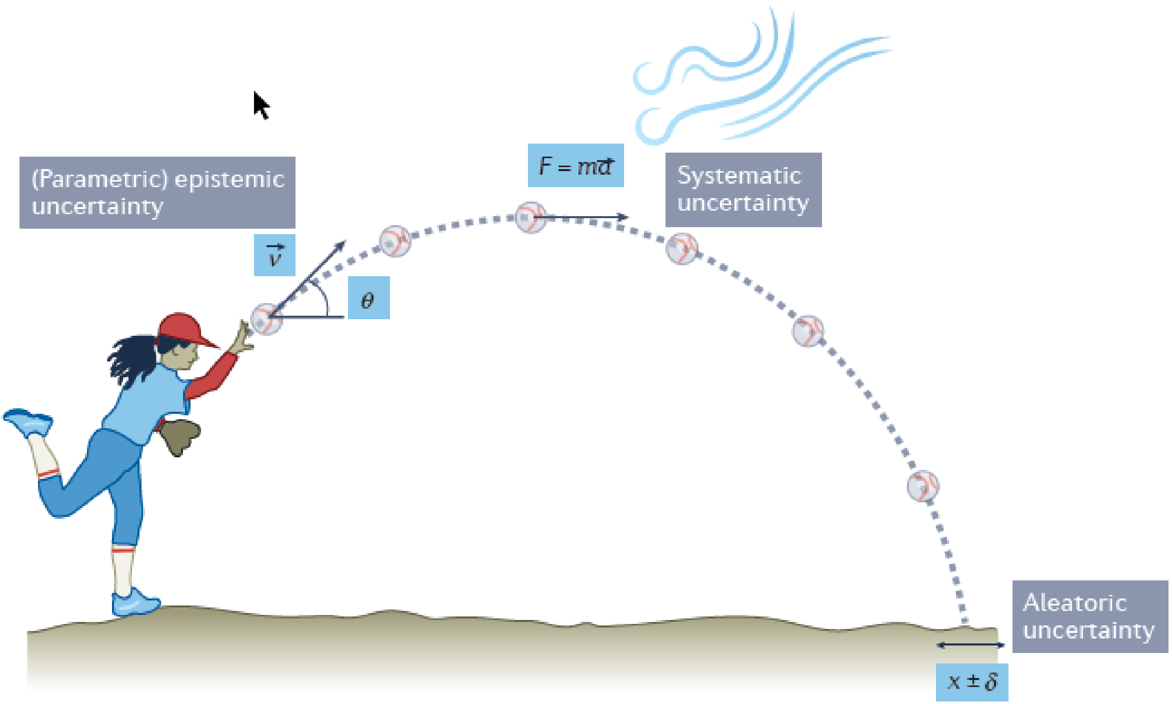
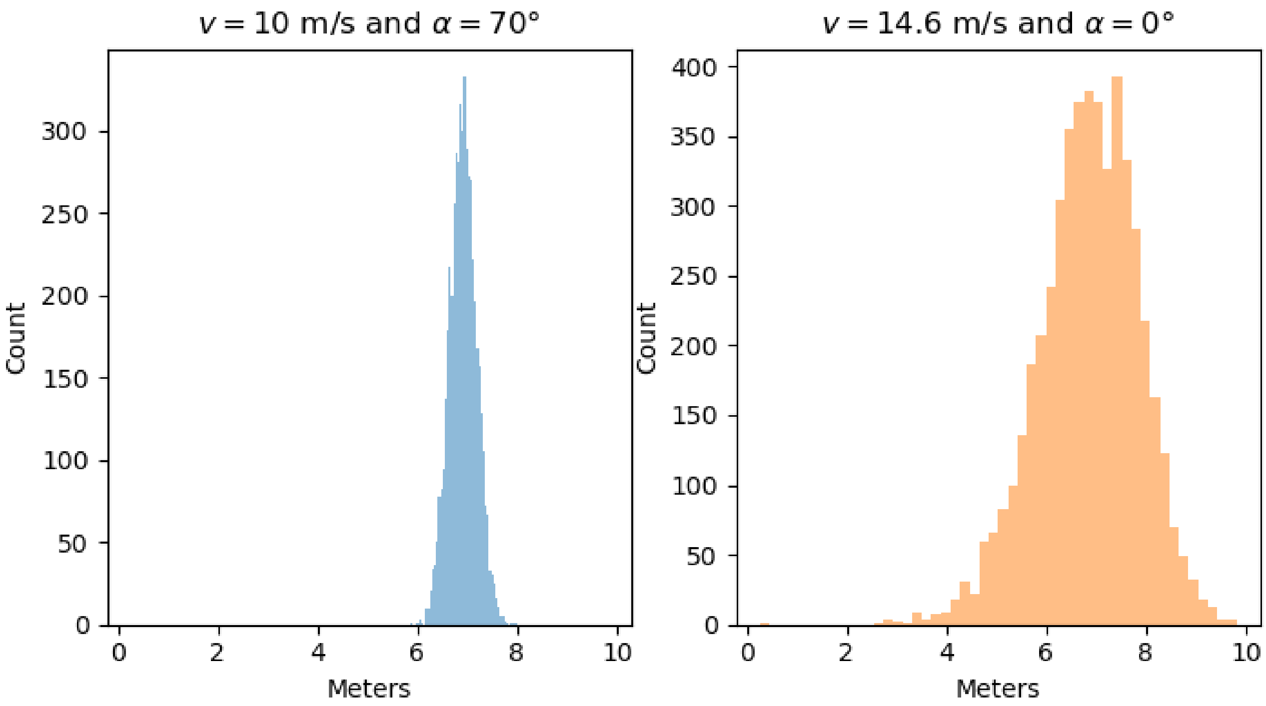


(Parametric) epistemic uncertainty
$\vec{v}$
θ
$F = m\vec{a}$
Systematic uncertainty
Aleatoric uncertainty
$x \pm \delta$

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

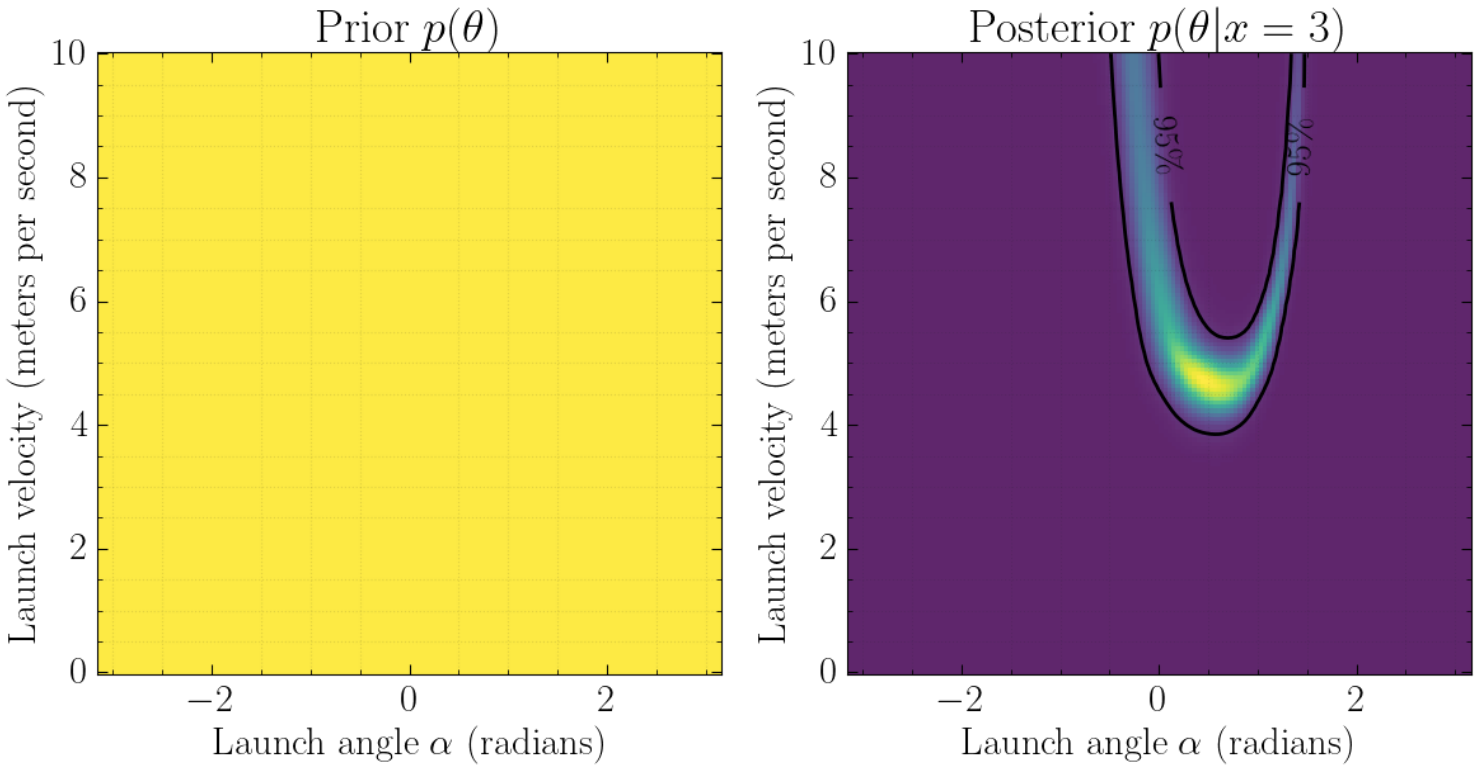
$$\frac{dx}{dt} = v_x\,, \quad \frac{dy}{dt} = v_y, \frac{dv_y}{dt} = -G.$$

```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 $\alpha = 70°$
Count
Meters
0
50
100
150
200
250
300
0
2
4
6
8
10
$v = 14.6$ 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 θ are the most plausible?



