An introduction to simulation-based inference

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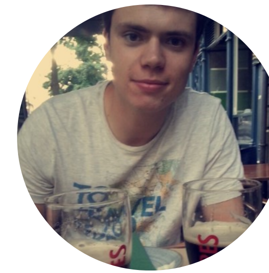
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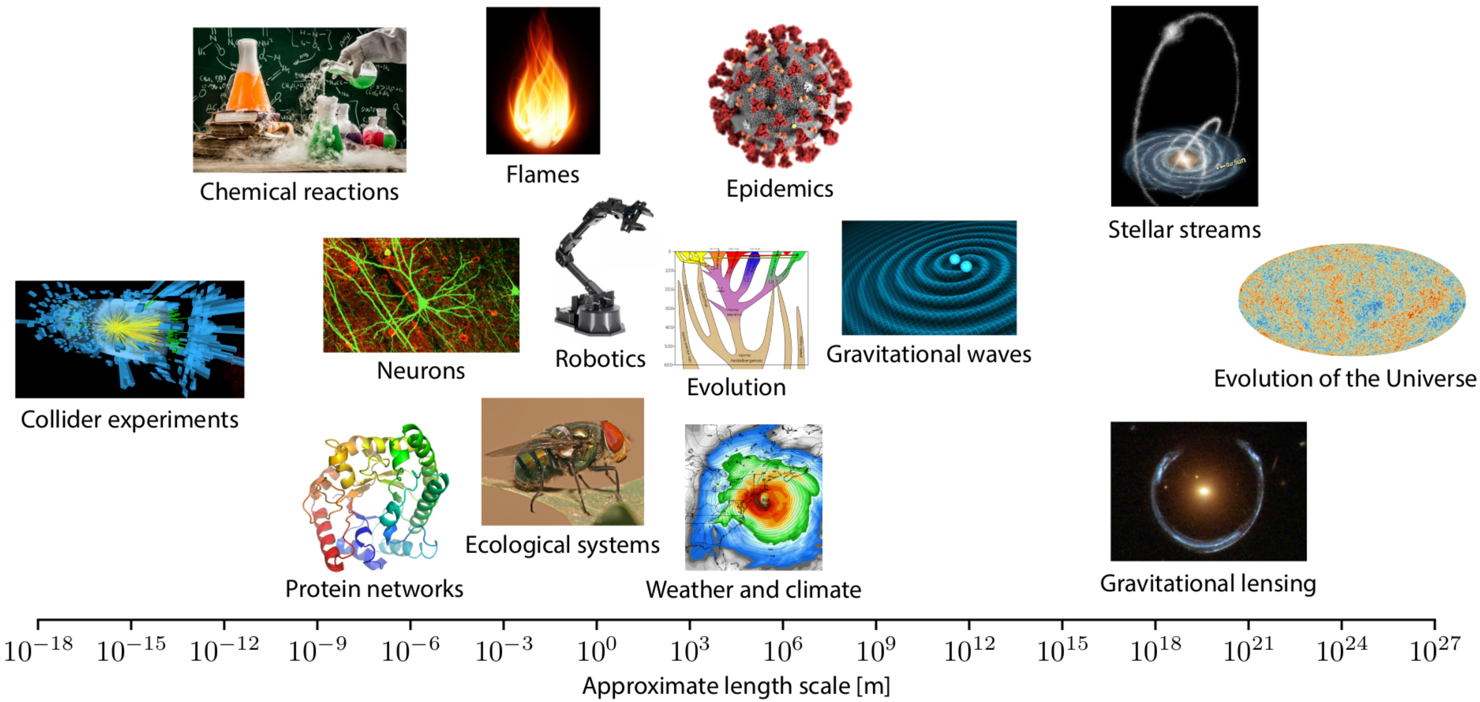
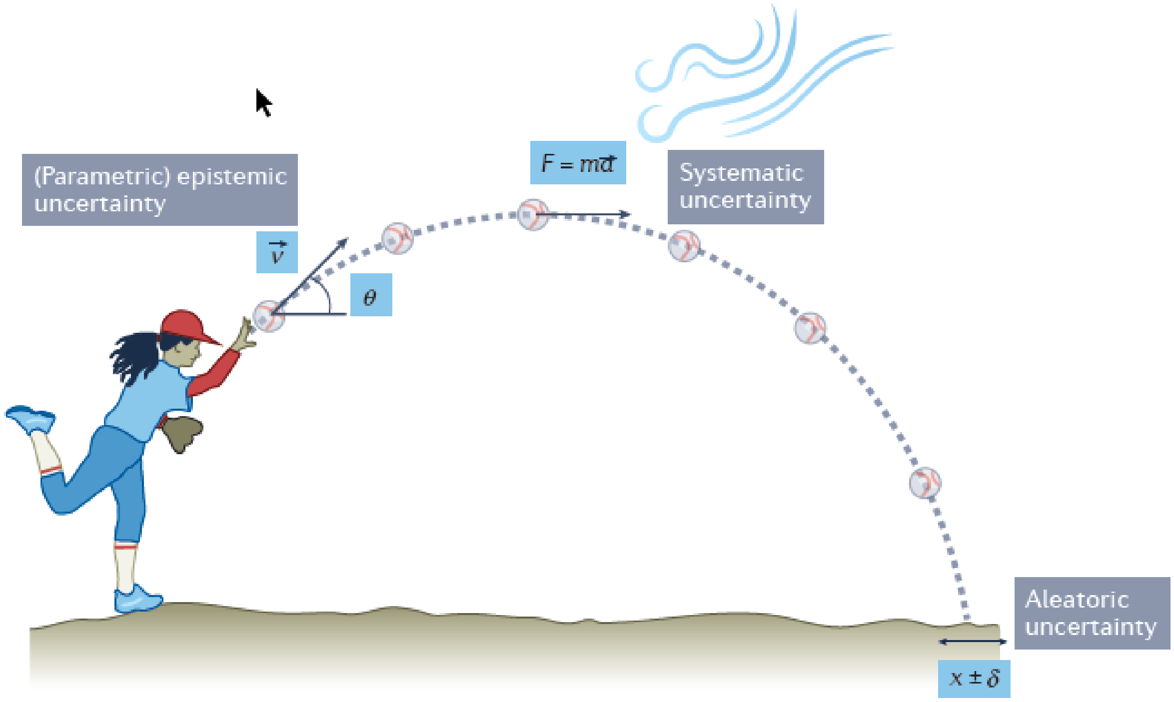

