# Simulation Based Inference

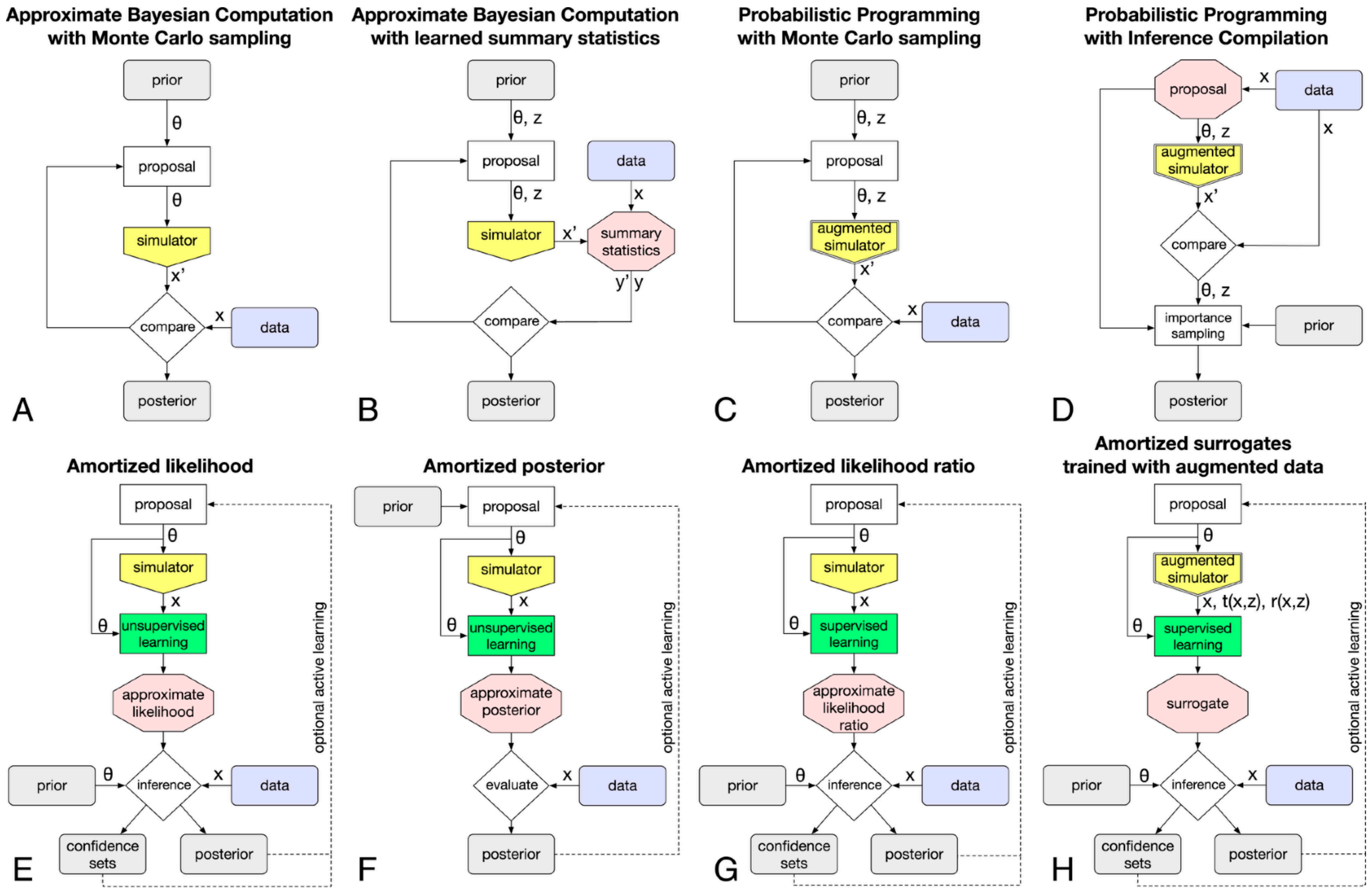
## Astro Data Science Discussion group

David Yallup - 28/02/24

# Building a mindmap of SBI

## Rather than analyse parameters (of models), analyse mock data (from models)

- NLE
- NPE
- NRE




Either using **classifiers** to distinguish between two piles of mock data, or using invertible **density estimators** to learn distributions over piles of mock data

[https://github.com/sbi-dev/sbi]

SBI Package `sbi`

Seems to be generally touted as one stop shop for all SBI needs

## Neural Posterior Estimation: amortized (NPE) and sequential (SNPE)

- `SNPE_A` (including amortized single-round `NPE`) from Papamakarios G and Murray I *Fast ε-free Inference of Simulation Models with Bayesian Conditional Density Estimation* (NeurIPS 2016).
- `SNPE_C` or `APT` from Greenberg D, Nonnenmacher M, and Macke J *Automatic Posterior Transformation for likelihood-free inference* (ICML 2019).
- `TSNPE` from Deistler M, Goncalves P, and Macke J *Truncated proposals for scalable and hassle-free simulation-based inference* (NeurIPS 2022).

## Neural Likelihood Estimation: amortized (NLE) and sequential (SNLE)

- `SNLE_A` or just `SNL` from Papamakarios G, Sterrat DC and Murray I *Sequential Neural Likelihood* (AISTATS 2019).

## Neural Ratio Estimation: amortized (NRE) and sequential (SNRE)

- `(S)NRE_A` or `AALR` from Hermans J, Begy V, and Louppe G. *Likelihood-free Inference with Amortized Approximate Likelihood Ratios* (ICML 2020).
- `(S)NRE_B` or `SRE` from Durkan C, Murray I, and Papamakarios G. *On Contrastive Learning for Likelihood-free Inference* (ICML 2020).
- `BNRE` from Delaunoy A, Hermans J, Rozet F, Wehenkel A, and Louppe G. *Towards Reliable Simulation-Based Inference with Balanced Neural Ratio Estimation* (NeurIPS 2022).
- `(S)NRE_C` or `NRE-C` from Miller BK, Weniger C, Forré P. *Contrastive Neural Ratio Estimation* (NeurIPS 2022).

These slides: bit.ly/ras-sbi-disc
Q&A: bit.ly/ras-sbi-qs

## Structure

- Why SBI?
- What are the limits?
- (When) Will SBI replace Likelihood-based?

https://ras.ac.uk/events-and-meetings/ras-meetings/simulation-based-inference-astrophysics

These slides: bit.ly/ras-sbi-disc
Q&A: bit.ly/ras-sbi-qs

## What are the limits?

- When not to use it?
- What is still missing from SBI frameworks?
- Is it only a matter of building trust in SBI techniques?
- Simulations are key, but what about compression?
- Are the emerging SBI methods multi-purpose enough that we now only need to worry about how we perform our simulations?

Thanks to organisers of RAS SBI meeting:
Alessio Spurio Mancini
Ian Harrison
Will Hartley

Watch out for community document summarising meeting and SBI outlook.

