Introduction to simulation-based inference (SBI)

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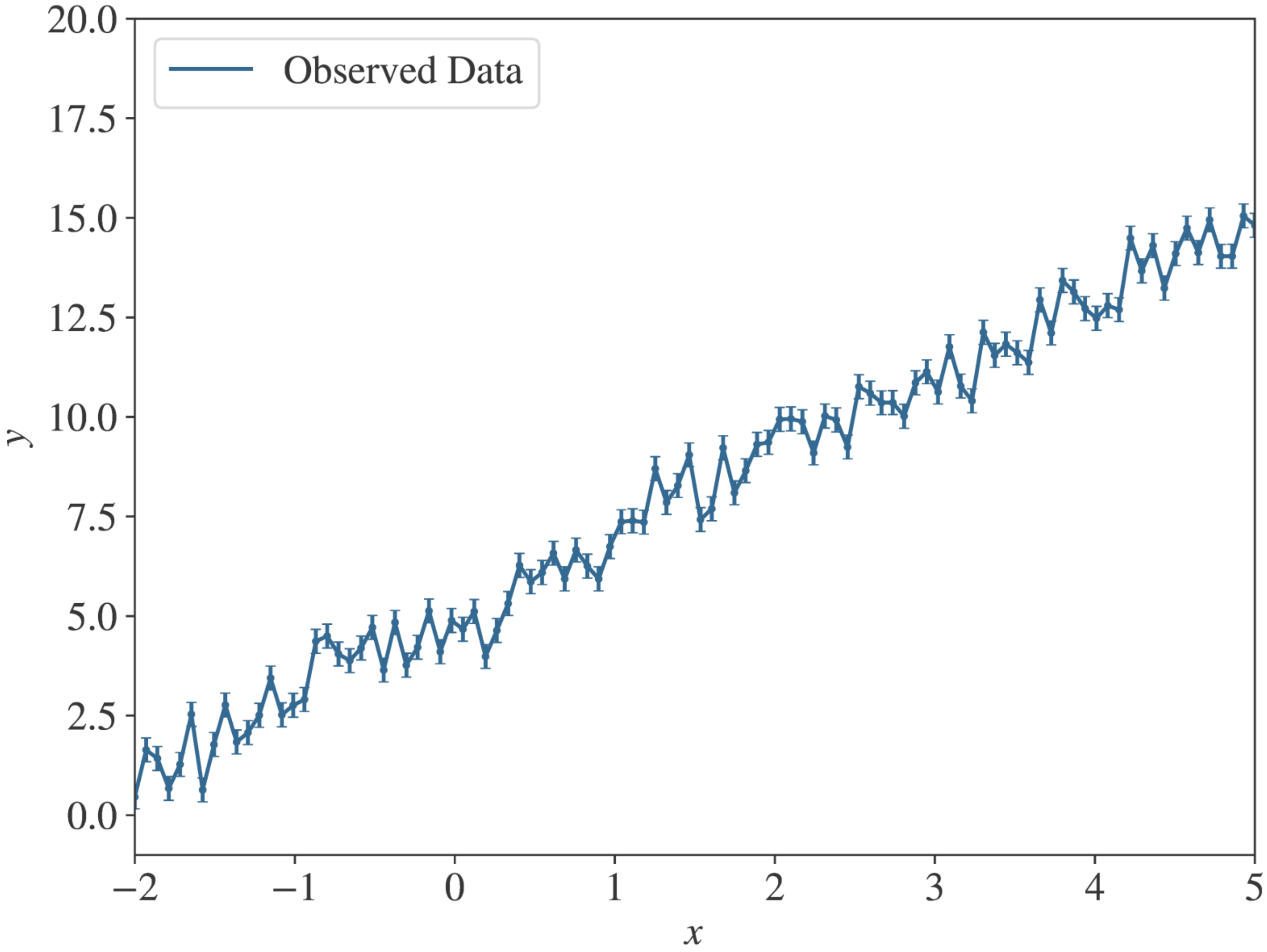
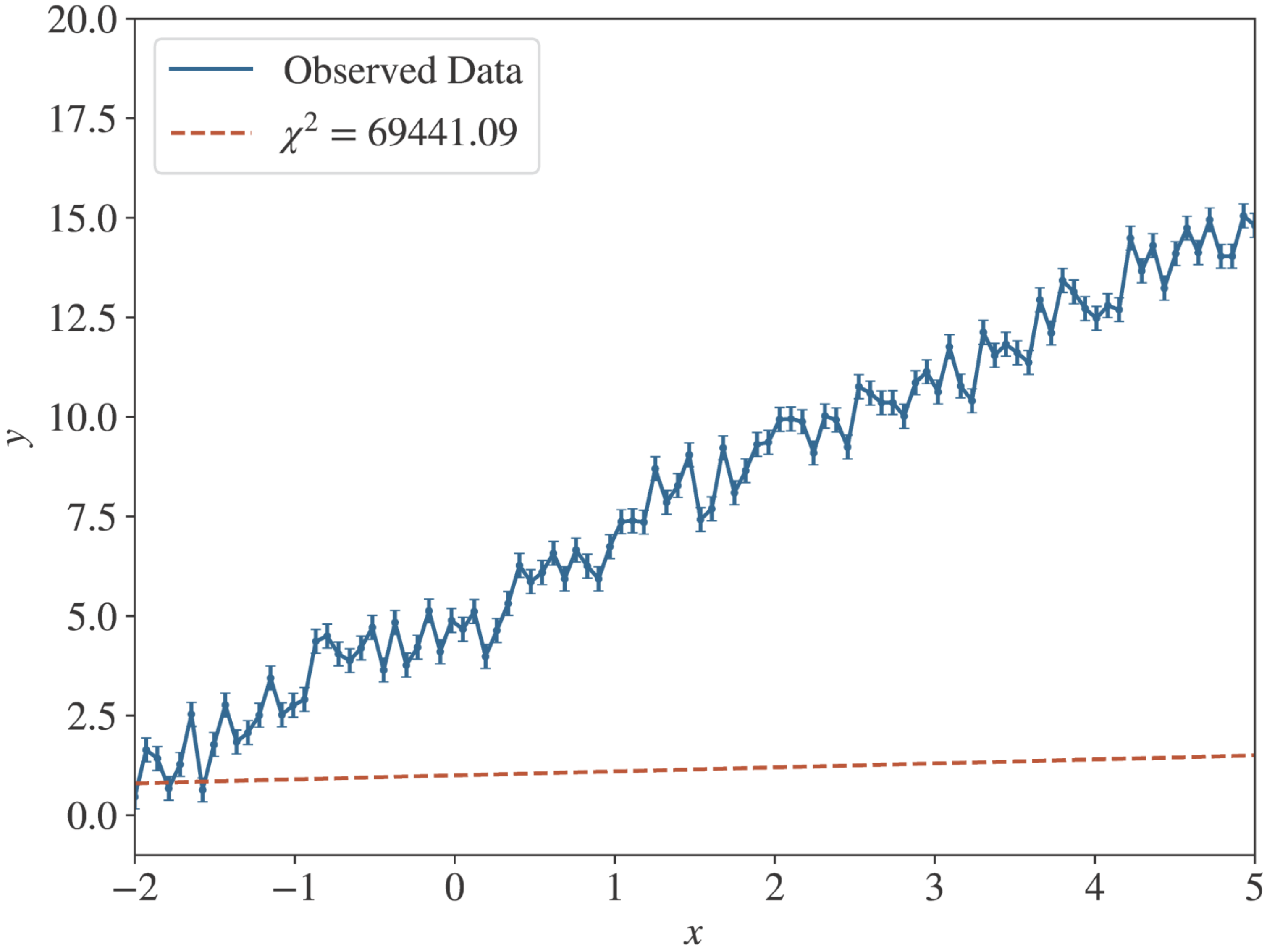
Accurate Likelihoods are hard

- Your likelihood probably is not Gaussian
- Observational systematics
  - Noise models (depth variability etc.)
  - Selection bias
- Complex physics is hard to cast into an analytic model