Chemical reactions
Flames
Epidemics
Stellar streams
Neurons
Robotics
Evolution
Gravitational waves
Evolution of the Universe
Collider experiments
Protein networks
Ecological systems
Weather and climate
Gravitational lensing
10^{-18} 10^{-15} 10^{-12} 10^{-9} 10^{-6} 10^{-3} 10^{0} 10^{3} 10^{6} 10^{9} 10^{12} 10^{15} 10^{18} 10^{21} 10^{24} 10^{27}
Approximate length scale [m]

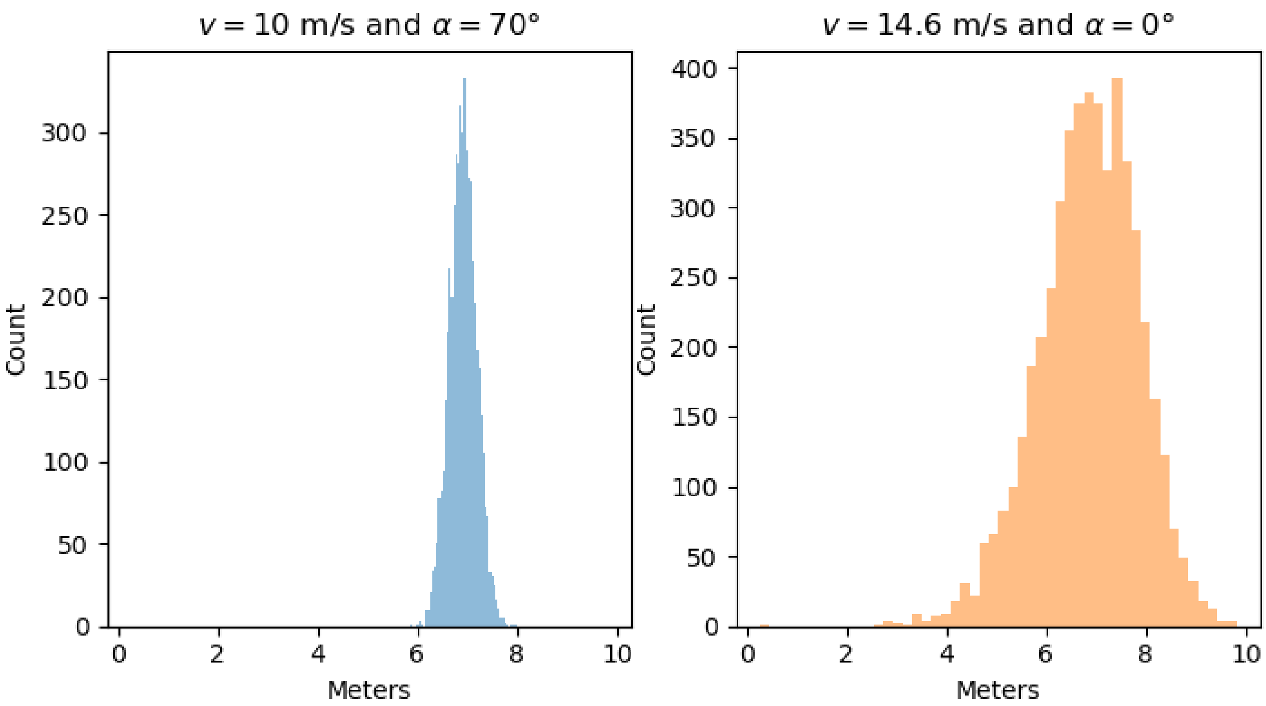

(Parametric) epistemic uncertainty
$\vec{v}$
θ
$F = m\vec{a}$
Systematic uncertainty
Aleatoric uncertainty
$x \pm \delta$

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

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

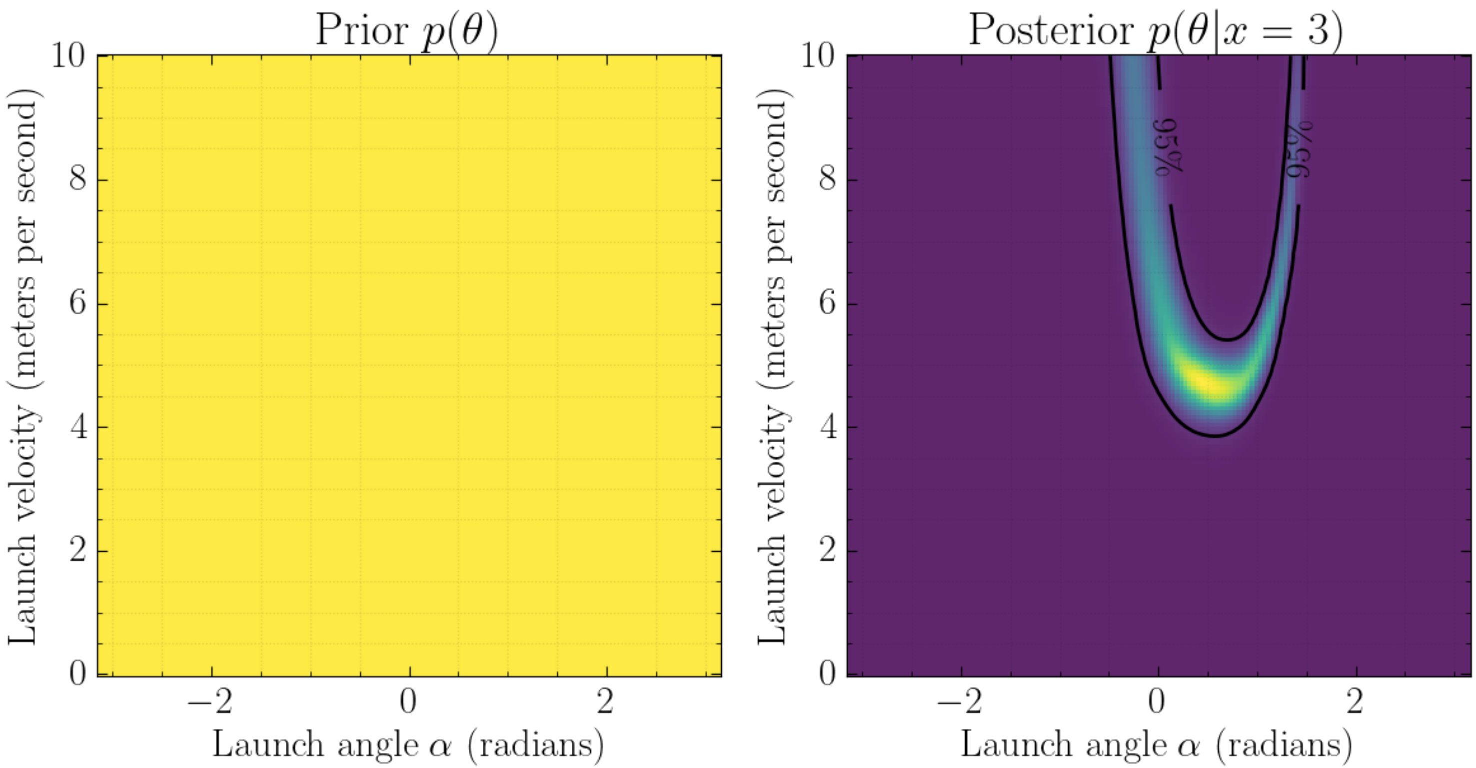
```python
def simulate(v, alpha, dt=0.001):
    v_x = v * np.cos(alpha)  # x velocity m/s
    v_y = v * np.sin(alpha)  # y velocity m/s
    y = 1.1 + 0.3 * random.normal()
    x = 0.0

    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()
```