*I know no other discipline where half of the principle equation is so widely ignored*

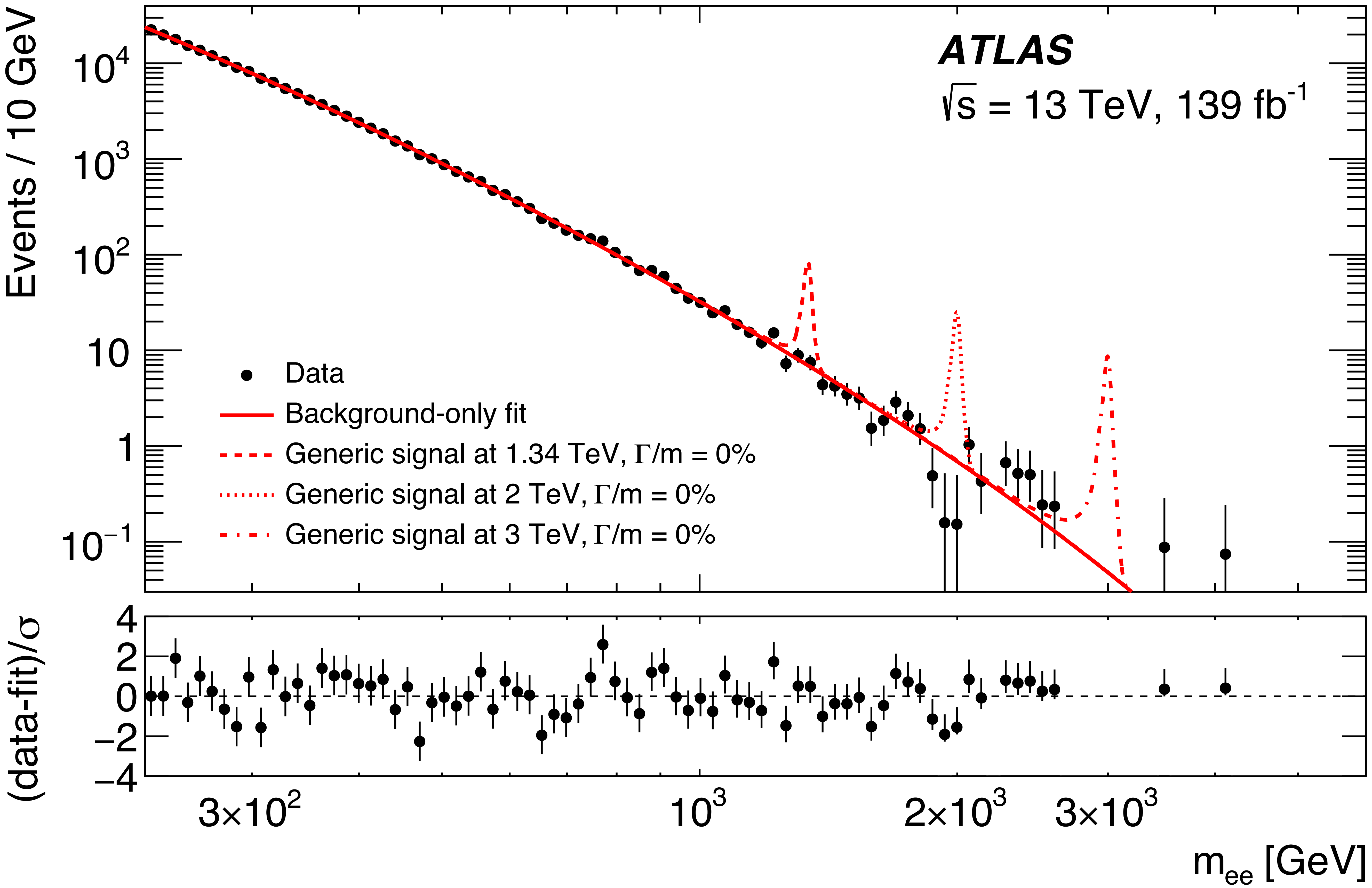
**John Skilling**

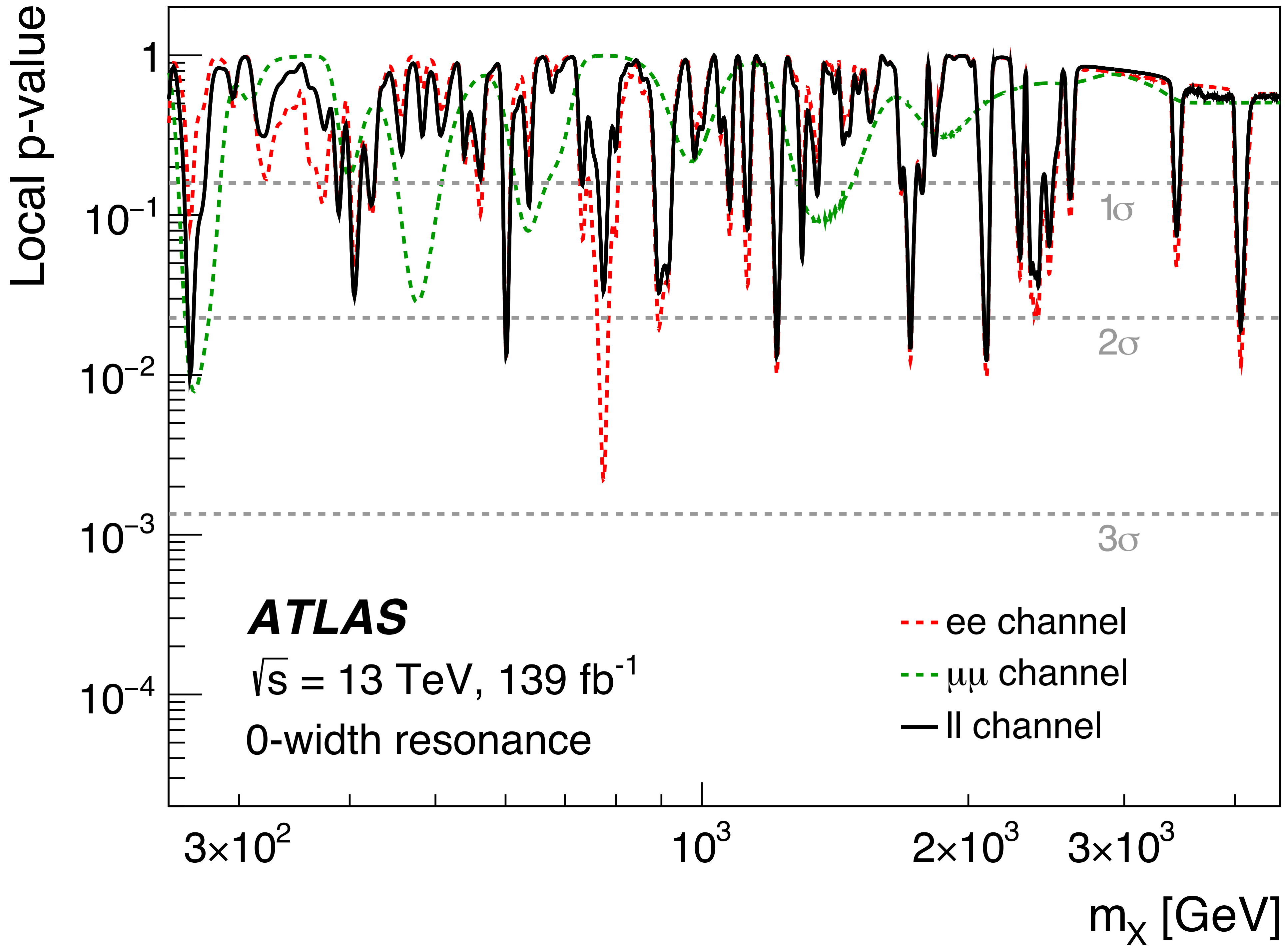
$$\mathscr{L} \times \Pi = Z \times P$$

Likelihood x Prior = Evidence x Posterior

***"Think of "Bayesian Inference" as generation of the Evidence, with the Posterior following if needed.***
***Evidence is primary."***