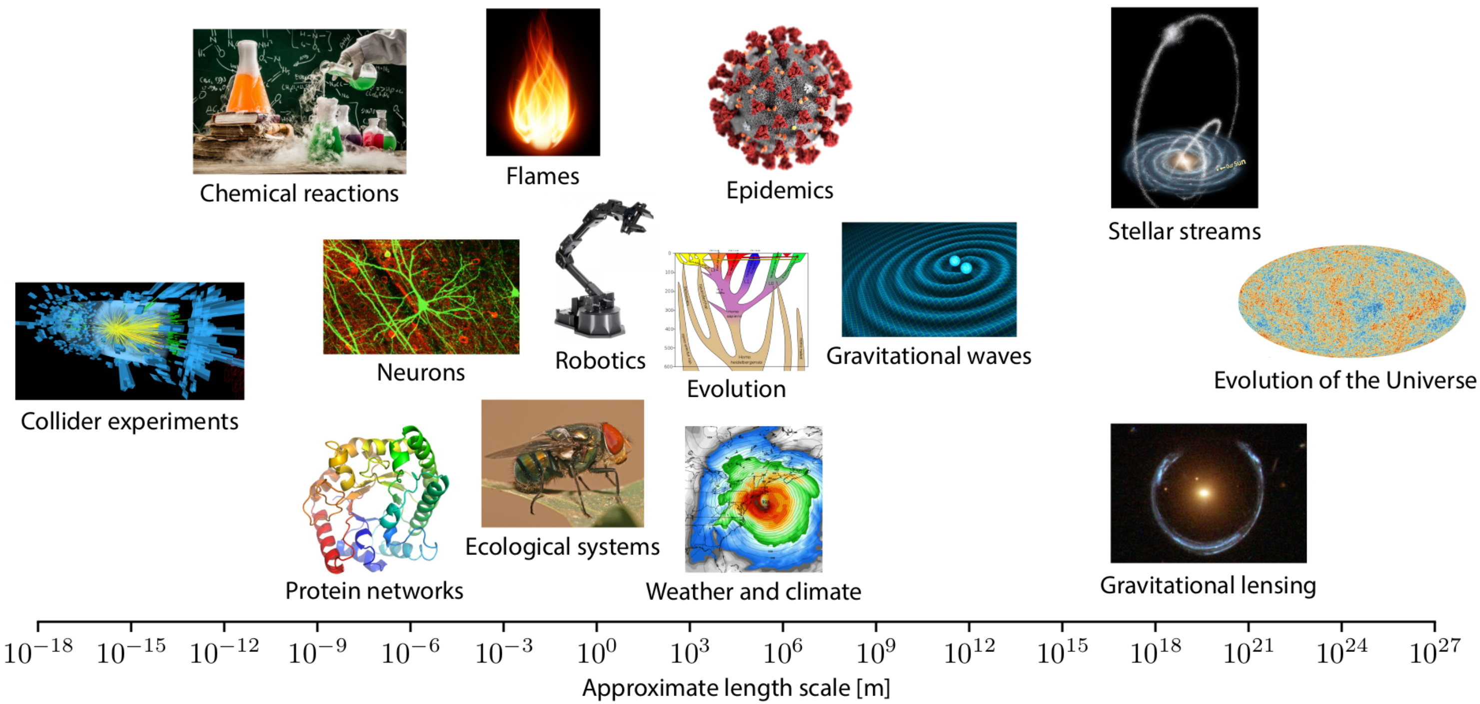
Prior $p(\theta)$
Posterior $p(\theta|x = 3)$
Launch velocity (meters per second)
Launch angle α (radians)
95%
95%
0
2
4
6
8
10
−2
0
2

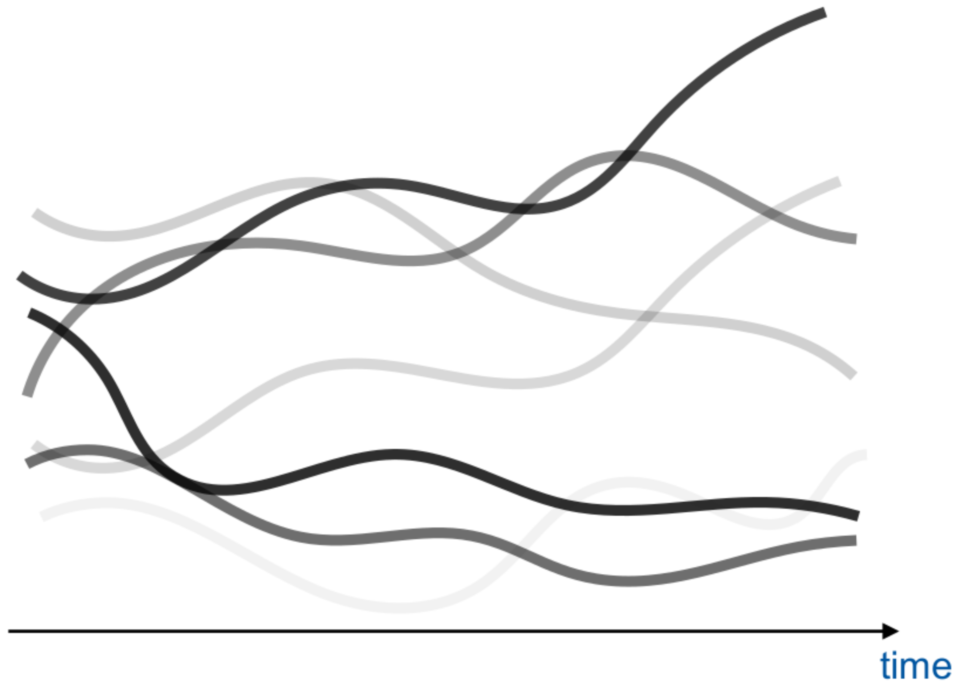
Outline

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

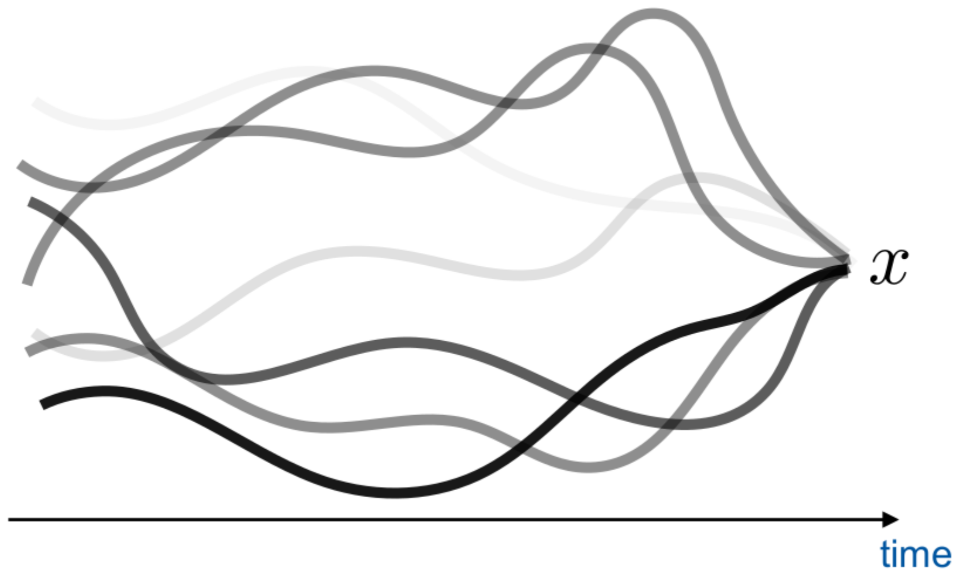
Simulation-based inference

Scientific simulators





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



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

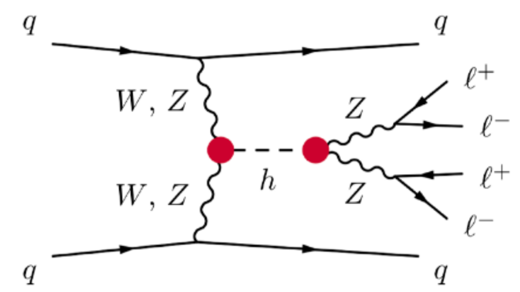
Latent variables

Parameters of interest

Parton-level momenta

Theory parameters

$$z_p \longleftarrow \theta$$



Latent variables

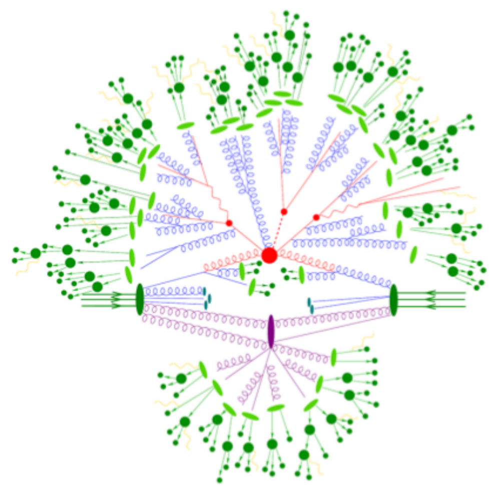
Parameters of interest

Shower splittings

Parton-level momenta

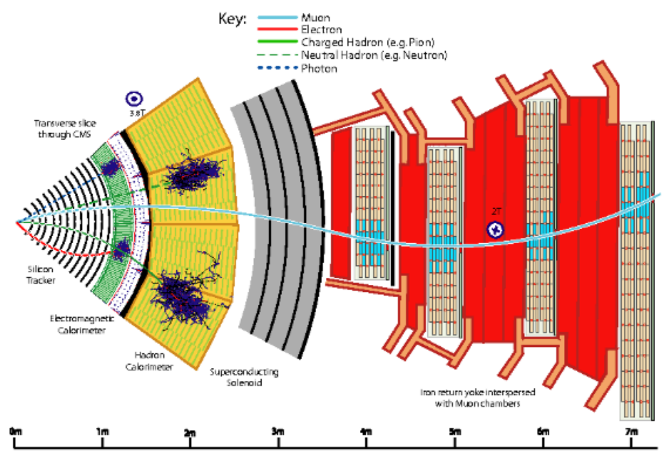
Theory parameters