Learn from simulations



Learn from simulations



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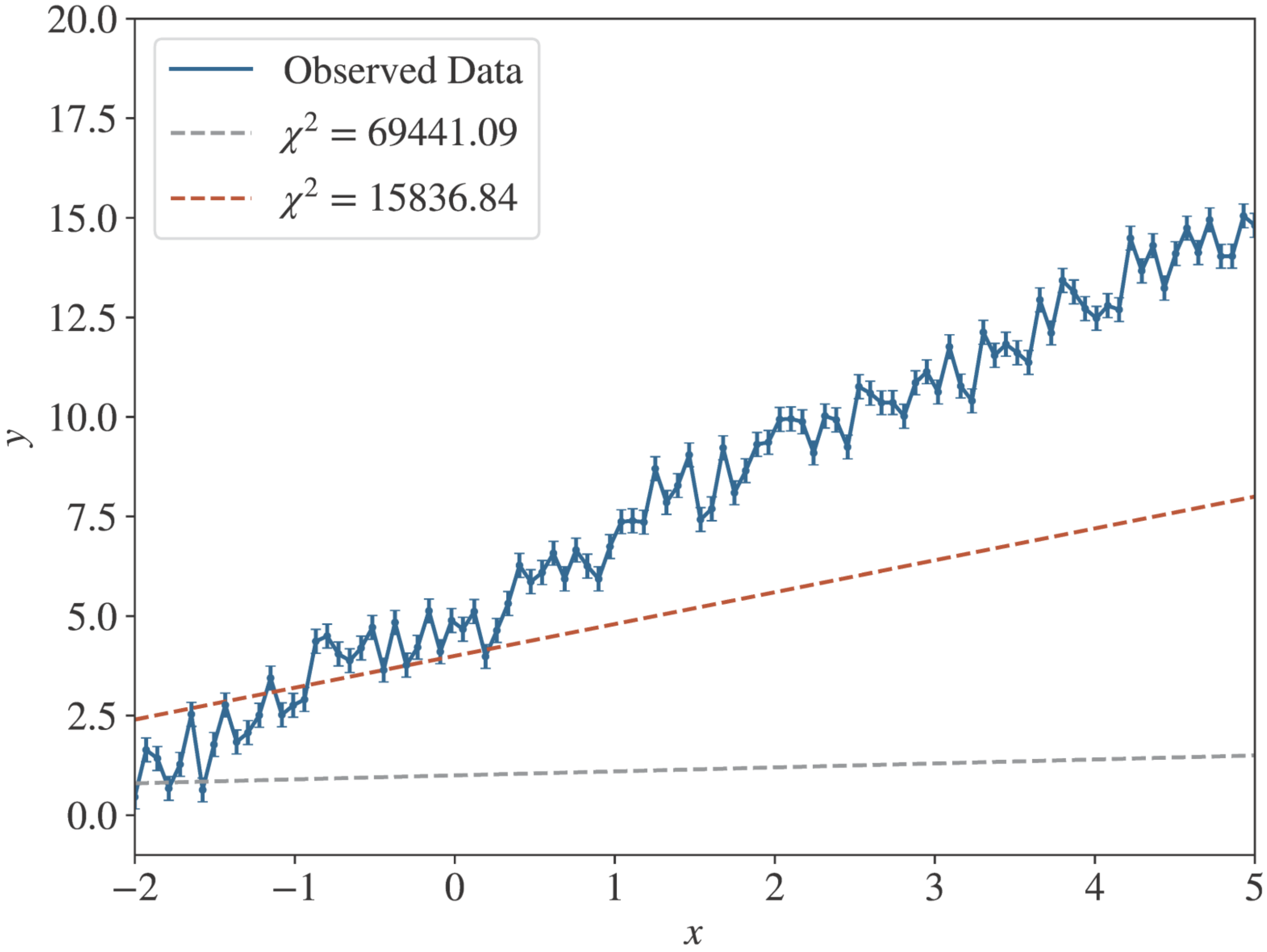
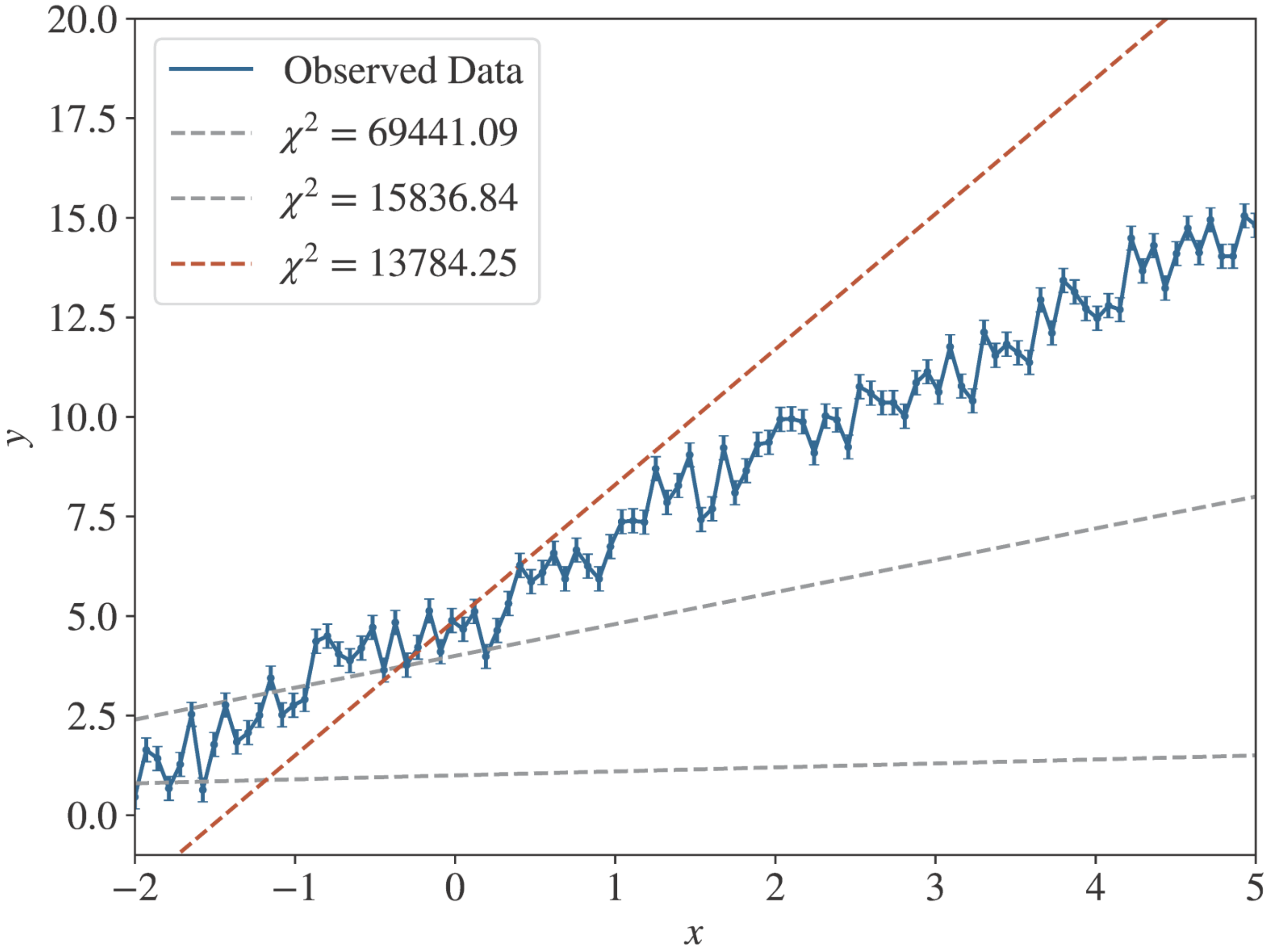
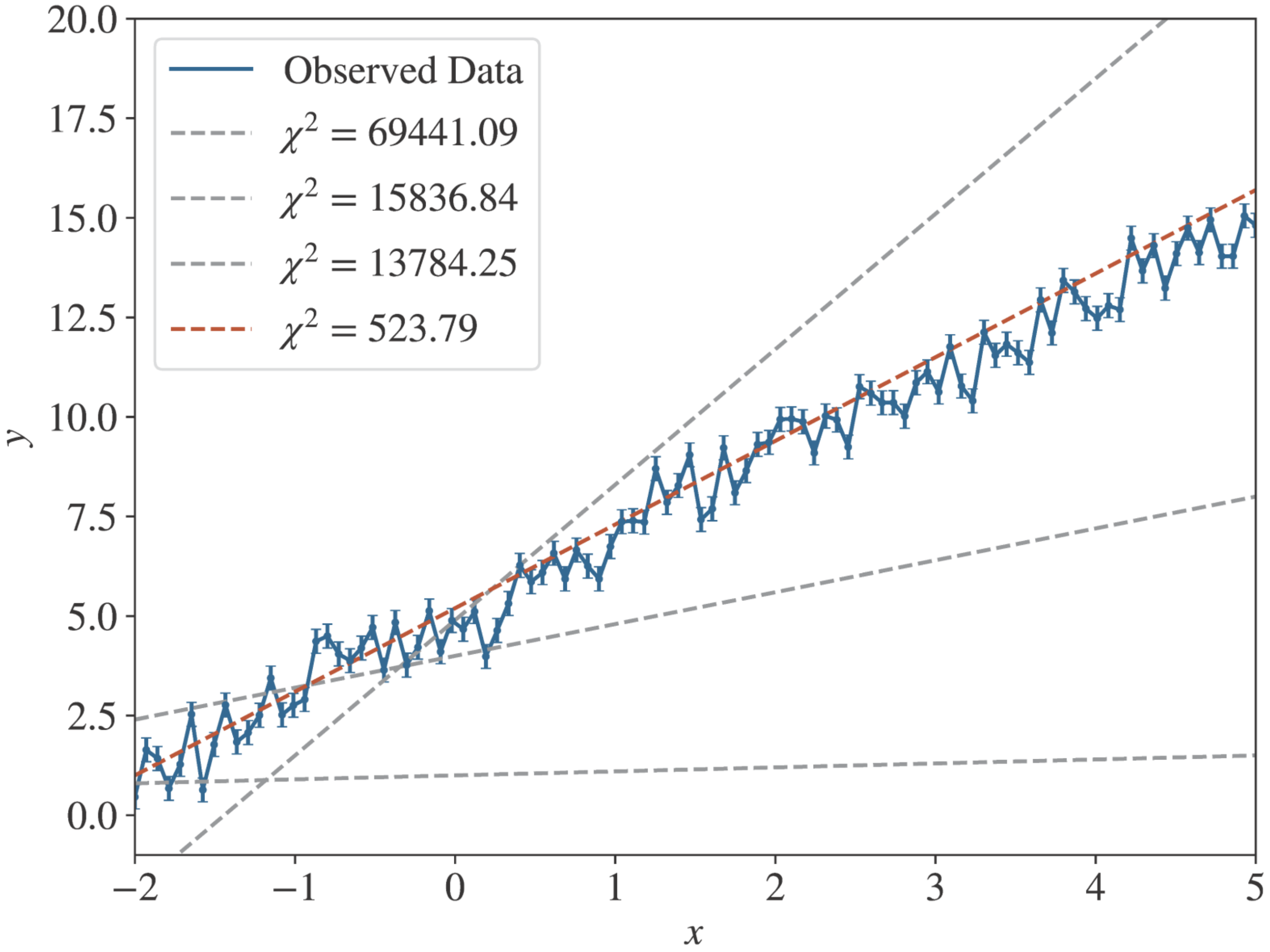


