

# Fast likelihood-free inference in the LSS Stage-IV era

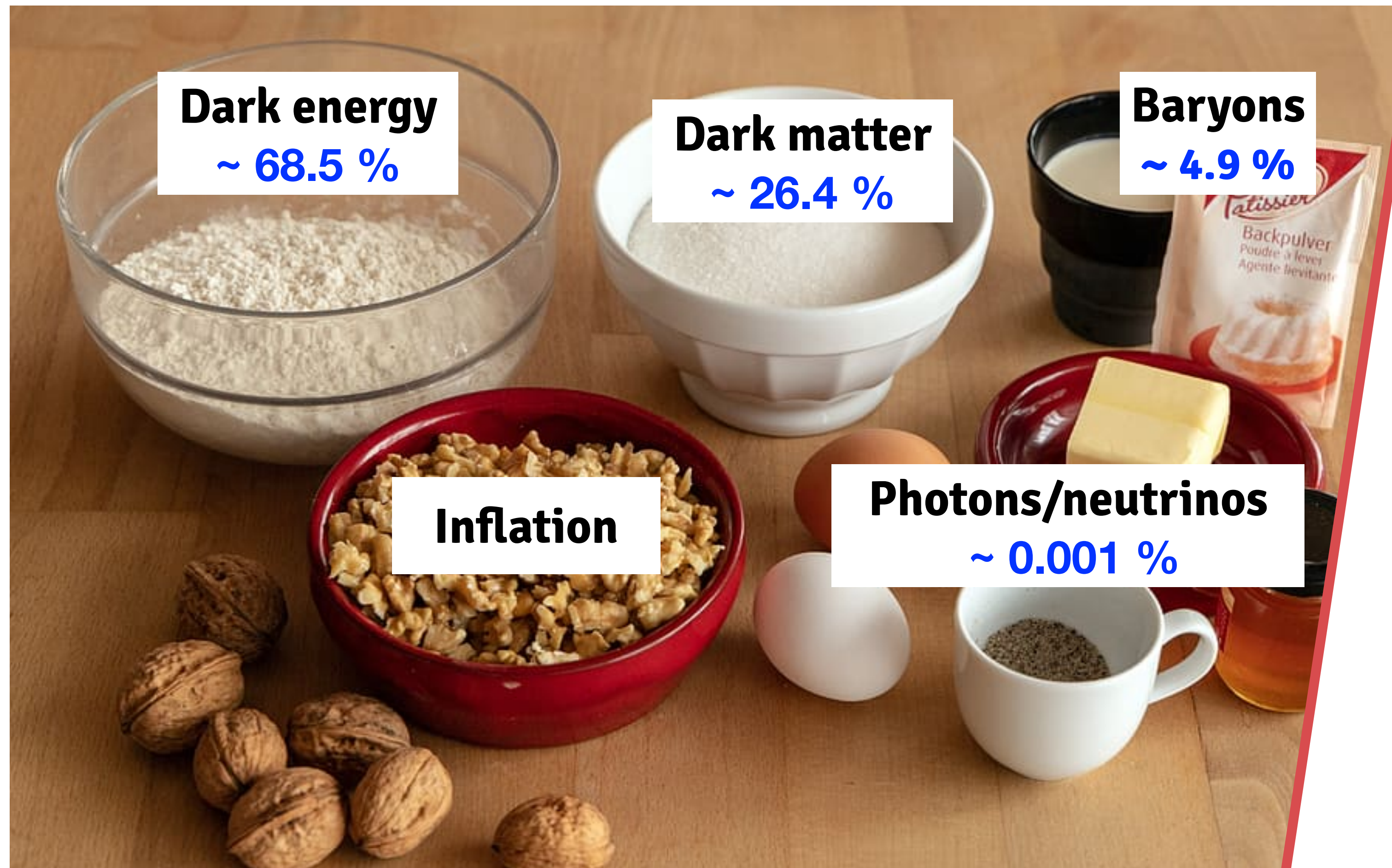
Guillermo Franco Abellán



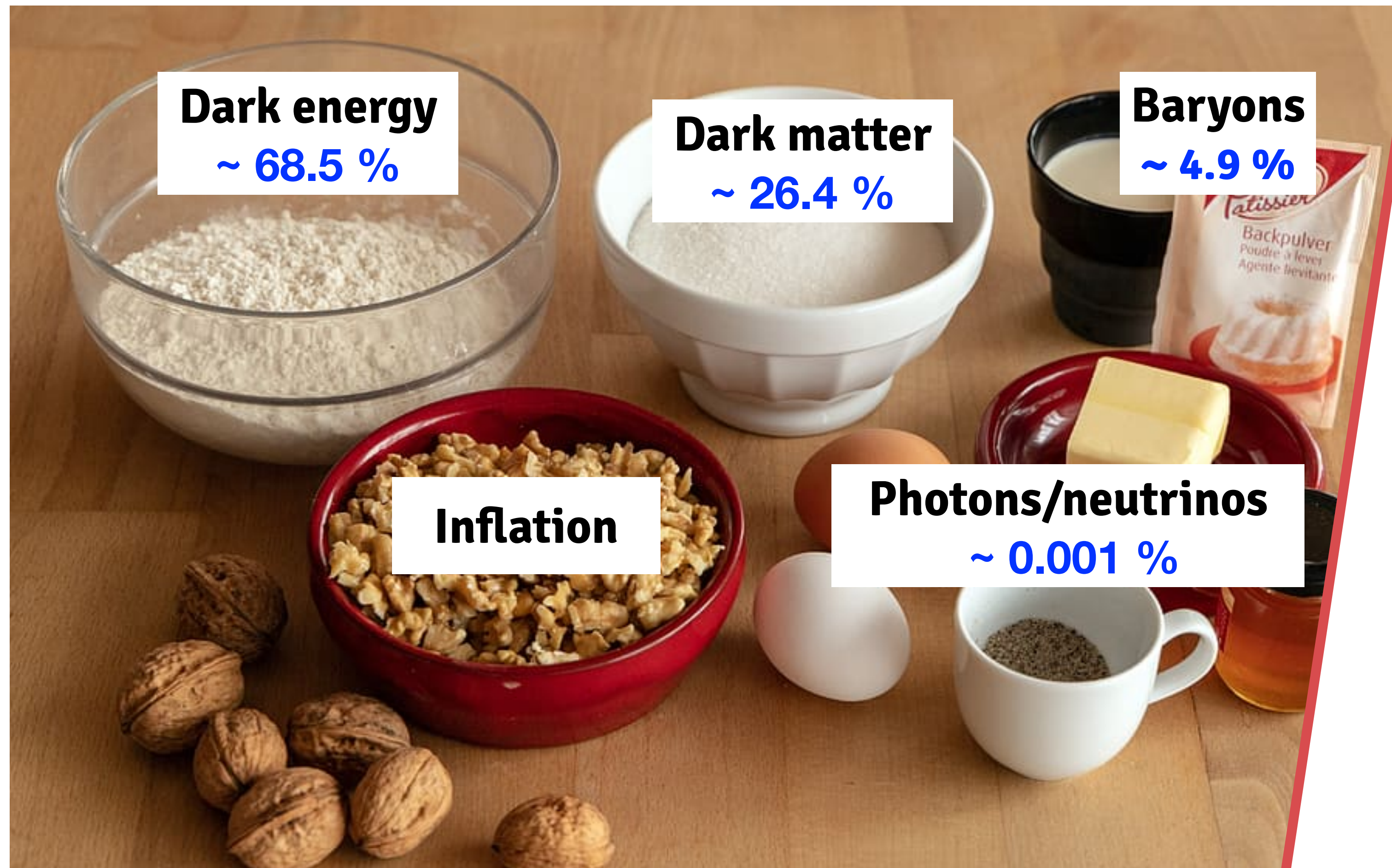
Based on [arXiv:2403.14750](https://arxiv.org/abs/2403.14750)  
with Guadalupe Cañas-Herrera,  
Matteo Martinelli,  
Oleg Savchenko,  
Davide Sciotti,  
& Christoph Weniger

Euclid TWG/WP17 - 26th April 2024

# Concordance $\Lambda$ CDM model of cosmology:

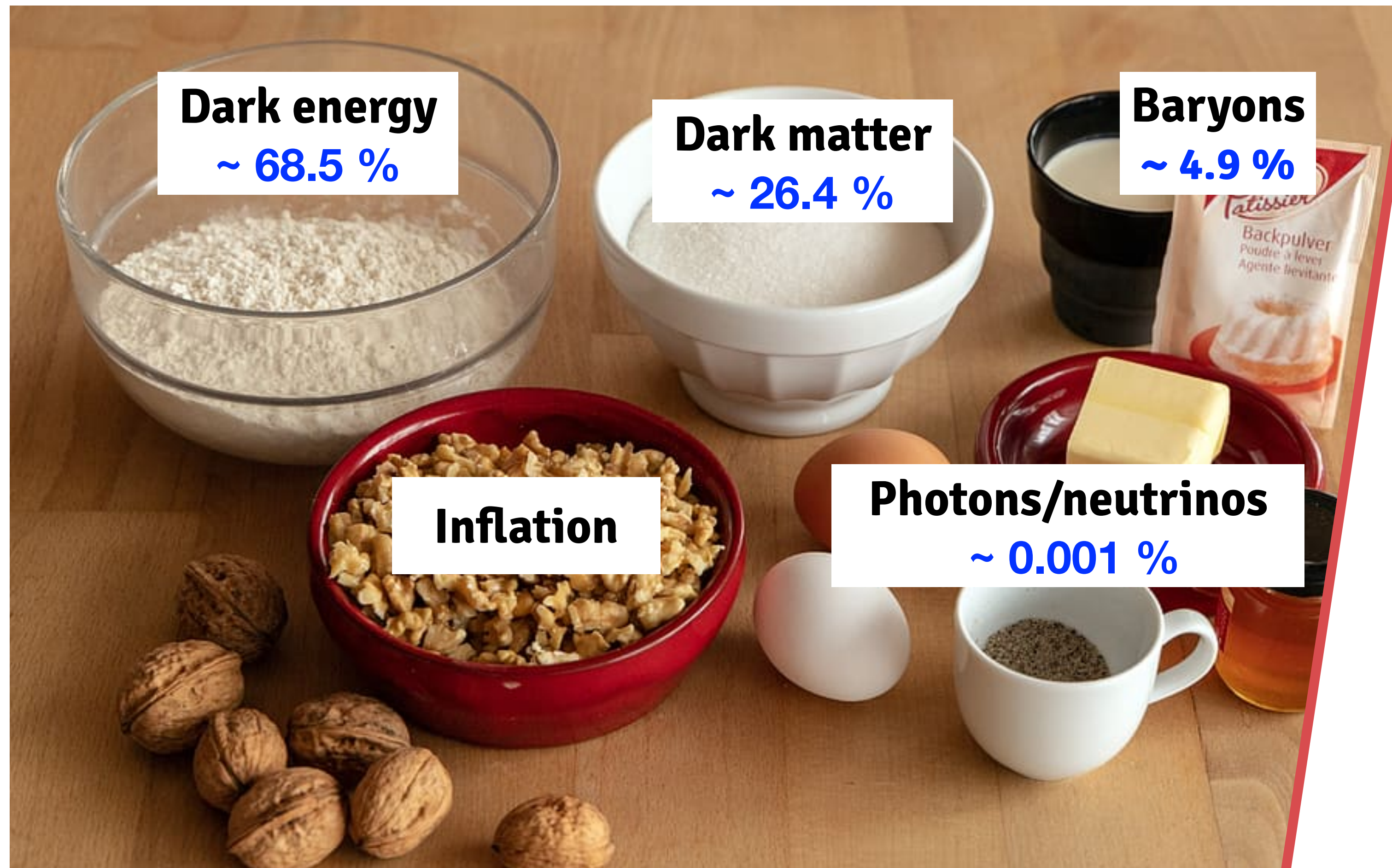


# Concordance $\Lambda$ CDM model of cosmology:



Some open problems:

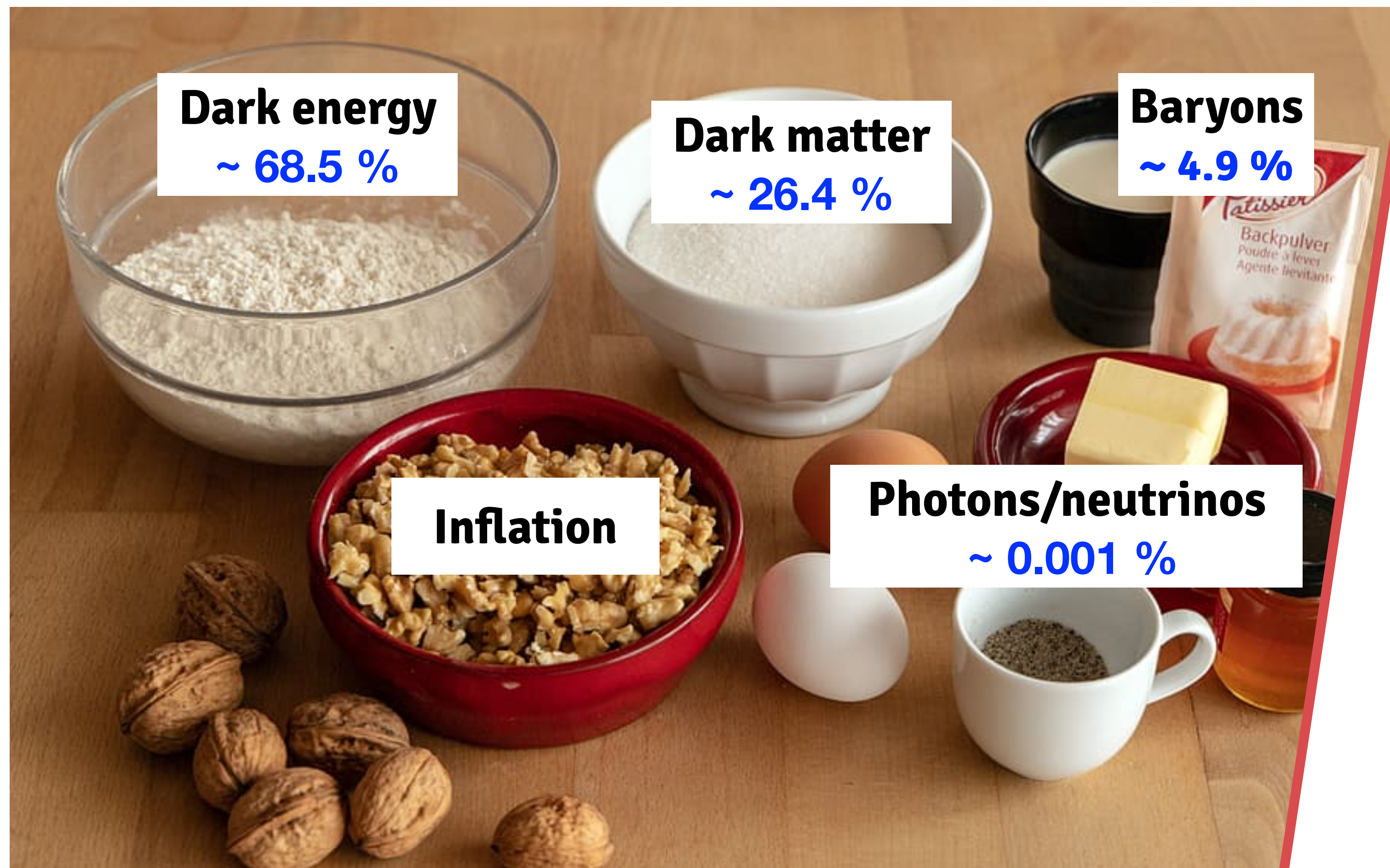
# Concordance $\Lambda$ CDM model of cosmology:



Some open problems:

■ **Nature of dark sector?**

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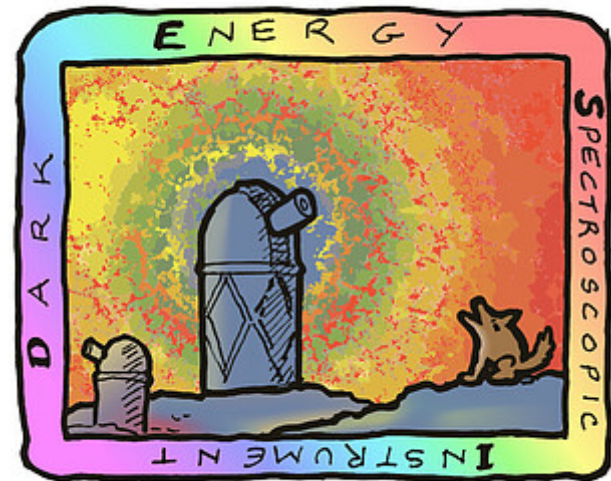
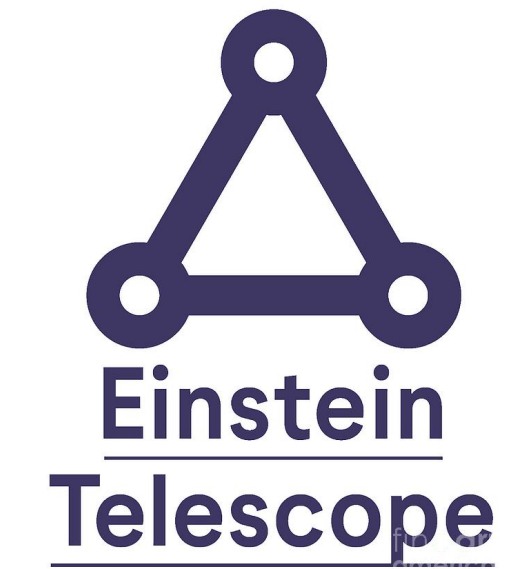
- Nature of dark sector?
- $H_0/S_8$  tensions?

Growing interest in testing  $\Lambda$ CDM extensions...

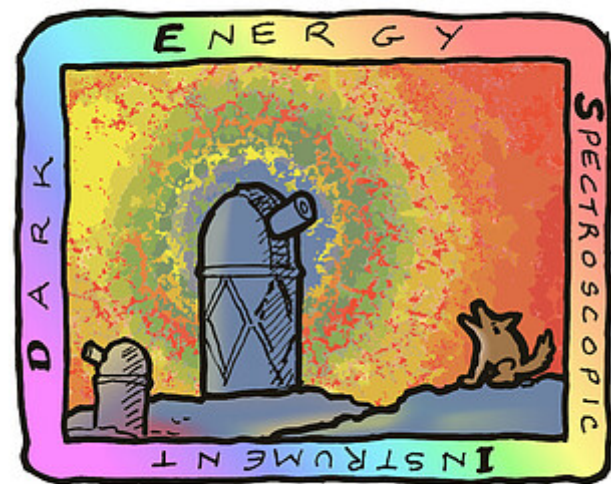
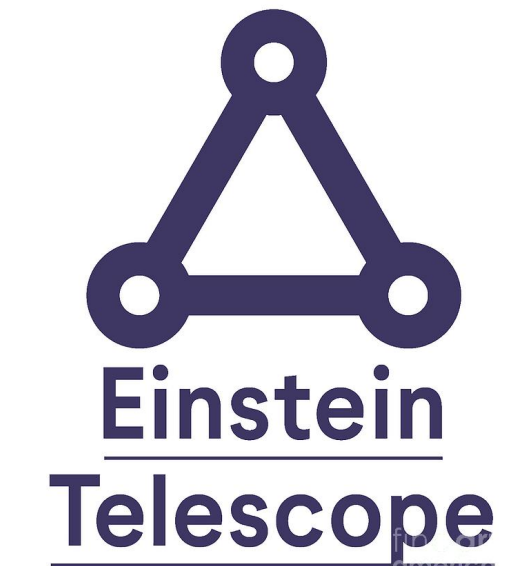
Growing interest in testing  $\Lambda$ CDM extensions...