The computer simulator defines the likelihood function $p(x|\theta)$ implicitly.



What parameter values θ are the most plausible?

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

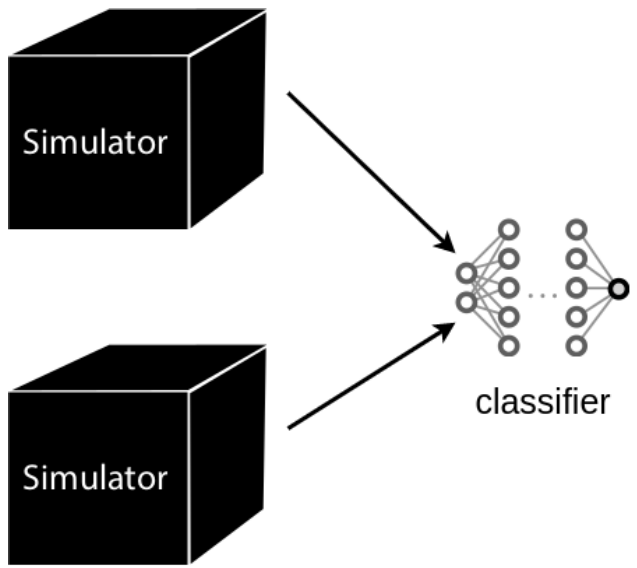

Prior $p(\theta)$
Posterior $p(\theta|x = 3)$
Launch velocity (meters per second)
Launch angle α (radians)
10
8
6
4
2
0
−2
0
2
95%
95%

Neural ratio estimation (NRE)

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:

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

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



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

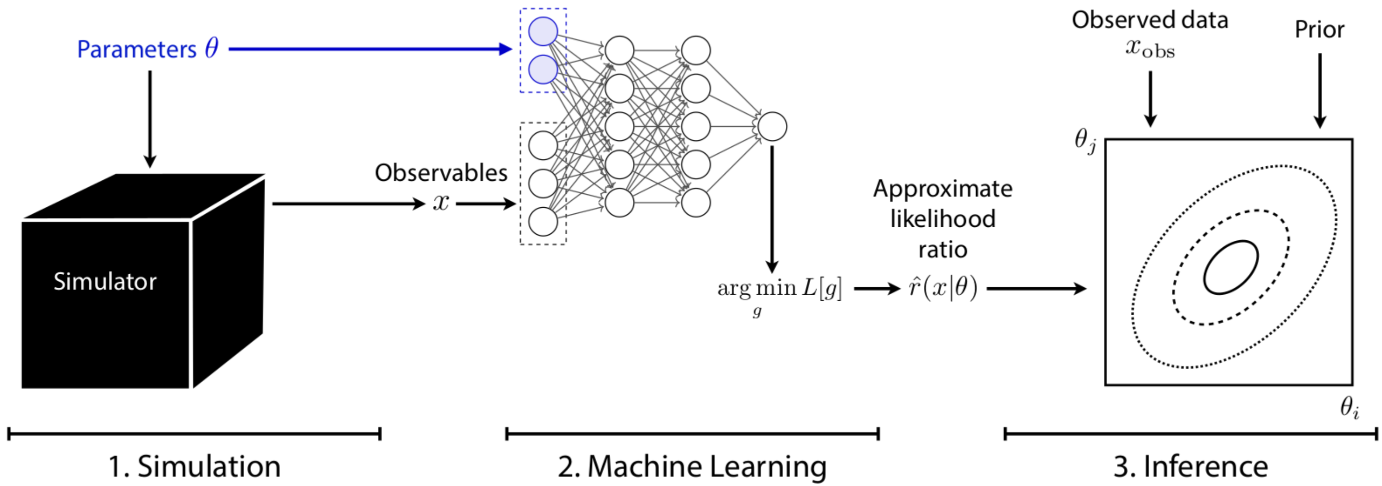
—
Credits: Cranmer et al, 2015; Hermans et al, 2020.