$z_s \longleftarrow z_p \longleftarrow \theta$



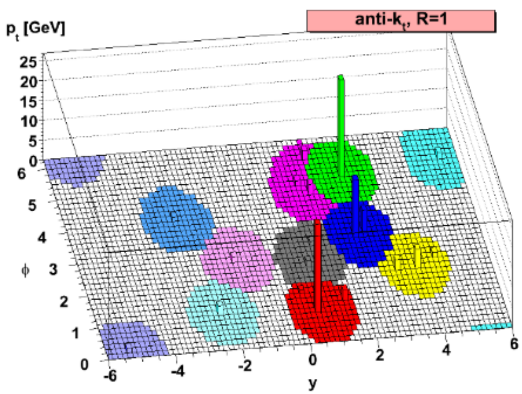
		Latent variables		Parameters of interest
	Detector interactions	Shower splittings	Parton-level momenta	Theory parameters

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



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]

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

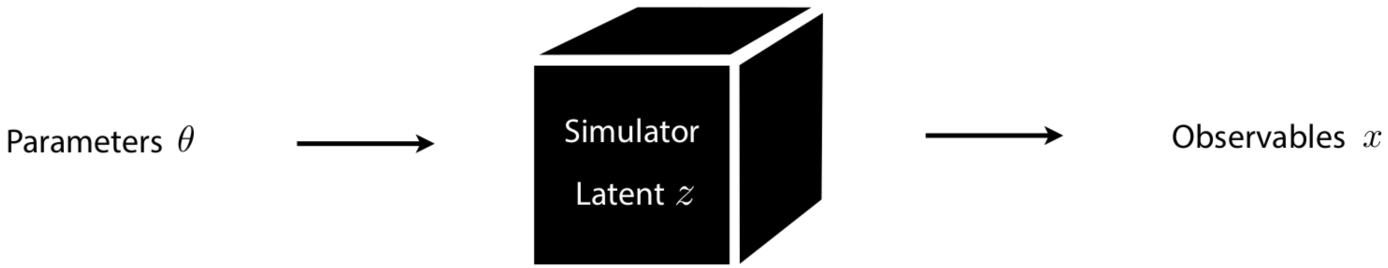
Bayesian inference

Start with

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

Then, estimate the posterior

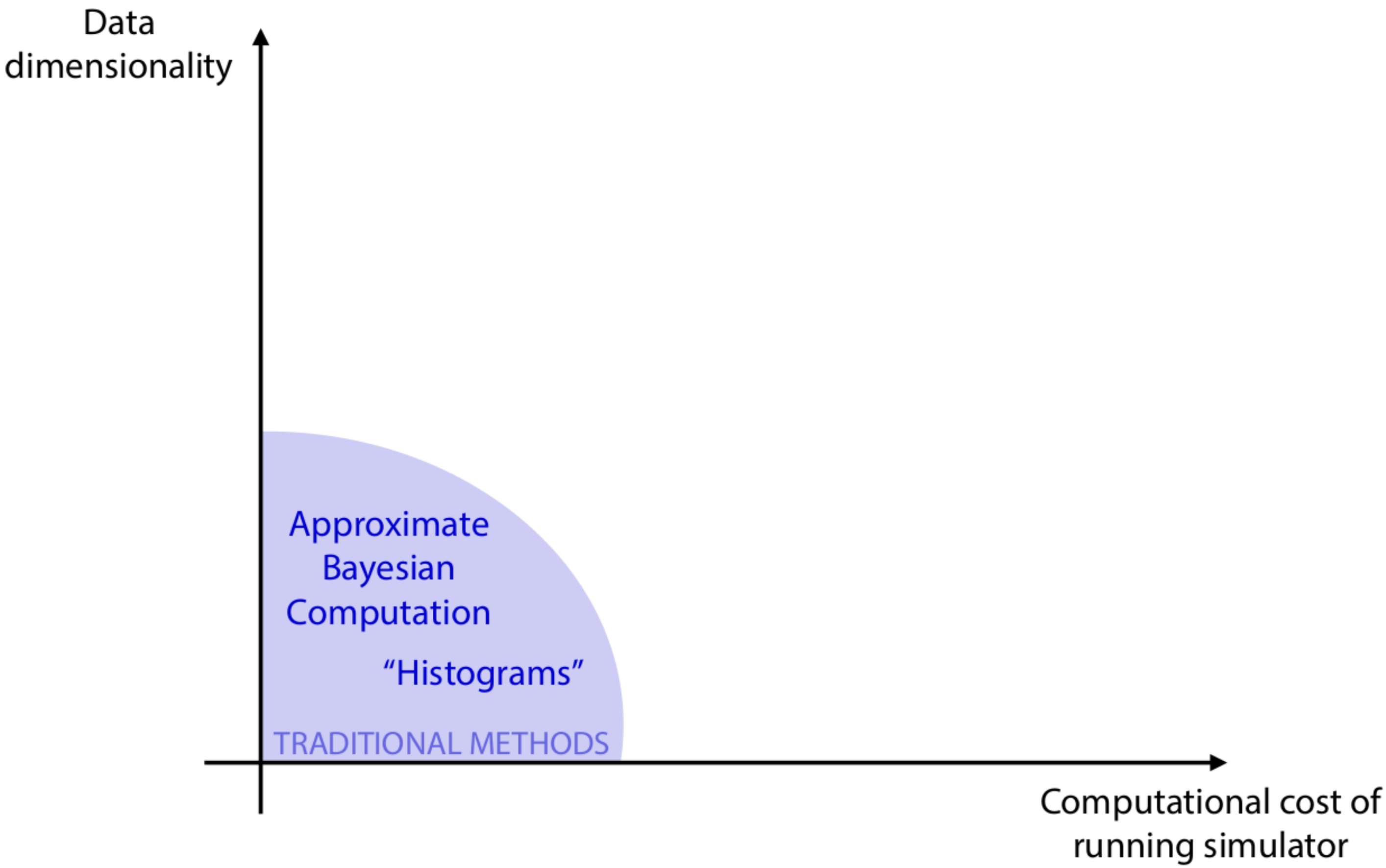
$$p(\theta|x_{\text{obs}}) = \frac{p(x_{\text{obs}}|\theta)p(\theta)}{p(x_{\text{obs}})}.$$



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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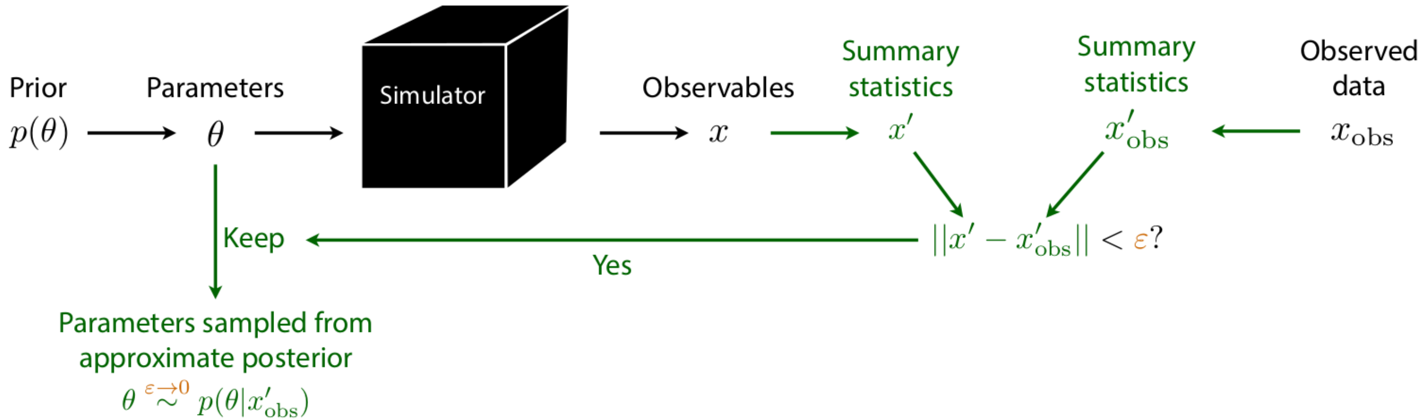
Credits: Cranmer, Brehmer and Louppe, 2020.