...but still no smoking-gun signature of new physics

# Next-generation cosmological data is becoming available



# Next-generation cosmological data is becoming available



Analysing these high-quality data will be extremely challenging with traditional methods

# Outline

I. Why we need to go **beyond MCMC**

II. Our new approach: **Marginal Neural Ratio Estimation**

III. Applying MNRE to **Stage IV** photometric observables

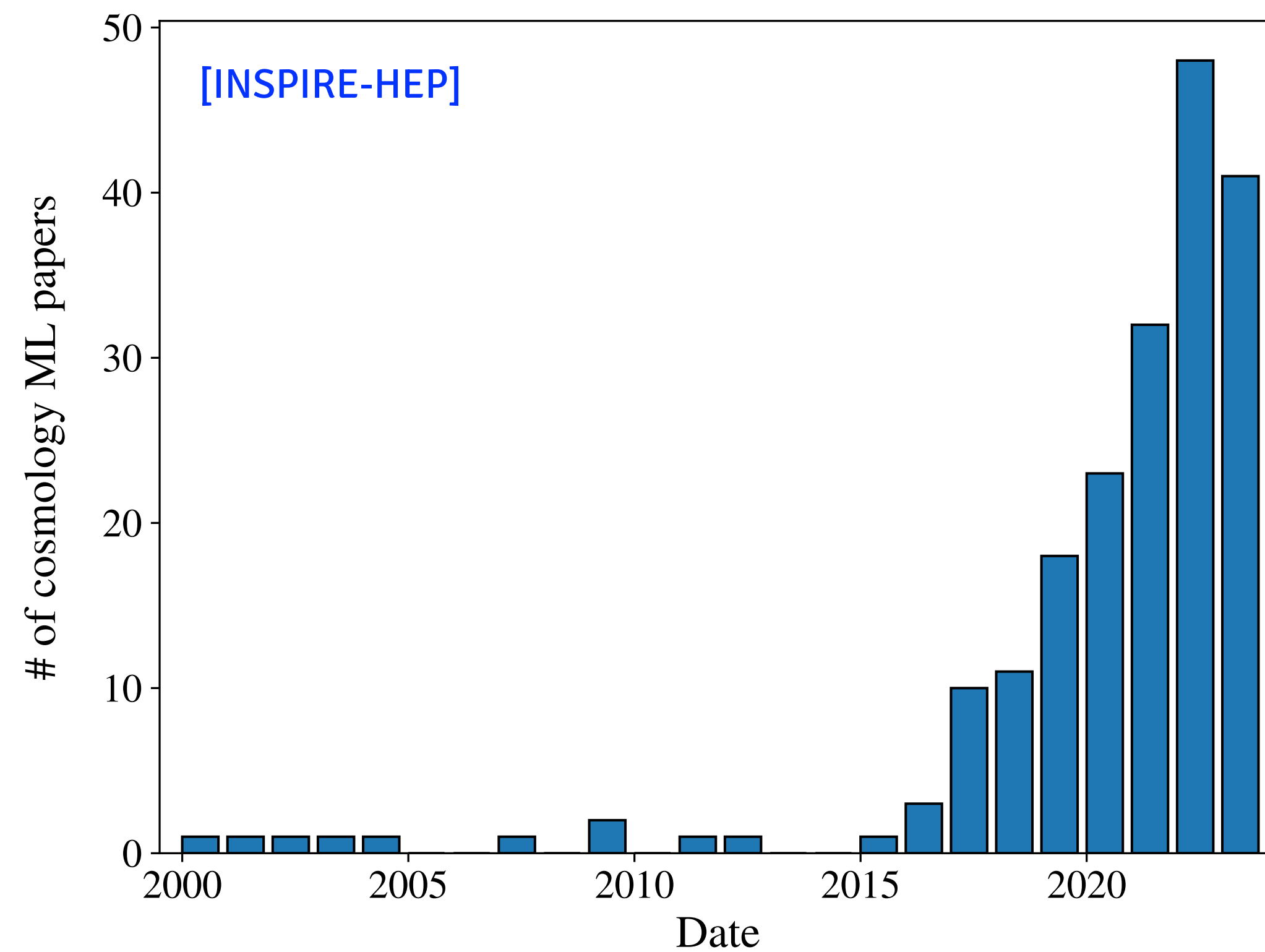
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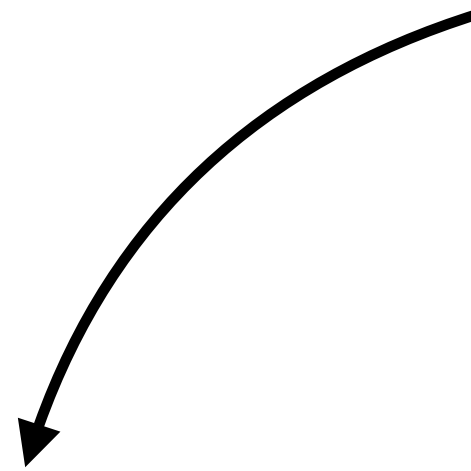
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Machine learning is  
having a **strong impact**  
in cosmology

# **Two main approaches in ML**

## Two main approaches in ML



### **Emulators**

to achieve **ultra-fast** evaluations  
of cosmological observables

## Two main approaches in ML



```
graph TD; A[Two main approaches in ML] --> B[Emulators]; A --> C[New statistical methods];
```

### Emulators

to achieve **ultra-fast** evaluations of cosmological observables

### New statistical methods

to improve the sampling in **high-dimensional** parameter spaces

## Two main approaches in ML



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### New statistical methods

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**This talk**

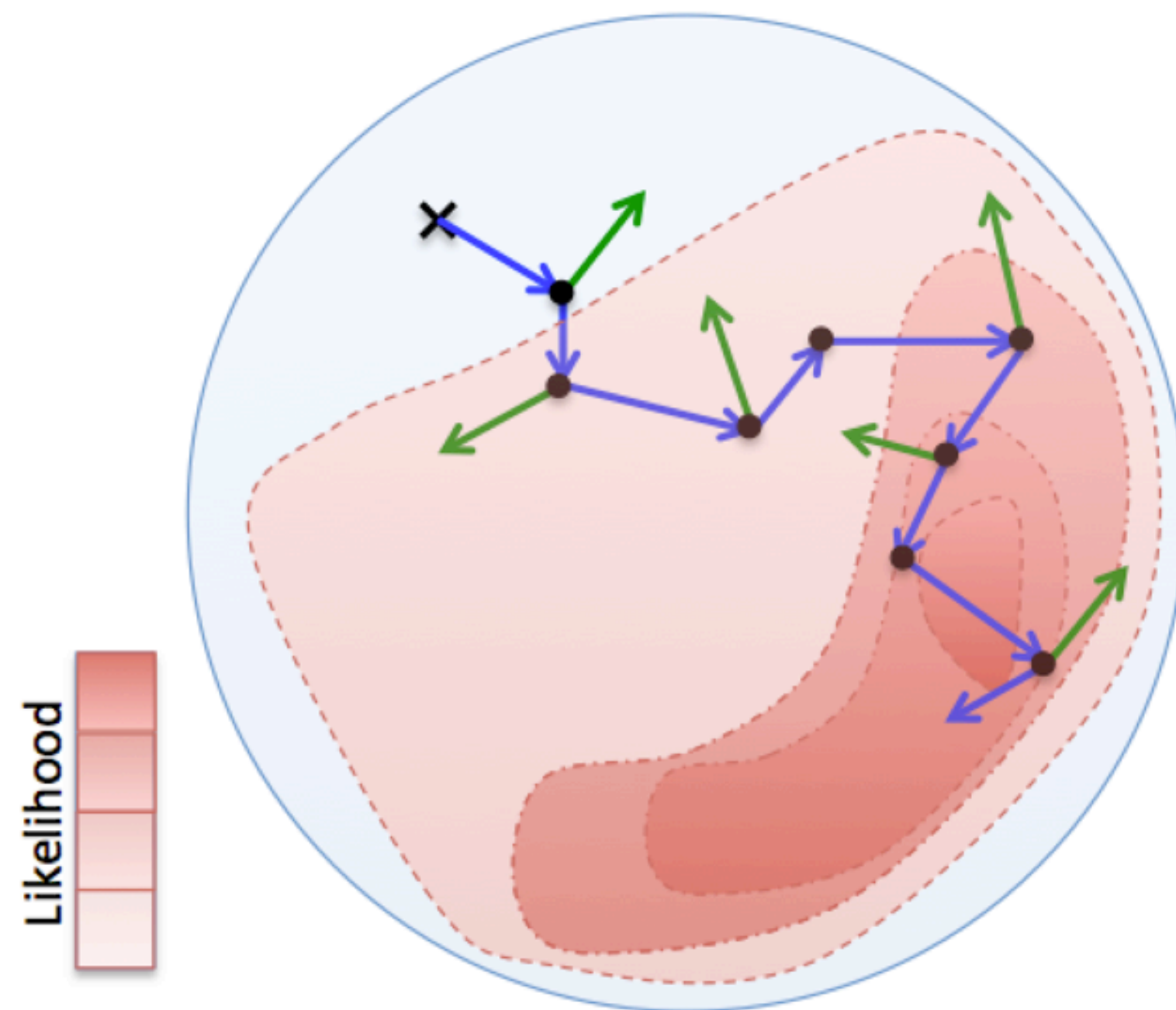
# Bayesian inference

$$\begin{array}{ccccc} & & \text{Likelihood} & & \\ & \text{Posterior} & & \text{Prior} & \\ & p(\theta | \mathbf{x}) & = & \frac{p(\mathbf{x} | \theta)}{p(\mathbf{x})} & p(\theta) \\ & & & \text{Evidence} & \end{array}$$

$\mathbf{x}$  : Data

$\theta$  : Parameters

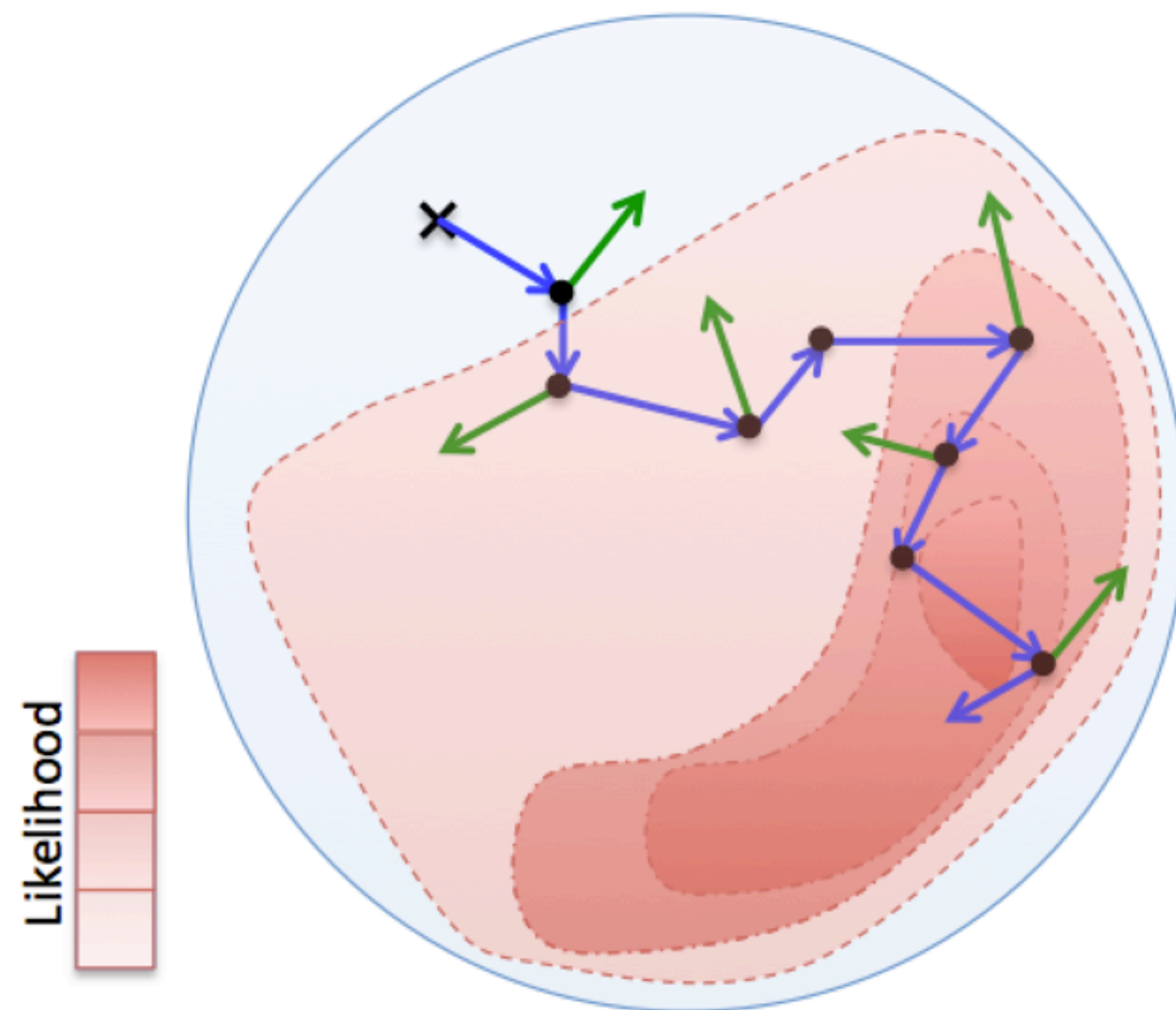
## Metropolis-Hastings algorithm



Traditional **likelihood-based** methods (MCMC, Nested Sampling,...) allow to get samples from the **full joint posterior**

$$\boldsymbol{\theta} \sim p(\boldsymbol{\theta} \mid \mathbf{x}), \quad \boldsymbol{\theta} \in \mathbb{R}^D$$

## Metropolis-Hastings algorithm



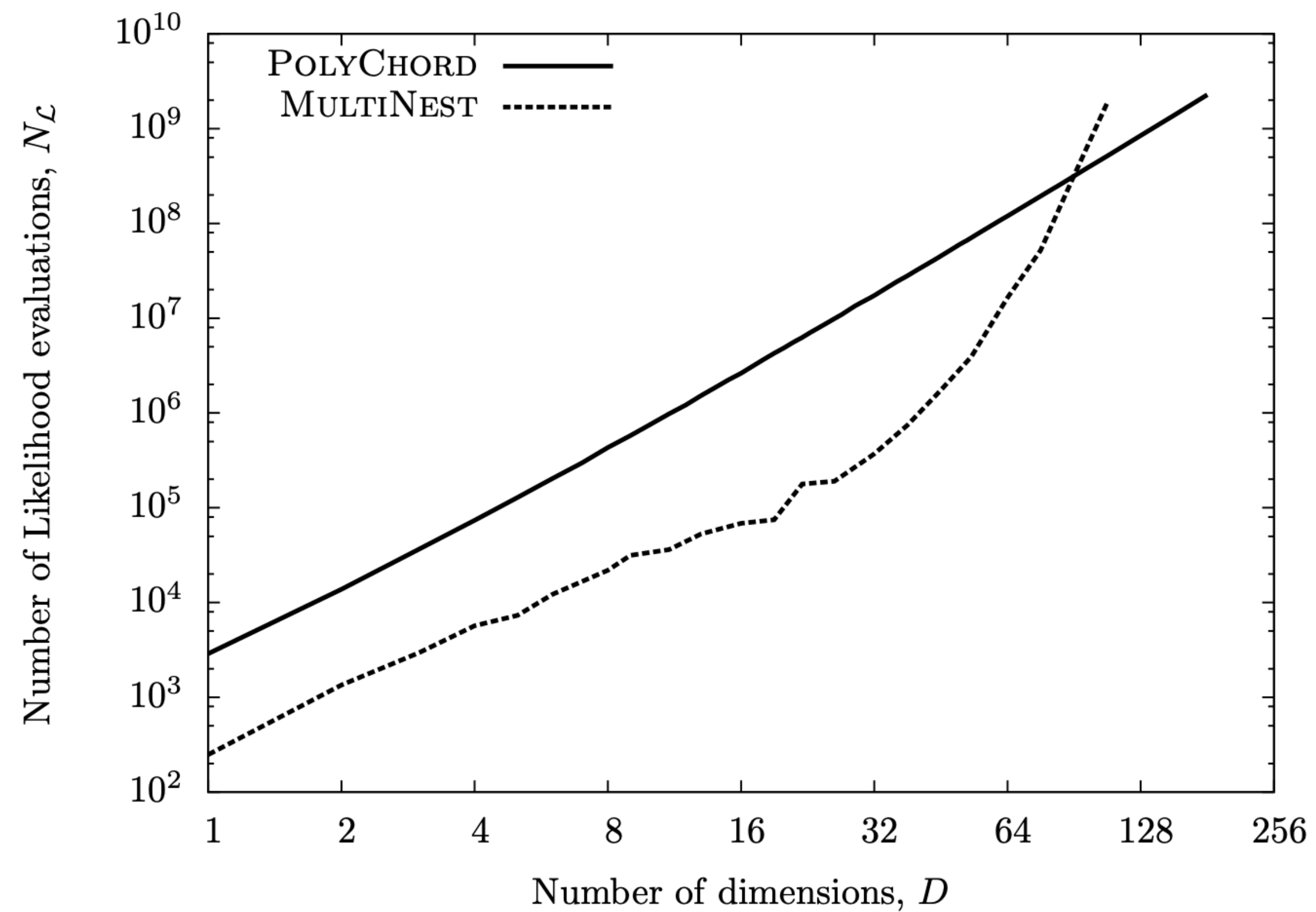
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Then we **marginalise** to get posteriors of interest

