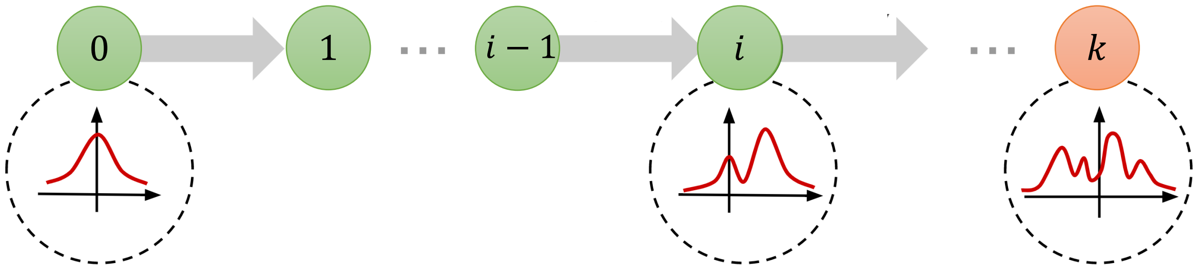
Normalizing flows for machine learning assisted Bayesian model comparison

Alicja Polanska, Matthew A. Price, Davide Piras, Alessio Spurio Mancini and Jason D. McEwen



Learned harmonic mean estimator

Estimator of the Bayesian evidence

Use with any MCMC sampler or on saved down chains

harmonic Python package

github.com/astro-informatics/harmonic

Outline of this talk

1. Learned harmonic mean estimator
2. Numerical experiments
3. High-dimensional model comparison for cosmology

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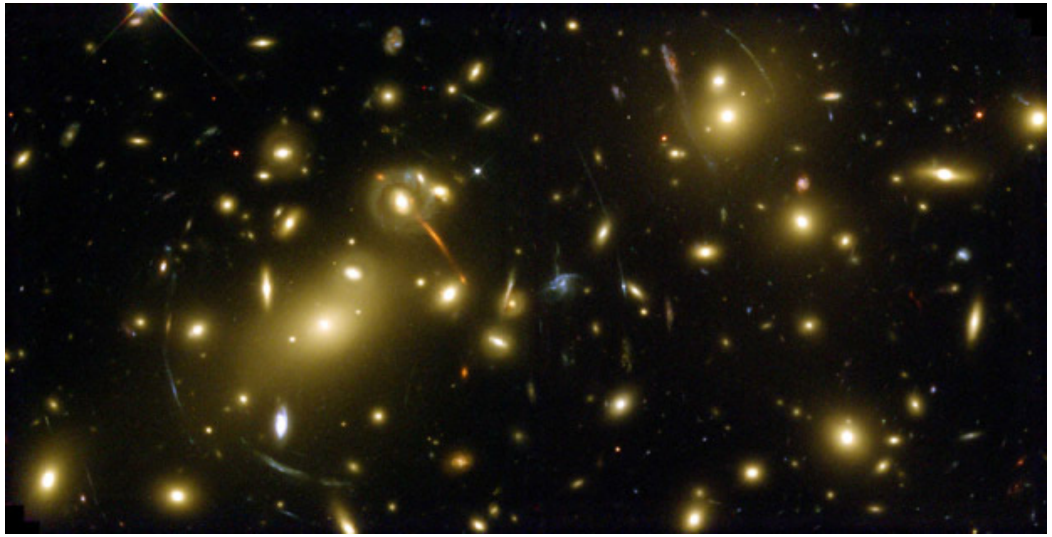
Model comparison

What model best describes the universe?



ΛCDM or wCDM?