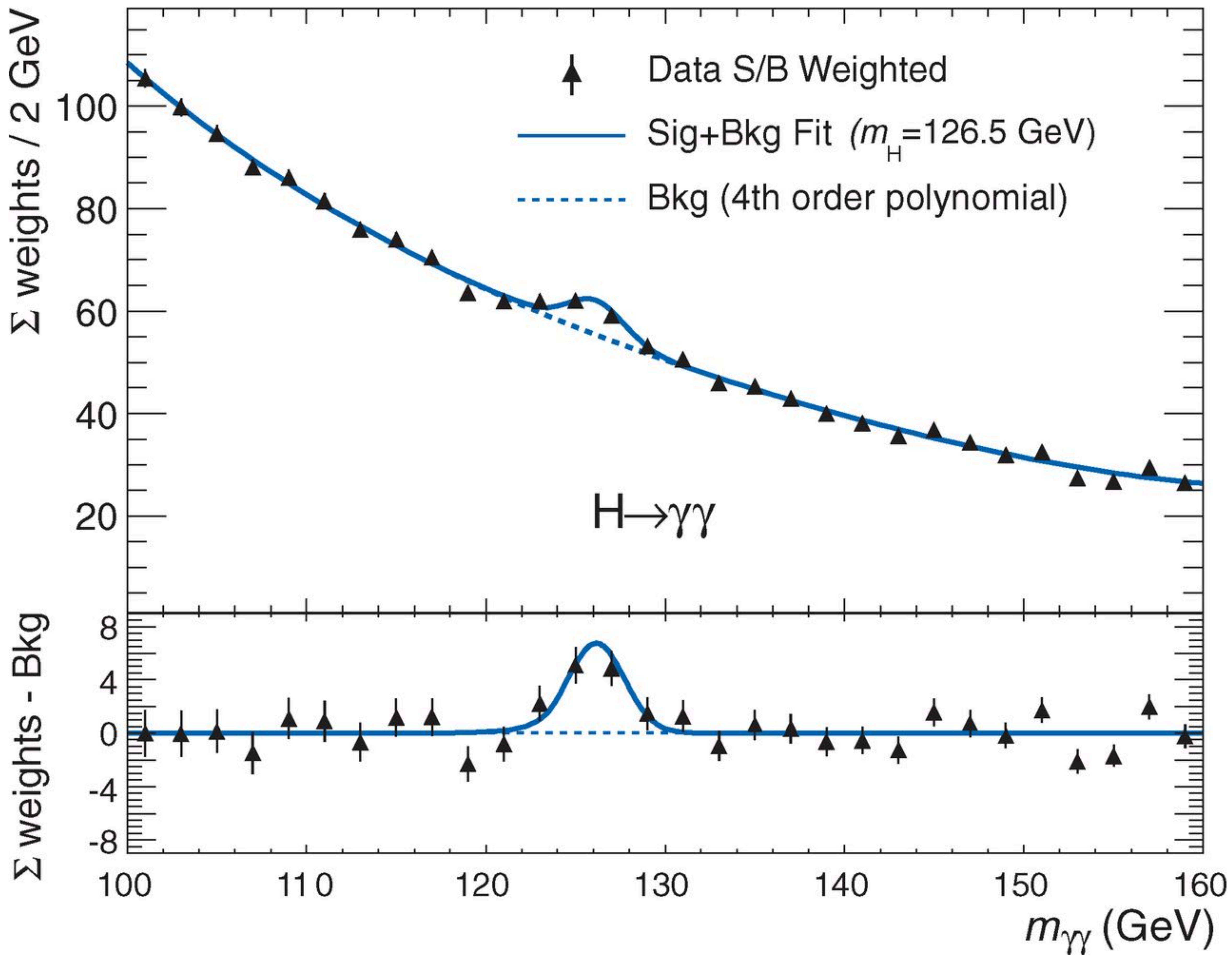
# Evidence is all you need

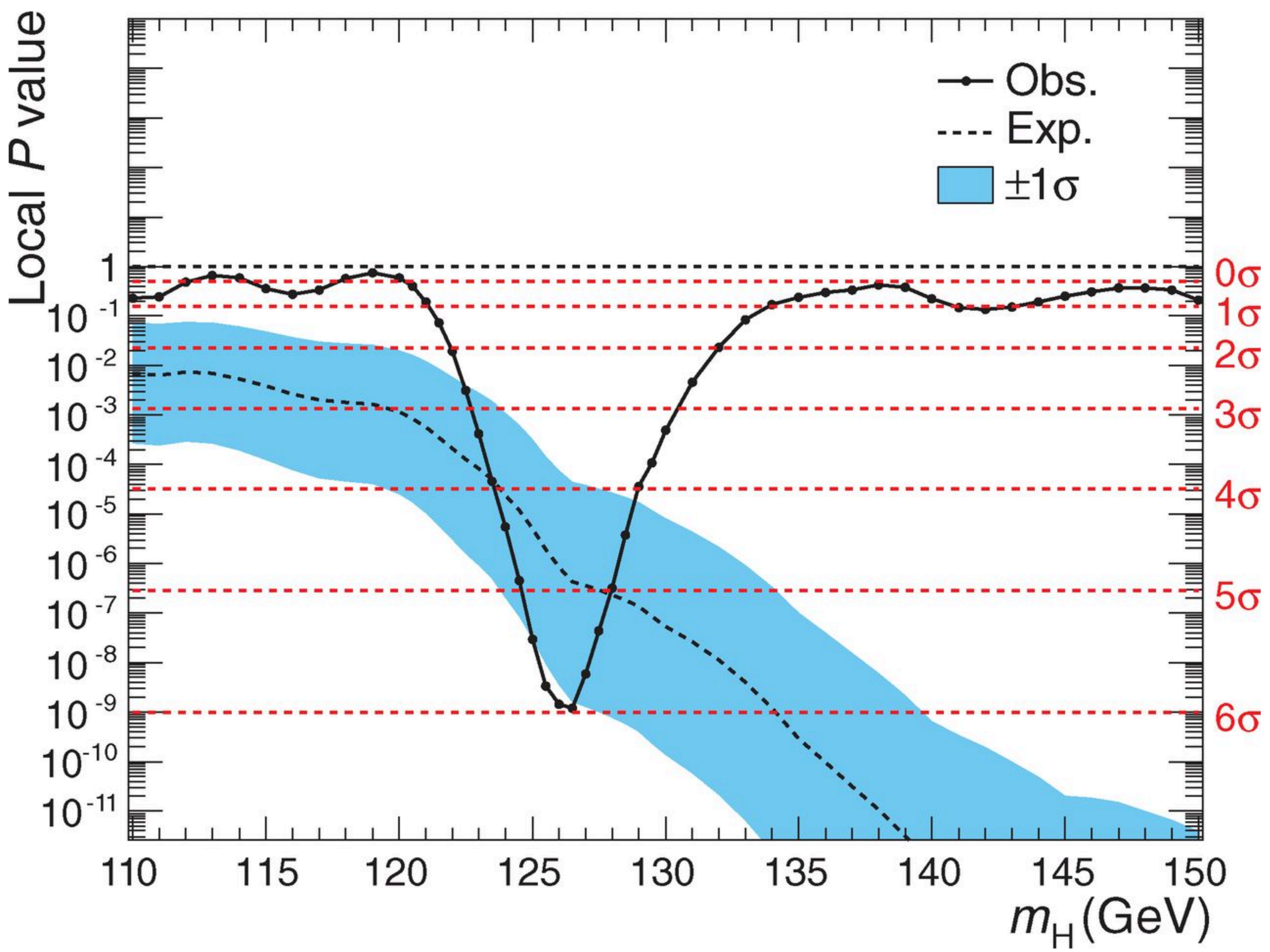


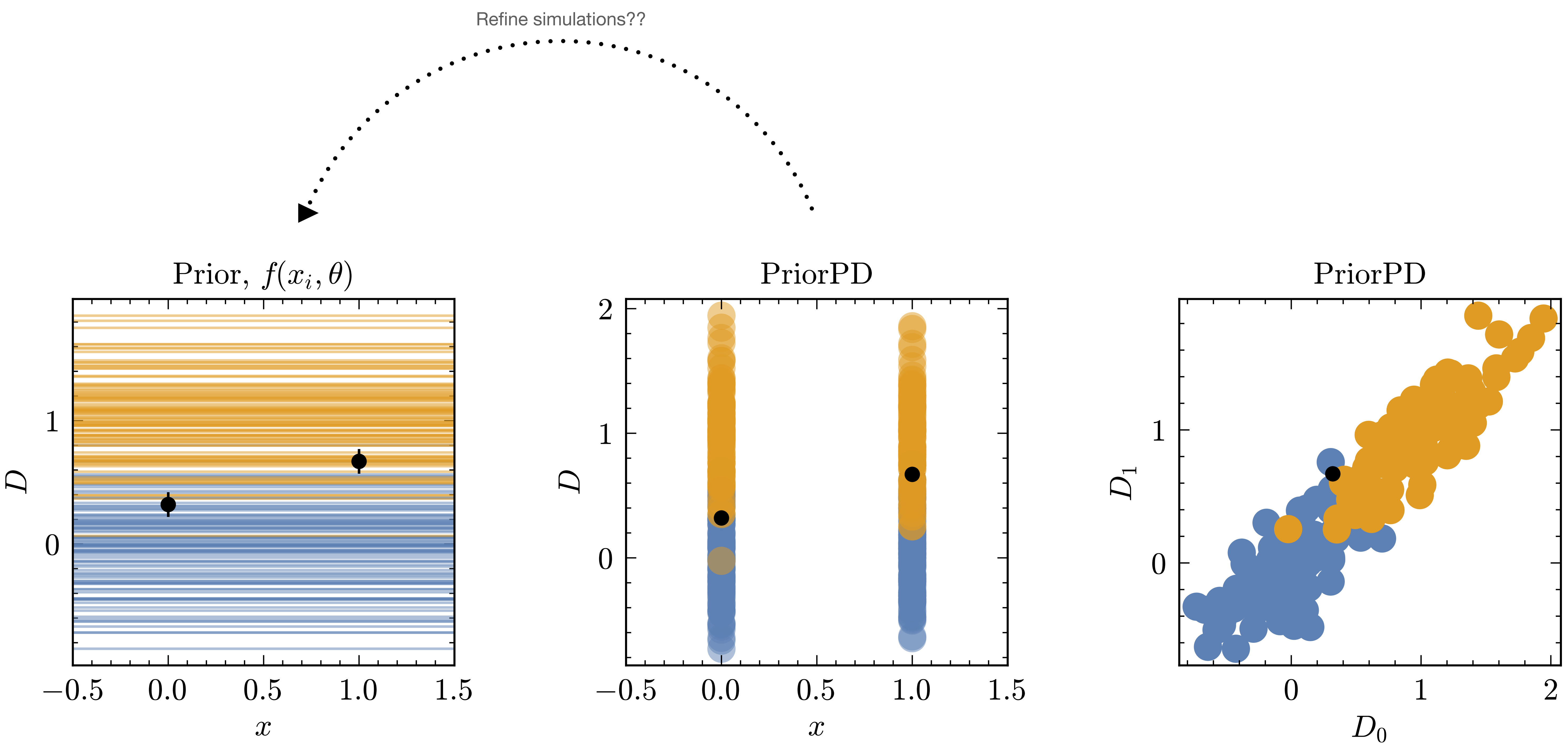




No significant excess is observed. The largest deviations from the background-only hypothesis in the dielectron, dimuon and combined dilepton