# The curse of dimensionality

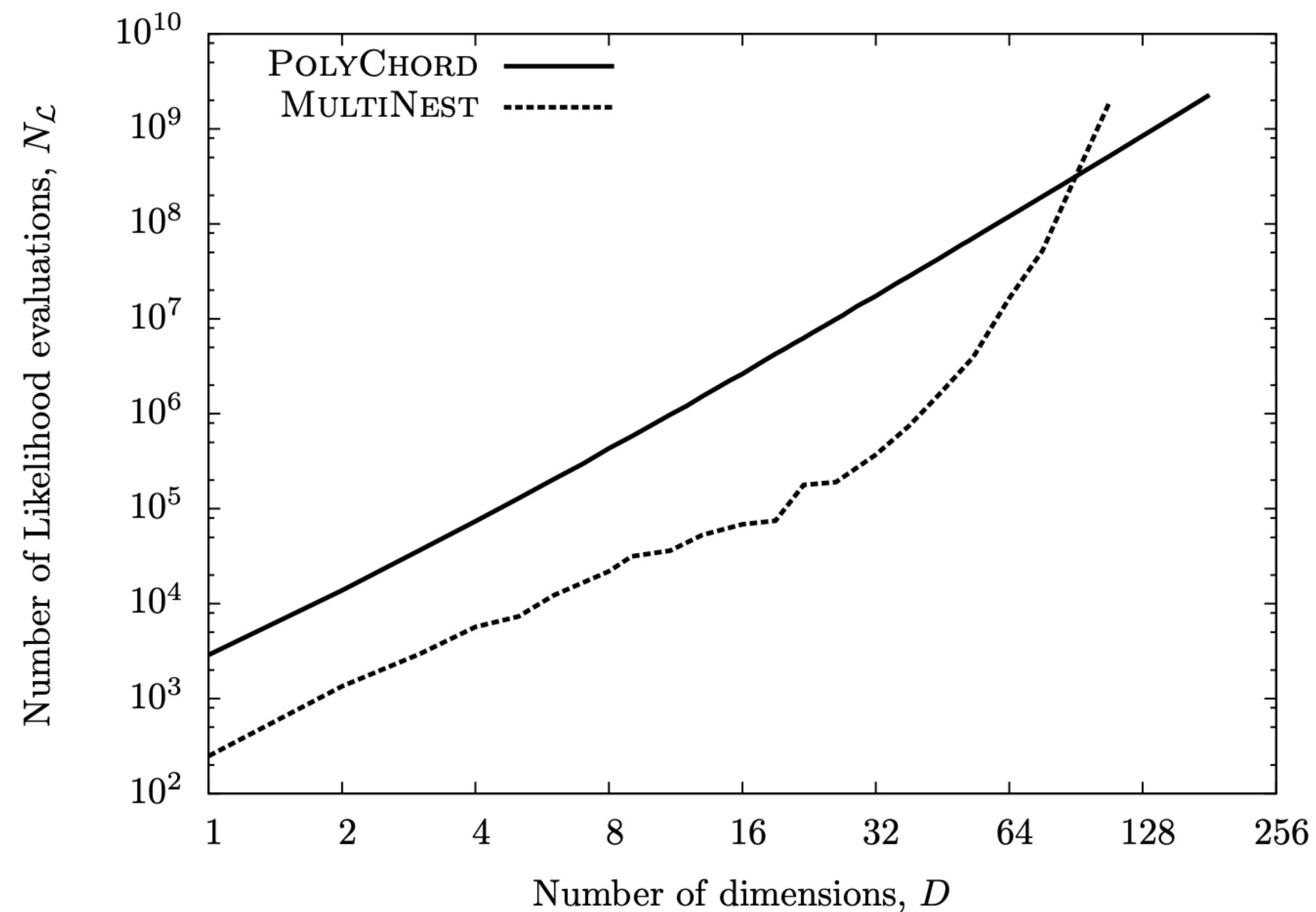
These methods **scale poorly** with the **dimensionality** of the parameter space



[Handley+ 15](#)

# The curse of dimensionality

These methods **scale poorly** with the **dimensionality** of the parameter space



[Handley+ 15](#)

**Ex: For Stage IV surveys, we expect  
~100 nuisance parameters**



Weeks...

**Are there methods to overcome this problem?**

**Are there methods to overcome this problem?**

**Can machine learning be helpful?**

# A NEW HOPE

**MNRE = Marginal Neural Ratio Estimation**

Implemented in [Swyft\\*](#) [\[Miller+ 20\]](#)

\* Stop Wasting Your Precious Time

I. Why we need to go **beyond MCMC**

II. Our new approach: **Marginal Neural Ratio Estimation**



III. Applying MNRE to **Stage IV** photometric observables

# 1. Simulation

**(generate training data)**

# 2. Inference

**(train networks to get posteriors)**

# 1. Simulation

- **Simulation-based inference**  
(or likelihood-free inference)

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■ **Simulation-based inference**  
(or likelihood-free inference)



**Stochastic simulator** that maps from  
model parameters  $\theta$  to data  $\mathbf{x}$

$$\mathbf{x} \sim p(\mathbf{x} | \theta) \quad (\text{implicit likelihood})$$

We can **simulate** N samples that can be used as **training data** for a neural network

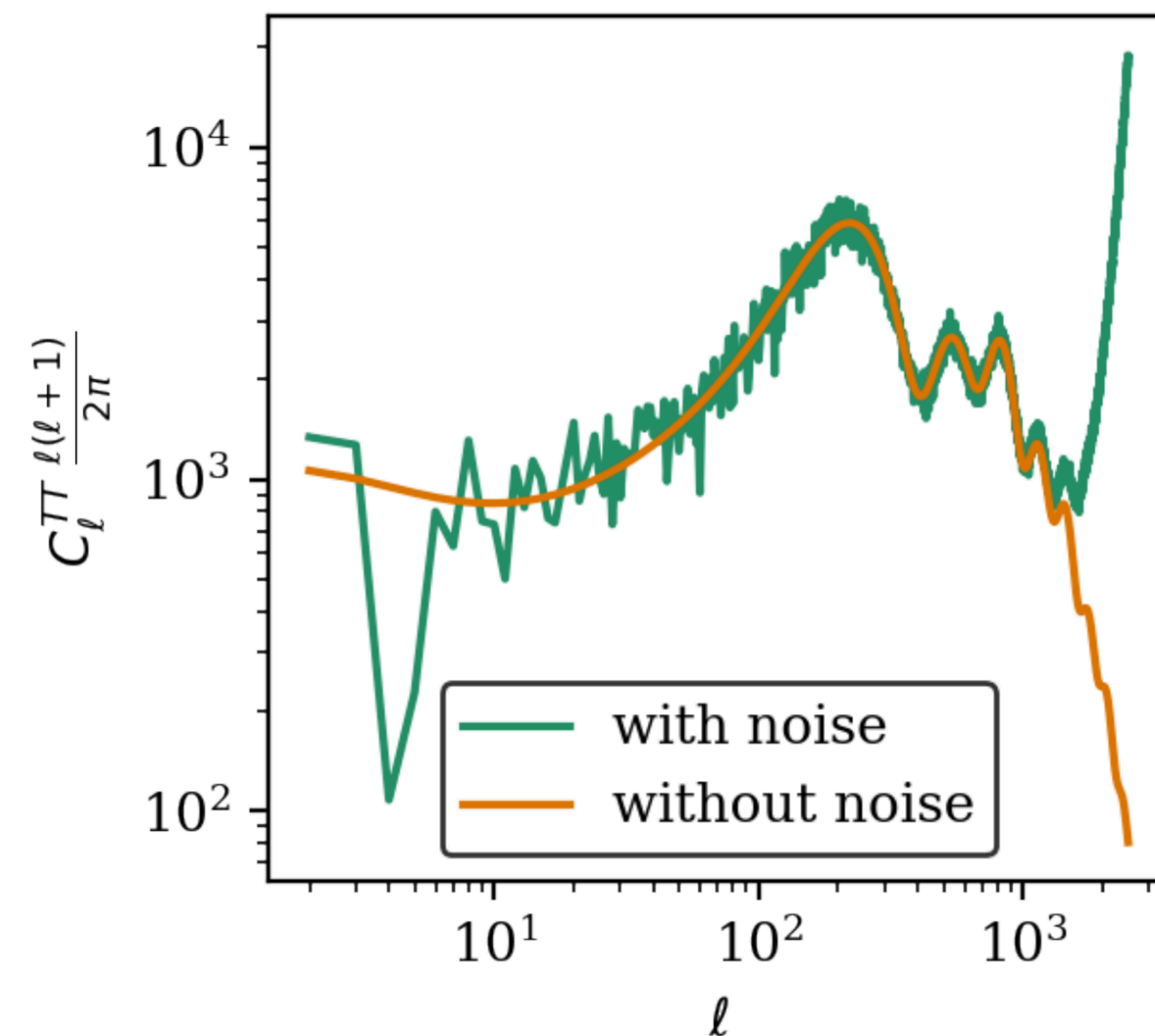
$$\{(\mathbf{x}^{(1)}, \boldsymbol{\theta}^{(1)}), (\mathbf{x}^{(2)}, \boldsymbol{\theta}^{(2)}), \dots, (\mathbf{x}^{(N)}, \boldsymbol{\theta}^{(N)})\}$$

We can **simulate** N samples that can be used as **training data** for a neural network

$$\{(\mathbf{x}^{(1)}, \boldsymbol{\theta}^{(1)}), (\mathbf{x}^{(2)}, \boldsymbol{\theta}^{(2)}), \dots, (\mathbf{x}^{(N)}, \boldsymbol{\theta}^{(N)})\}$$

**Ex:** CMB simulator

$$\boldsymbol{\theta} \rightarrow C_\ell(\boldsymbol{\theta}) \rightarrow C_\ell(\boldsymbol{\theta}) + N_\ell$$



[Cole+ 22](#)

## Neural Ratio Estimation

Instead of directly estimating the posterior, estimate:

$$r(\mathbf{x}; \boldsymbol{\theta}) = \frac{p(\mathbf{x}, \boldsymbol{\theta})}{p(\mathbf{x})p(\boldsymbol{\theta})}$$

## 2. Inference

## Neural Ratio Estimation

Instead of directly estimating the posterior, estimate:

$$r(\mathbf{x}; \boldsymbol{\theta}) = \frac{p(\mathbf{x}, \boldsymbol{\theta})}{p(\mathbf{x})p(\boldsymbol{\theta})}$$

It's easy to show that:

$$\frac{p(\mathbf{x}, \boldsymbol{\theta})}{p(\mathbf{x})p(\boldsymbol{\theta})} = \frac{p(\boldsymbol{\theta} | \mathbf{x})}{p(\boldsymbol{\theta})} \quad (\text{posterior-to-prior ratio})$$

## 2. Inference

$$\boldsymbol{\theta} \sim p(\boldsymbol{\theta}) \quad (\mathbf{ex:} \Omega_b \text{ and } \Omega_c)$$

$$\boldsymbol{x} \sim p(\boldsymbol{x}) \quad (\mathbf{ex:} \text{CMB spectra})$$

$$\frac{p(\mathbf{x}, \boldsymbol{\theta})}{p(\mathbf{x})p(\boldsymbol{\theta})} = \frac{p(\boldsymbol{\theta} | \mathbf{x})}{p(\boldsymbol{\theta})}$$

$\theta \sim p(\theta)$  (ex:  $\Omega_b$  and  $\Omega_c$ )

$x \sim p(x)$  (ex: CMB spectra)

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

$\Omega_b =$  5%

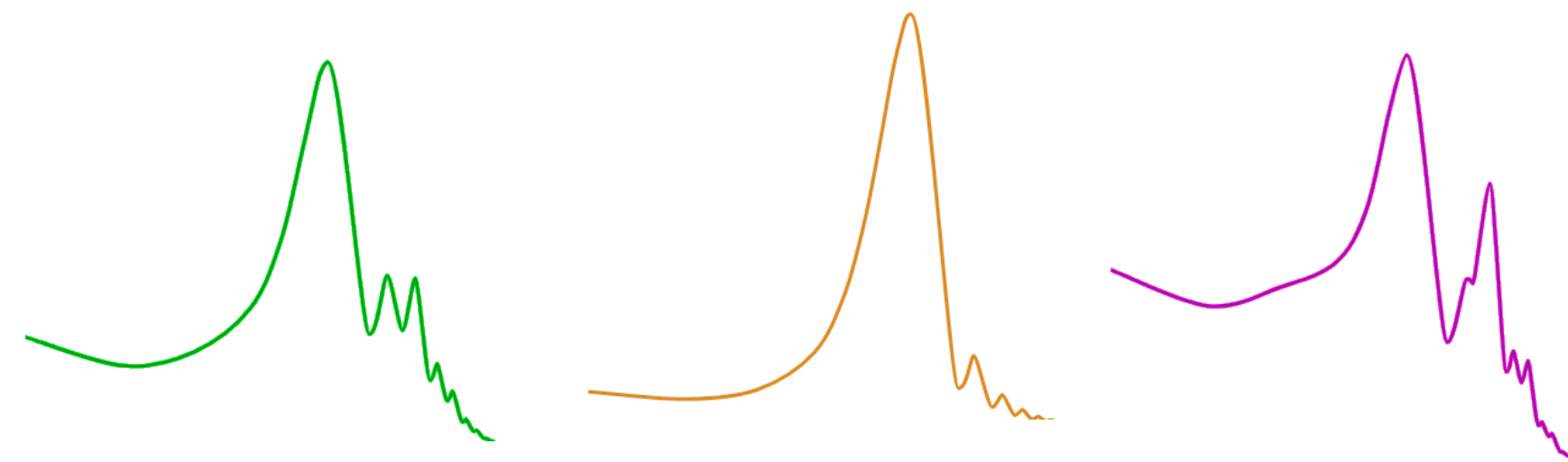
30%

5%

$\Omega_c =$  25%

0%

95%



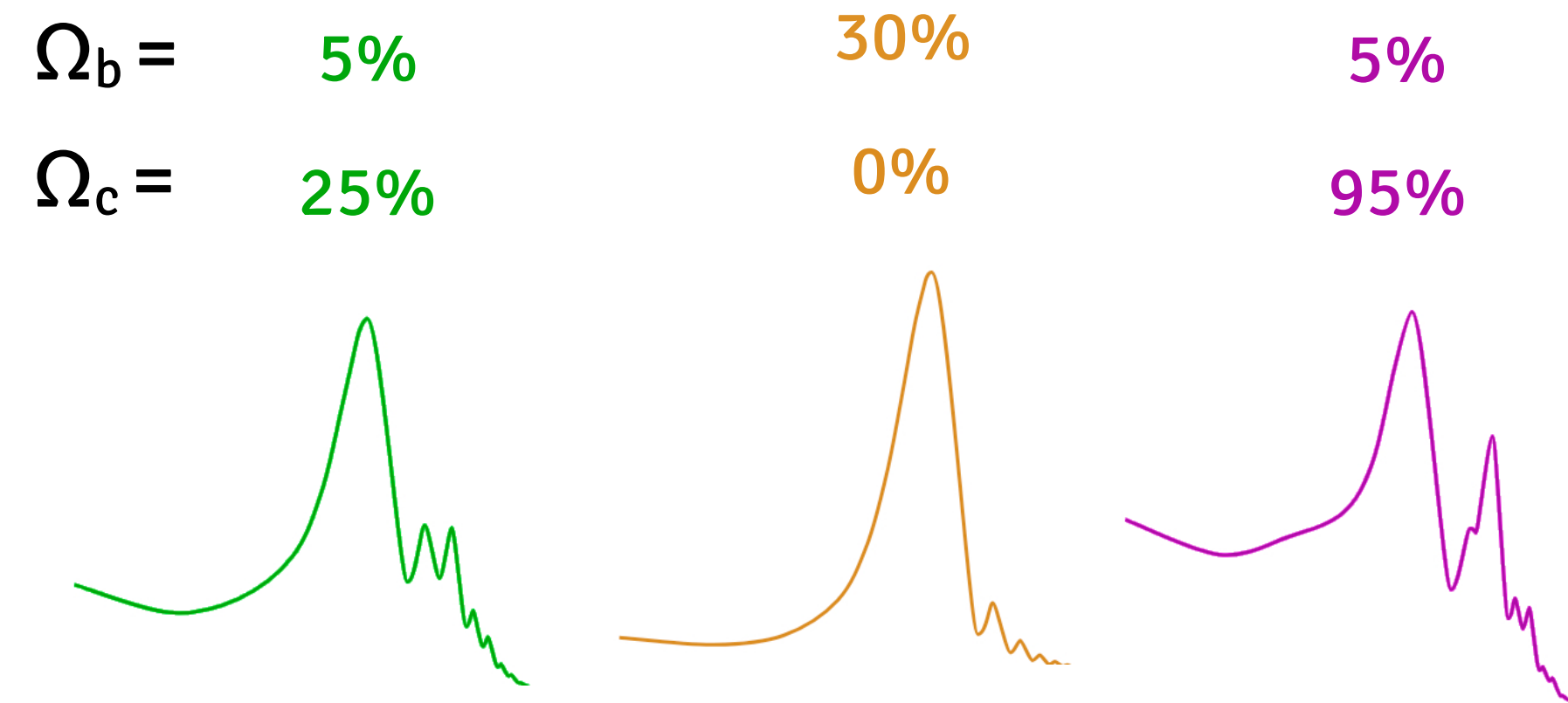
$$\frac{p(\mathbf{x}, \theta)}{p(\mathbf{x})p(\theta)} = \frac{p(\theta | \mathbf{x})}{p(\theta)}$$

$\theta \sim p(\theta)$  (ex:  $\Omega_b$  and  $\Omega_c$ )