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

$$p(\theta|x) \approx r(x|\theta)p(\theta)$$

Constraining dark matter with stellar streams (Bayesian)

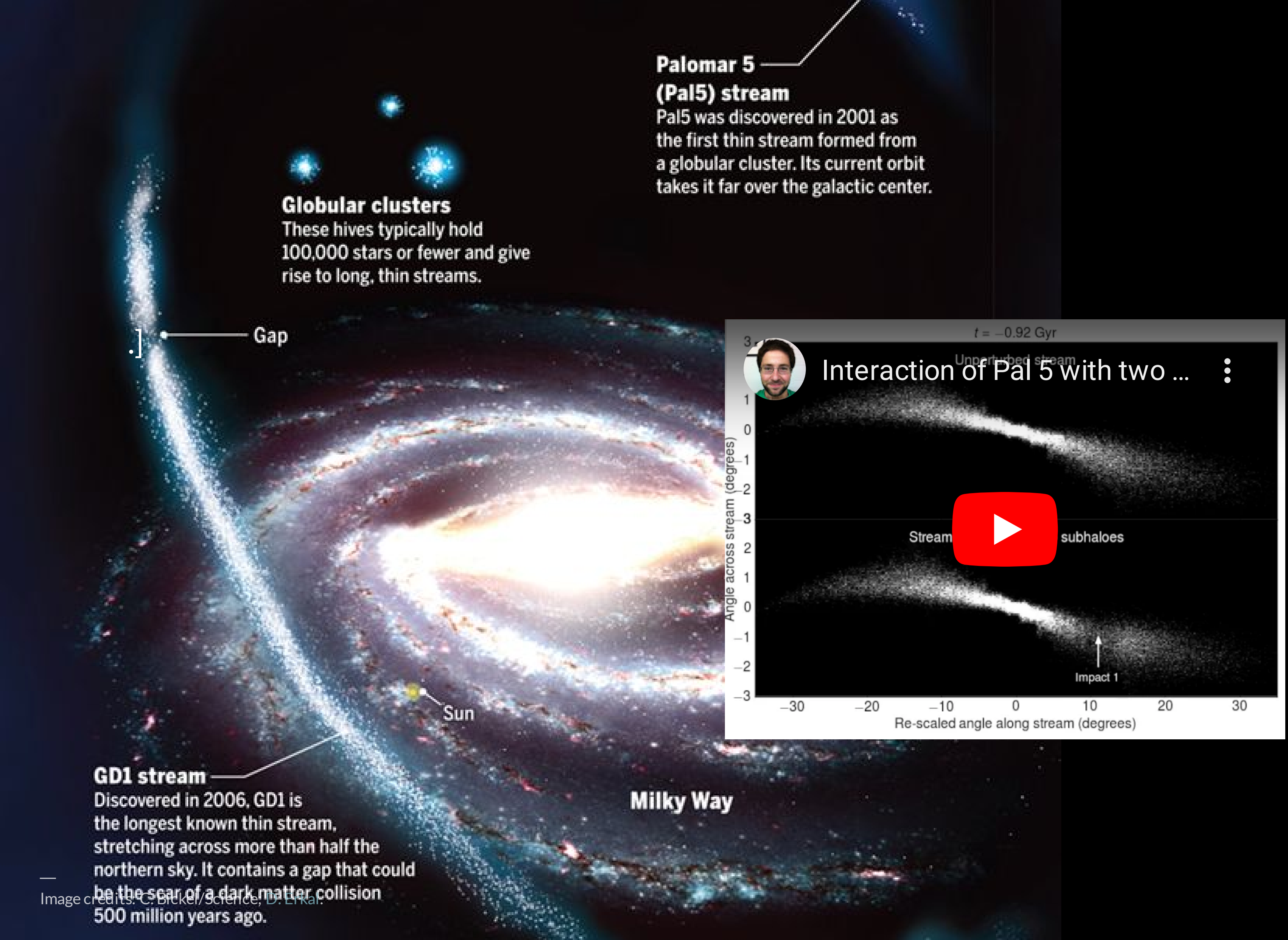
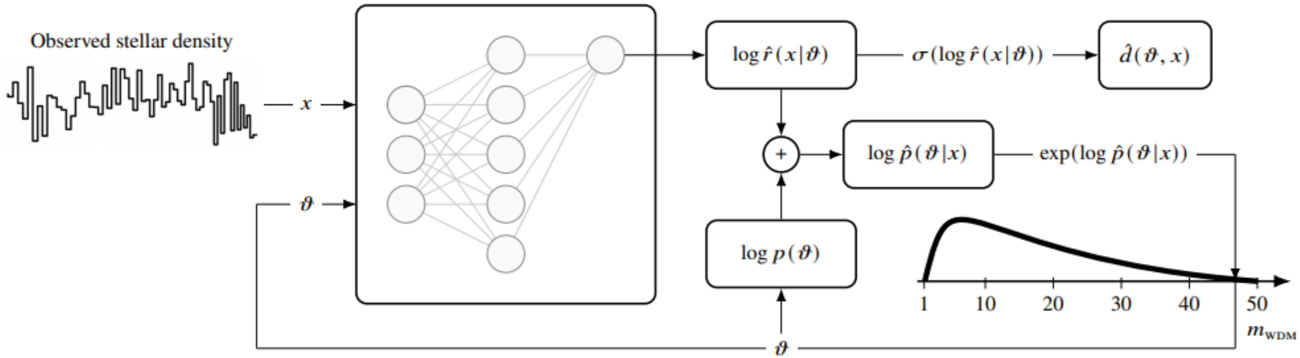
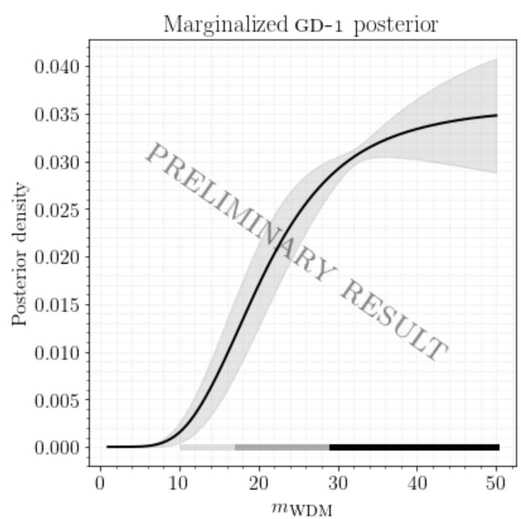
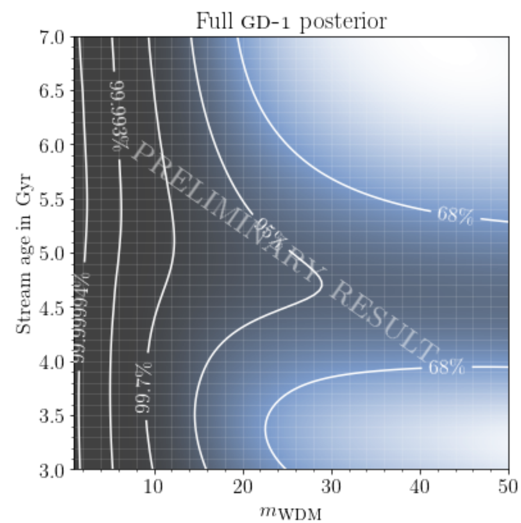