Approximate Bayesian Computation (ABC)



Issues:

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

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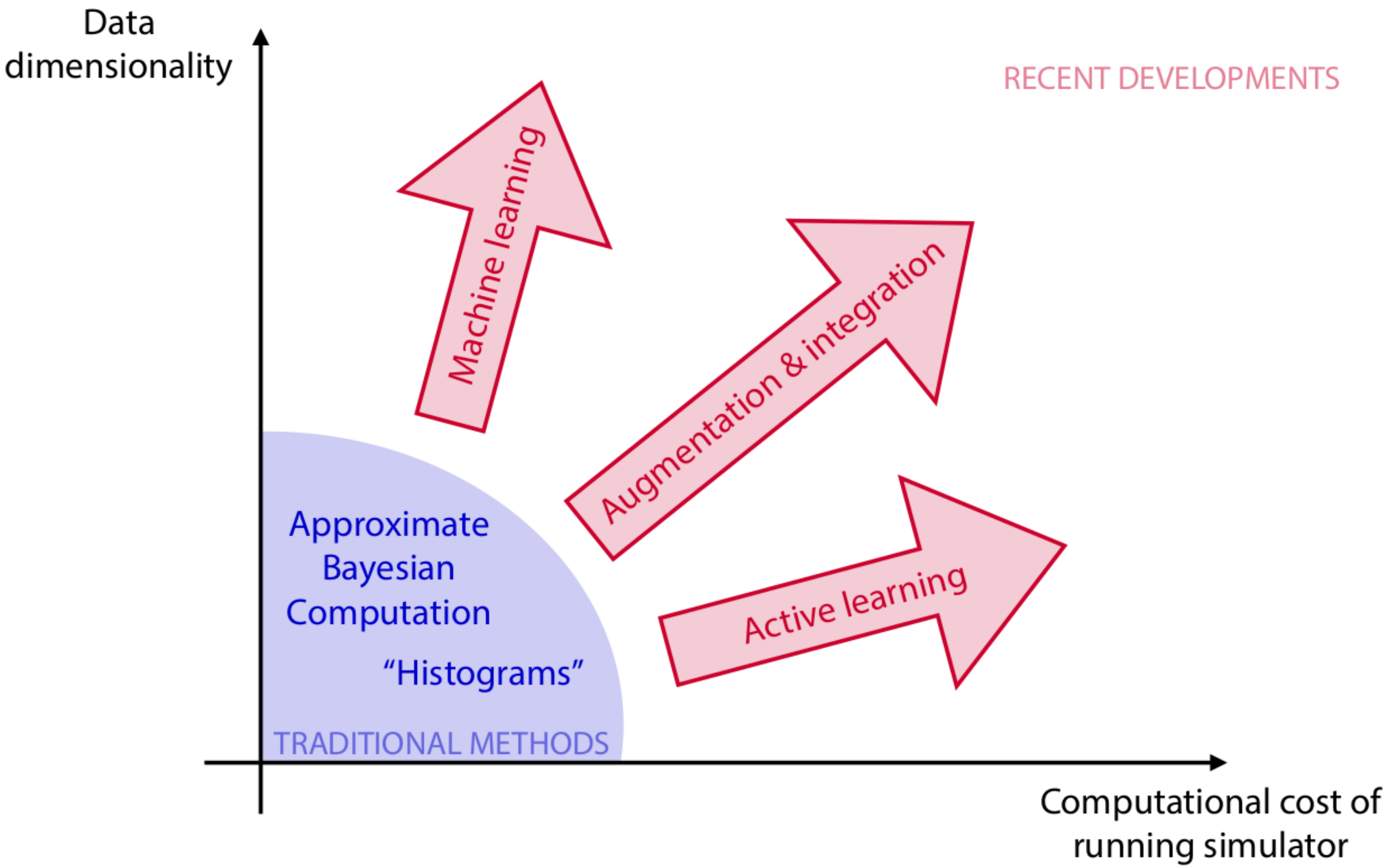
Credits: Johann Brehmer.



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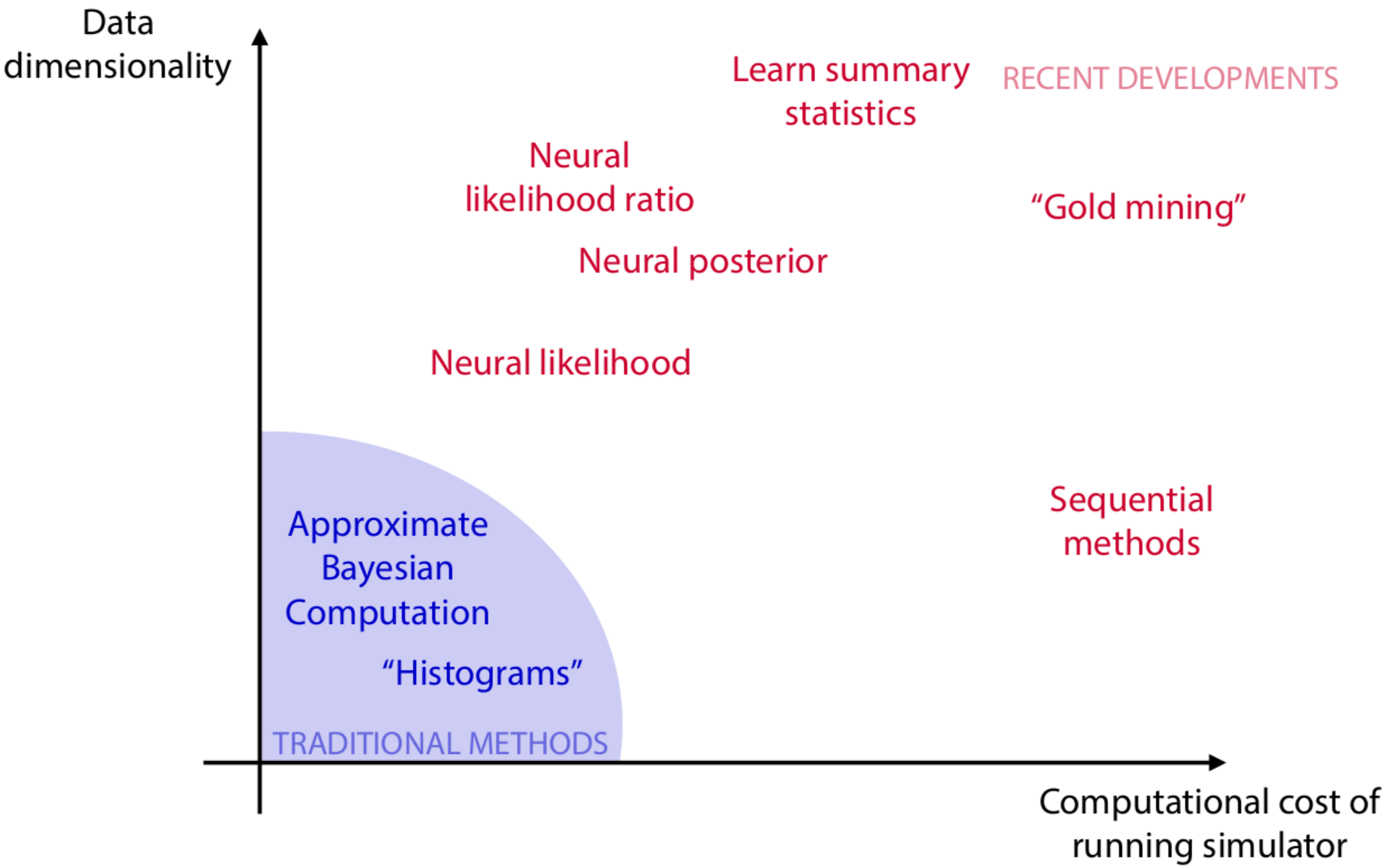

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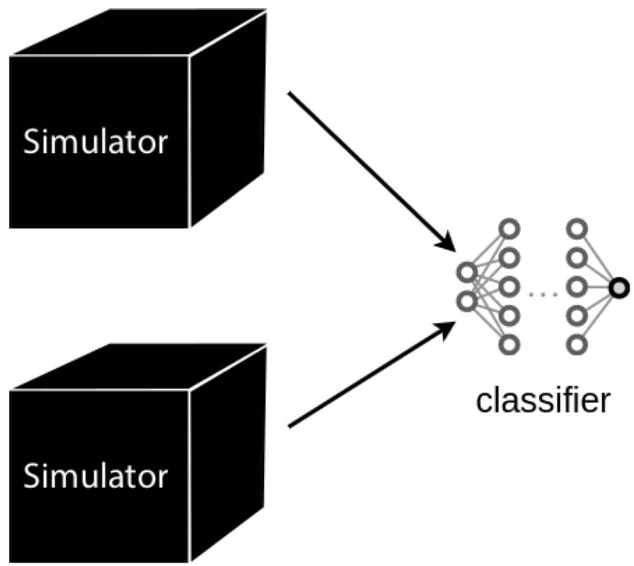
Credits: Cranmer, Brehmer and Louppe, 2020.