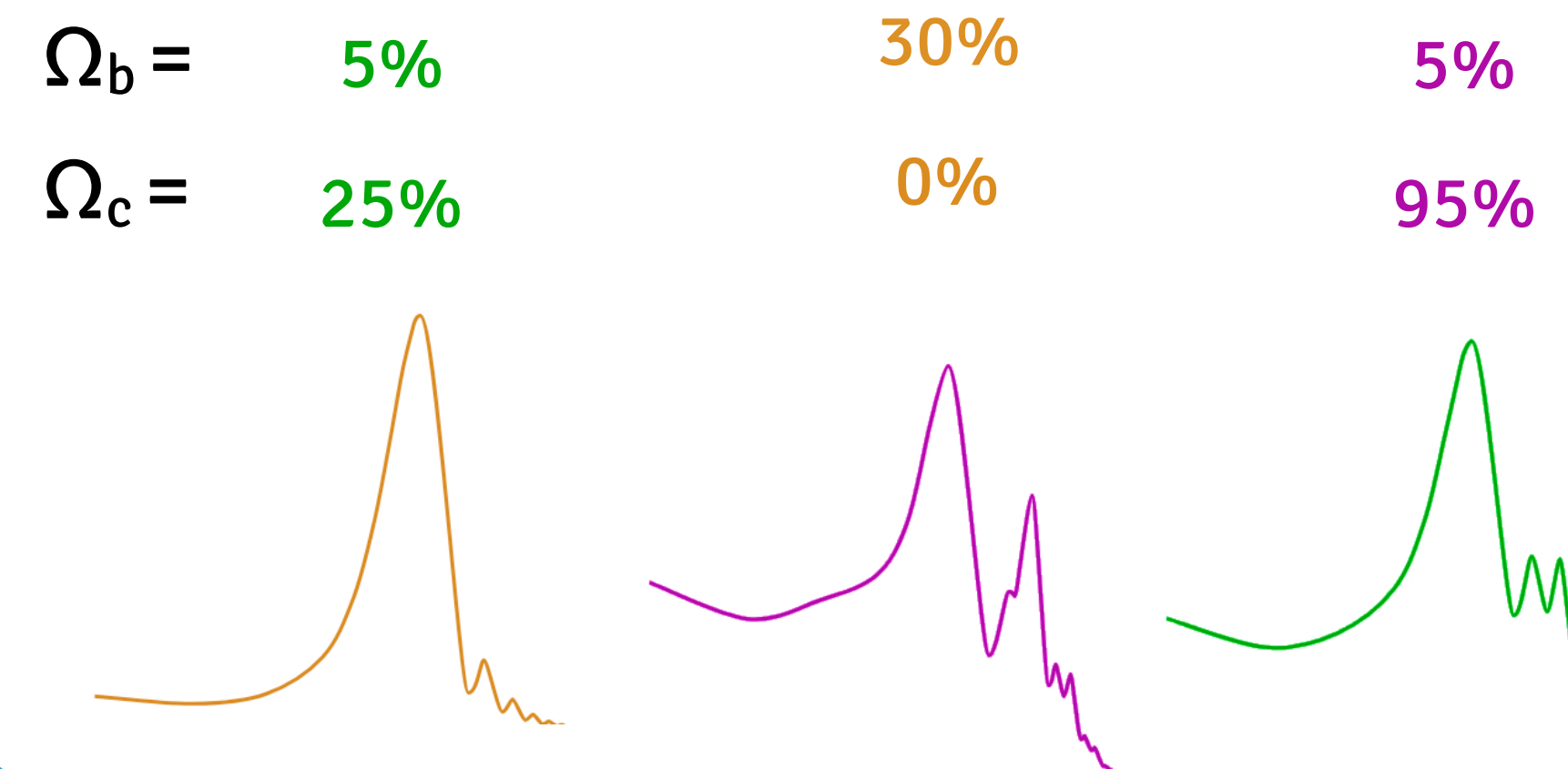
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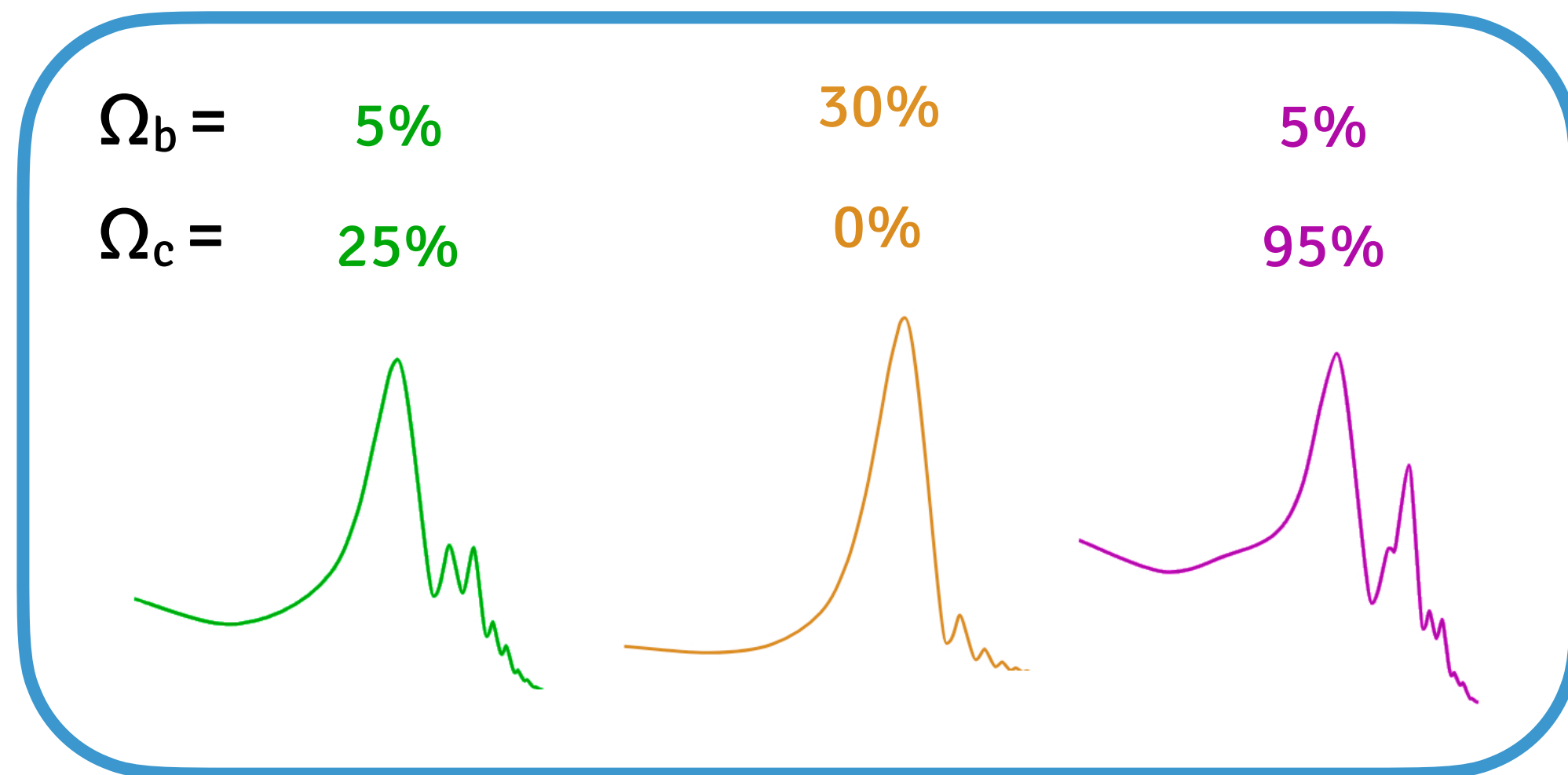


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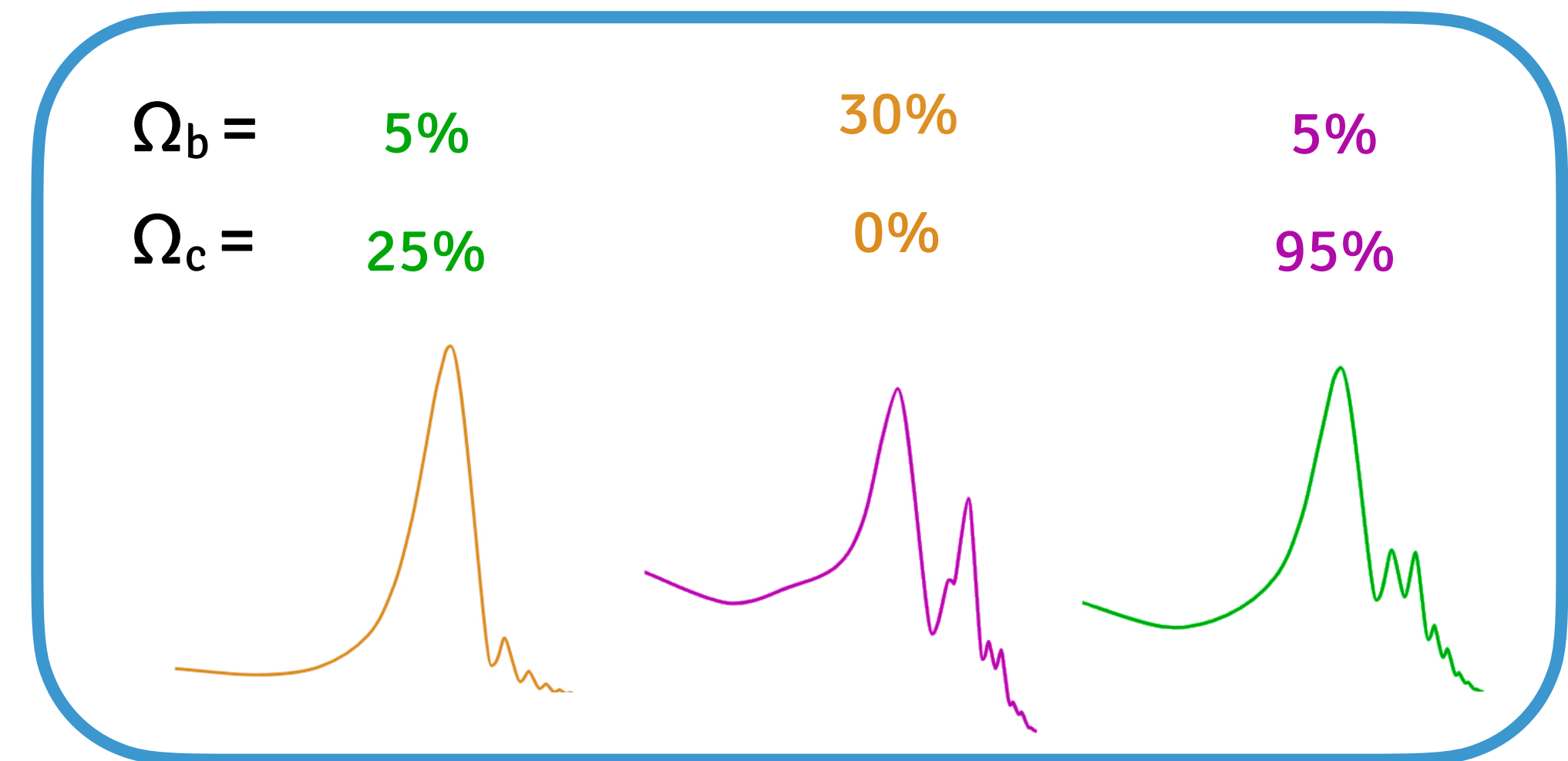
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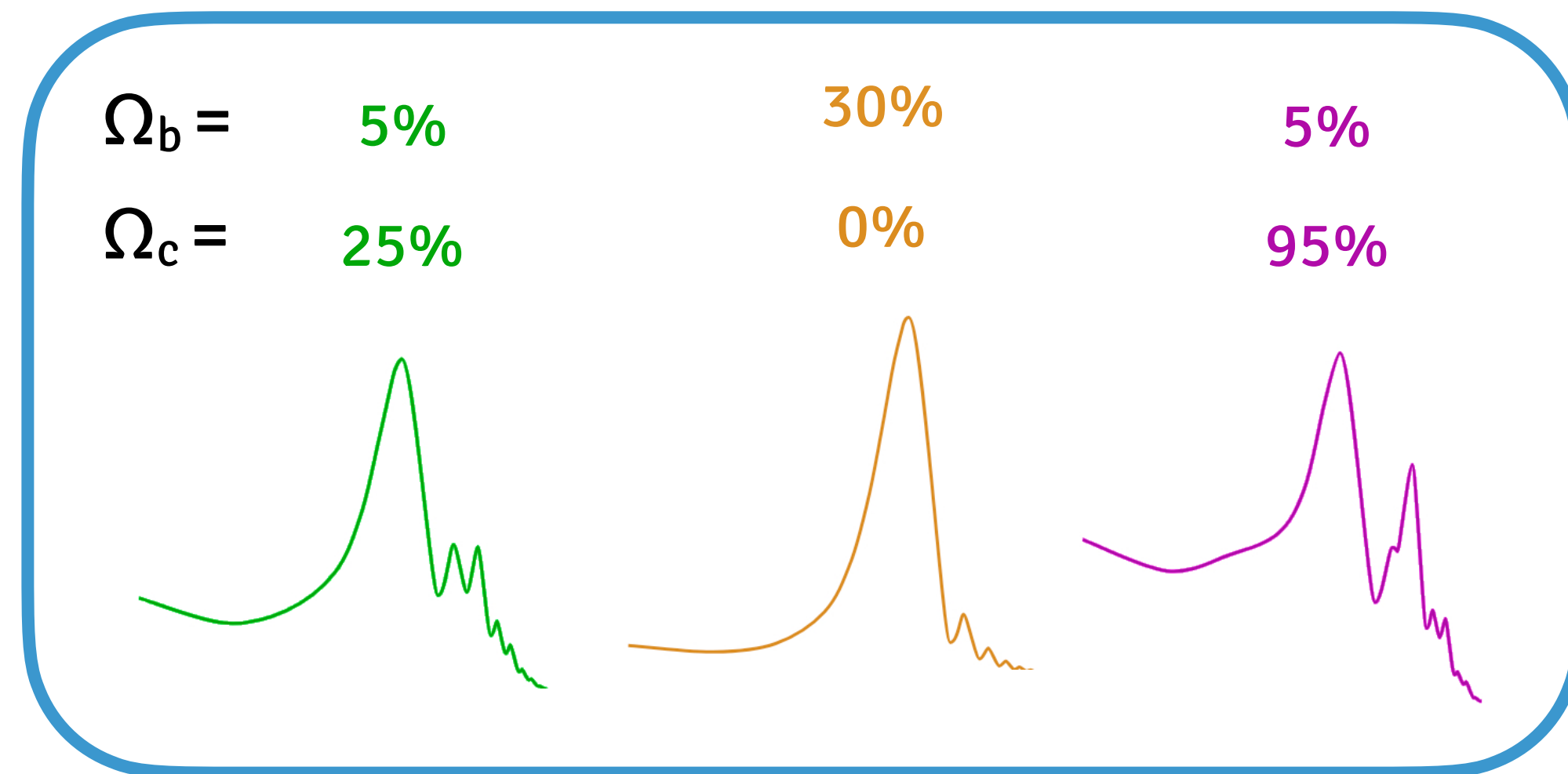


Given some  $(x, \theta)$  pair, are they drawn jointly or marginally?

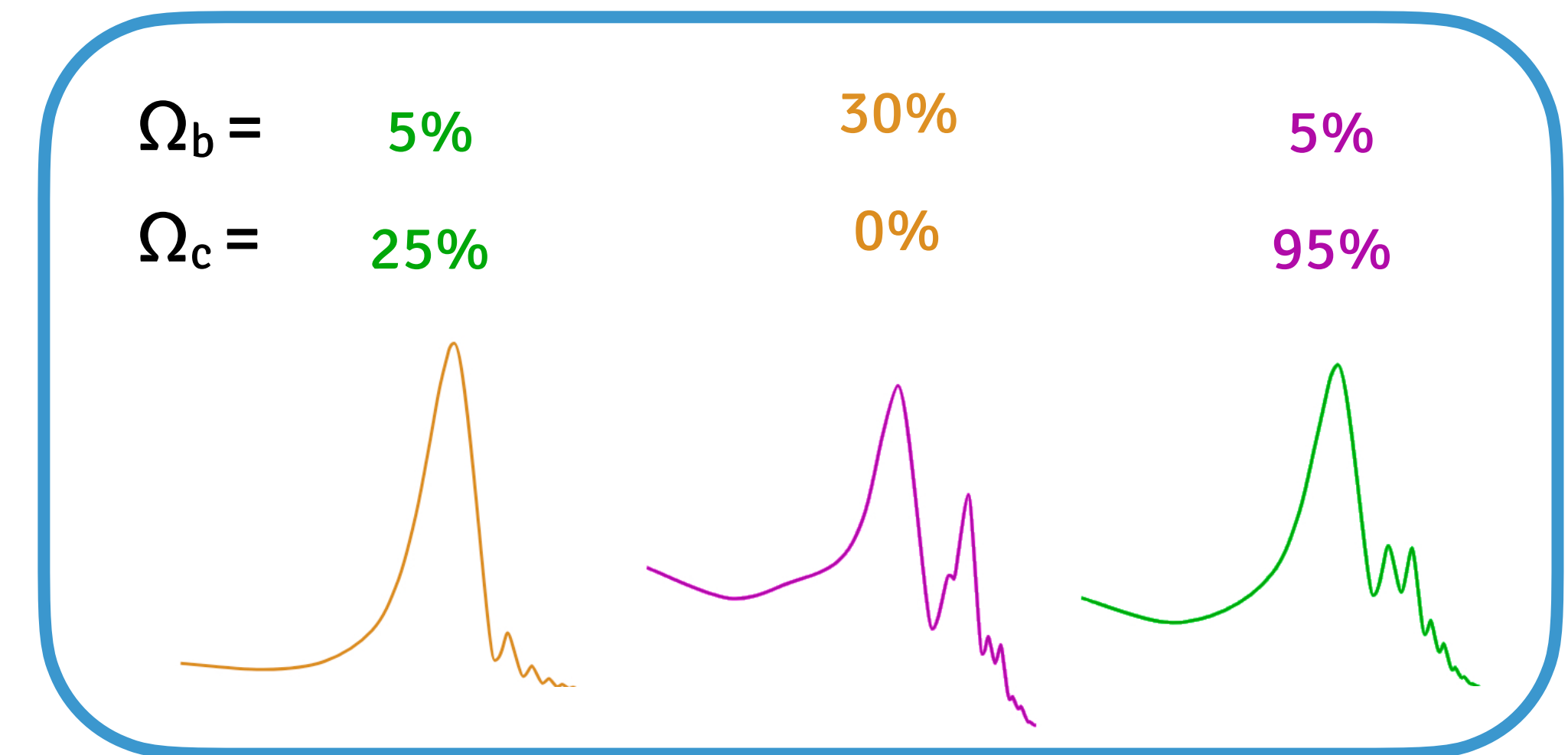
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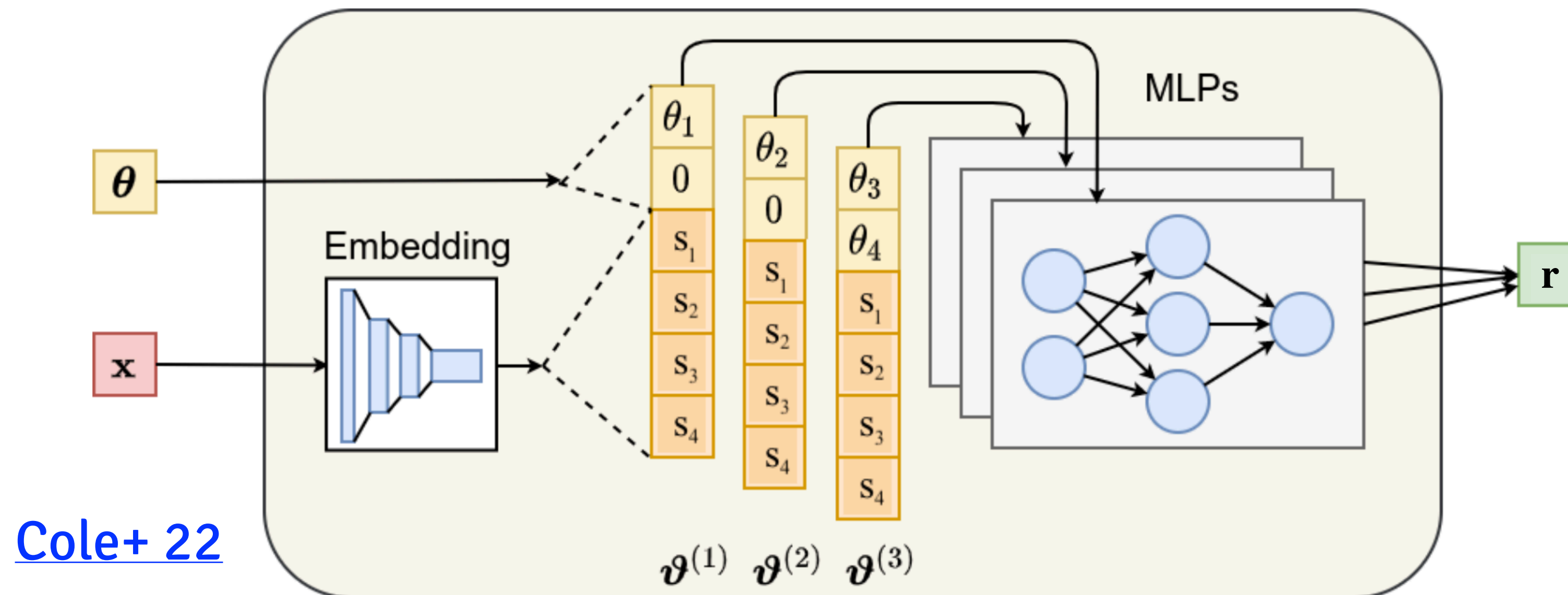
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Rephrase inference as a **binary classification problem**