channels are observed at masses of 774 GeV, 267 GeV and 264 GeV for zero-width signals with a local p0 of 2.9 σ, 2.4 σ and 2.3 σ and a **global significance of 0.1 σ, 0.3 σ, and zero**, respectively

# Evidence is all you need (sort of)





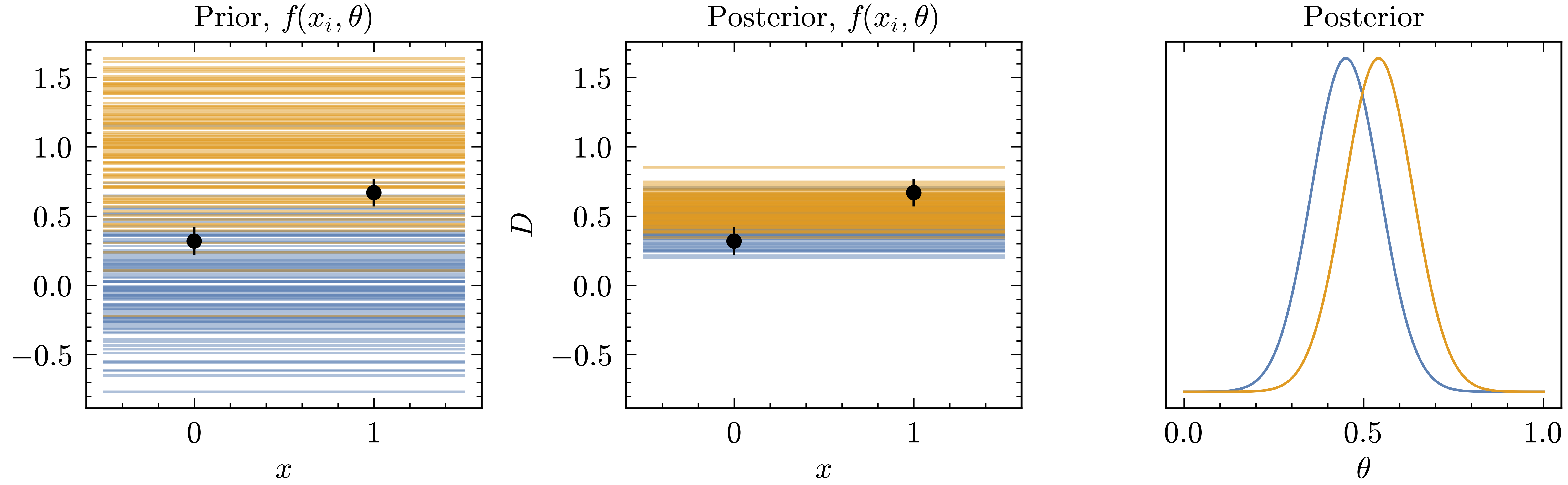

Ingredients:

Model for your data: $f(x_i, \theta)$

Noise model for your data e.g.: $n_i \leftarrow \mathcal{N}(0,\sigma)$

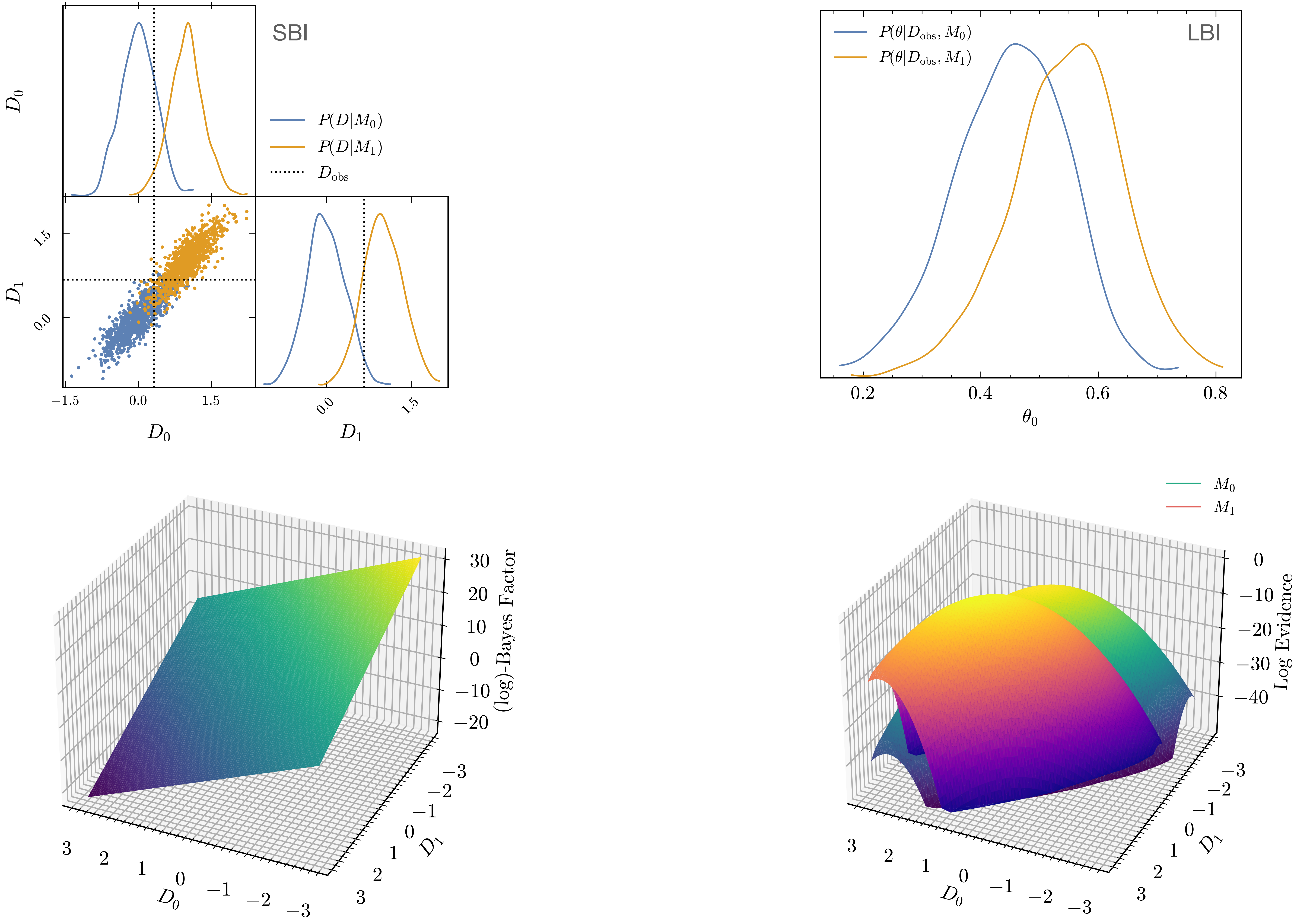
$$D_i = f(x_i, \theta) + n_i$$

SBI




$$L(D\,|\,\theta, M) = \prod_i \frac{1}{\sqrt{2\pi\sigma}} e^{\frac{-(f(x_i,\theta) - D_i^{obs})^2}{2\sigma^2}}$$

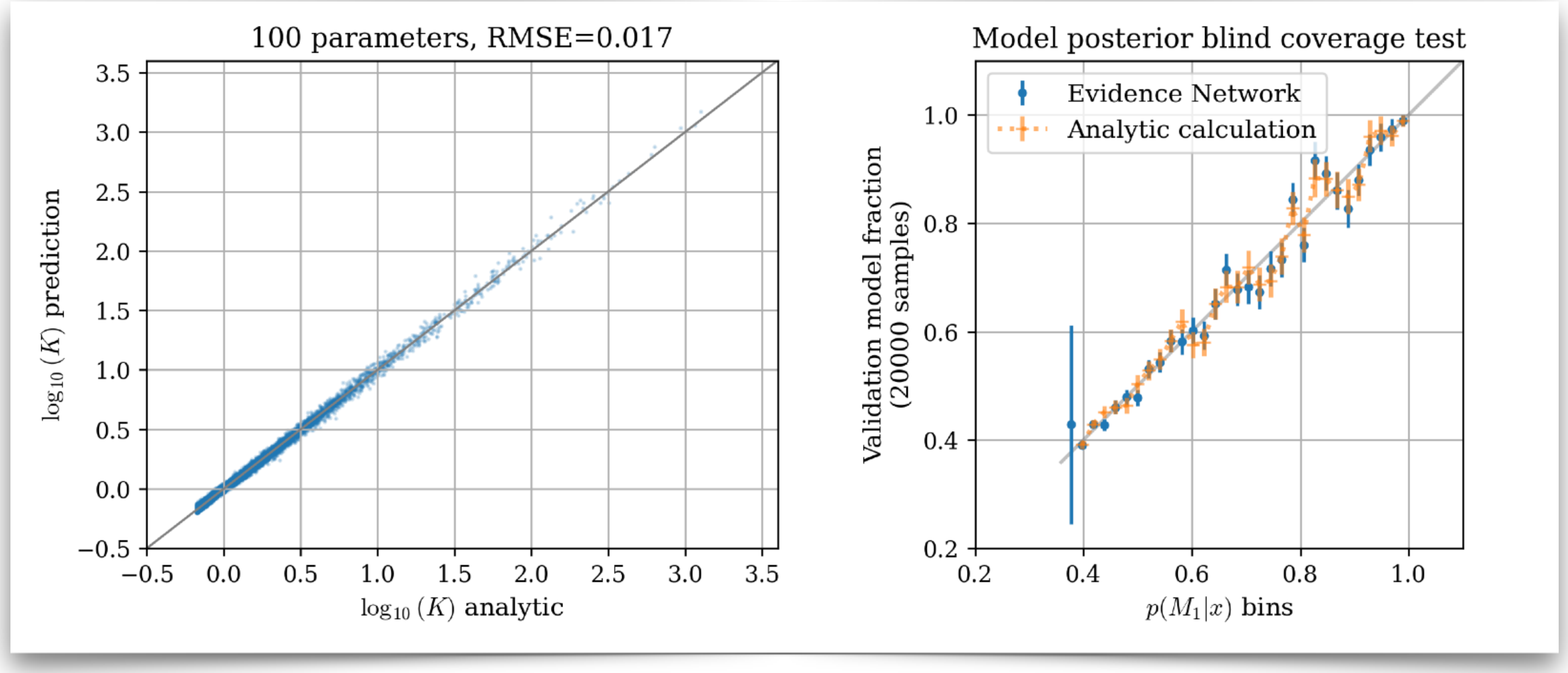
LBI



SBI
$P(D|M_0)$
$P(D|M_1)$
$D_{obs}$
$D_0$
$D_1$
LBI
$P(\theta|D_{obs}, M_0)$
$P(\theta|D_{obs}, M_1)$
$\theta_0$
(log)-Bayes Factor
$M_0$
$M_1$
Log Evidence

# The likelihood ratio trick appears to imply model comparison is "easier" than parameter estimation in SBI.

This is what I find most interesting about SBI!




[2305.11241]

Evidence Networks:

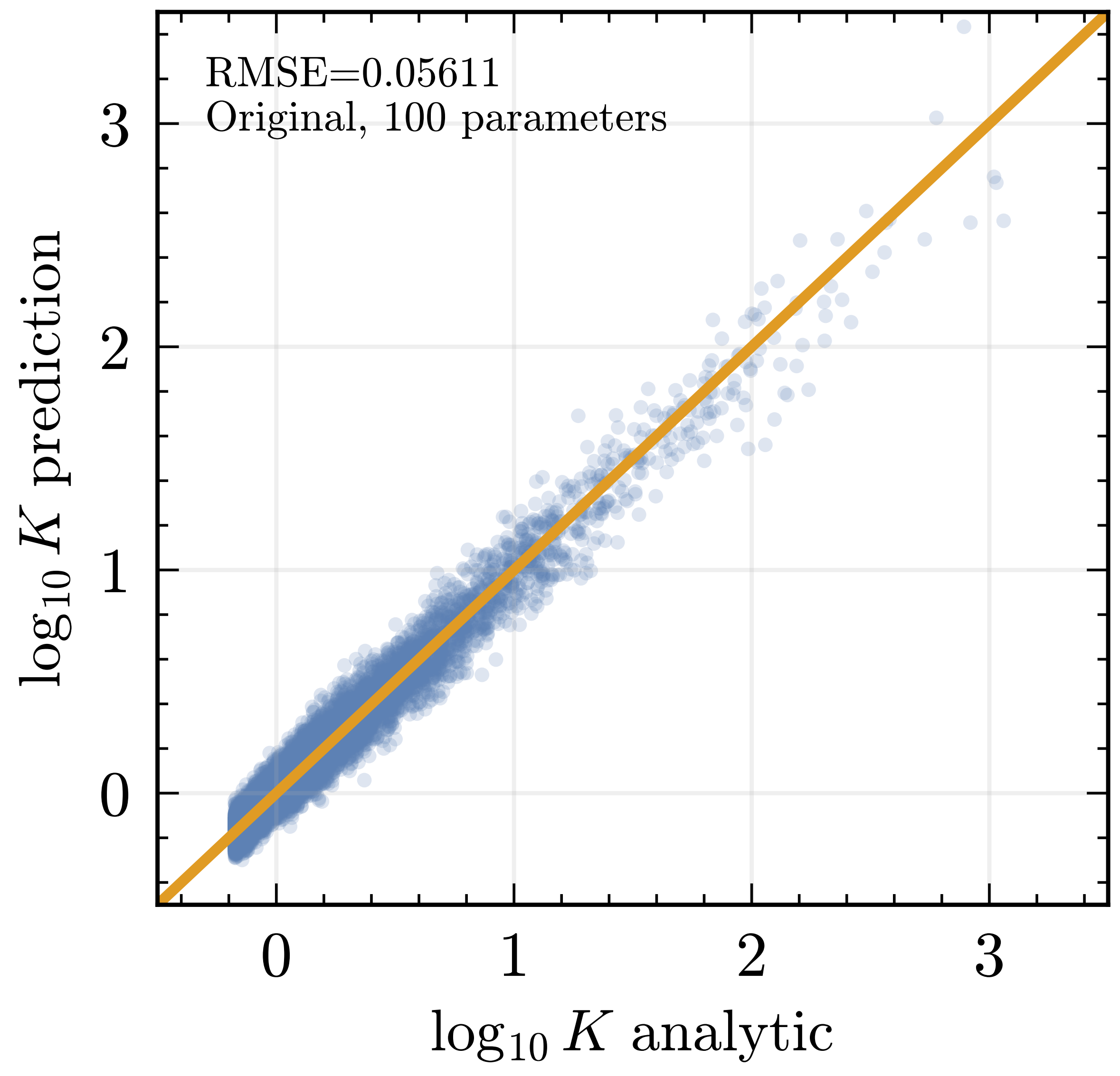
Take the "Likelihood ratio trick" seriously with generation of data from a prior distribution.