Bayesian model comparison

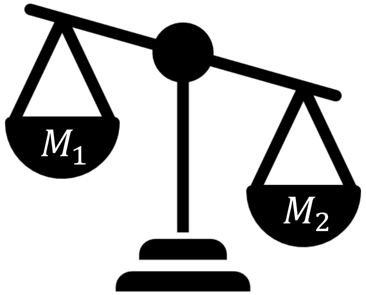
In the Bayesian framework probability distributions provide a quantification of uncertainty.

$$P(\theta|\boldsymbol{y}, M) = \frac{\overbrace{P(\boldsymbol{y}|\theta, M)}^{\text{Likelihood}}\,\overbrace{P(\theta|M)}^{\text{Prior}}}{\underbrace{P(\boldsymbol{y}|M)}_{\text{Bayesian Evidence}}} = \frac{\mathcal{L}(\theta)\pi(\theta)}{z}$$

$$z = \mathrm{P}(\boldsymbol{y}|M) = \int \mathrm{d}\theta\, \mathcal{L}(\theta)\pi(\theta)$$

Which model to choose?

Bayesian evidence tells us which scientific model is more plausible



Very useful but hard to compute!

Harmonic mean estimator

Estimator of evidence (Newton and Raftery, 1994)

$$\rho = \mathbb{E}_{P(\theta|\boldsymbol{y})}\left[\frac{1}{\mathcal{L}(\theta)}\right] = \frac{1}{z}$$

☺ It's agnostic to sampling method $\longrightarrow$ It's flexible

☹ But…. fails catastrophically

Why does it fail?

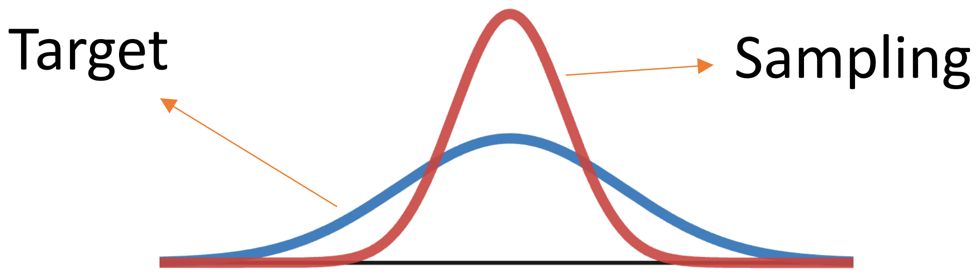
Can be interpreted as importance sampling

$$\rho = \int \mathrm{d}\theta \, \frac{1}{\mathcal{L}(\theta)} \, \mathrm{P}(\theta \,|\, y)$$

$$= \int \mathrm{d}\theta \, \frac{1}{z} \, \frac{\pi(\theta)}{\mathrm{P}(\theta \,|\, y)} \, \mathrm{P}(\theta \,|\, y)$$

Target density

Sampling density



Target density has fatter tails than sampling density

Harmonic mean estimator fails

Learned harmonic mean estimator

Introduce arbitrary normalized target density $\varphi(\theta)$ (Gelfand and Dey, 1994)

$$\rho = \mathbb{E}_{P(\theta|\boldsymbol{y})}\left[\frac{1}{\mathcal{L}(\theta)}\right] = \frac{1}{z} \quad \Rightarrow \quad \boxed{\rho = \mathbb{E}_{P(\theta|\boldsymbol{y})}\left[\frac{\varphi(\theta)}{\mathcal{L}(\theta)\pi(\theta)}\right]}$$

Learned harmonic mean estimator

Introduce **learned harmonic mean estimator** (McEwen et al., 2021) :

$\varphi(\theta)$ is learned from posterior samples

$$\psi^{\text{ML}} \approx \psi^{\text{optimal}}(\theta) = \frac{\mathcal{L}(\theta)\pi(\theta)}{z}$$

$$\rho = \mathbb{E}_{P(\theta|\boldsymbol{y})}\left[\frac{\varphi(\theta)}{\mathcal{L}(\theta)\pi(\theta)}\right]$$