We can directly **target marginal posteriors of interest,**  
and forget about the rest

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[Cole+ 22](#)

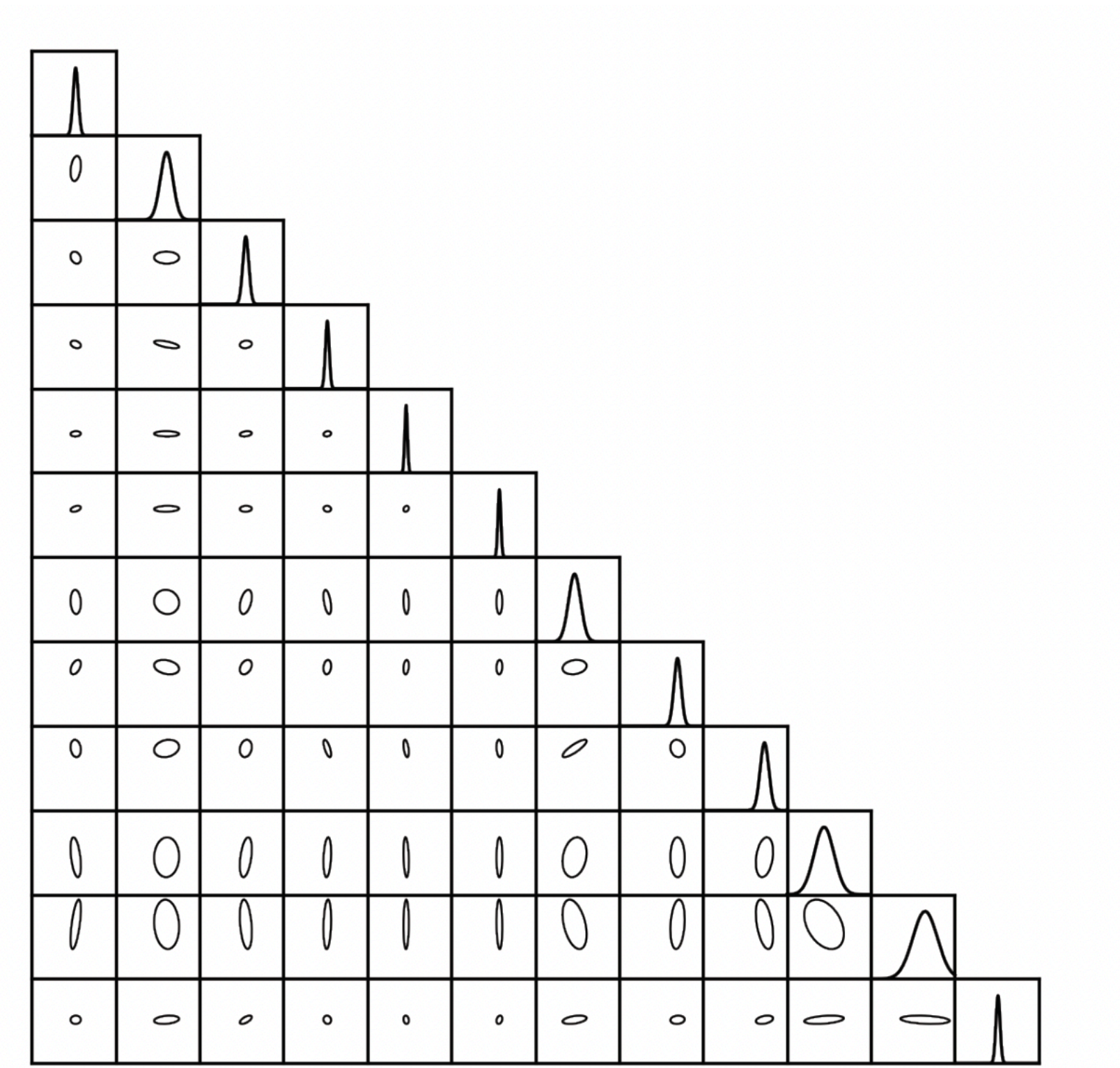
**Estimates**

$$p(\theta_1 | \mathbf{x}), \quad p(\theta_2 | \mathbf{x}), \quad p(\theta_3, \theta_4 | \mathbf{x})$$

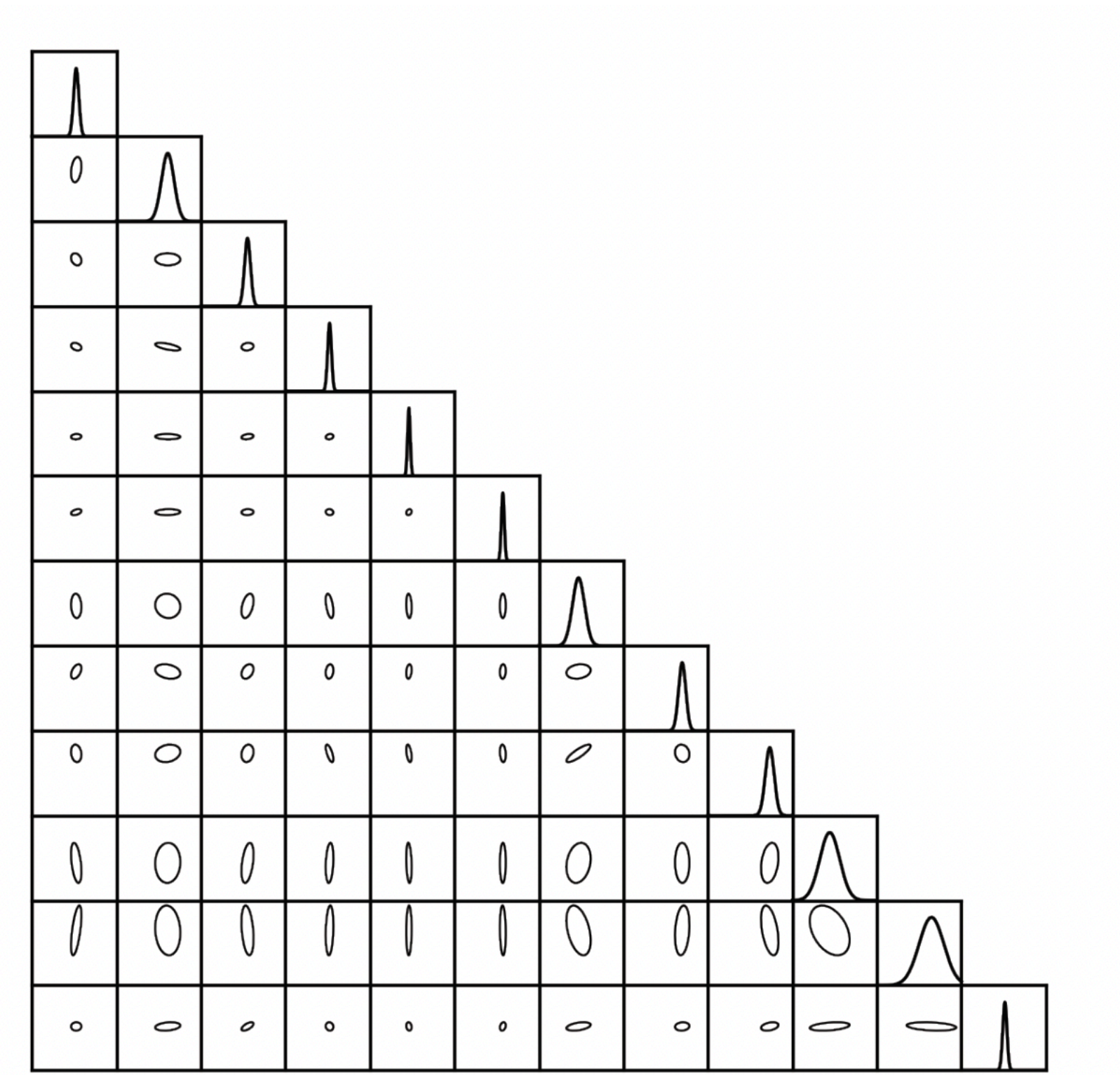
**Does not estimate**

$$p(\theta_1, \theta_2 | \mathbf{x}), \quad p(\theta_1, \theta_2, \theta_3 | \mathbf{x}), \dots$$

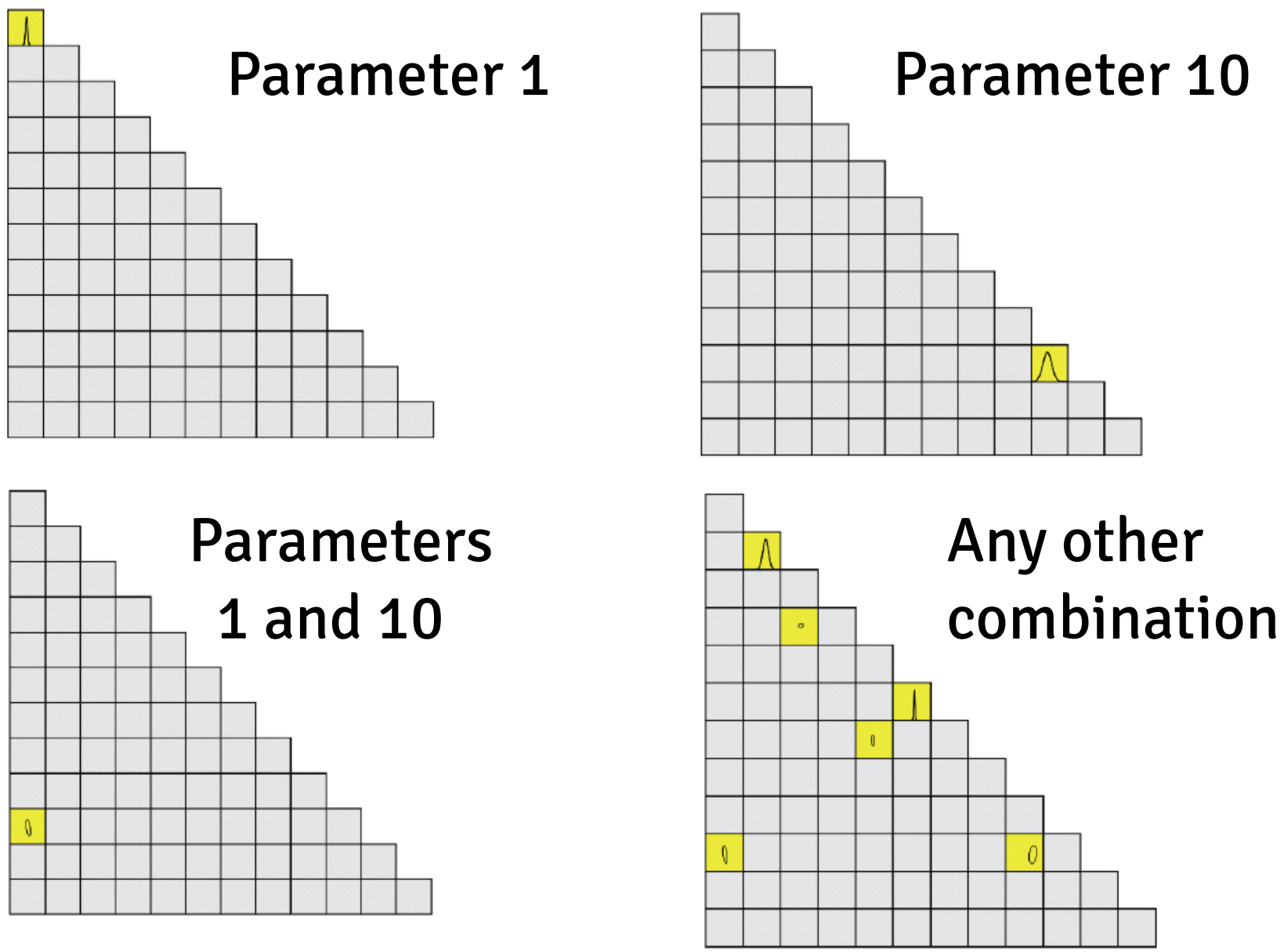
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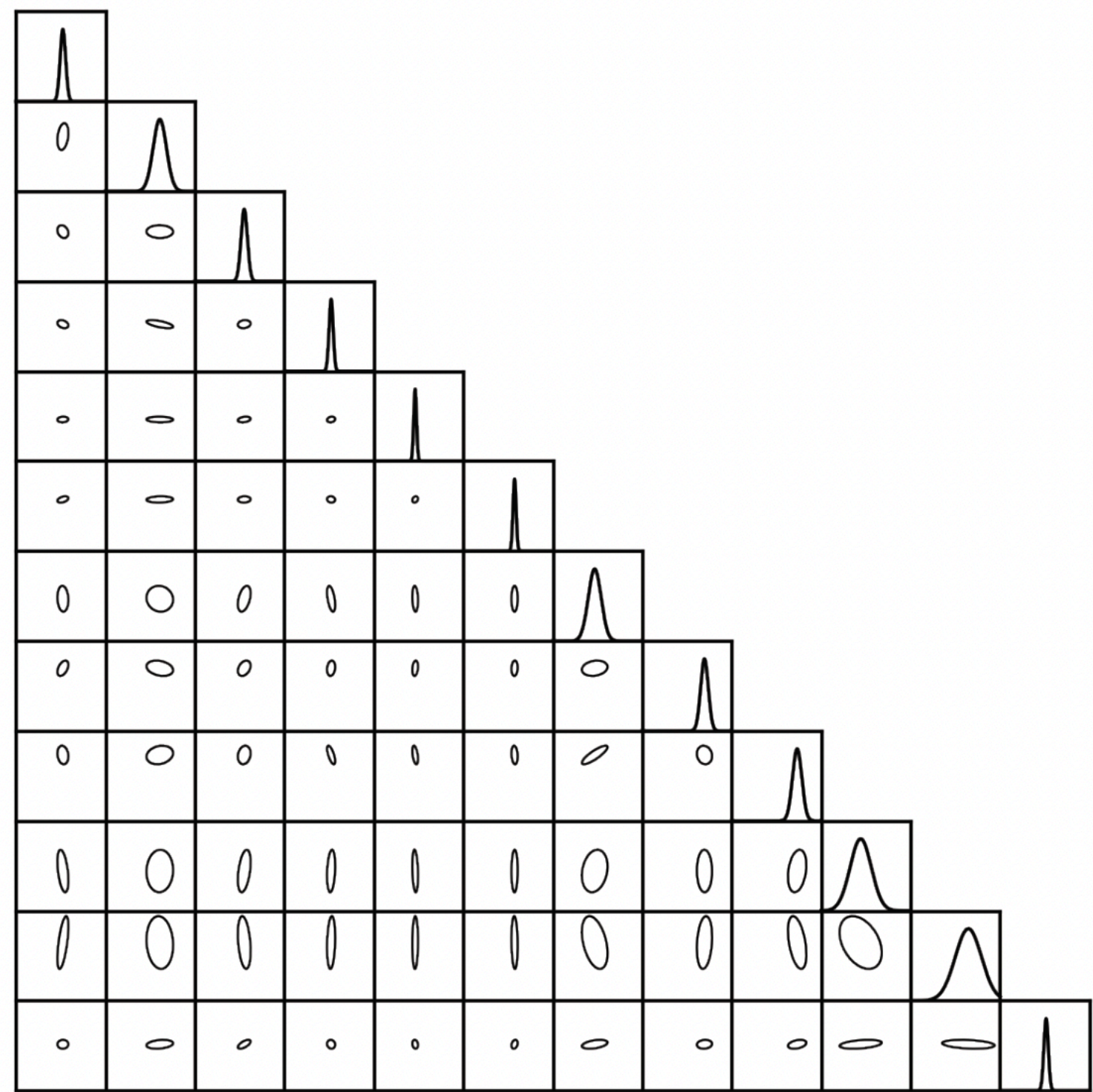
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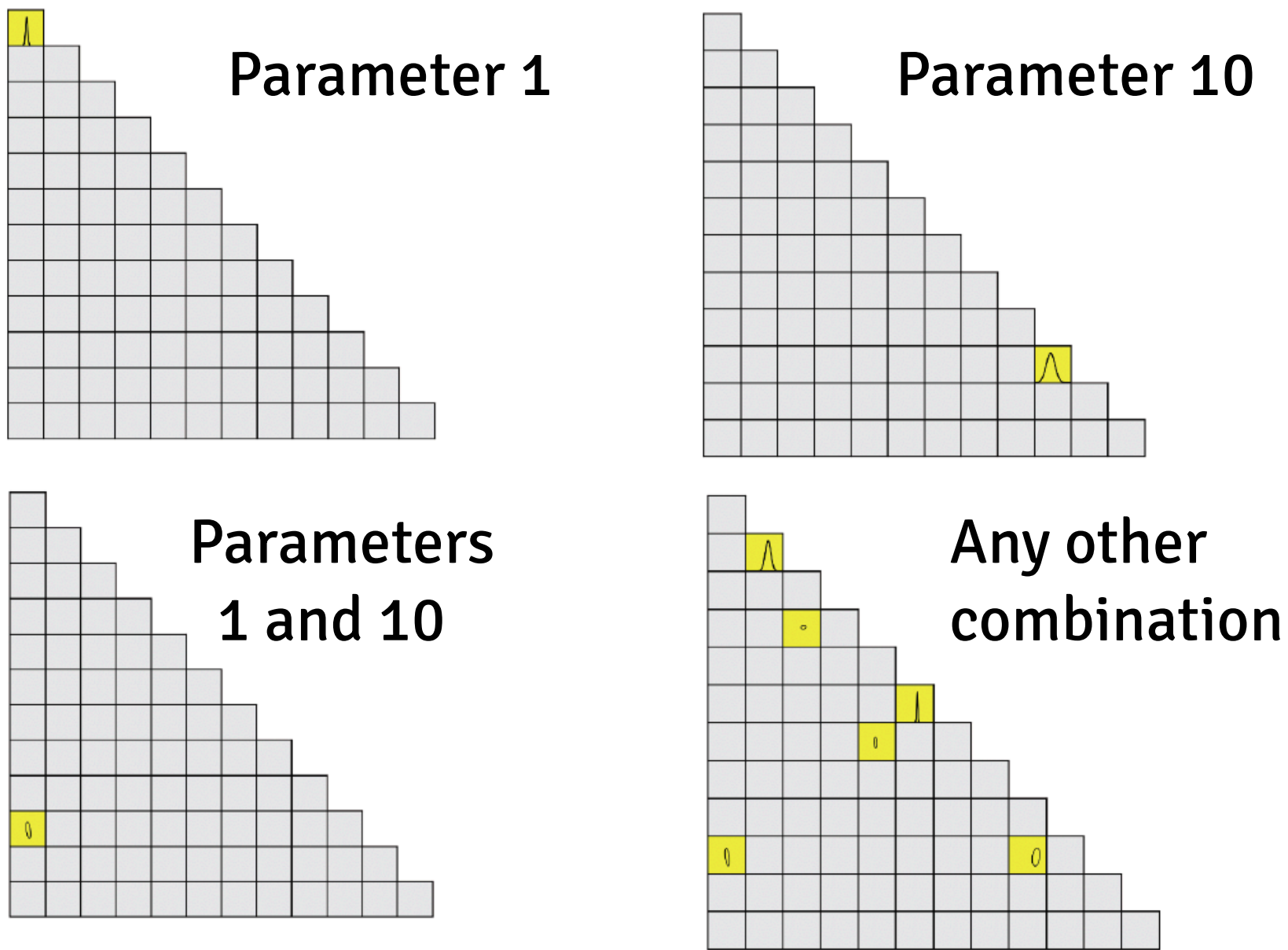
... we can cherry-pick what we care about



Instead of estimating all parameters...