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:

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



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

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

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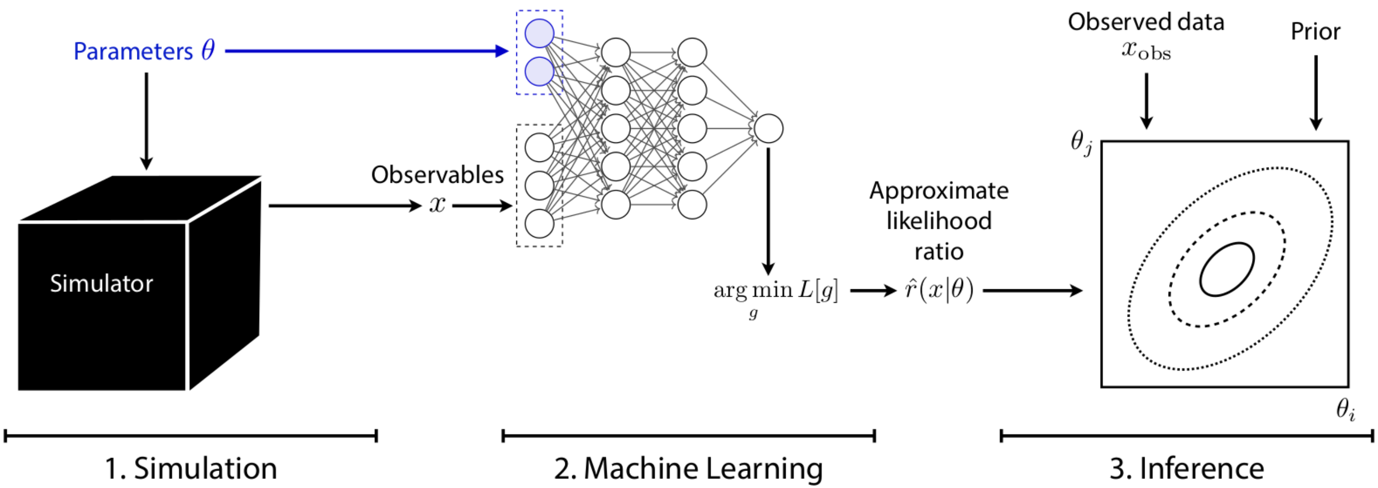
Credits: Cranmer et al, 2015; Hermans et al, 2020.

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,

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



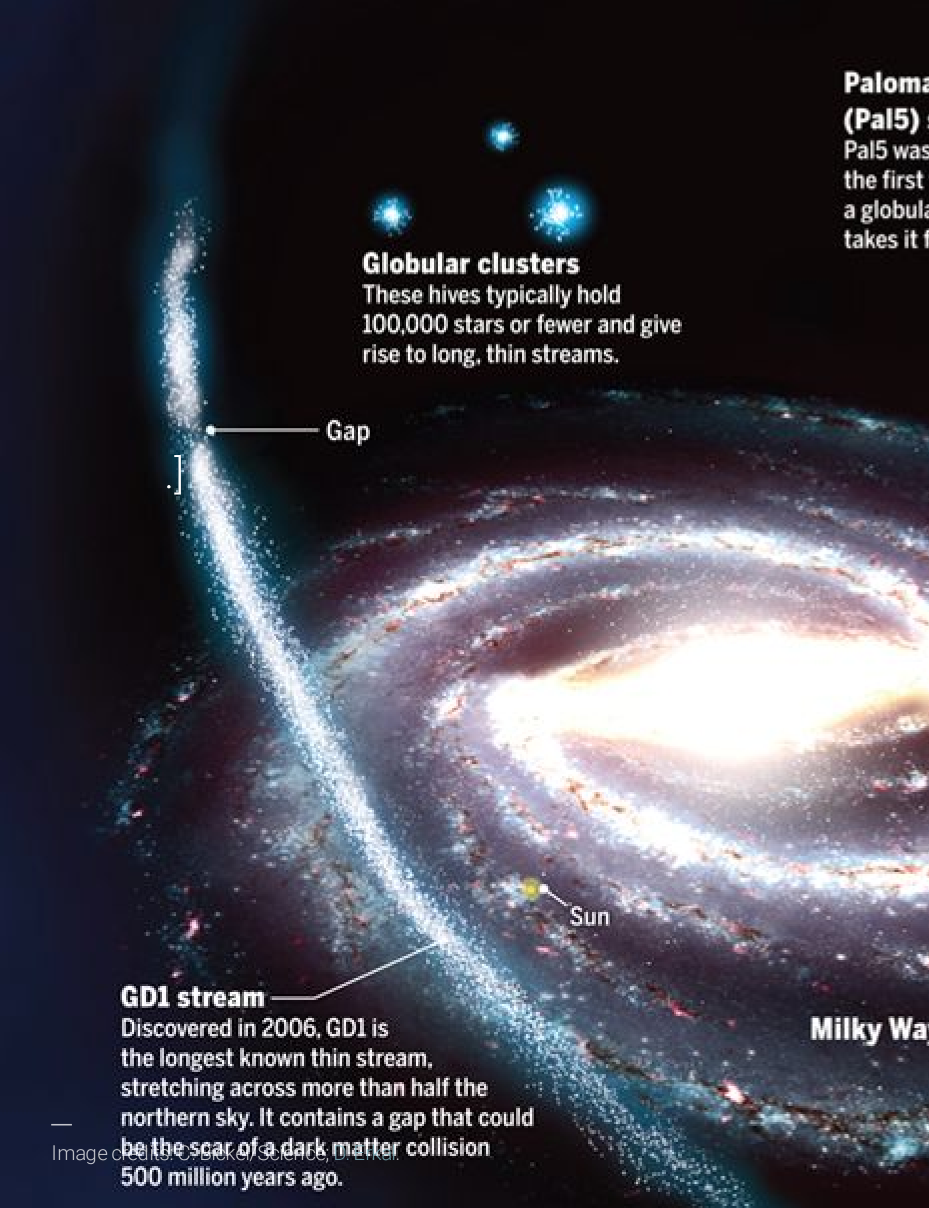
Run simulator and save data

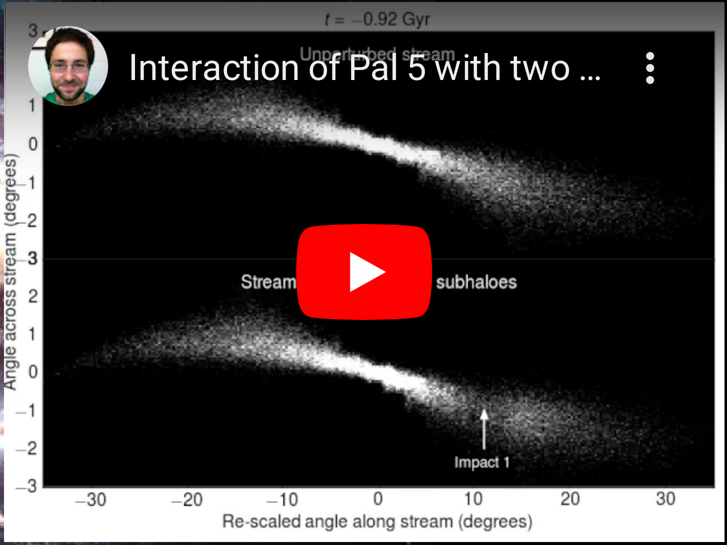
Train NN classifier, interpret as likelihood ratio estimator

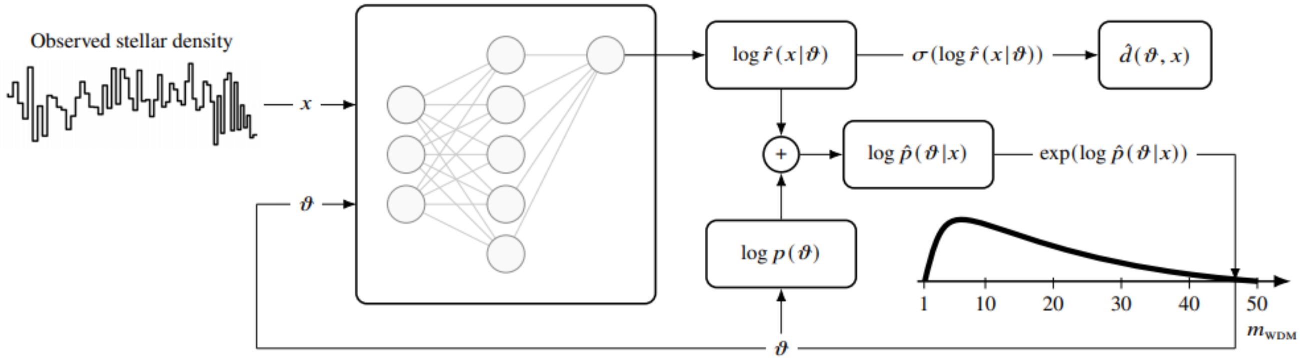
Amortized: cheap to repeat for new data

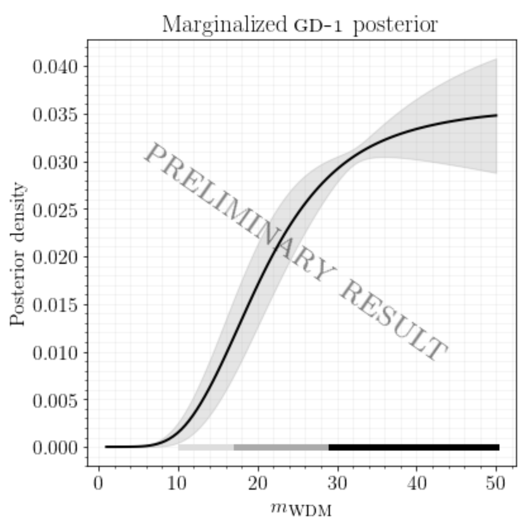