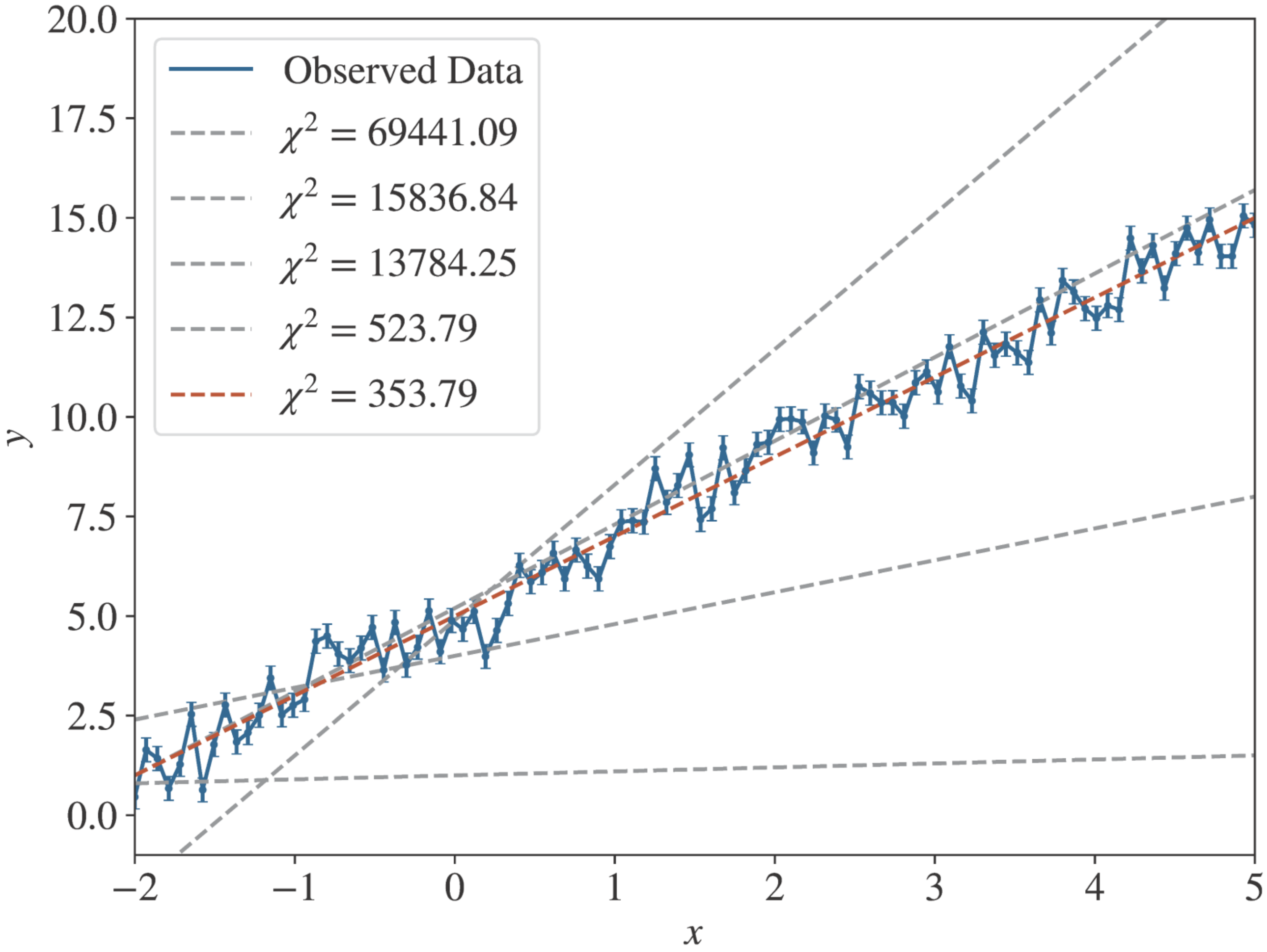
Learn from simulations



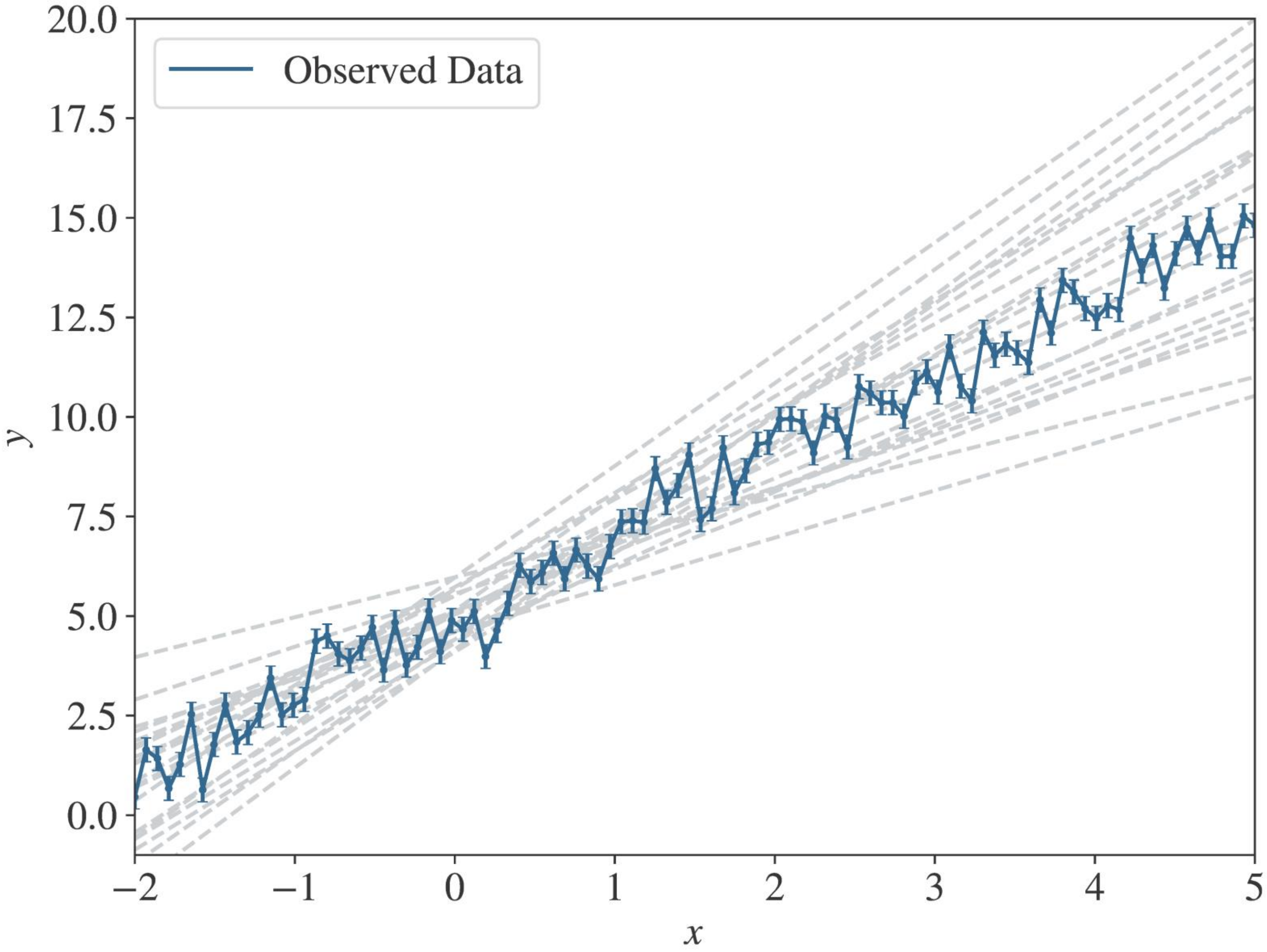
Learn from simulations



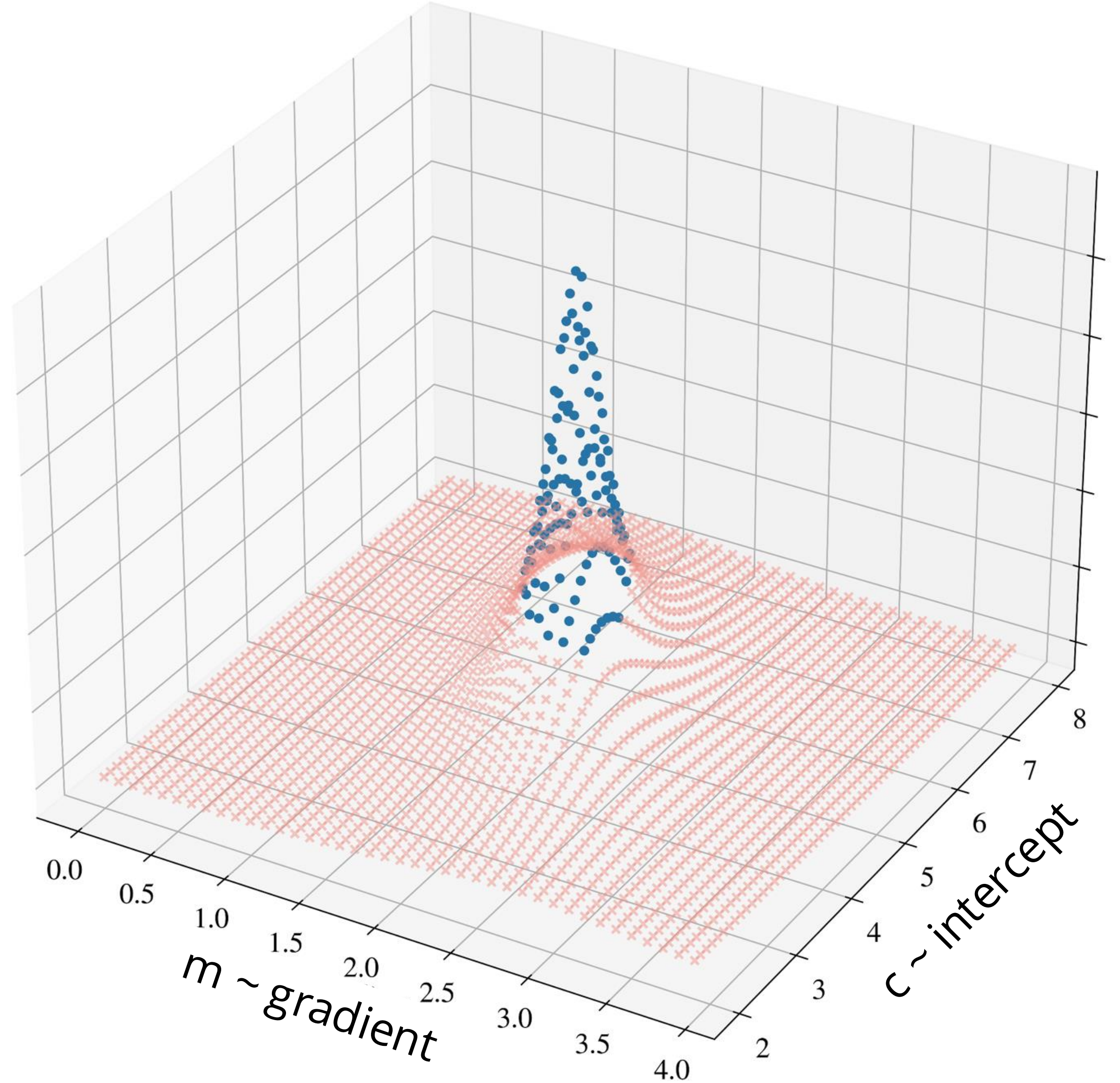
Learn from simulations



Learn from simulations

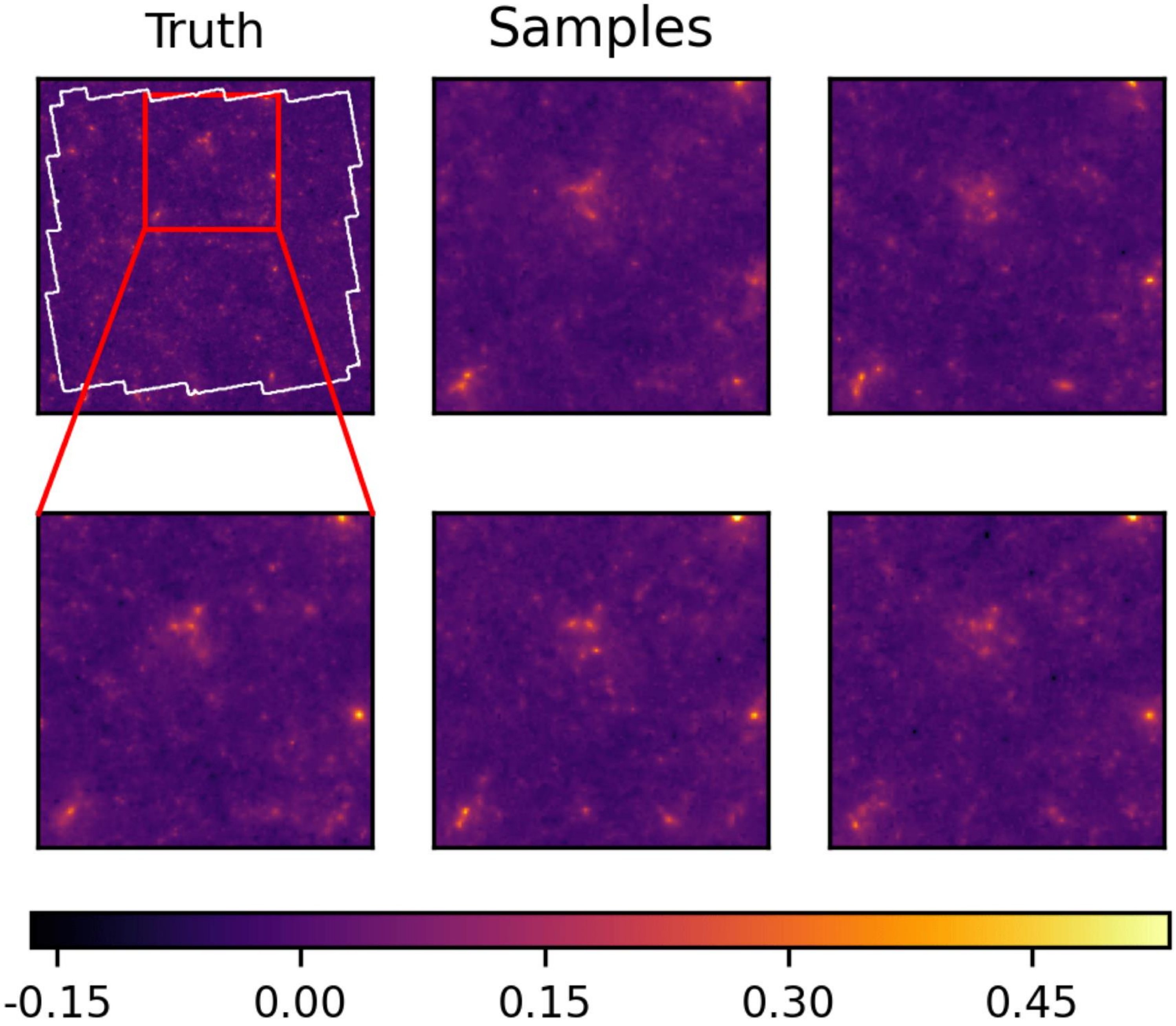


Learn from simulations



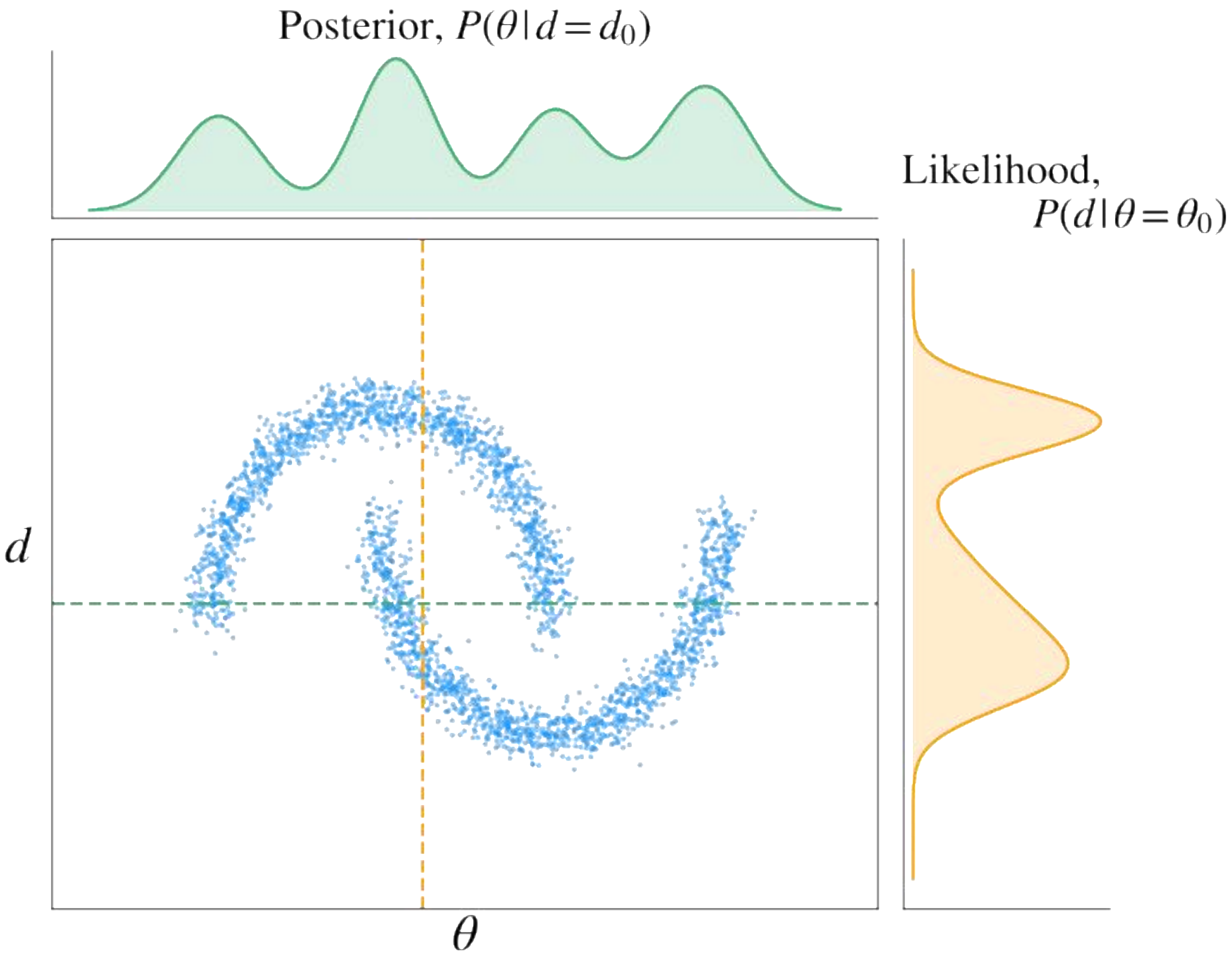
Learn from simulations

- Approximate Bayesian computation (ABC)
  - How do you define closeness
  - Incredibly inefficient



Whitney et al. (2024)

Joint probability is everything $p(\theta, d)$



SBI – Neural methods

- Neural Posterior
- Neural Likelihood
- Neural Ratio

Neural SBI, the premise

- Have a simulator such that one can draw samples from the joint distribution

$$p(\theta, d)$$

SBI – Training

- Train a neural density estimator (NDE) such that $q_\phi(\theta|\mathrm{d}) \rightarrow p(\theta|d)$
- Minimise Kullback-Leibler (KL) Divergence

$$KL\left(p(\theta|d)||q_\phi(\theta|d)\right) = \mathrm{E}_{p(\theta,d)}\left[\log\frac{p(\theta|d)}{q_\phi(\theta|d)}\right]$$

$$KL = \mathrm{E}_{p(\theta,d)}[\log p(\theta|d)] - \mathrm{E}_{p(\theta,d)}\left[\log q_\phi(\theta|d)\right]$$

SBI – Training

$$KL = \mathrm{E}_{p(\theta,d)}[\log p(\theta|d)] - \mathrm{E}_{p(\theta,d)}\left[\log q_\phi(\theta|d)\right]$$