... we can cherry-pick what we care about



**Much more flexible  
much more efficient!**

MNRE has been successfully applied in many contexts:

- **Strong lensing** [\[Montel+ 22\]](#)
- **Stellar Streams** [\[Alvey+ 23\]](#)
- **Gravitational Waves** [\[Bhardwaj+ 23\]](#) [\[Alvey+ 23\]](#)
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**Our goal:** apply MNRE to **Stage IV** photometric observables

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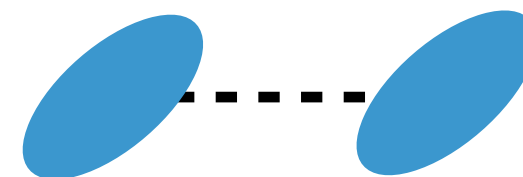


# 3x2pt photometric probes

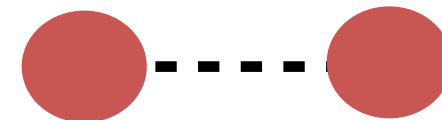
Summarise maps of galaxy **positions/shapes** using three 2-point statistics (**3x2pt**) measured at **10 tomographic redshift bins**



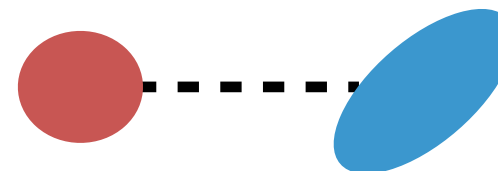
**Cosmic Shear**



**Galaxy clustering**

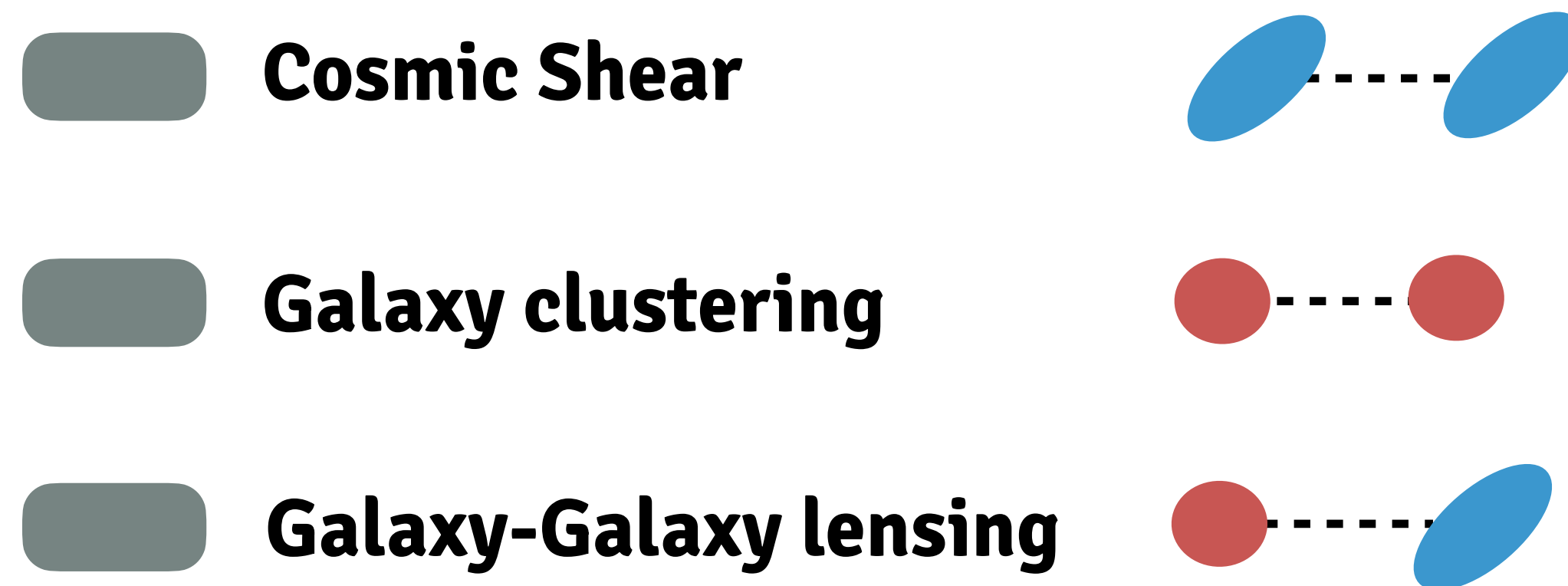


**Galaxy-Galaxy lensing**



# 3x2pt photometric probes

Summarise maps of galaxy **positions/shapes** using three 2-point statistics (**3x2pt**) measured at **10 tomographic redshift bins**



...described by angular **power spectra**  $C_{ij}^{XY}(\ell) = \int dz W_i^X(z) W_j^Y(z) P_m(k_\ell, z)$


# Swyft 3x2pt analysis

## 1. Simulator

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We generate 50k realisations of  
3x2pt spectra with gaussian noise

$$\hat{C}_{ij}^{AB}(\ell) = C_{ij}^{AB}(\ell) + n_{ij}^{AB}(\ell)$$

$$\mathcal{N}(0, \mathbf{C})$$

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**12 nuisance params**

$$\{A_{\text{IA}}, \eta_{\text{IA}}, b_1, \dots, b_{10}\}$$

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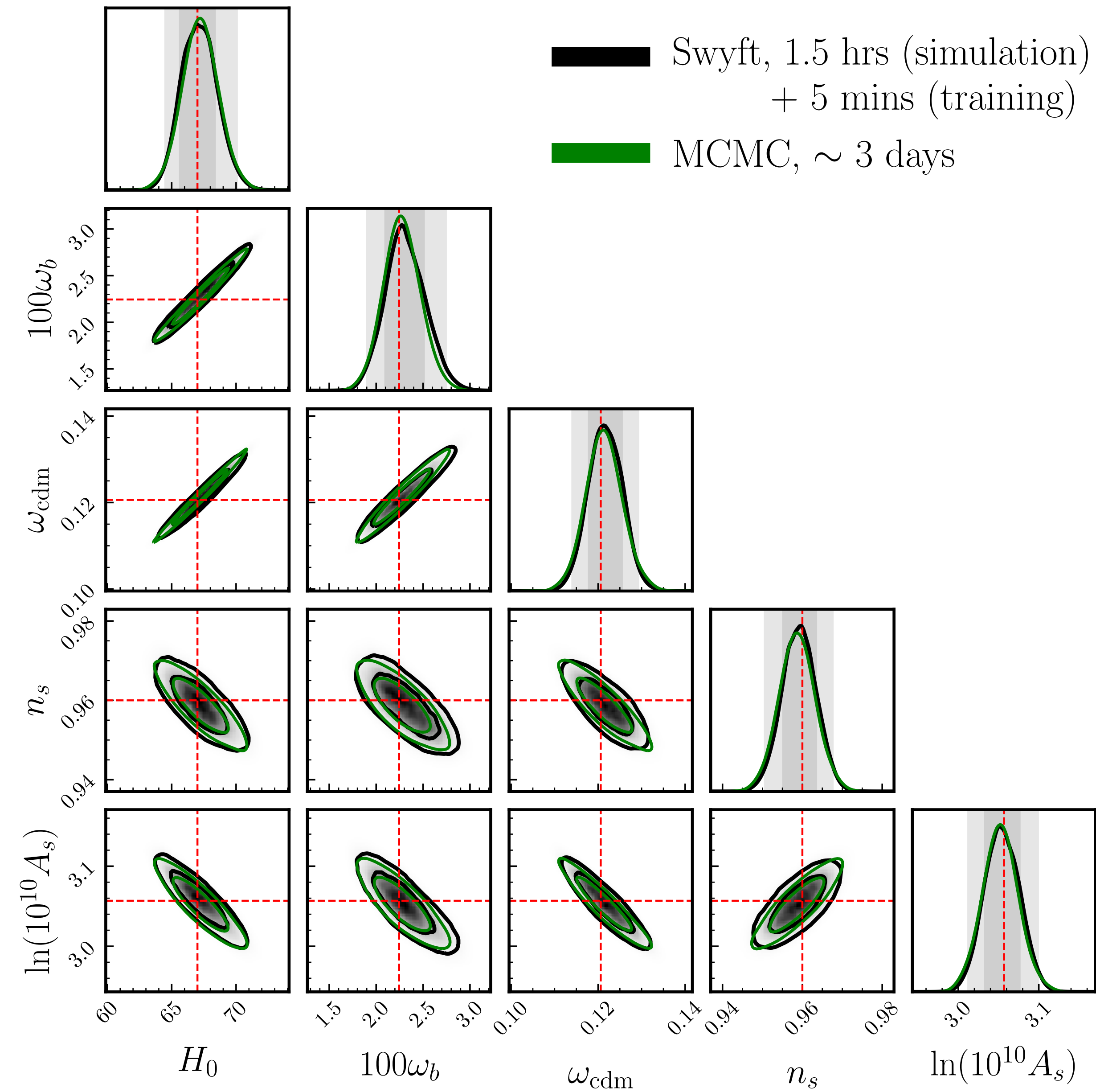
**12 nuisance params**

$$\{A_{\text{IA}}, \eta_{\text{IA}}, b_1, \dots, b_{10}\}$$

## 2. Network

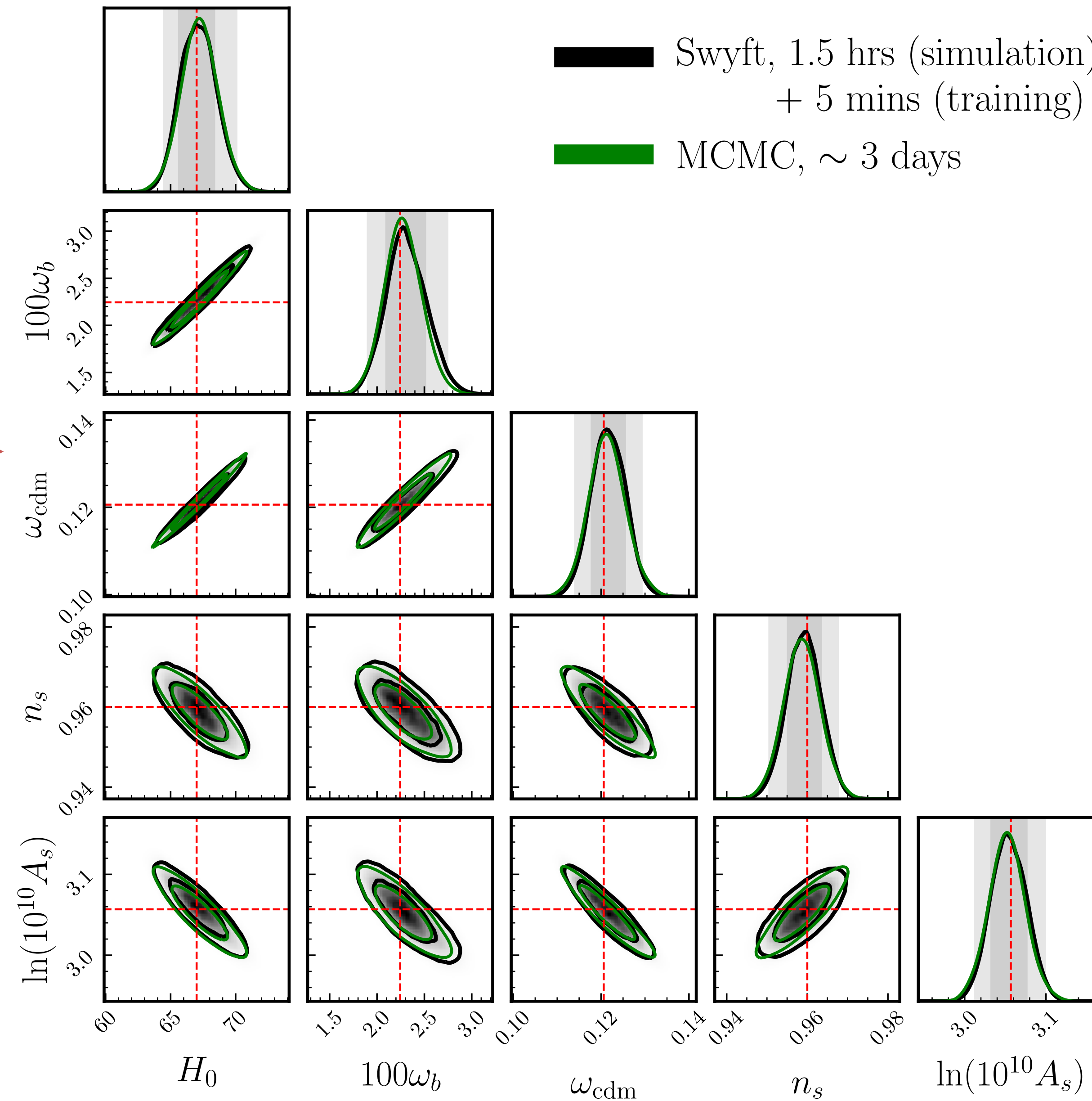
We do a **pre-compression** of data using **PCA** and parameter-specific data summaries

# Forecast $\Lambda$ CDM posteriors



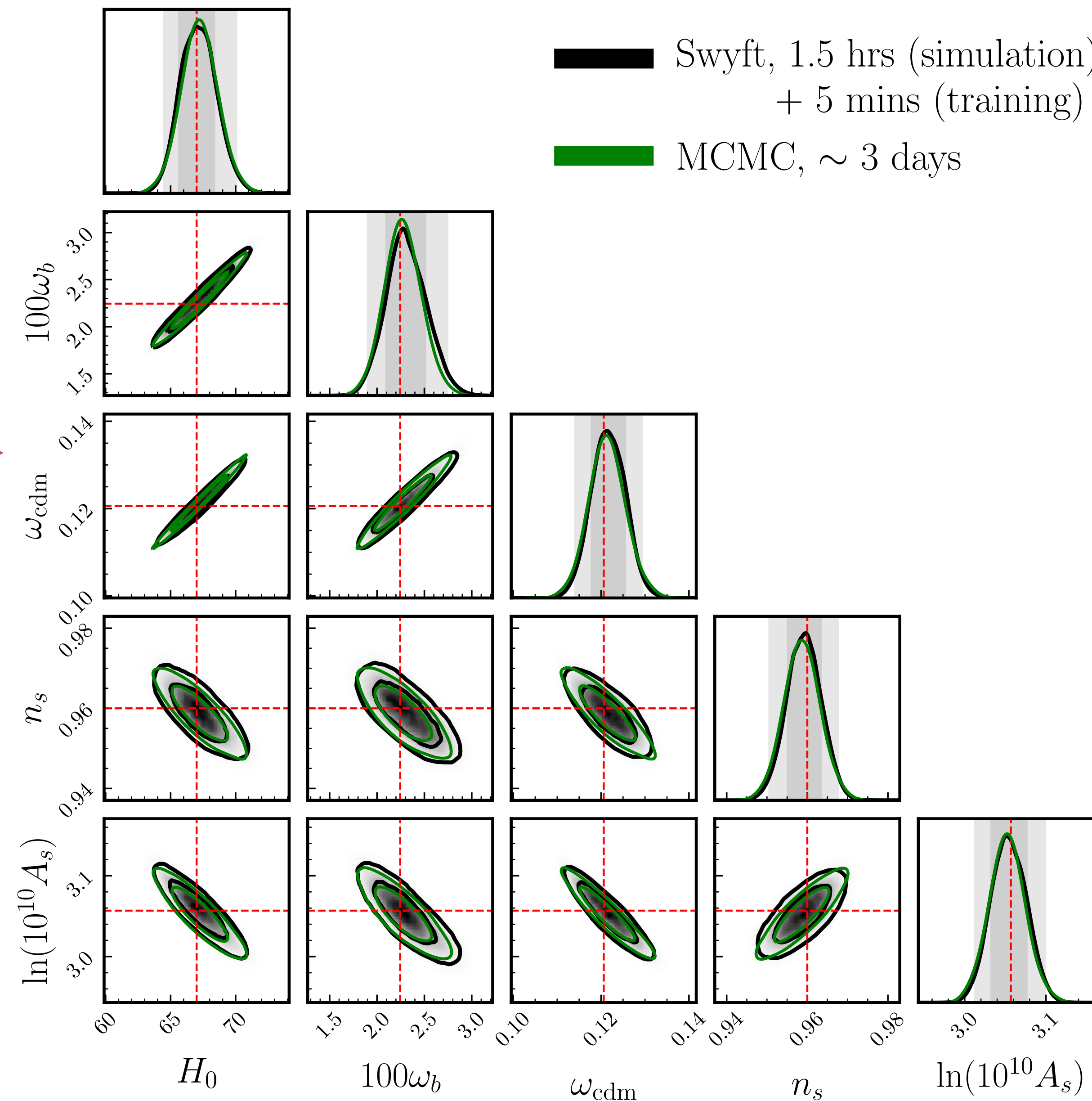
# Forecast $\Lambda$ CDM posteriors

— Swyft, 1.5 hrs (simulation)  
+ 5 mins (training)  
— MCMC,  $\sim 3$  days



MNRE & MCMC are in excellent agreement!

# Forecast $\Lambda$ CDM posteriors



MNRE & MCMC are in excellent agreement!

Dramatic reduction in CPU time!