Image credits: C. Bickel/Science, D. Erkal.







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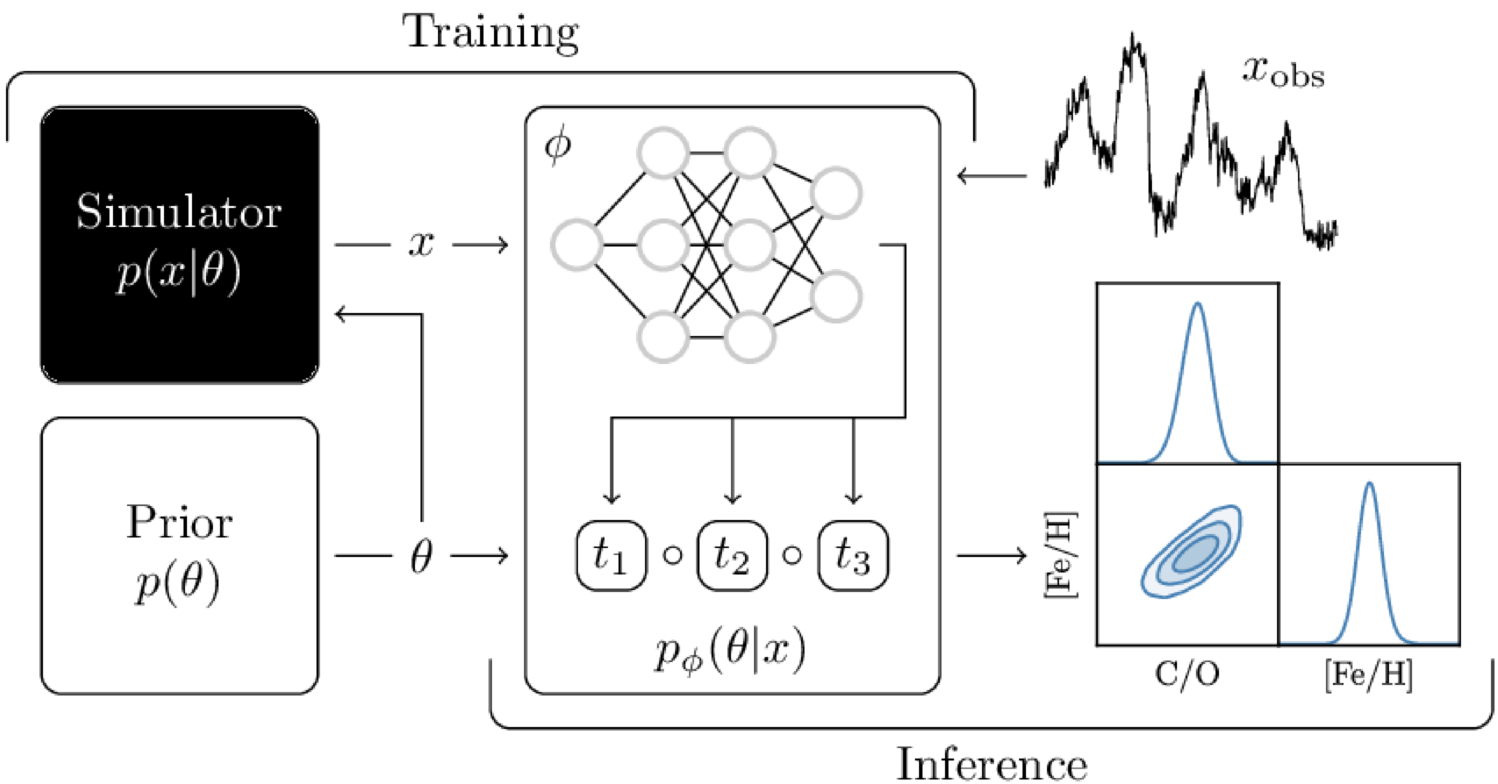
Credits: Hermans et al, 2021.

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

Neural Posterior Estimation (NPE)