Learned harmonic mean estimator

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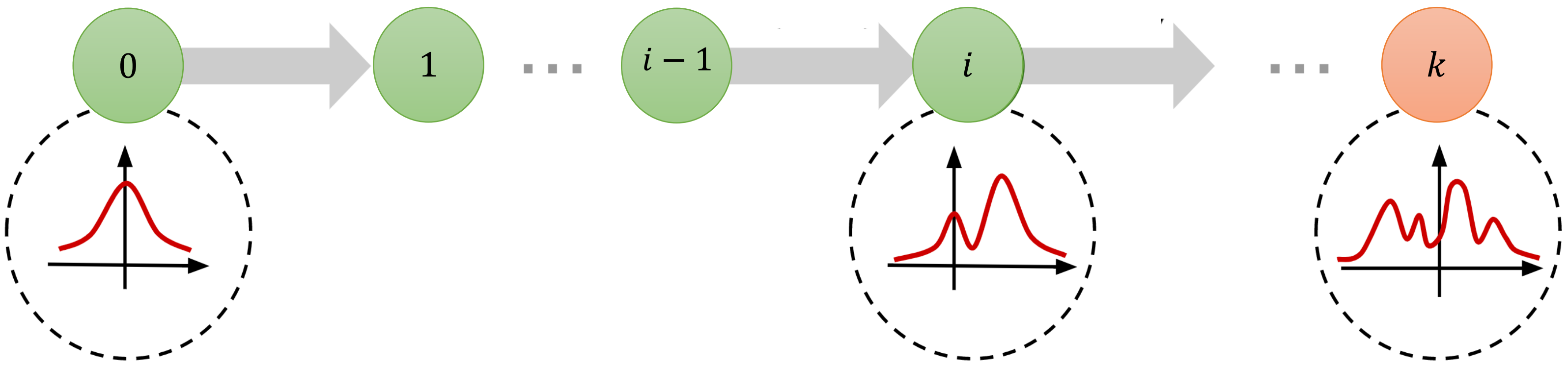
☹ Requires bespoke training approach and fine-tuning

➡ Use normalizing flows to solve these issues!

(Polanska et al., 2024)
arXiv:2405.05969

Normalizing flows

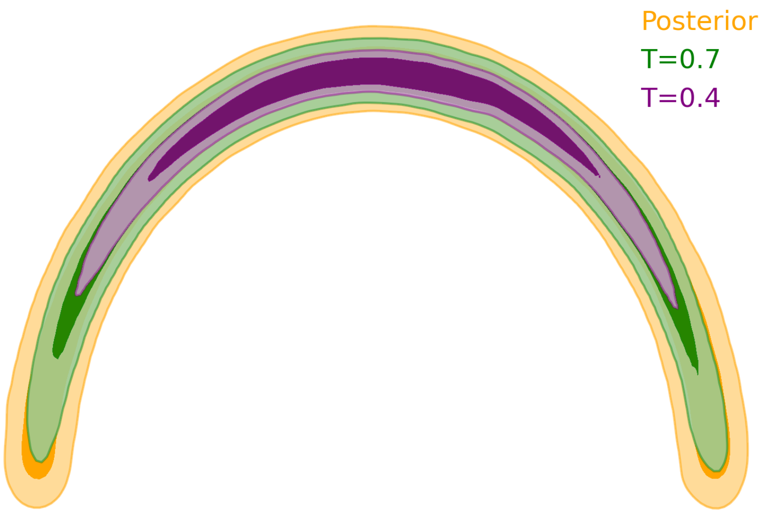
Normalizing flows take a simple base distribution through a series of reversible transformations to approximate a complex distribution



Adapted from lilianweng.github.io/posts/2018-10-13-flow-models

We use real non-volume preserving and rational-quadratic spline flows

Concentrating the target distribution



We train a flow on samples from the posterior and introduce temperature parameter T to concentrate the probability density

The base distribution variance is scaled by

$$0 < T < 1$$

Learned harmonic mean estimator

Train normalizing flow on posterior samples

Concentrate probability density

Use concentrated flow as $\varphi(\theta)$

Evidence estimate

$$\rho = \mathbb{E}_{P(\theta|\boldsymbol{y})}\left[\frac{\varphi(\theta)}{\mathcal{L}(\theta)\pi(\theta)}\right]$$

Learned harmonic mean estimator

Our method provides a tool for Bayesian model comparison that is:

- ☑ Accurate
- ☑ Scalable
- ☑ Robust
- ☑ Flexible

SciAI UCL

harmonic software

harmonic Python package[1] has been made available in the new release of harmonic on PyPi and GitHub

HARMONIC

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[1]github.com/astro-informatics/harmonic

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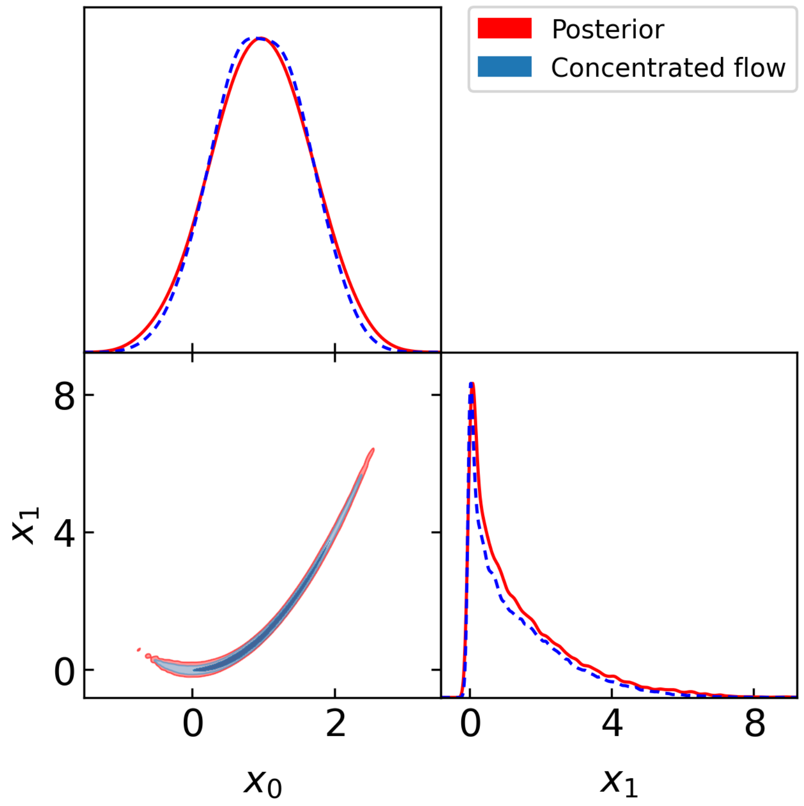
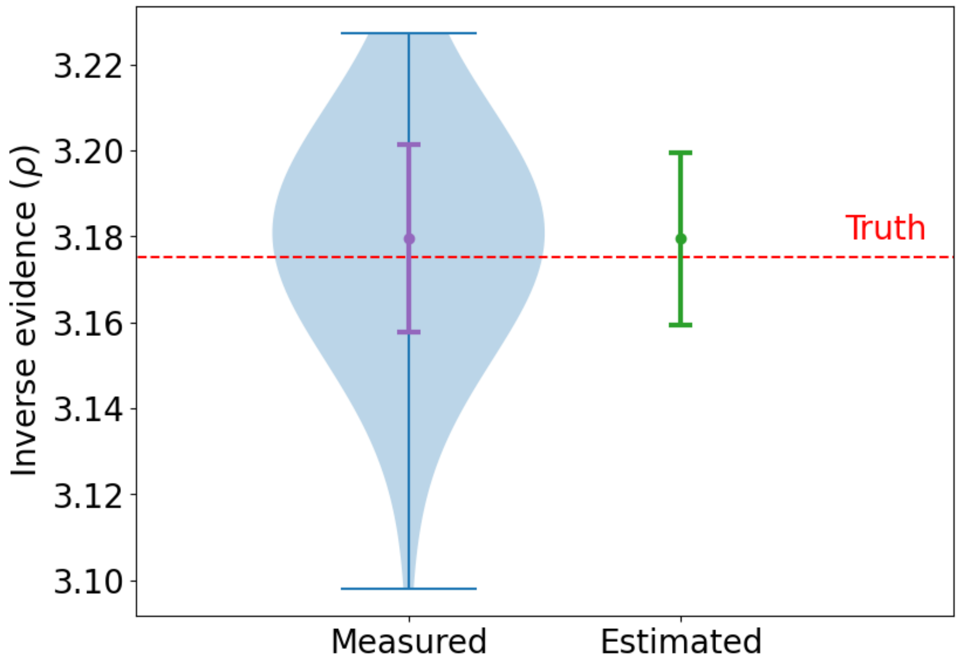
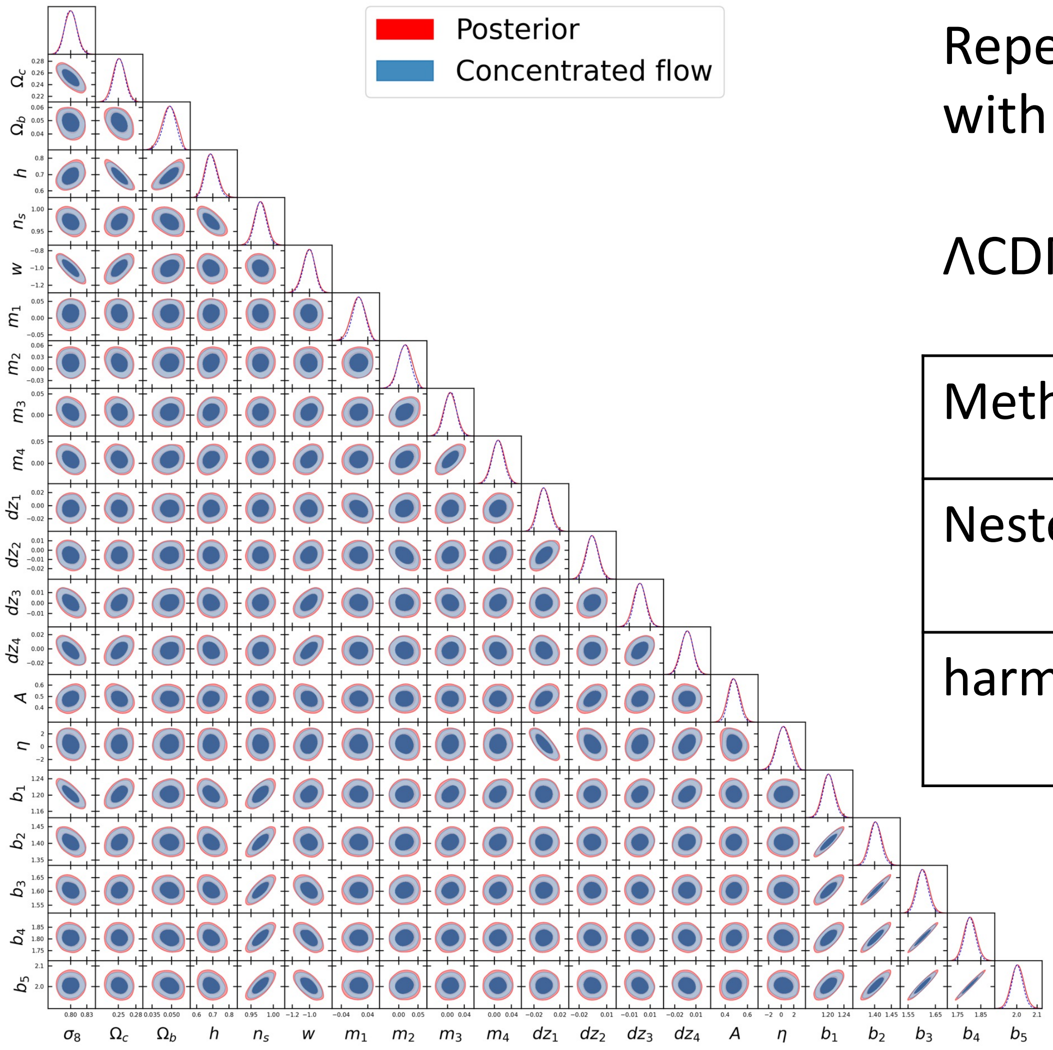
Rosenbrock example