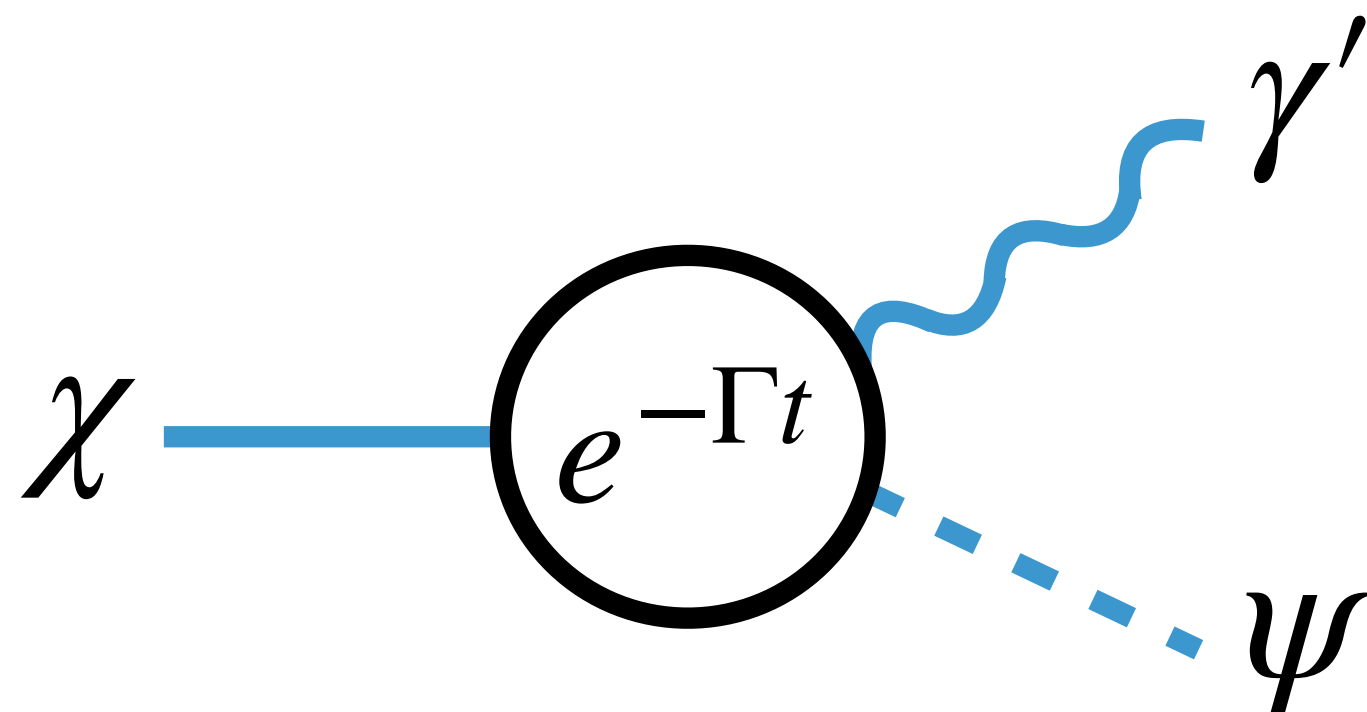
■ With MNRE, we can also test models with highly non-Gaussian posteriors

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As an example, we consider a model of **CDM decaying to DR + WDM**  
(proposed to explain the  $S_8$  tension)

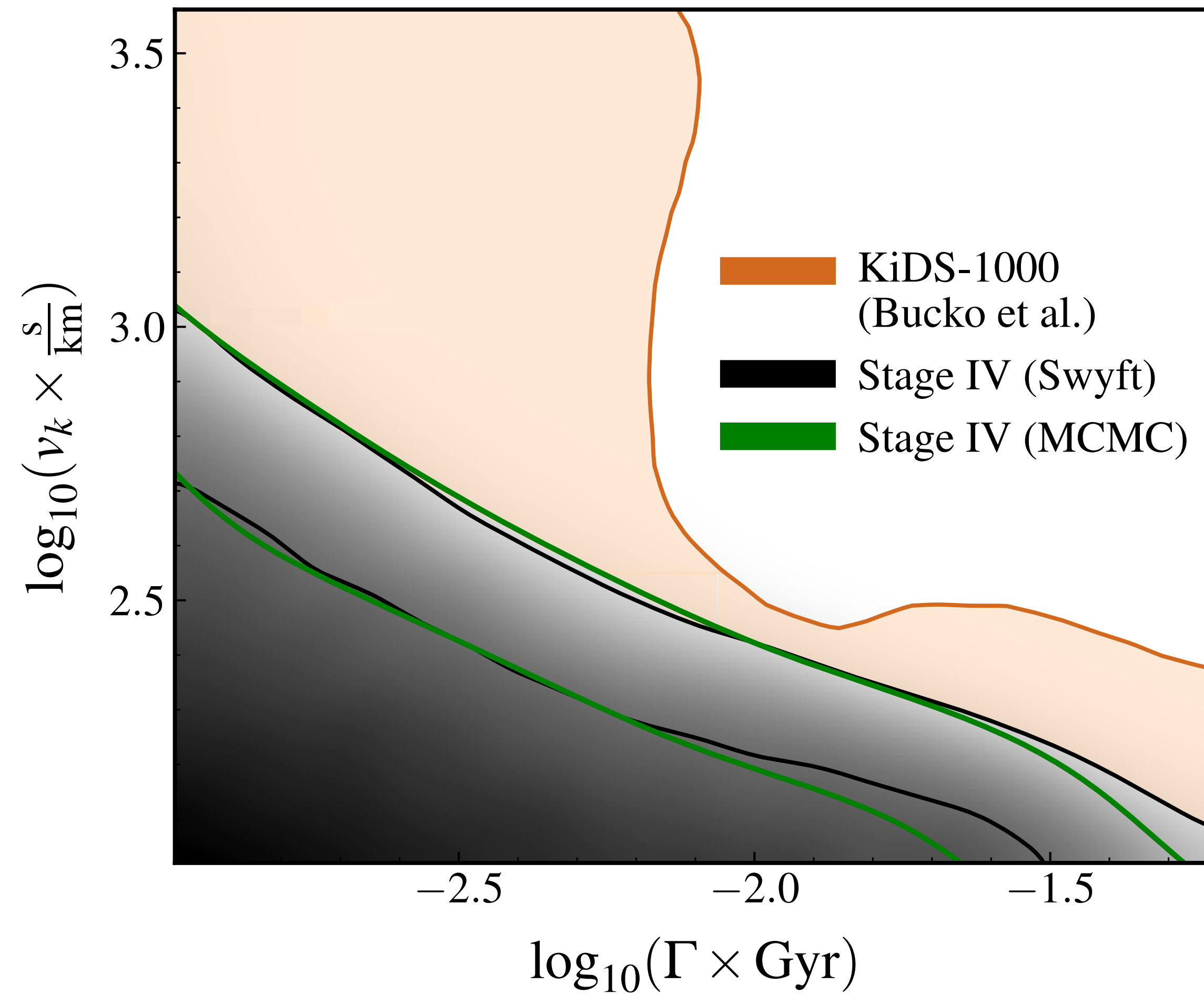
[\[Abellan+ 21\]](#)

[\[Bucko+ 23\]](#)

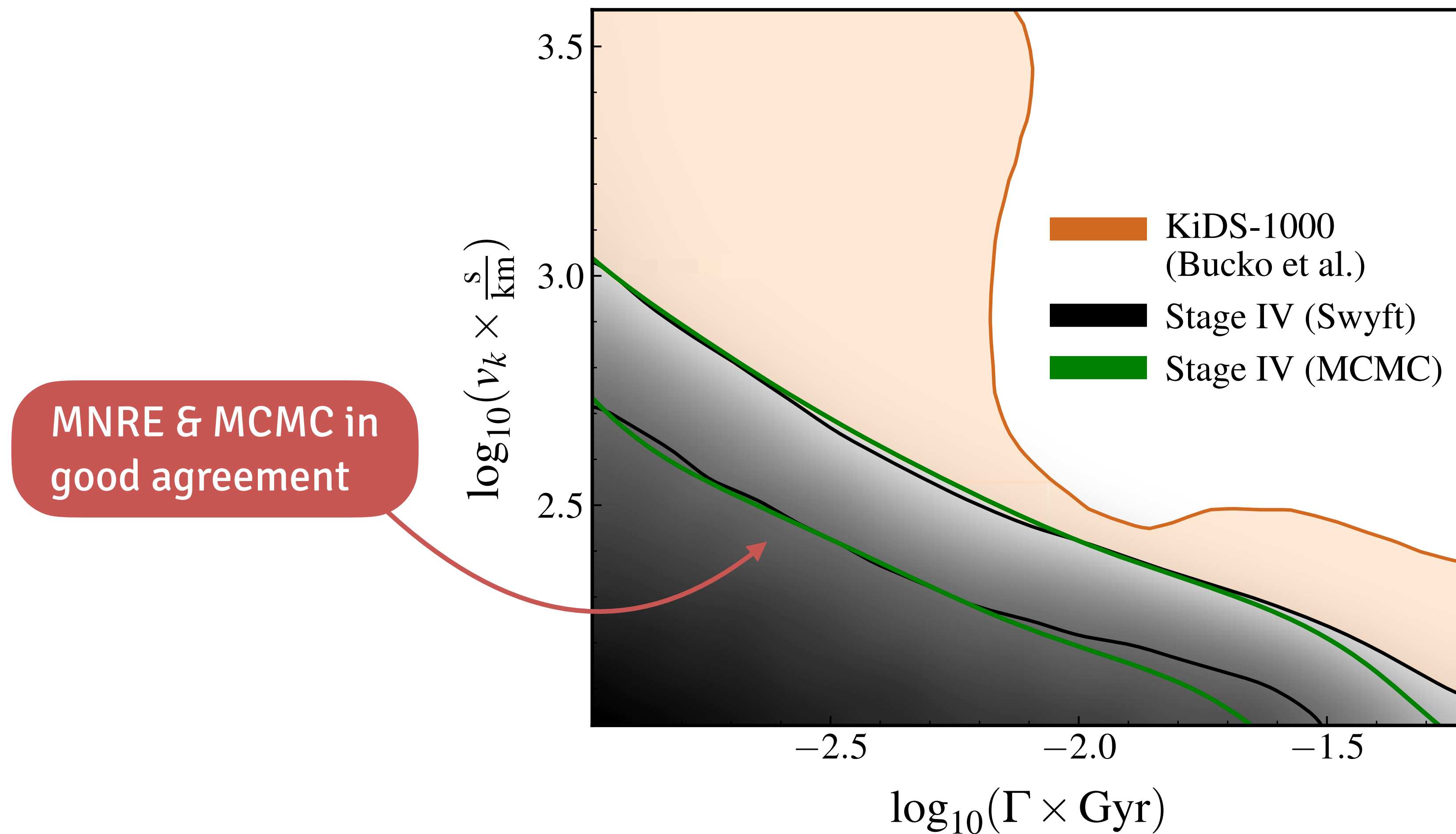


Decay rate  $\Gamma$   
WDM velocity kick  $v_k$

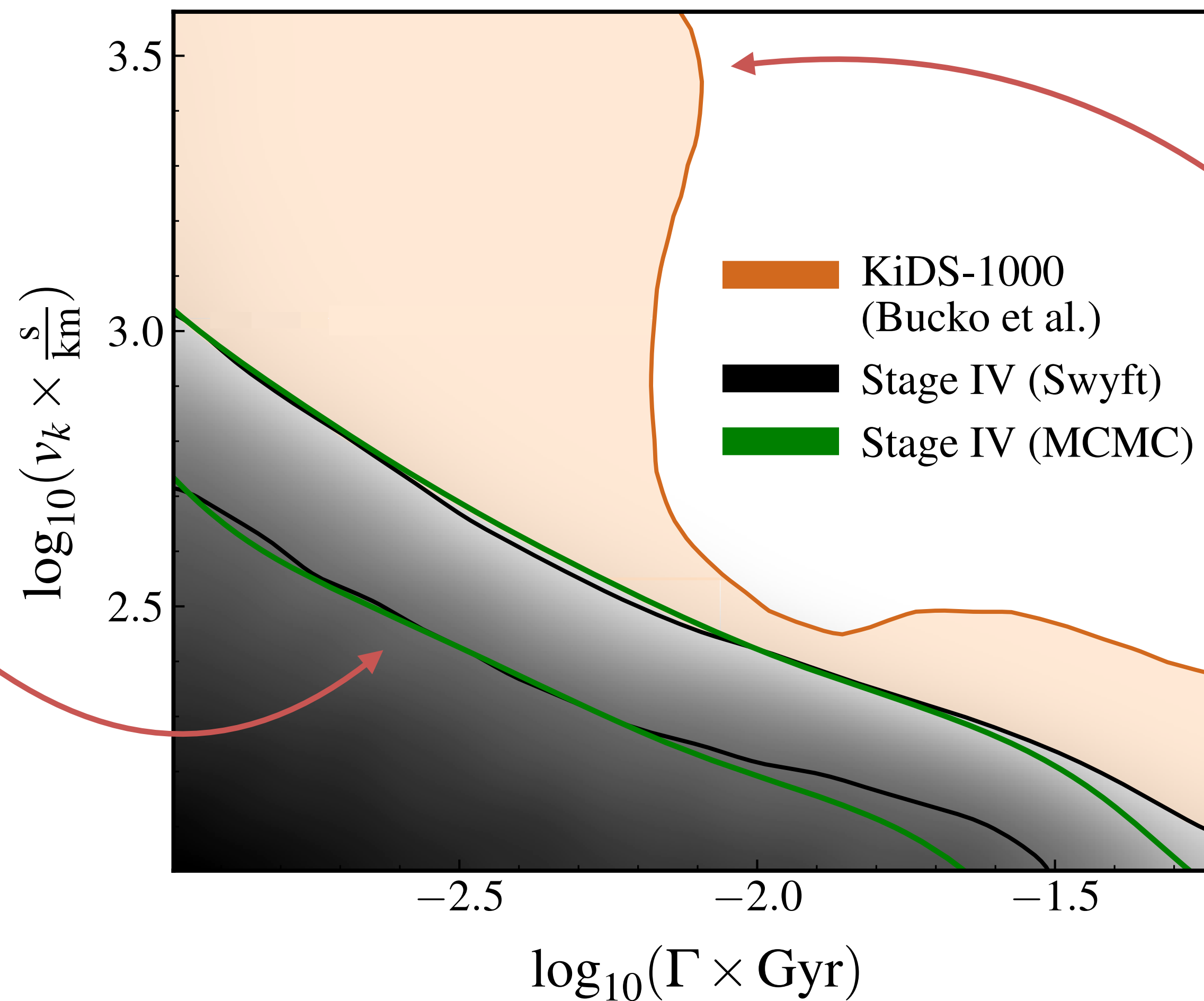
# Forecast constraints on decaying DM



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MNRE & MCMC in  
good agreement

Improve current limits by  
~1 order of magnitude!

# Next steps

- Use **simulator based on CLOE** (many more nuisance params.)

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- Use **simulator based on CLOE** (many more nuisance params.)
- Consider **other observables**, like spectroscopic galaxy clustering
- Perform **field-level inference** to extract all possible information  
[\[Lemos+ 23\]](#)  
[\[Jeffrey+ 24\]](#)

## Conclusions

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**THANKS FOR YOUR ATTENTION**

[g.francoabellan@uva.nl](mailto:g.francoabellan@uva.nl)

**BACK-UP**

**Strategy:** train a neural network  $d_\phi(\mathbf{x}, \boldsymbol{\theta}) \in [0,1]$  as a binary classifier, so that

■  $d_\phi(\mathbf{x}, \boldsymbol{\theta}) \simeq 1$  if  $(\mathbf{x}, \boldsymbol{\theta}) \sim p(\mathbf{x}, \boldsymbol{\theta}) = p(\mathbf{x} | \boldsymbol{\theta})p(\boldsymbol{\theta})$

■  $d_\phi(\mathbf{x}, \boldsymbol{\theta}) \simeq 0$  if  $(\mathbf{x}, \boldsymbol{\theta}) \sim p(\mathbf{x})p(\boldsymbol{\theta})$

**Note:**  $\Phi$  denotes all the network parameters

We have to **minimise a loss function** w.r.t. the network params.  $\Phi$

$$L[d_\phi(\mathbf{x}, \boldsymbol{\theta})] = - \int d\mathbf{x} d\boldsymbol{\theta} \left[ p(\mathbf{x}, \boldsymbol{\theta}) \ln(d_\phi(\mathbf{x}, \boldsymbol{\theta})) + p(\mathbf{x})p(\boldsymbol{\theta}) \ln(1 - d_\phi(\mathbf{x}, \boldsymbol{\theta})) \right]$$

which yields

$$d_\phi(\mathbf{x}, \boldsymbol{\theta}) \simeq \frac{p(\mathbf{x}, \boldsymbol{\theta})}{p(\mathbf{x}, \boldsymbol{\theta}) + p(\mathbf{x})p(\boldsymbol{\theta})} = \frac{r(\mathbf{x}; \boldsymbol{\theta})}{r(\mathbf{x}; \boldsymbol{\theta}) + 1}$$

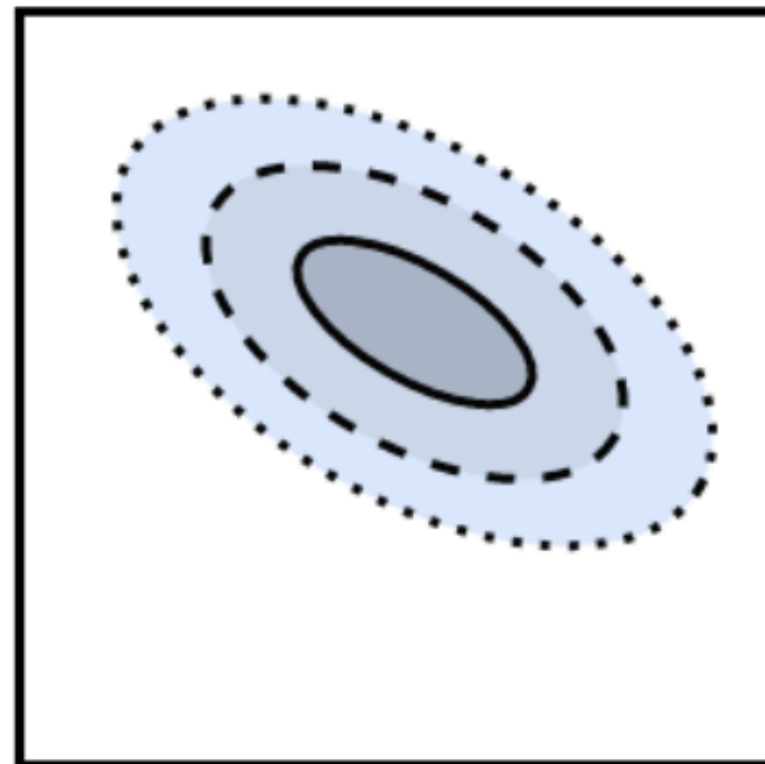
## But can we trust our results?