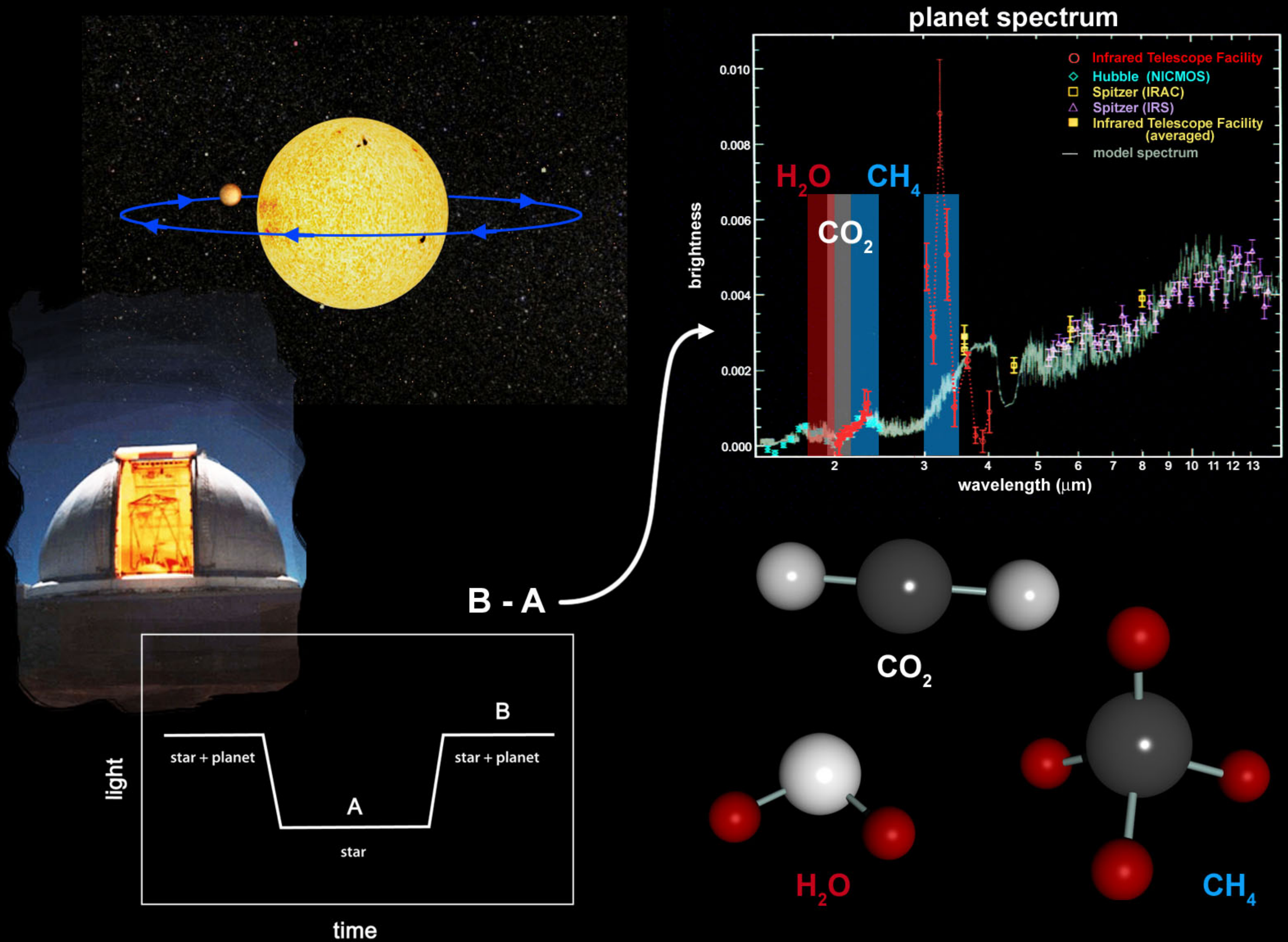


Use variational inference to directly estimate the posterior, by solving

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

where q_ϕ is a neural density estimator, such as a normalizing flow.

Exoplanet atmosphere characterization (Bayesian)



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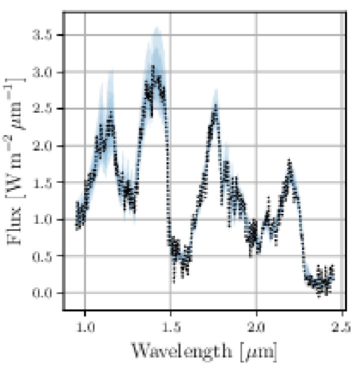
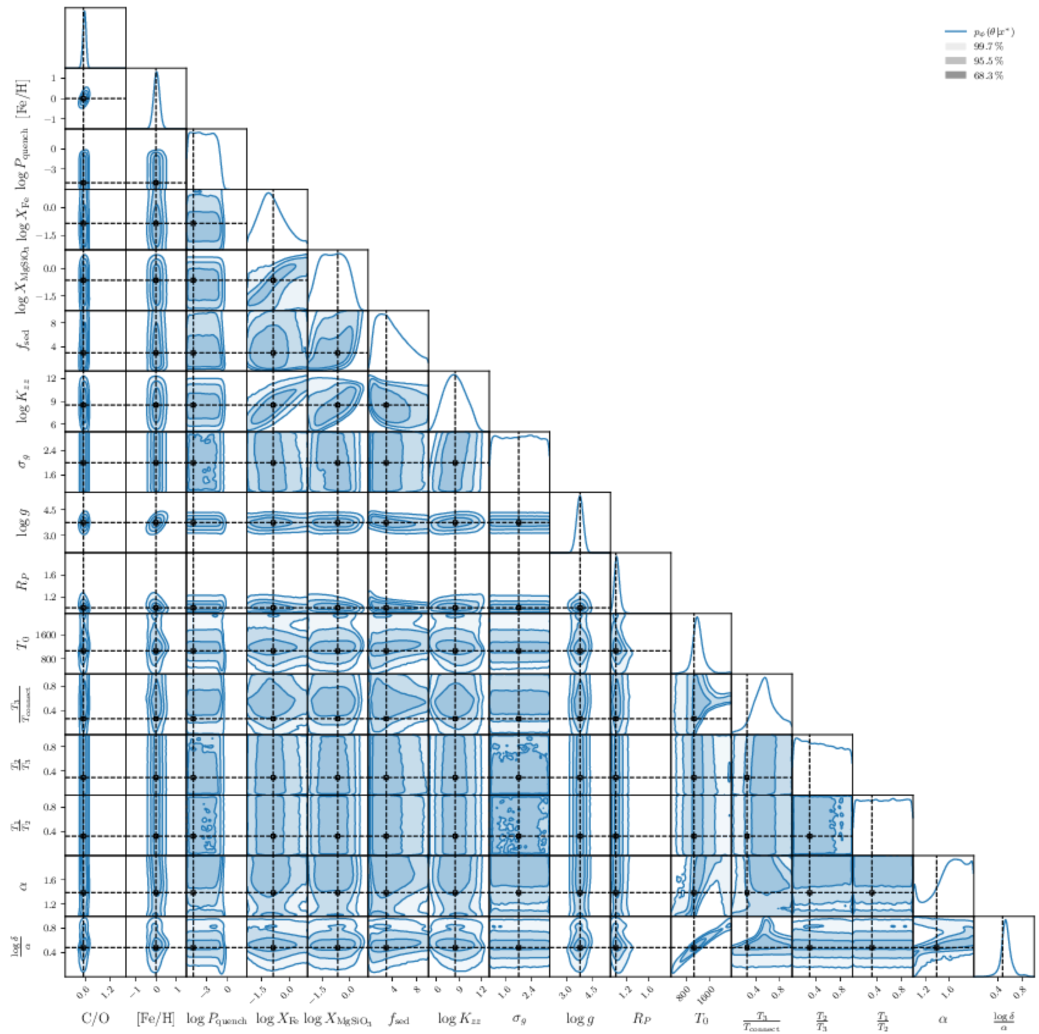
Credits: NSA/JPL-Caltech, 2010.