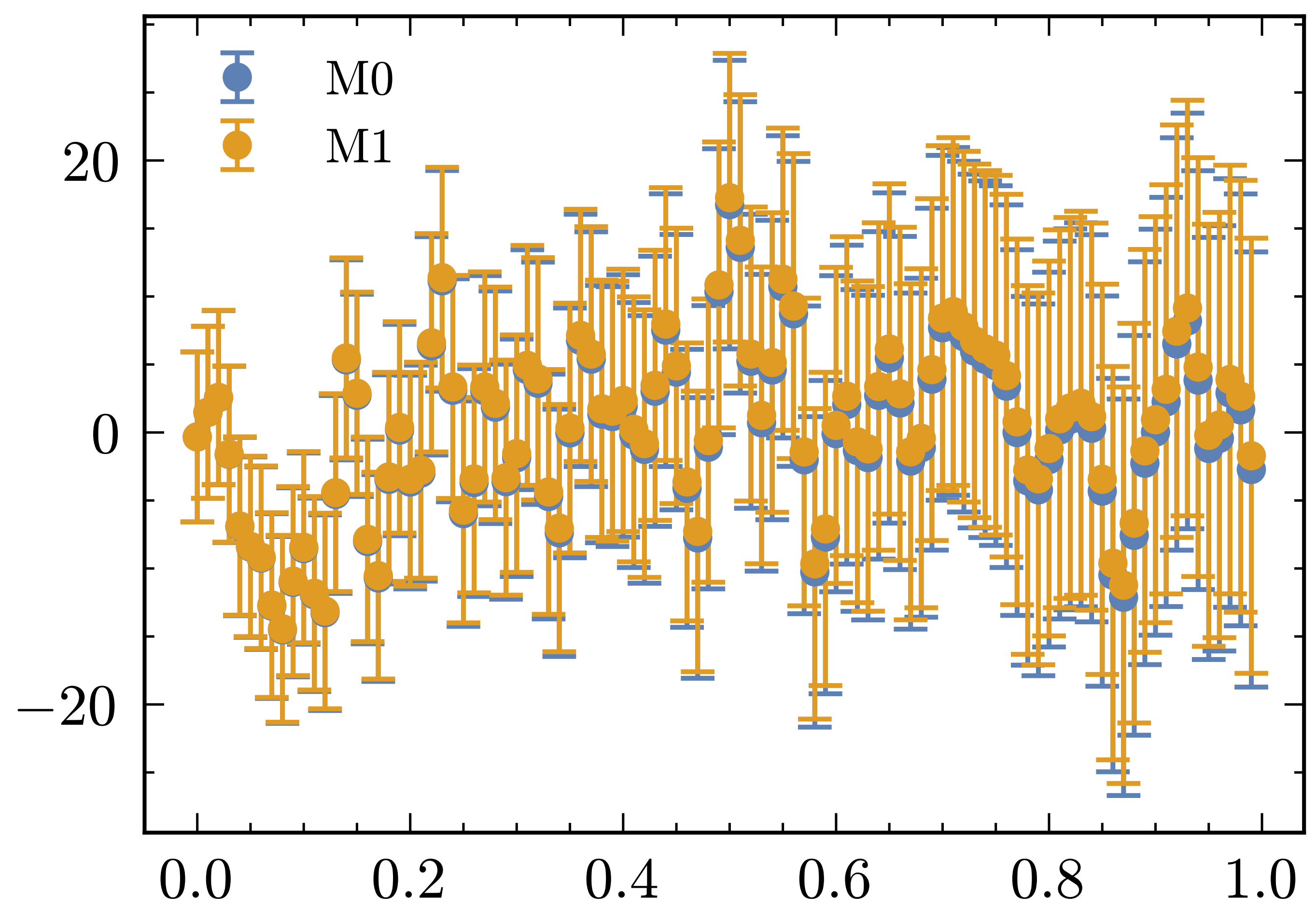
[1805.12244]

**The likelihood ratio trick (LRT).** A surrogate model for the likelihood ratio $\hat{r}(x|\theta_0,\theta_1)$ can be defined by training a probabilistic classifier to discriminate between two equal-sized samples $\{x_i\} \sim p(x|\theta_0)$ and $\{x_i\} \sim p(x|\theta_1)$. The binary cross-entropy loss