$$p(\theta|x) \approx \hat{r}\,(x|\theta)p(\theta)$$

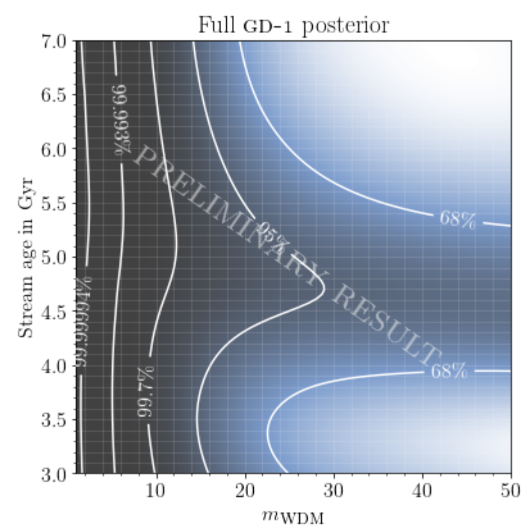
Constraining dark matter with stellar streams











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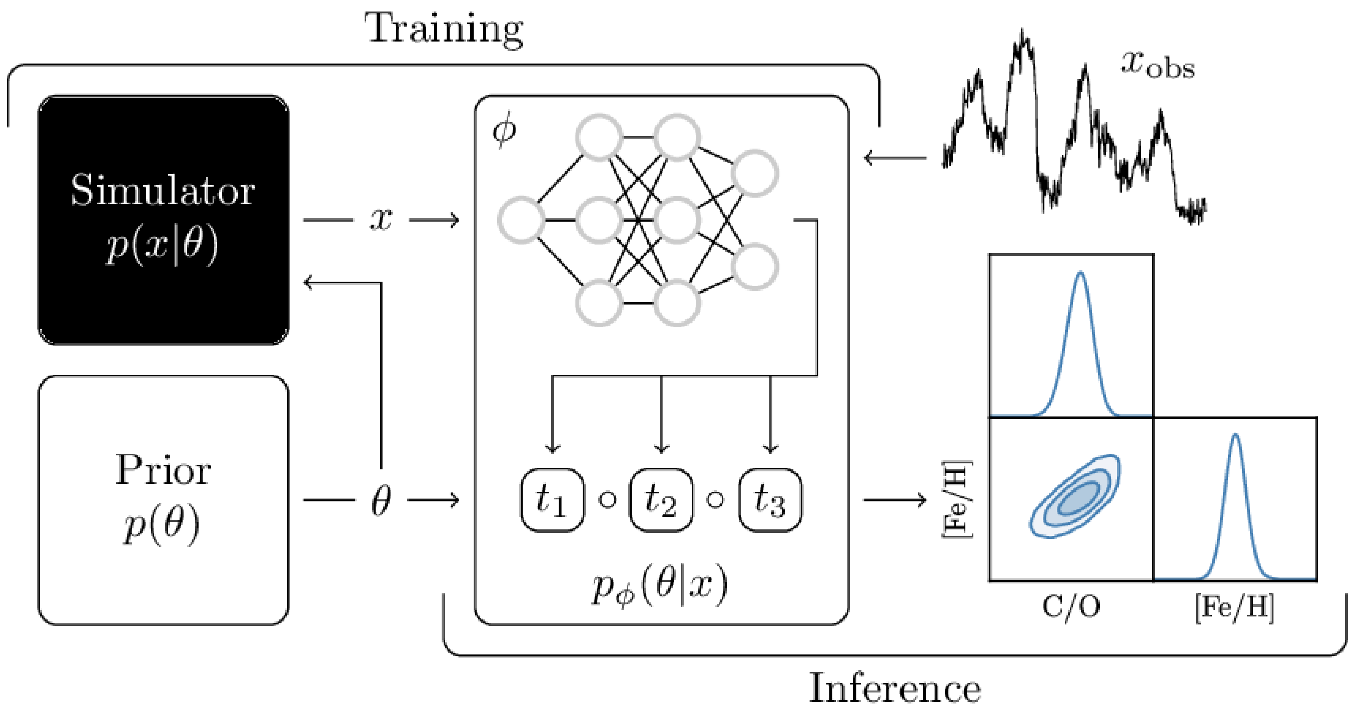
Credits: Hermans et al, 2021.

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

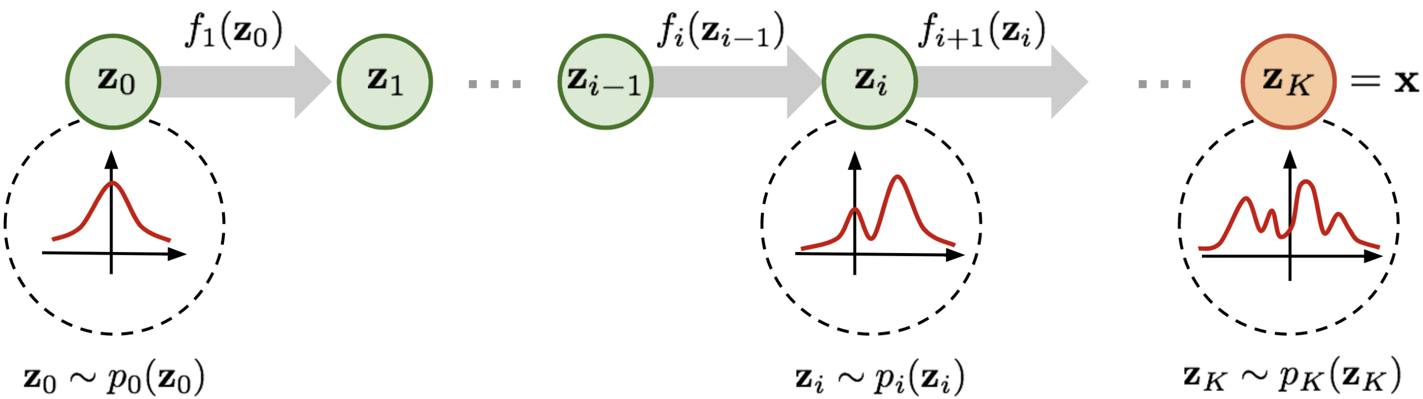
Neural Posterior Estimation



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

Normalizing flows

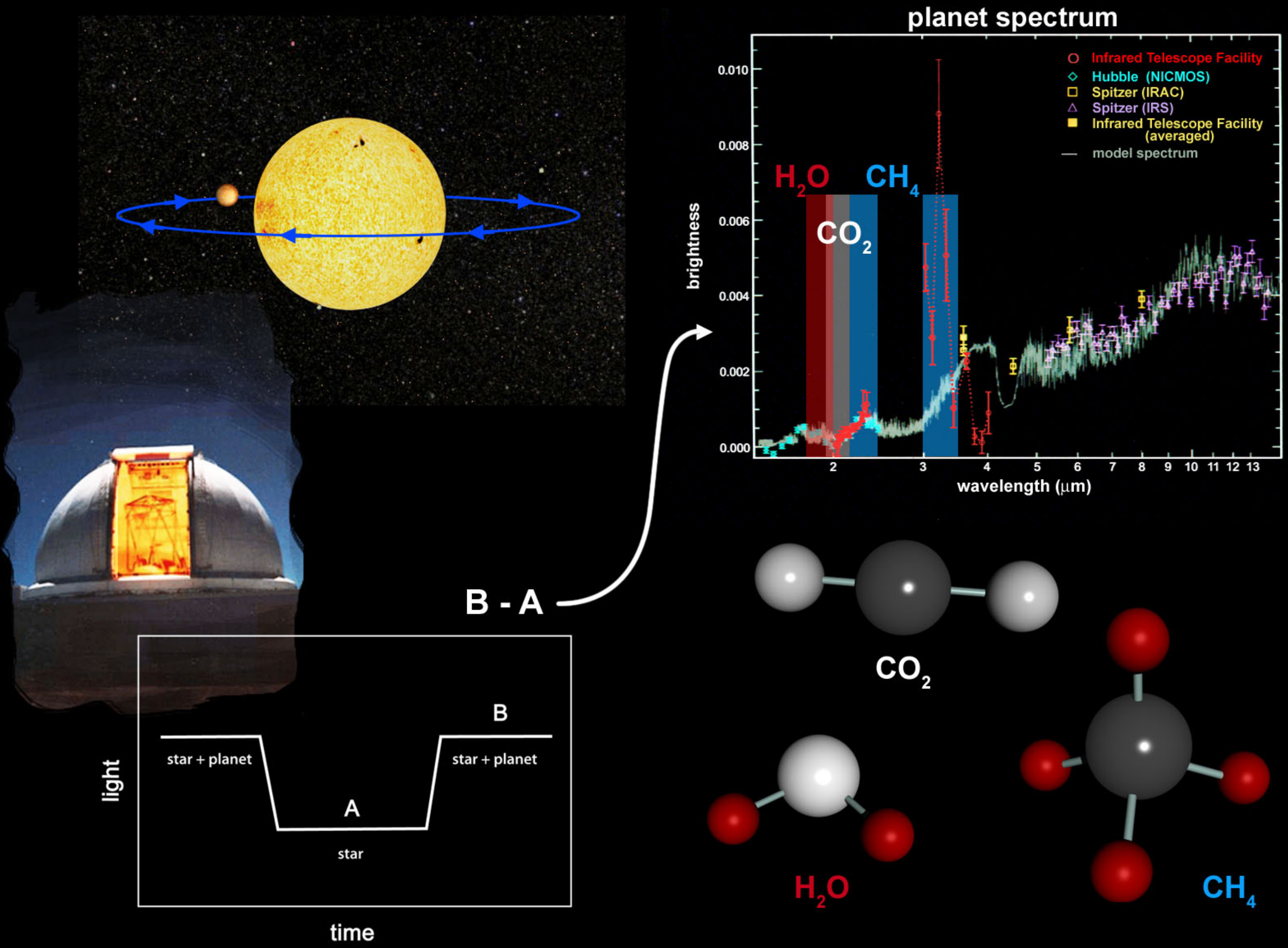
A normalizing flow is a sequence of invertible transformations f_k that map a simple distribution p_0 to a more complex distribution p_K:



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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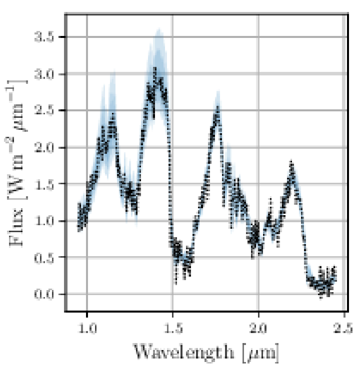