DES Y1 Example



Repeat DES Y1 3x2pt analysis from (Campagne et al., 2023) with harmonic

ΛCDM vs wCDM in 20D

Method	$\Delta \log z$	Computation time
Nested sampling	2.23 ± 0.64	94h on 64 CPU
harmonic	2.15 ± 0.01	16h on 64CPU + 16min

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High-dimensional model comparison for cosmology

Emulation (CosmoPower-JAX)

+

Differentiable and probabilistic programming

+

Scalable sampling (NUTS)

+

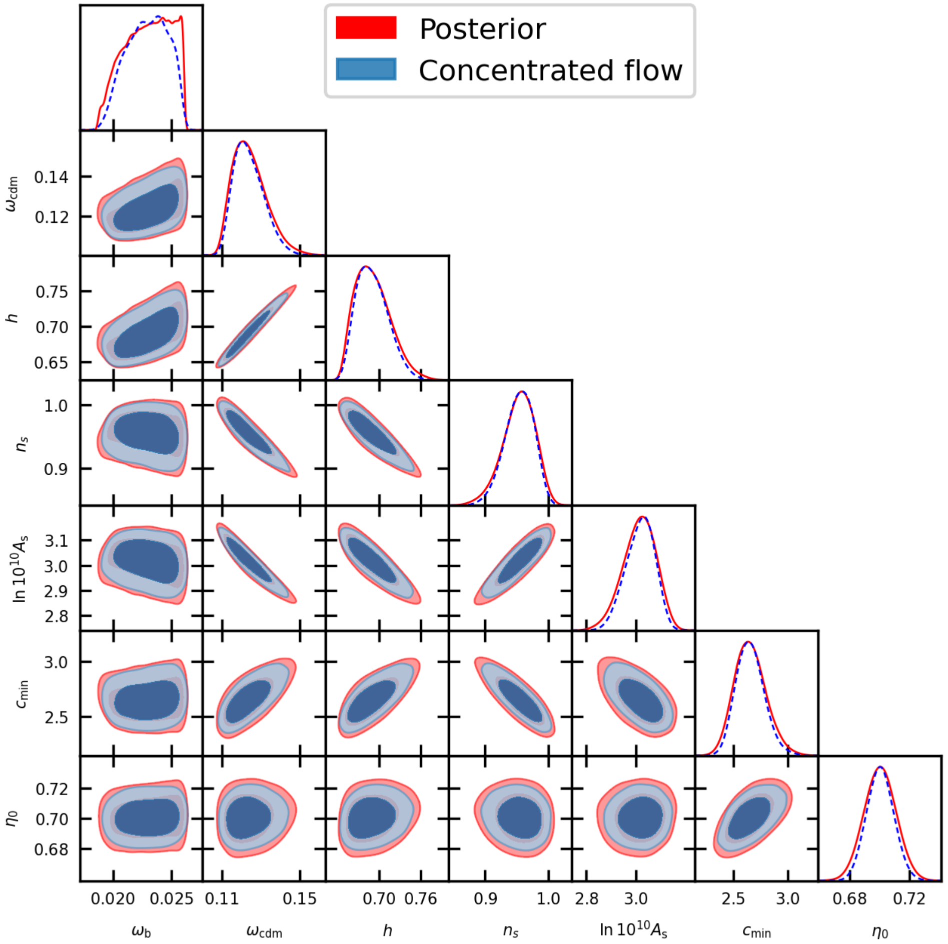
Decoupled and scalable evidence (*harmonic)*