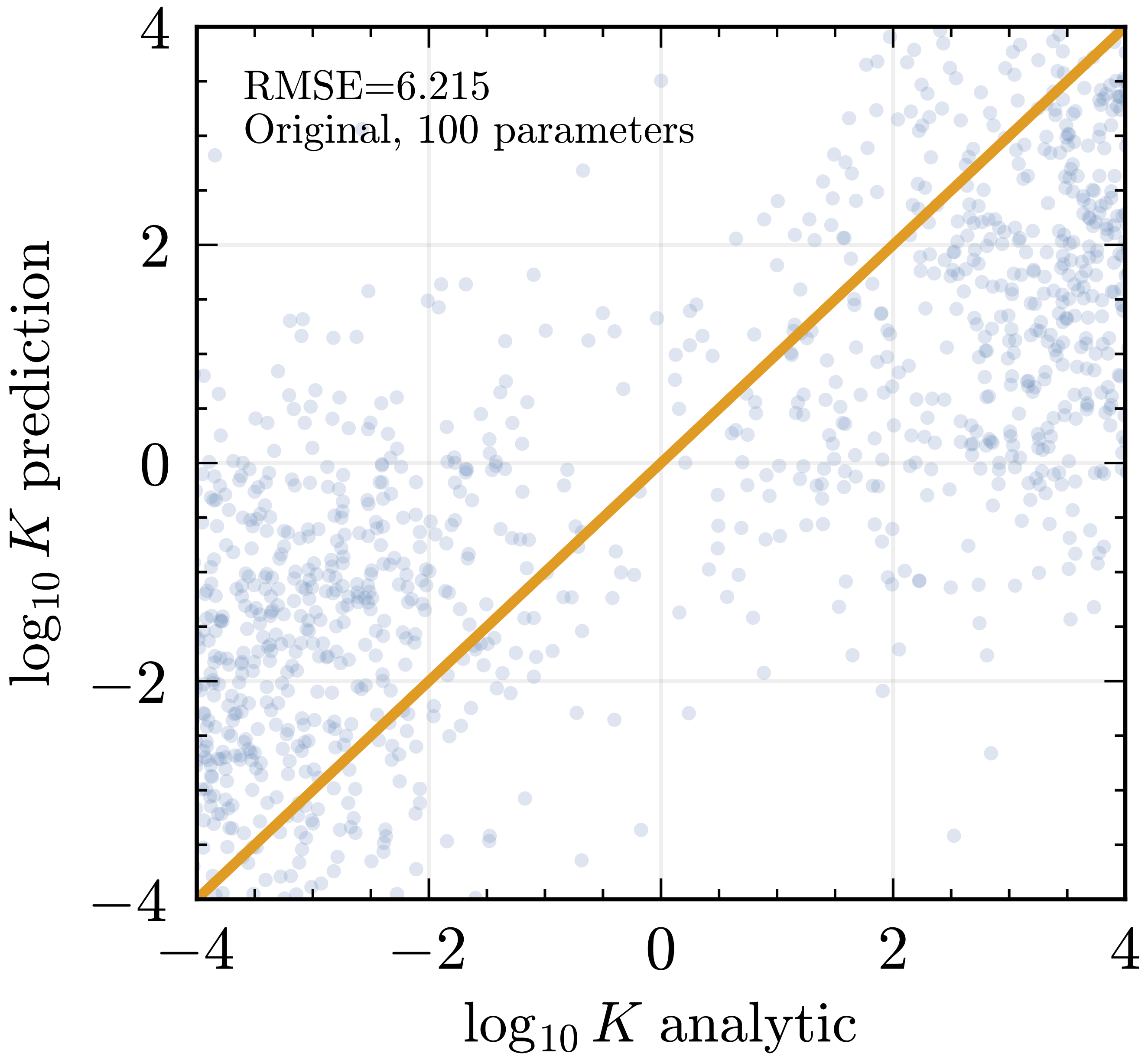
$$L_{\mathrm{XE}} = -\mathbb{E}[\mathbb{1}(\theta=\theta_1)\log \hat{s}(x|\theta_0,\theta_1) + \mathbb{1}(\theta=\theta_0)\log(1-\hat{s}(x|\theta_0,\theta_1))] \tag{1}$$

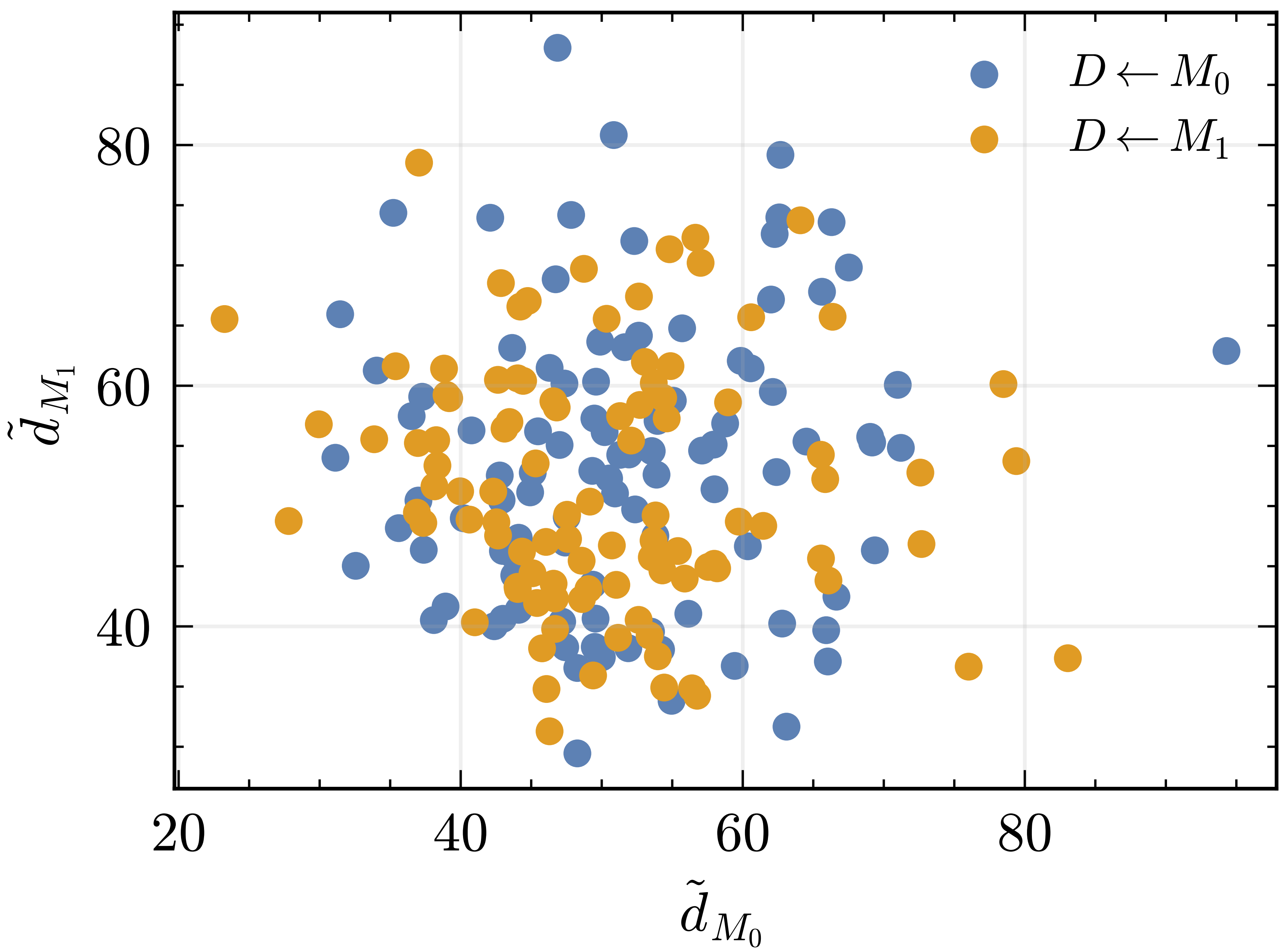
is minimized by the optimal decision function $s(x|\theta_0,\theta_1) = p(x|\theta_1)/(p(x|\theta_0)+p(x|\theta_1))$. Inverting this relation, the likelihood ratio can be estimated from the classifier decision function $\hat{s}(x)$ as $\hat{r}(x|\theta_0,\theta_1) = (1-\hat{s}(x|\theta_0,\theta_1))/\hat{s}(x|\theta_0,\theta_1)$. This "likelihood ratio trick" is widely appreciated [5–