- Minimise the log likelihood of θ

$$\mathcal{L}(\phi) = \mathrm{E}_{p(\theta,d)}\left[-\log q_\phi(\theta|d)\right]$$

SBI – Neural Posterior

- Curse of dimensionality
- $\tilde{p}(\theta|d) \propto \frac{\tilde{p}(\theta)}{p(\theta)} p(\theta|d)$

SBI – Neural Posterior

- $\tilde{p}(\theta|d) \propto \frac{\tilde{p}(\theta)}{p(\theta)} p(\theta|d)$
- NPE-A – Papamakarios & Murray 2016
  - Post-hoc analytical correction needed
- NPE-B – Lueckmann et al. 2017
  - Proposal embedded as an importance weight
- NPE-APT – Greenberg et al. 2019
  - Automatic Posterior Transformations

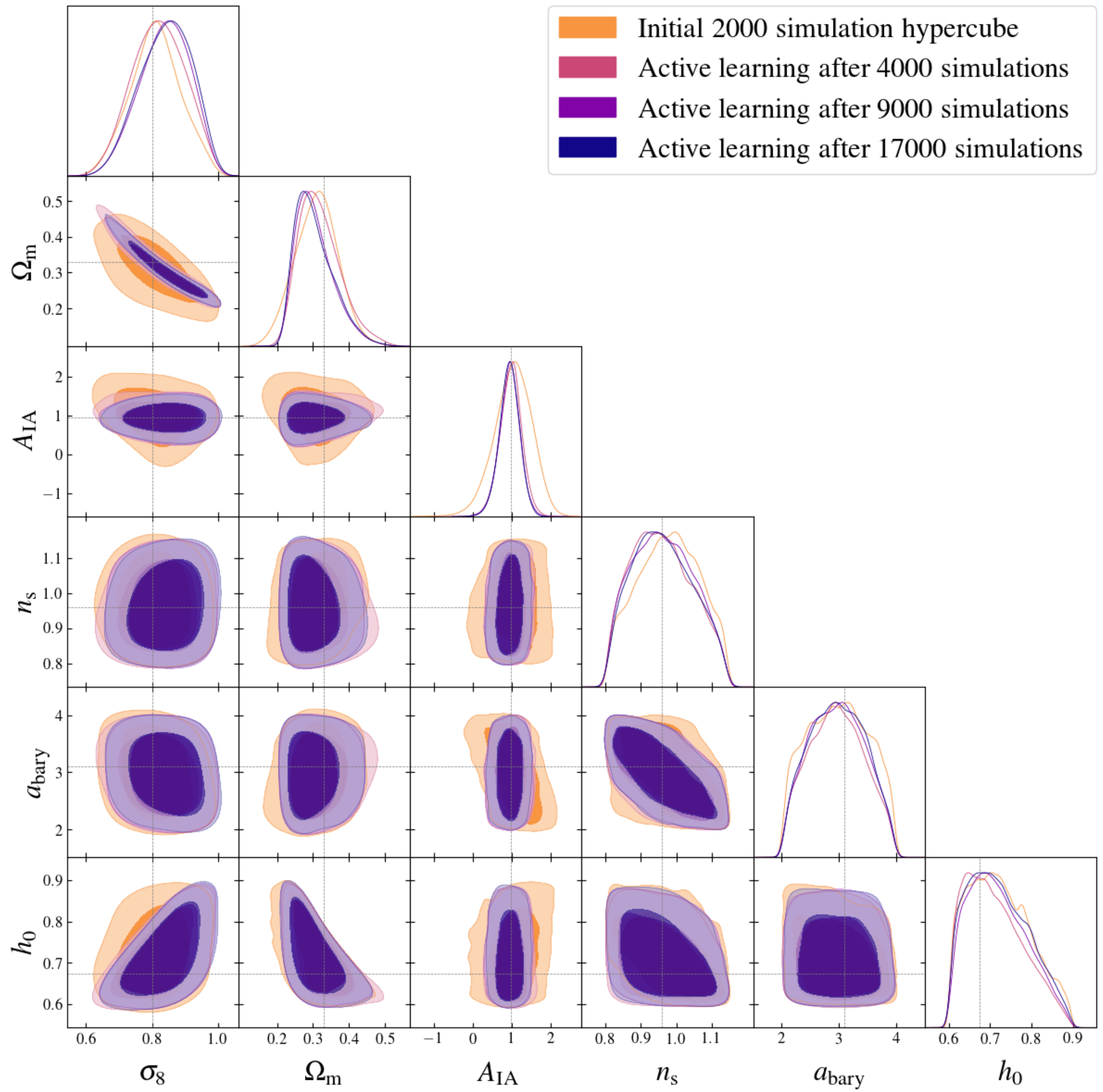
SBI – Neural Posterior

- NPE-APT is the standard approach now
- Amortized for data, but is prior dependent
- Can be sequential

SBI jargon

- Amortization
  - Learned model *not* specific to one data vector
- Sequential
  - Adaptively acquire simulations

Active learning posteriors



SBI – Neural Likelihood

- Learn conditional likelihood as a function of θ
- Minimise the conditional log likelihood

$$\mathcal{L}(\phi) = \mathrm{E}_{p(\theta,d)}\left[-\log q_{\phi}(d|\theta)\right]$$

SBI – Neural Likelihood

- Can draw simulations any way we want
- Gives access to the likelihood!
- Need sampling for final posterior
- Amortized
- Can be sequential

SBI - Neural Ratio

- Train a classifier to distinguish samples drawn from the joint distribution vs. marginal distribution
- Likelihood ratio trick:

$$r_\phi(d|\theta) = \frac{\boldsymbol{d}^*(d,\theta)}{1-\boldsymbol{d}^*(d,\theta)} \approx \frac{p(\theta|d)}{p(\theta)}$$

- Need sampling for final posterior

Hermans et al. (2020)

SBI – Neural Ratio

- In practice, little overlap between joint and marginal distributions to use as training data set.
- Truncated marginal neural ratio estimation exists to only learn the marginals
- Can be amortized
- Can be sequential

Hermans et al. (2020)