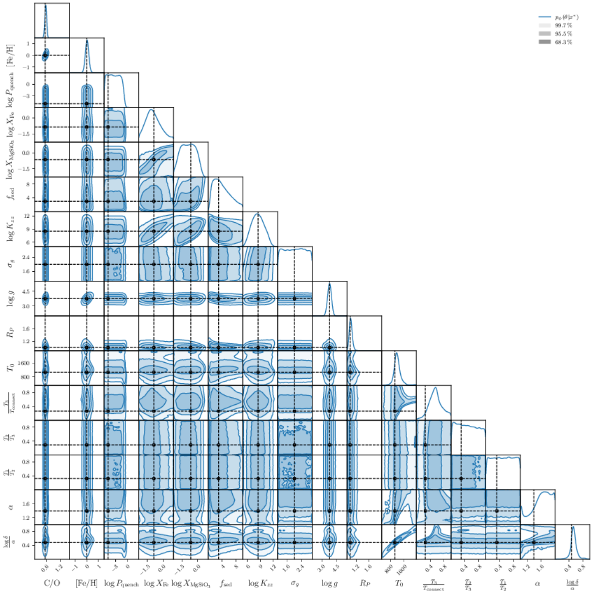

Flux [W m⁻² μm⁻¹]
Wavelength [μm]


p_φ(θ|x*)
99.7 %
95.5 %
68.3 %
C/O
[Fe/H]
log P_quench
log X_Fe
log X_MgSiO3
f_sed
log K_zz
σ_g
log g
R_P
T_0
T_3/T_connect
T_2/T_3
T_1/T_2
α
log δ/α

Computational faithfulness

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

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

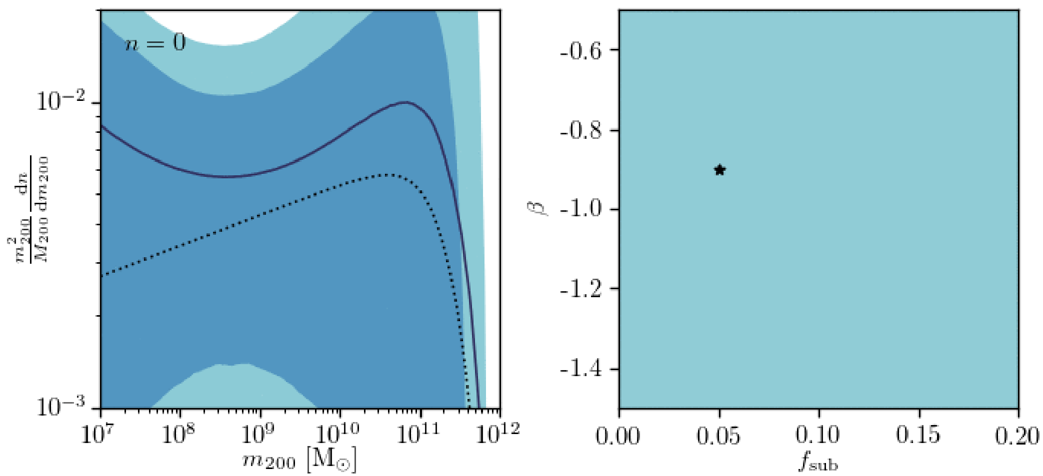


How do we know this is good enough?

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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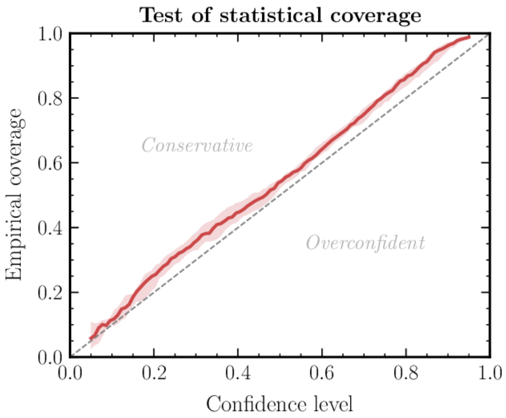
Credits: Brehmer et al, 2019.

A common observation at the root of several other diagnostics is to check for the **self-consistency** of the Bayesian joint distribution,