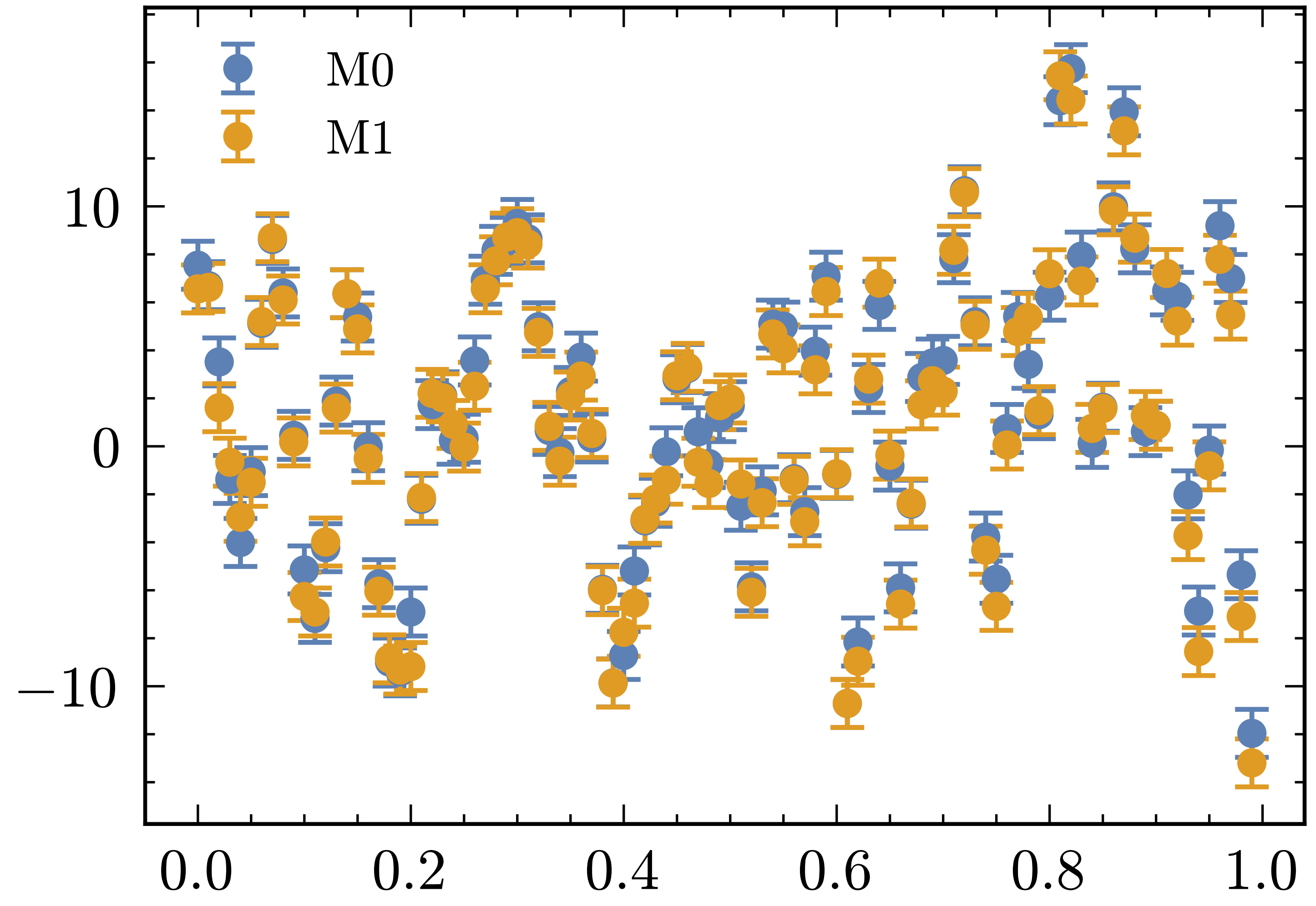



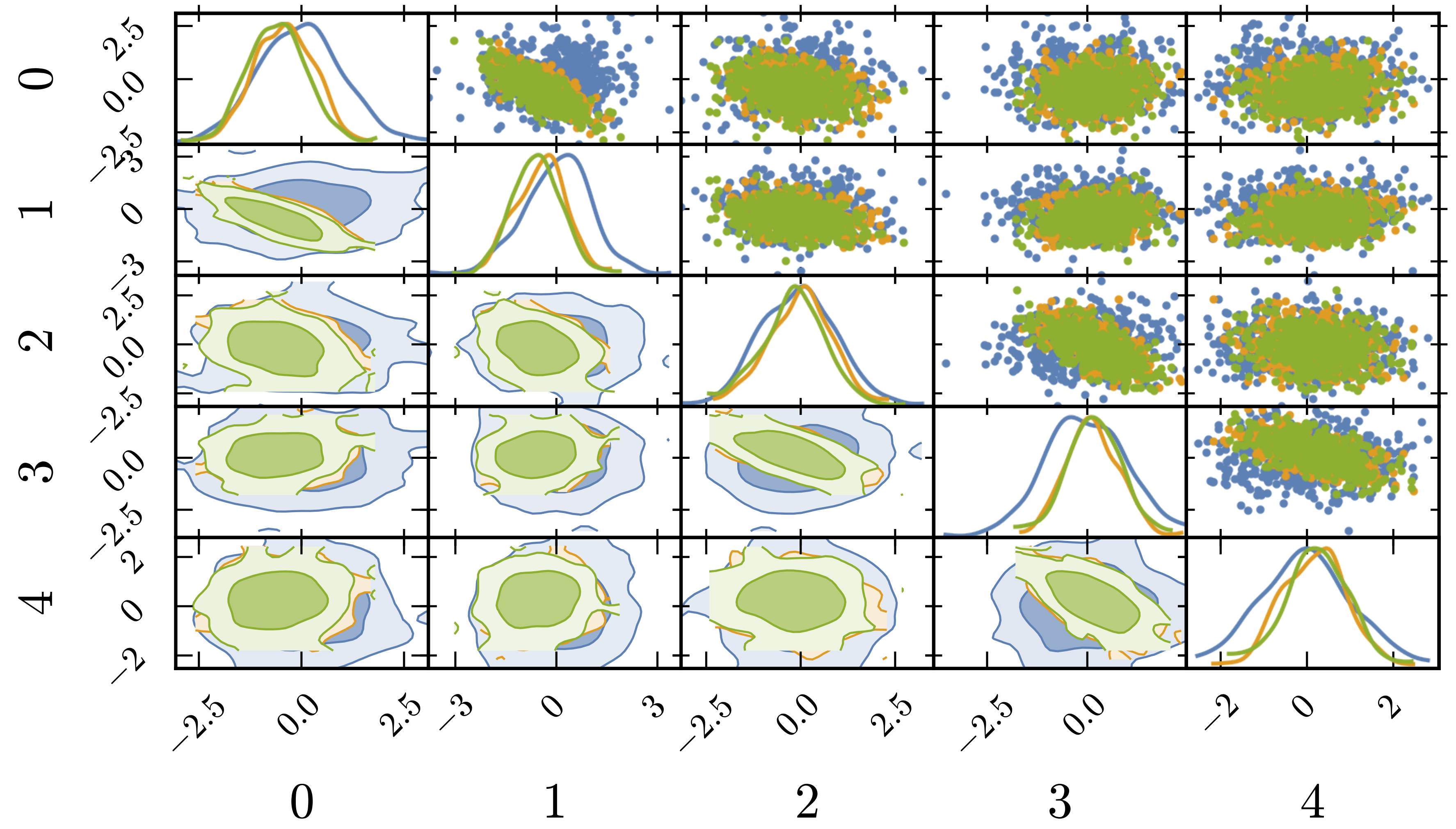

$$A_{i0} = 2x_i\,,$$
$$A_{ij} = \cos(j-1/2)x_i\,,$$
$$n_i \leftarrow \mathcal{N}(0,\{2,\ldots,4.5\})\,,$$
$$\theta_i \leftarrow \mathcal{N}(0,1)\,.$$
$$D_i = A_{ij}\theta_j + n_i$$




$$A^0_{ij} = \cos(j - 1/2)x_i\,,$$
$$A^1_{ij} = A^0_{ij} \cdot R$$
$$R \leftarrow O(N, \epsilon)$$
$$n_i \leftarrow \mathcal{N}(0,1)$$



# How good do your simulations have to be?

- Model misspecification — *“All models are wrong some are useful”*, expect data we analyse will *never* be drawn from the model we are proposing
    - How well can neural techniques extrapolate

- Relevance of simulation data to observed data
    - A lot of the really juicy parts of SBI are gaining from being apparently vastly more economical here, amortization over all data?
    - **How good do your {simulations} have to be?**

# Assorted thoughts

- How different is using a GP acquisition to get a new set of sims for my amortized SBI pipeline from using a GP surrogate in parameter space?
- What regime are we in: $$\mathcal{O}(D) \ll \mathcal{O}(\theta), \quad \mathcal{O}(D) = \mathcal{O}(\theta), \quad \mathcal{O}(D) \gg \mathcal{O}(\theta)$$
- It's very hard to think of something analytic, non-linear, representative of real problems! Writing good test problems is a lot harder than it seems

# Conclusions

- Ratios are interesting, potential cancellation that simplifies problems
- How we [sequential] or [amortize] + [active learning??] is for my money the open problem
- The above can be mapped onto traditional methods?
- SBI is here to stay