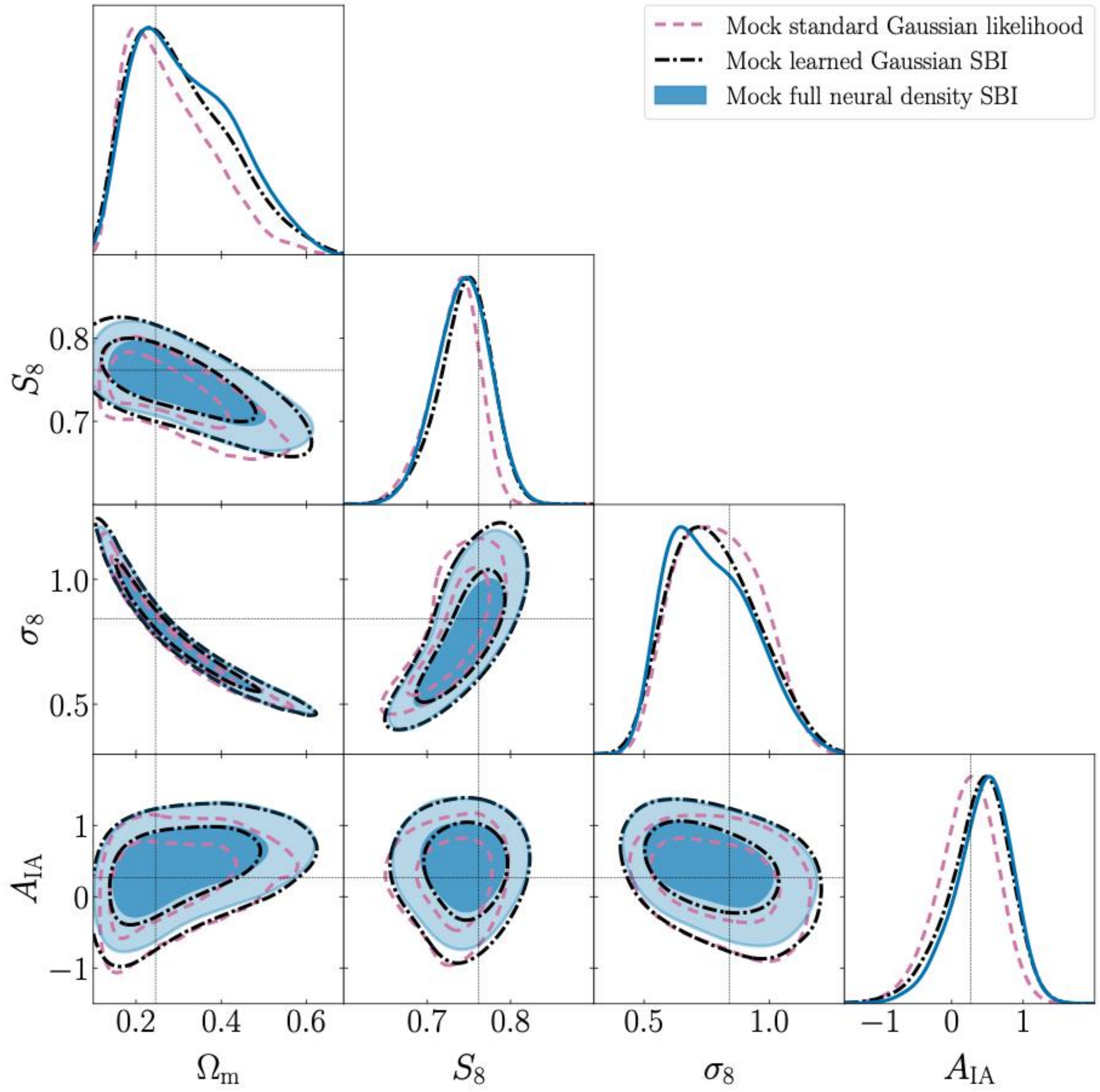
SBI – Software

Github links	NPE	NLE	NRE
https://github.com/sbi-dev/sbi	✅	✅	✅
https://github.com/probabilists/lampe	✅	❌	❌
https://github.com/maho3/ltu-ili	✅	✅	✅
https://github.com/undark-lab/swyft	❌	❌	✅ TMNRE
https://github.com/justinalsing/pydelfi	❌	✅	❌

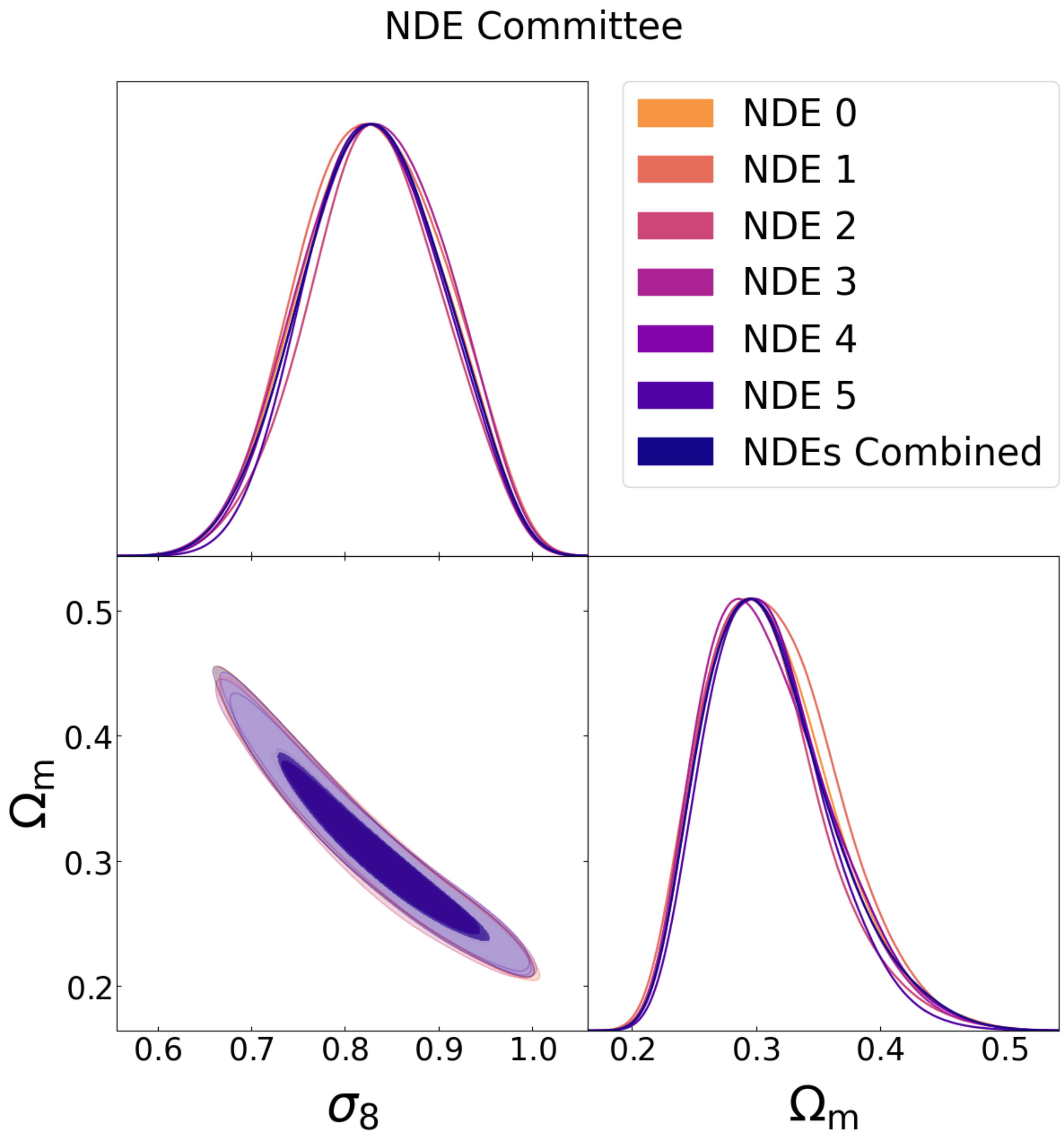
SBI – NDEs

- Mixture density networks
- Masked autoregressive flows
- Neural spline flows
- Real-valued non-volume preserving flows

Papamakarios et al. (2021)



Mock standard Gaussian likelihood
Mock learned Gaussian SBI
Mock full neural density SBI
Ω_m
S_8
σ_8
A_IA
0.2
0.4
0.6
0.7
0.8
0.5
1.0
−1
0
1