$$p(\theta) = \int p(\theta')p(x|\theta')p(\theta|x)d\theta'\,dx.$$

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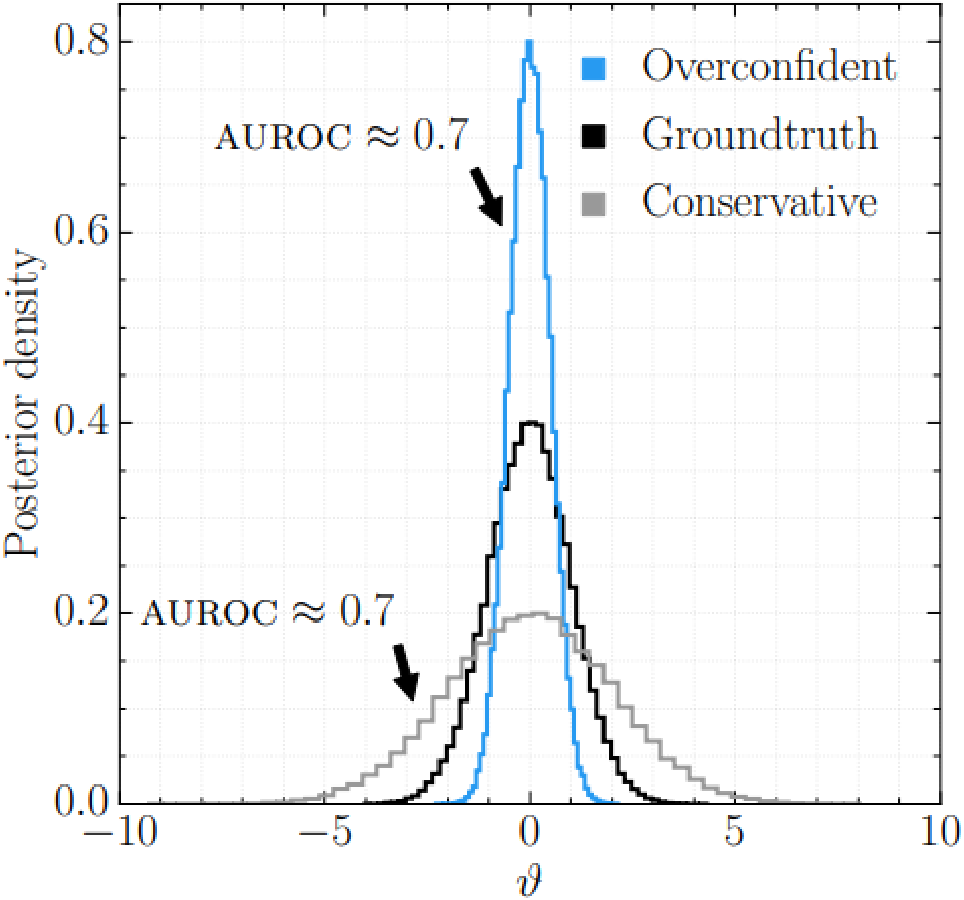
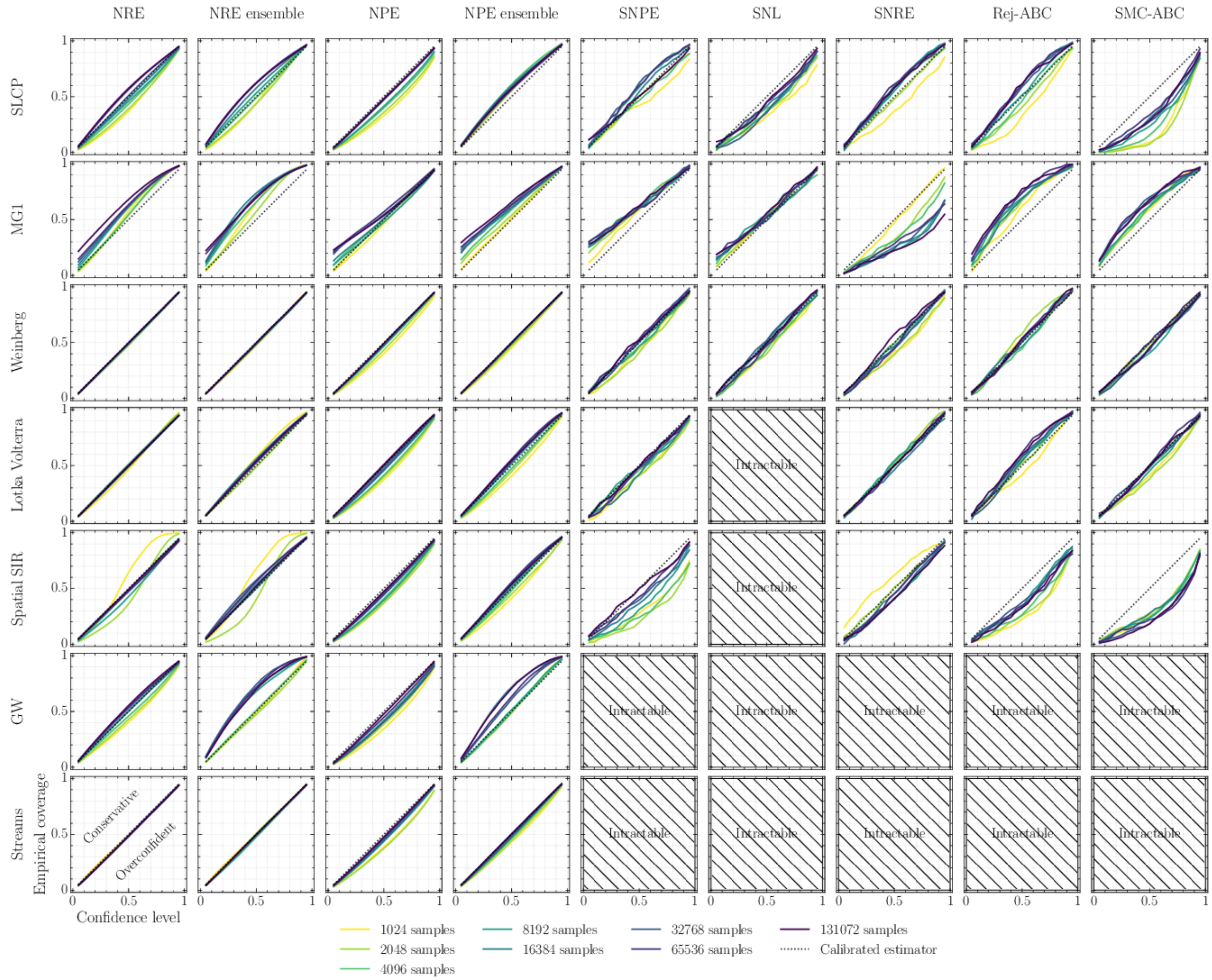
Credits: Hermans et al, 2021; Siddharth Mishra-Sharma, 2021.



Overconfident
Groundtruth
Conservative
AUROC ≈ 0.7
AUROC ≈ 0.7
Posterior density
0.0
0.2
0.4
0.6
0.8
−10
−5
0
5
10
ϑ



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Credits: Hermans et al, 2021.

What if diagnostics fail?

Summary

Simulation-based inference is a major evolution in the statistical capabilities for science, enabled by advances in machine learning.

Need to reliably and efficiently evaluate the quality of the posterior approximations.

The end.