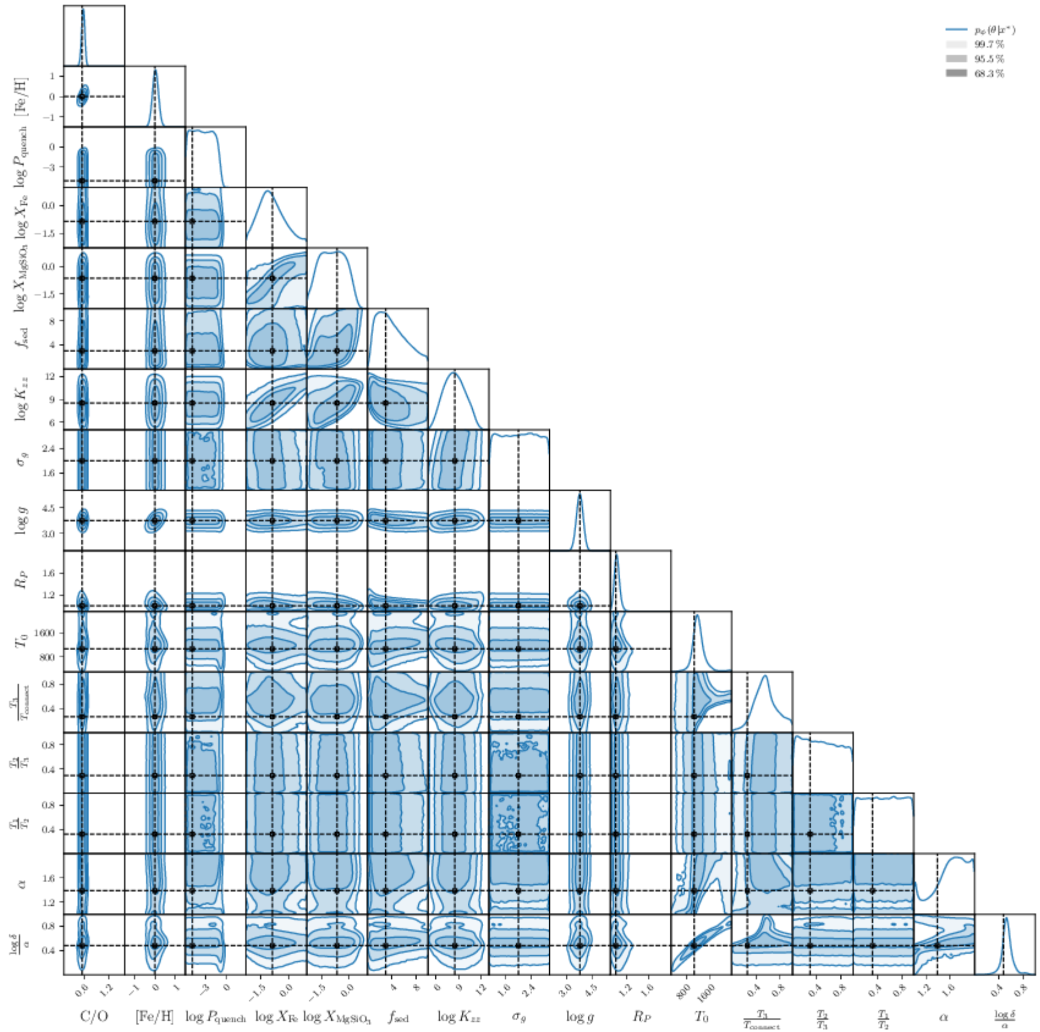
Credits: NSA/JPL-Caltech, 2010.





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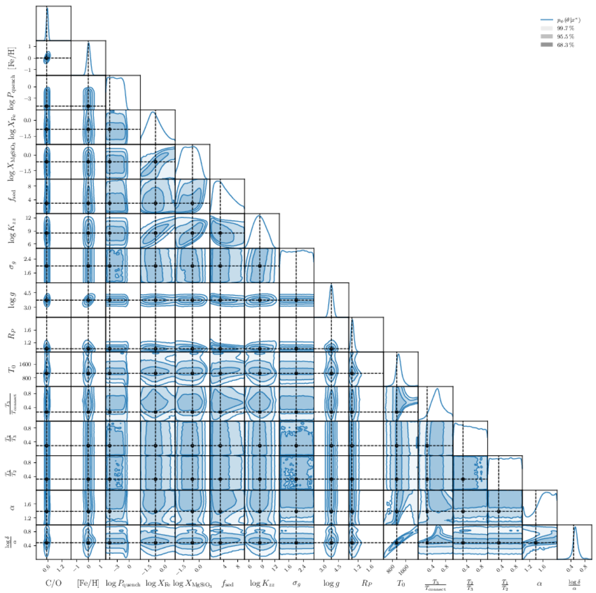
Credits: Vasist et al, 2023.

Diagnostics

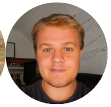
$$\hat{p}(\theta|x) = \mathrm{sbi}(p(x|\theta), p(\theta), x)$$

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



How do we know this is good enough?

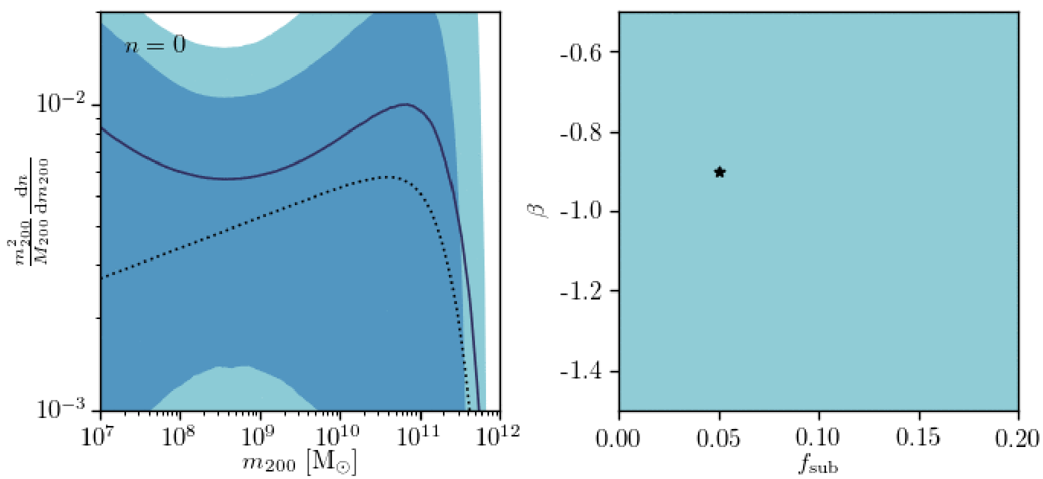


Mode convergence

The maximum a posteriori estimate converges towards the nominal value θ^* 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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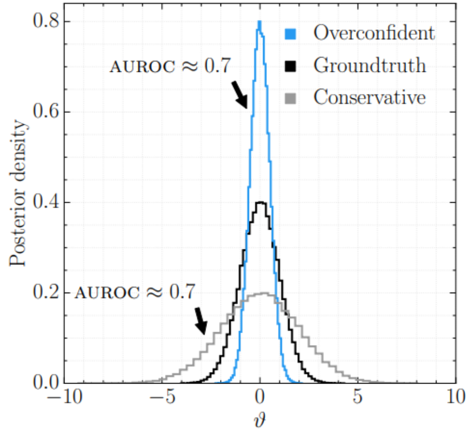
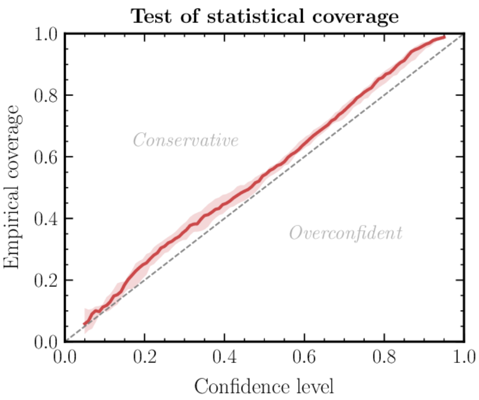
Credits: Brehmer et al, 2019.