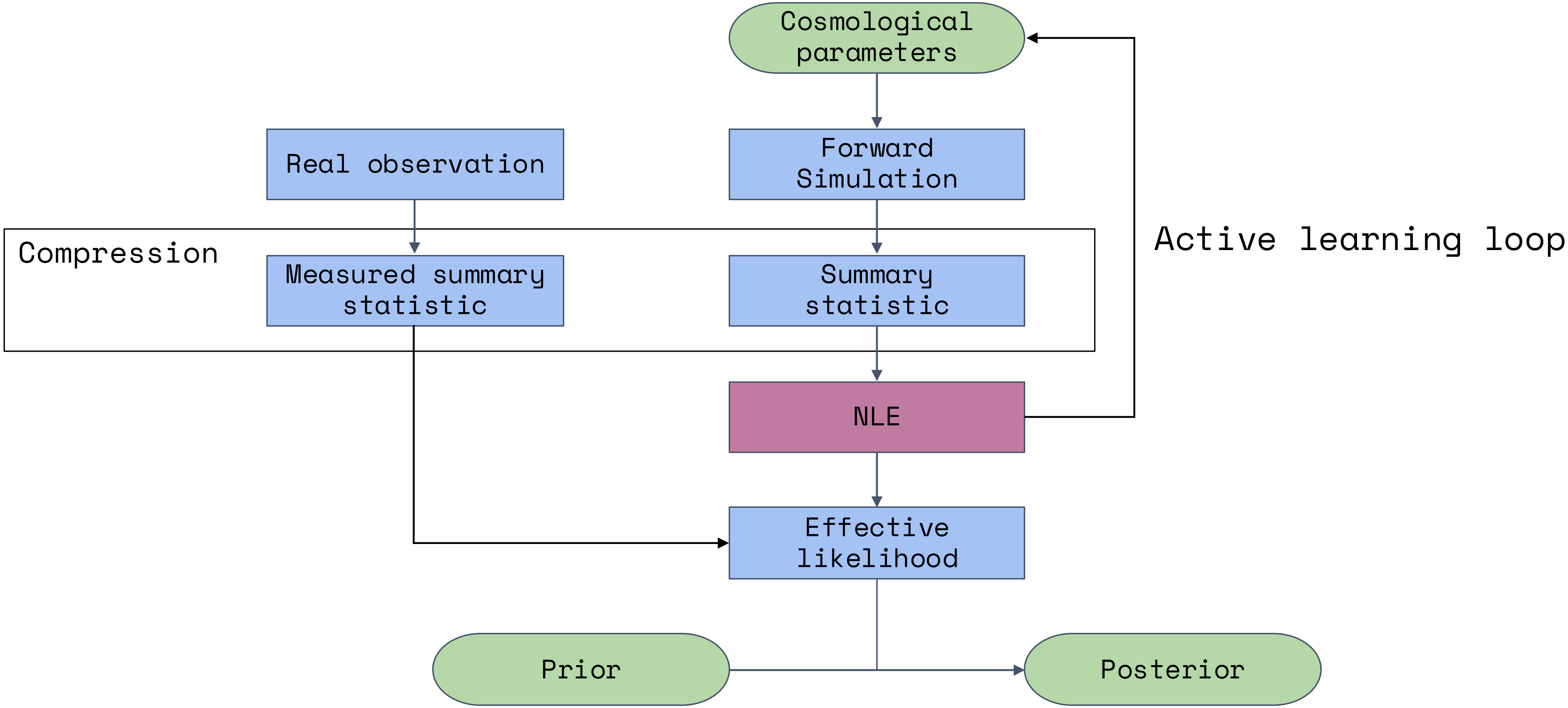


NDE Committee
NDE 0
NDE 1
NDE 2
NDE 3
NDE 4
NDE 5
NDEs Combined
0.5
0.4
0.3
0.2
Ω_m
0.6
0.7
0.8
0.9
1.0
σ_8
0.2
0.3
0.4
0.5
Ω_m

SBI – Compression

- Analytical compression
  - MOPED
  - Score
  - CCA
  - PCA
- Neural compression
  - IMNN
  - Fishnets

SBI – The loop


Cosmological parameters
Real observation
Forward Simulation
Compression
Measured summary statistic
Summary statistic
Active learning loop
NLE
Effective likelihood
Prior
Posterior

SBI – Challenges

- Dimensionality
- Speed
- Validation and Accuracy

SBI – Evidence

- $p(\theta|d,\mathcal{M}) = \frac{p(d|\theta,\mathcal{M})p(\theta|\mathcal{M})}{p(d|\mathcal{M})}$
- $\frac{p(\mathcal{M}_1|d)}{p(\mathcal{M}_2|d)} = \frac{p(d|\mathcal{M}_1)p(\mathcal{M}_1)}{p(d|\mathcal{M}_2)p(\mathcal{M}_2)}$
- Nested Sampling
- Learned Harmonic Mean (McEewen et al 2021)
- Evidence Networks (Jeffrey & Wandelt 2023)

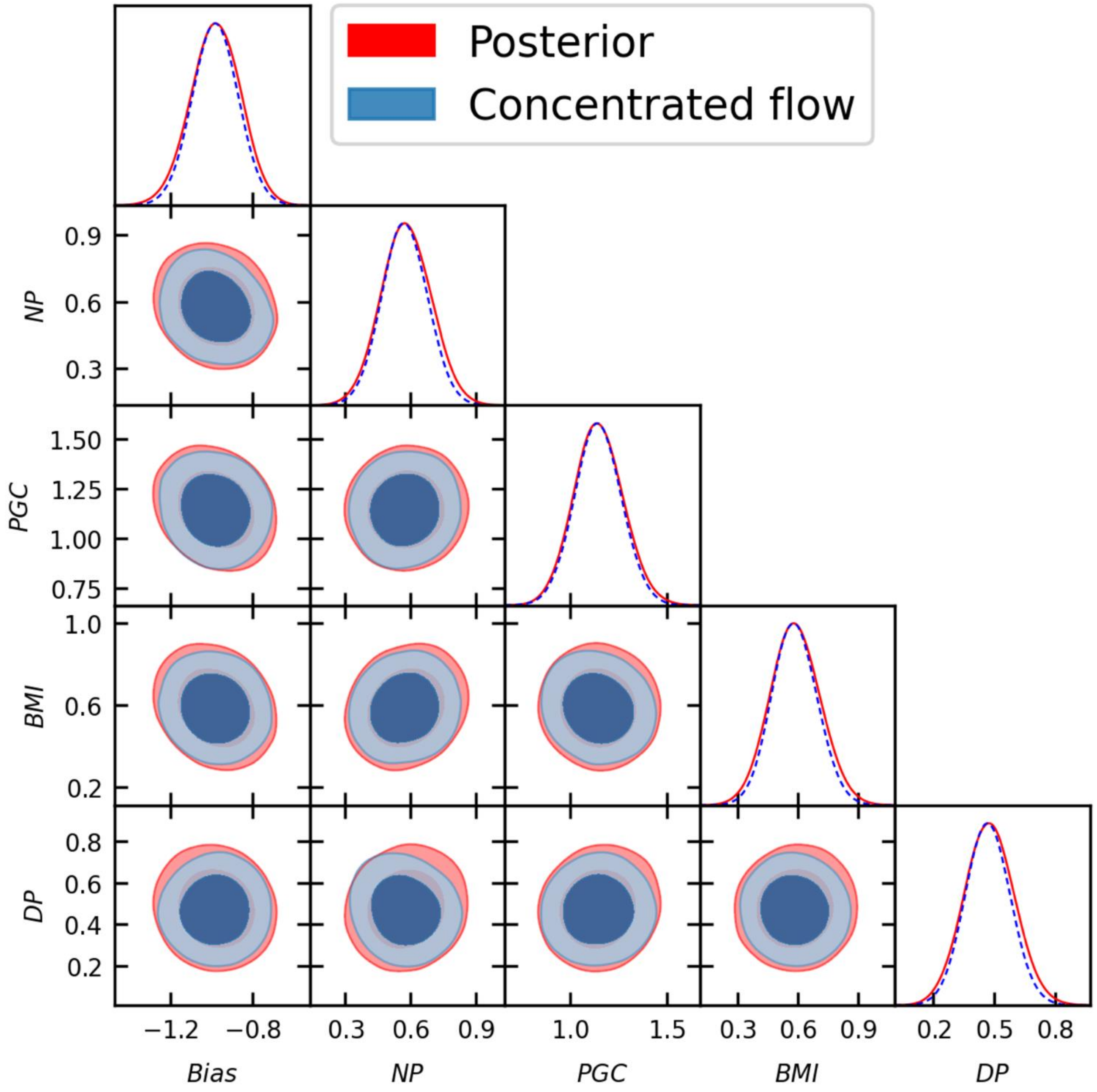
SBI – Evidence

- Learned Harmonic mean –
  - Get evidence directly from posterior samples!

In practice, a shrunk posterior!

$$\frac{1}{z} = \frac{1}{N}\sum_{i=1}^{N} \frac{\varphi(\theta_i)}{\mathcal{L}(d|\theta_i)\pi(\theta_i)}, \qquad \theta_i \sim p(\theta|d)$$

Mcewen et al. (2021), Polanska et al. (2024)



Polanska et al. (2024)

Savage-Dickey density ratio

- SDDR for nested models

$$\frac{z_1}{z_2} = \frac{p(\eta_1|d, M_2)}{\pi(\eta_1|M_2)}$$

- For high dimensional marginals, can make use of normalizing flows!
- Both implemented in harmonic package:
  - https://github.com/astro-informatics/harmonic

Demo notebook

https://github.com/Kiyam/astrodat-2025

Thank you for listening, questions?