=

The future of cosmological likelihood-based inference…

(Piras et al., 2024) arXiv:2405.12965

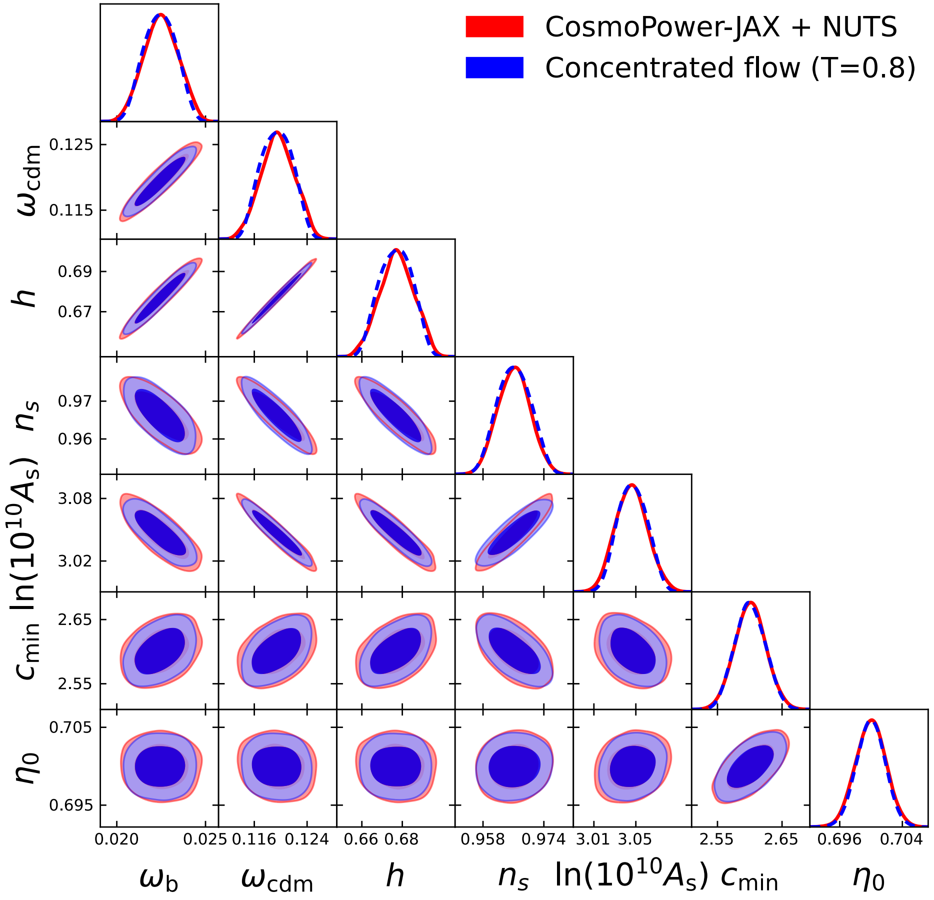
High-dimensional model comparison for cosmology



ΛCDM vs $w_0 w_a$CDM in 37/39D

Method	$\Delta \log z$	Computation time
CAMB + Nested sampling	0.78 ± 0.79	8 months on 48 CPUs
CosmoPower-JAX + NUTS + harmonic	$1.53^{0.07}_{-0.07}$	2 days on 12 GPUs

High-dimensional model comparison for cosmology



ΛCDM vs $w_0 w_a$CDM in 157/159D

Method	$\Delta \log z$	Computation time
CAMB + Nested sampling	Not feasible	Estimated 12 years on 48 CPUs
CosmoPower-JAX + NUTS + harmonic	$1.9^{0.7}_{-0.5}$	8 days on 24 GPUs

Summary: Learned harmonic mean

Method to estimate the evidence that is

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- ☑ **Accurate:** based on a principled statistical framework
- ☑ **Robust:** no fine-tuning
- ☑ **Scalable:** analysis in 159 dimensions
- ☑ **Flexible:** use with any MCMC sampler, saved down chains, or any variational inference approach…

Summary: Learned harmonic mean

Method to estimate the evidence that is

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- **Robust:** no fine-tuning
- **Scalable:** analysis in 159 dimensions
- **Flexible:** use with any MCMC sampler, saved down chains, or any variational inference approach…

… or your application!

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References

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