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 θ 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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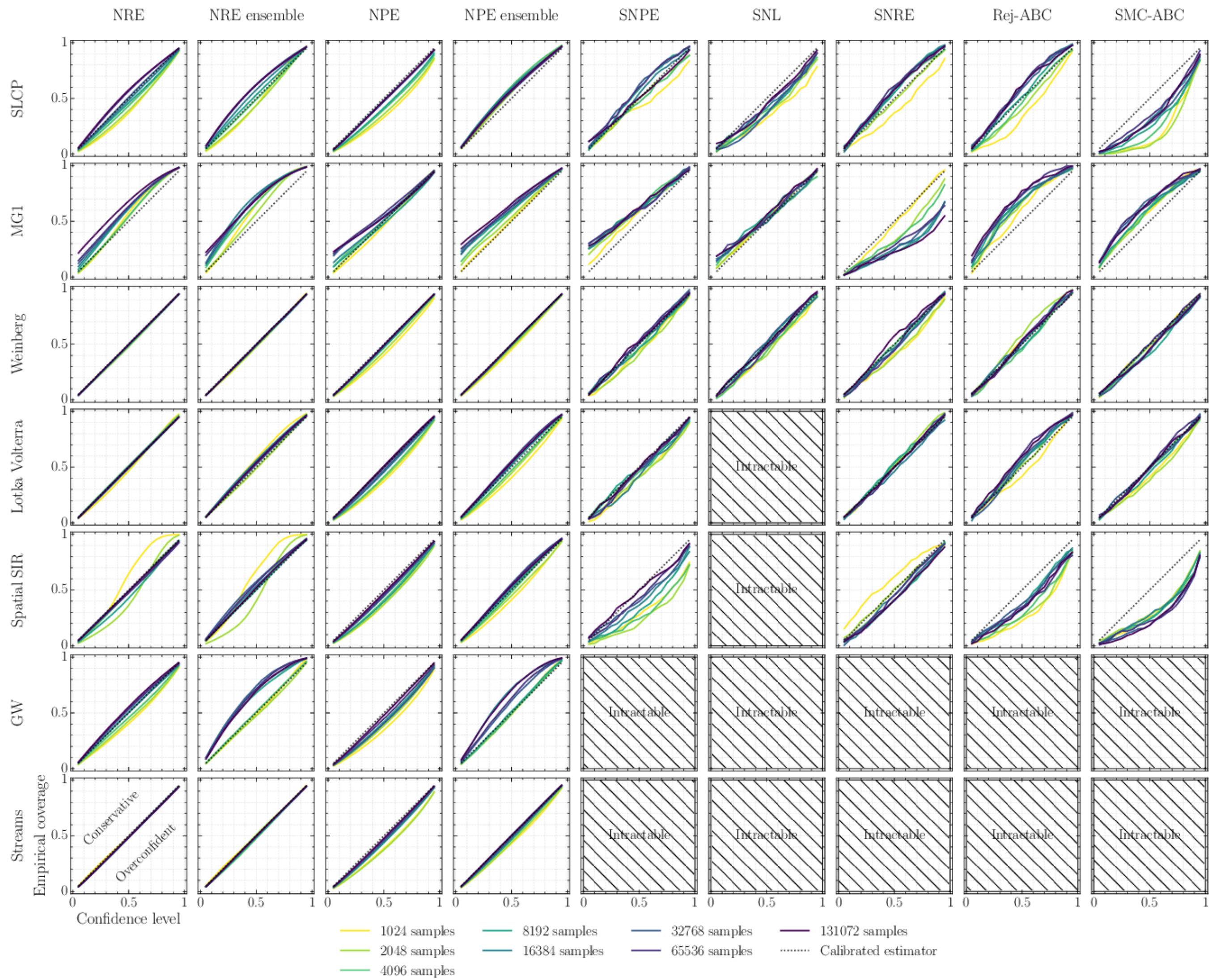
Credits: Hermans et al, 2021; Siddharth Mishra-Sharma, 2021.



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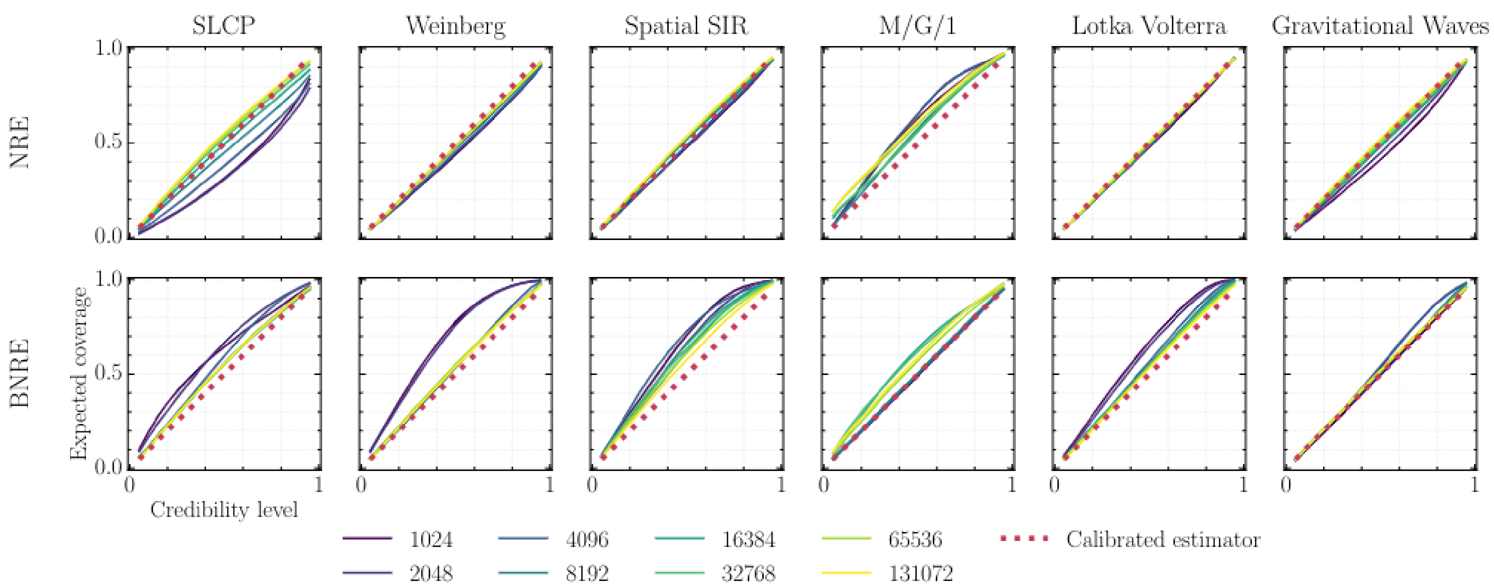
Credits: Hermans et al, 2021.

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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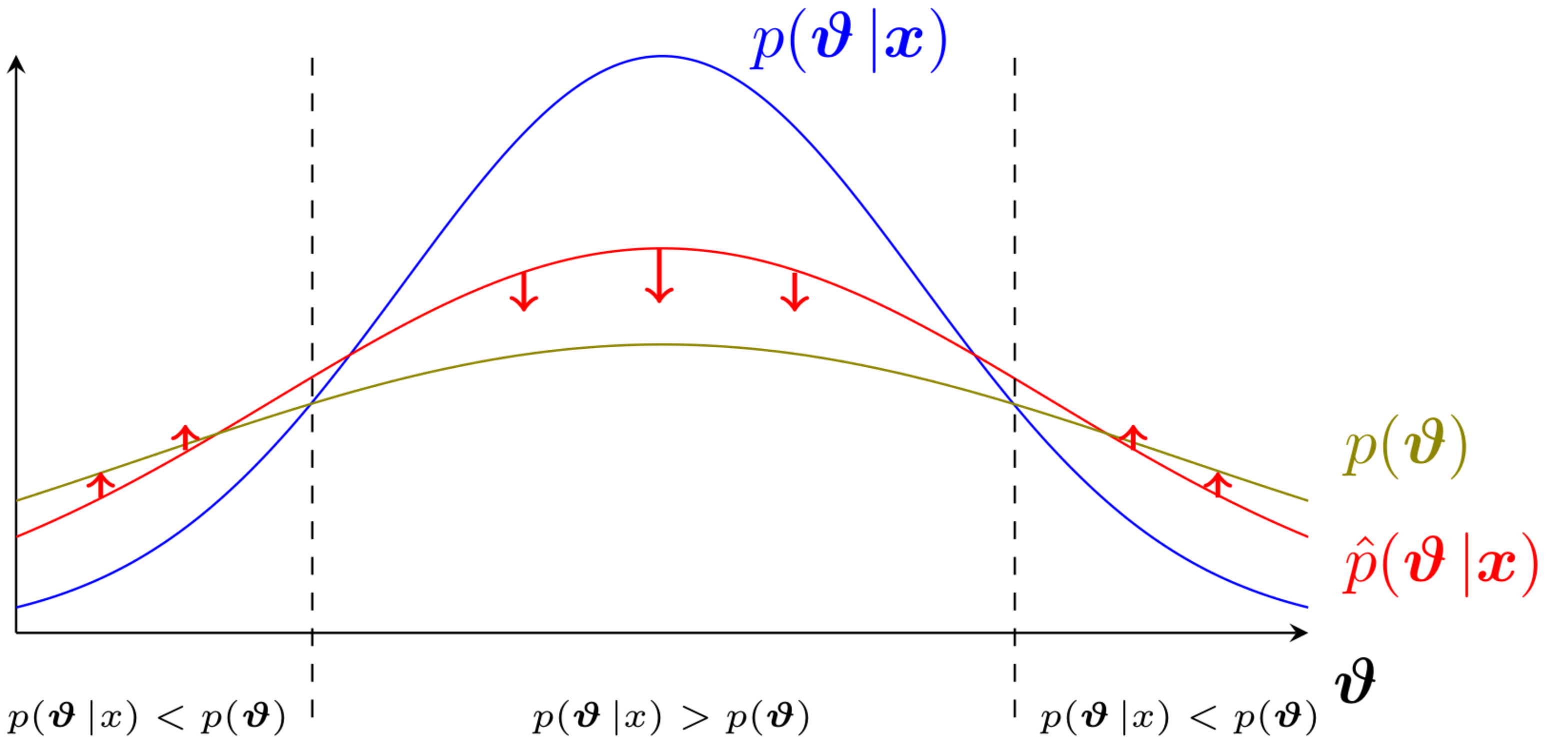
Credits: Delaunoy et al, 2022.



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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.