...even if NNs are often seen as "black boxes", it is possible to perform statistical consistency tests which are impossible with MCMC

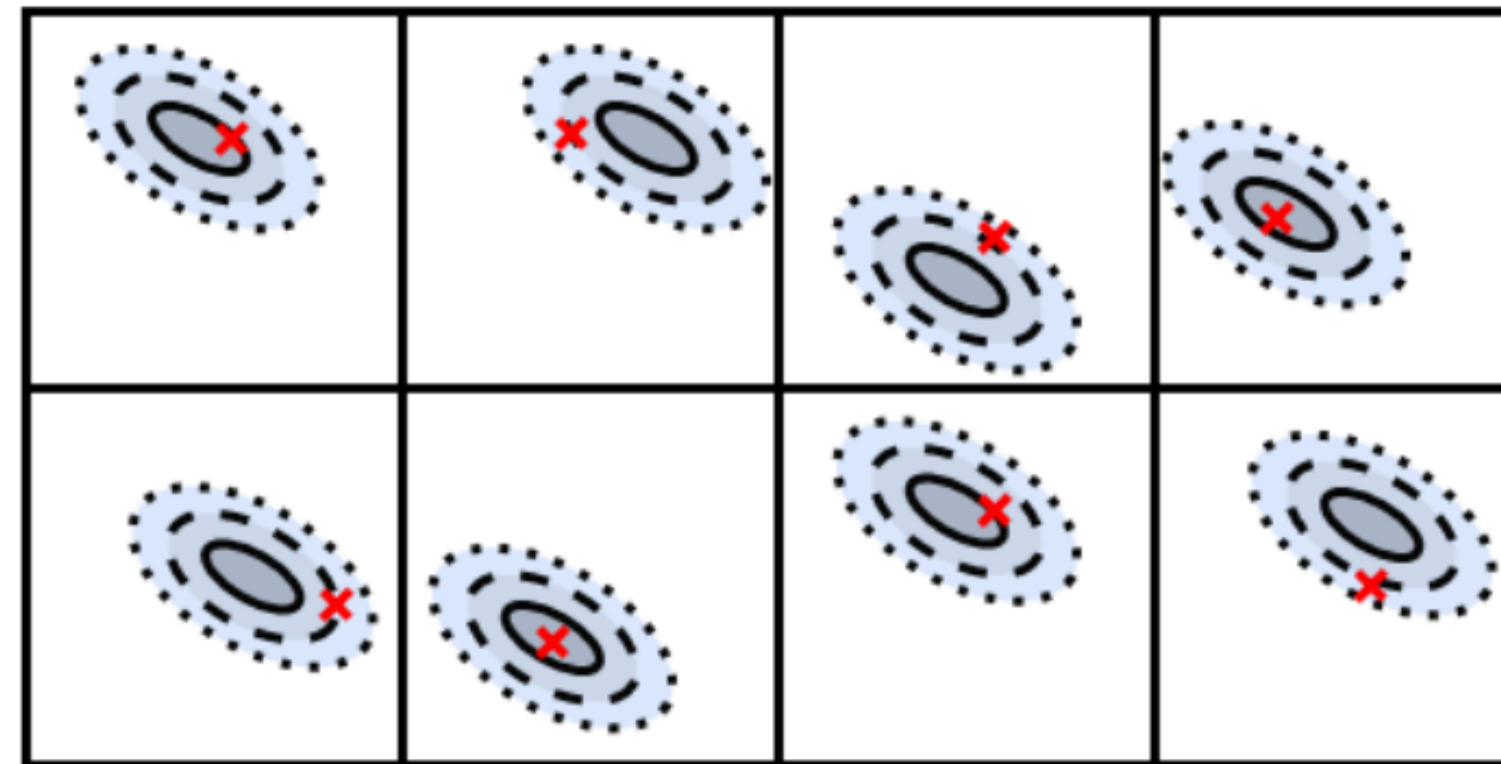
Trained networks can estimate effortlessly  
the posteriors for all simulated observations

MCMC



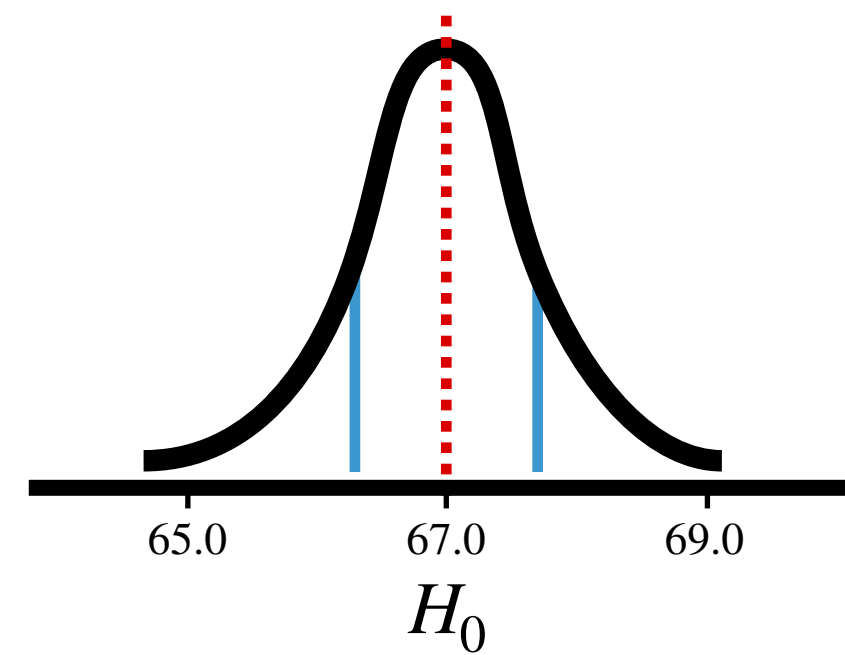
$$p(\theta|\mathbf{x}_o)$$

MNRE with swyft

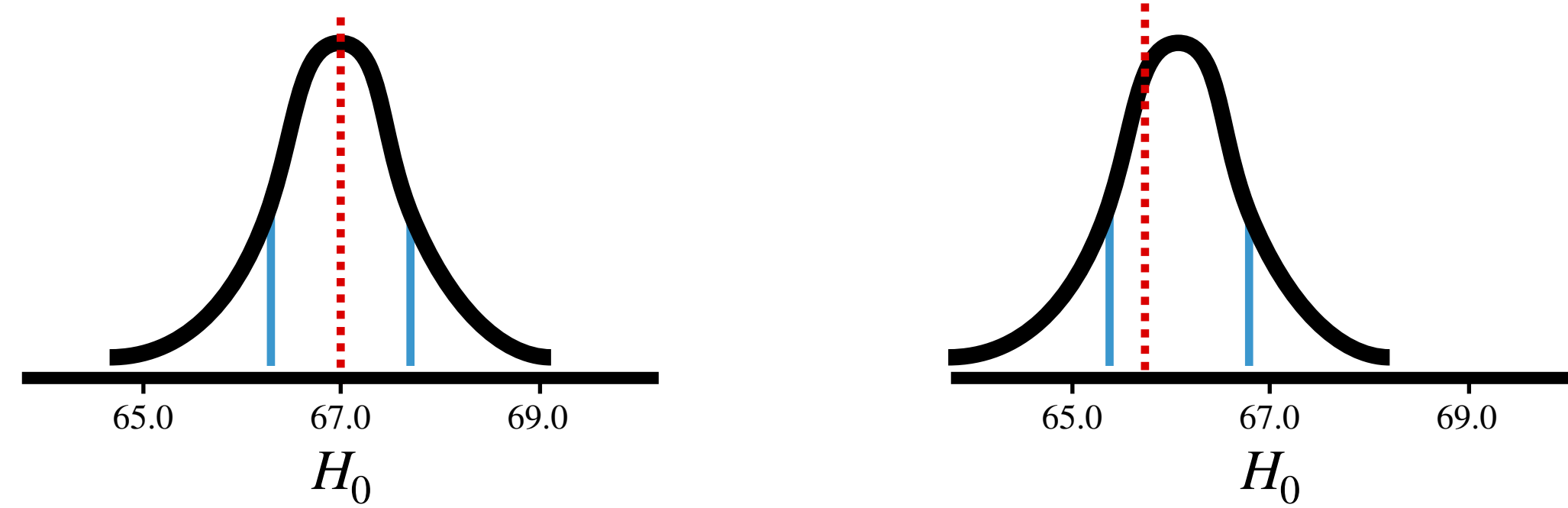


$$p(\theta|\mathbf{x}) \quad \forall \mathbf{x} \sim p(\mathbf{x})$$

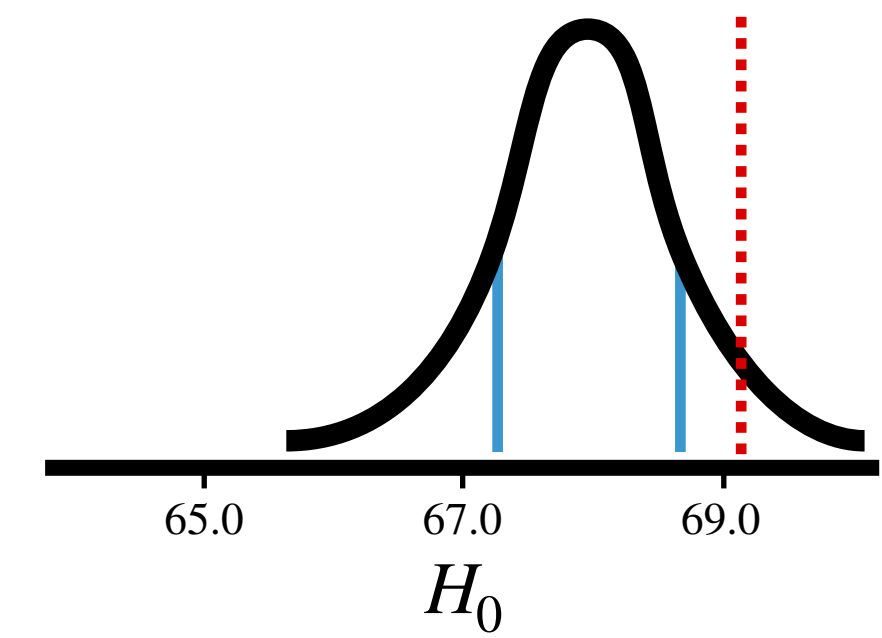
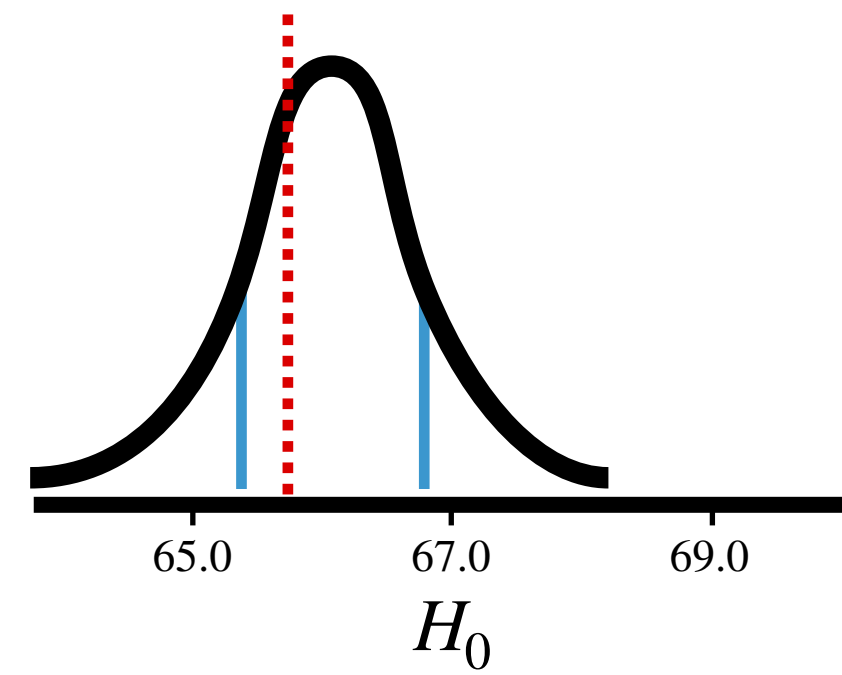
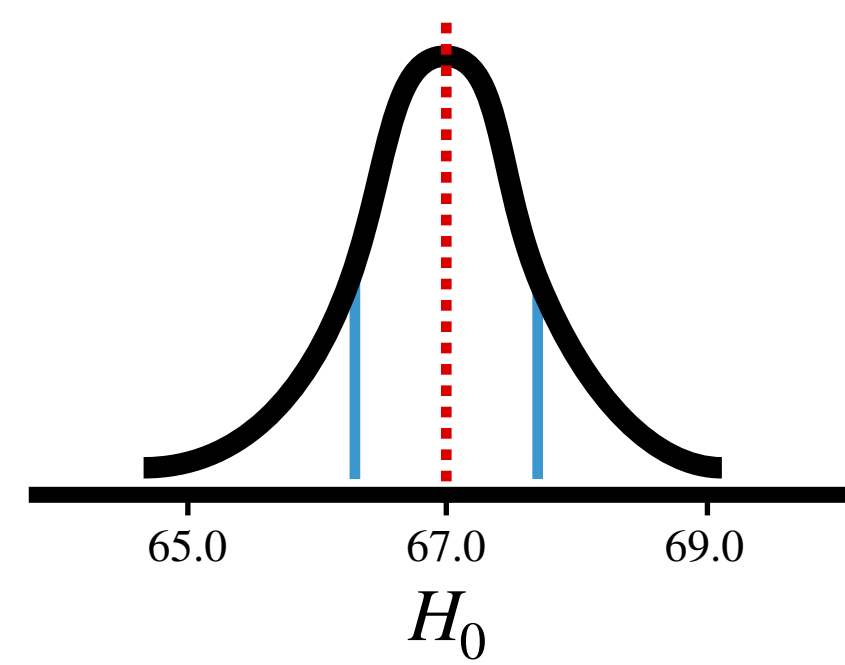
**Ex:** Is the estimated **68.27% interval** covering the **ground truth** in ~68% of the cases?



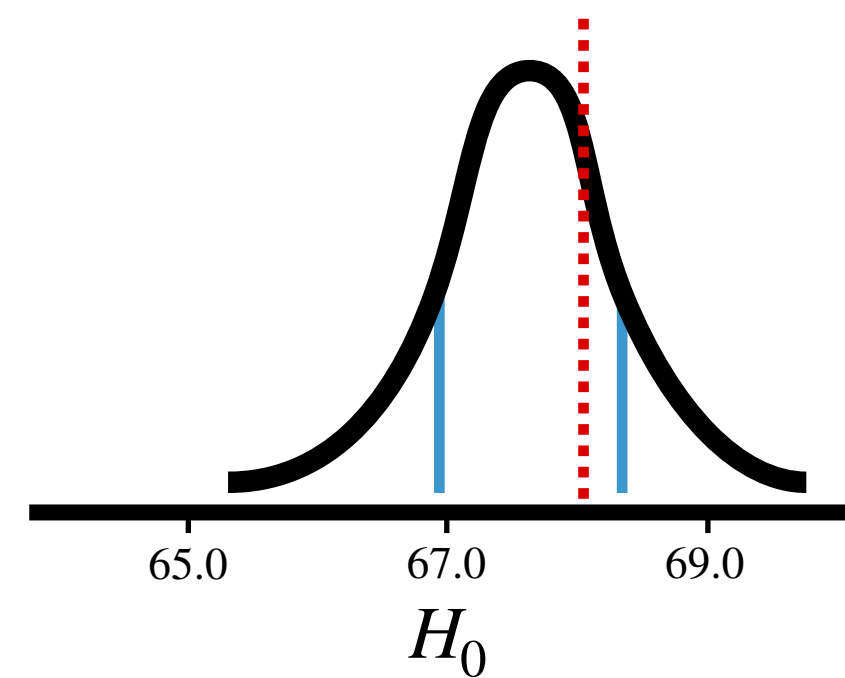
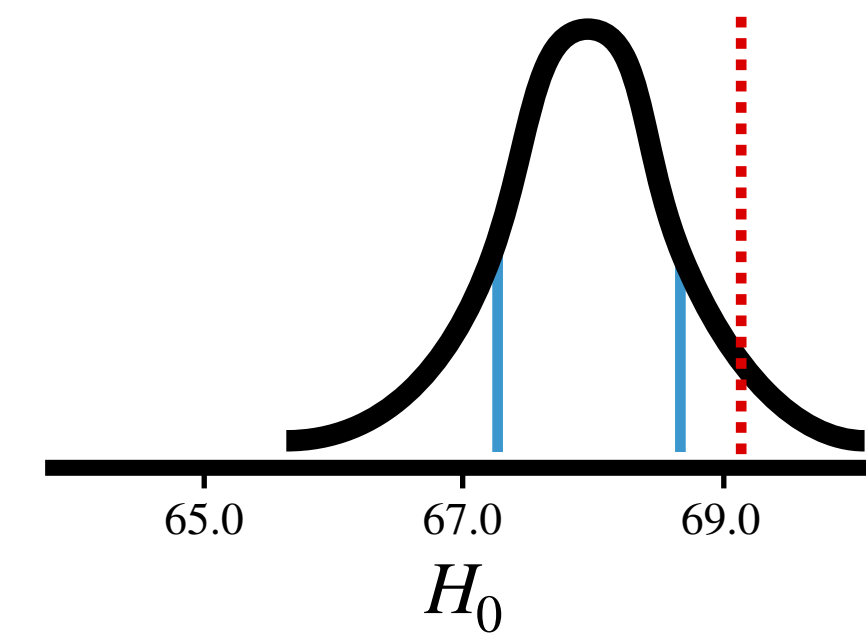
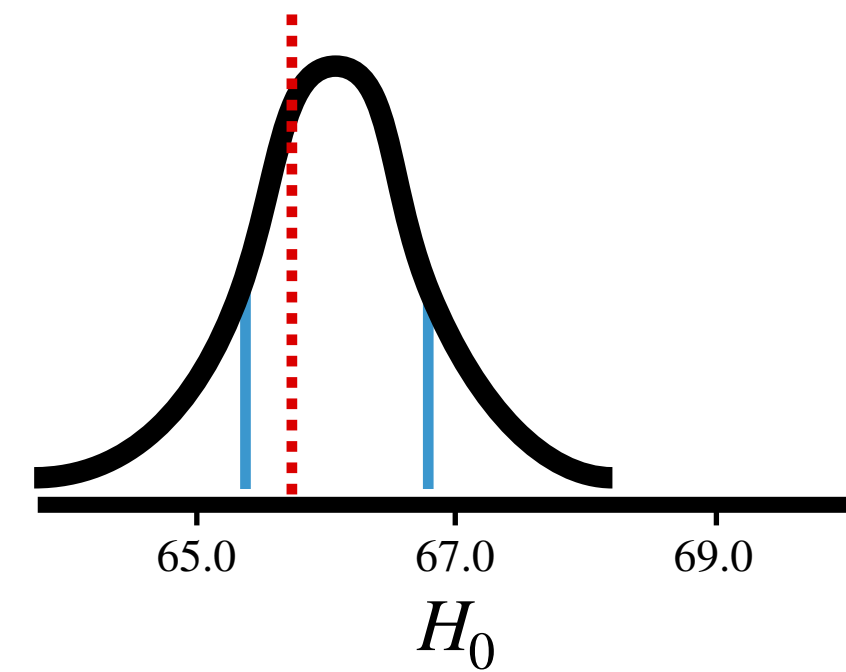
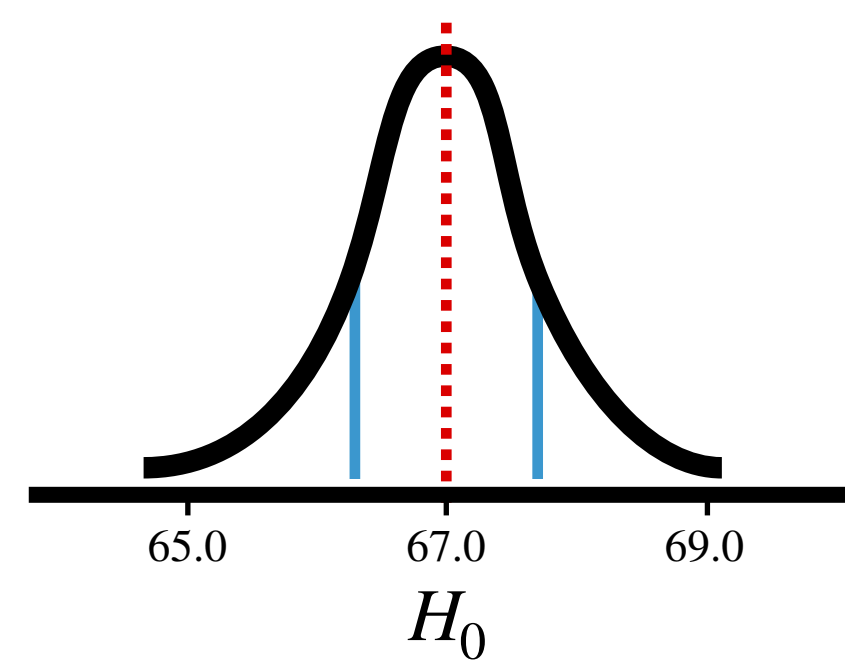
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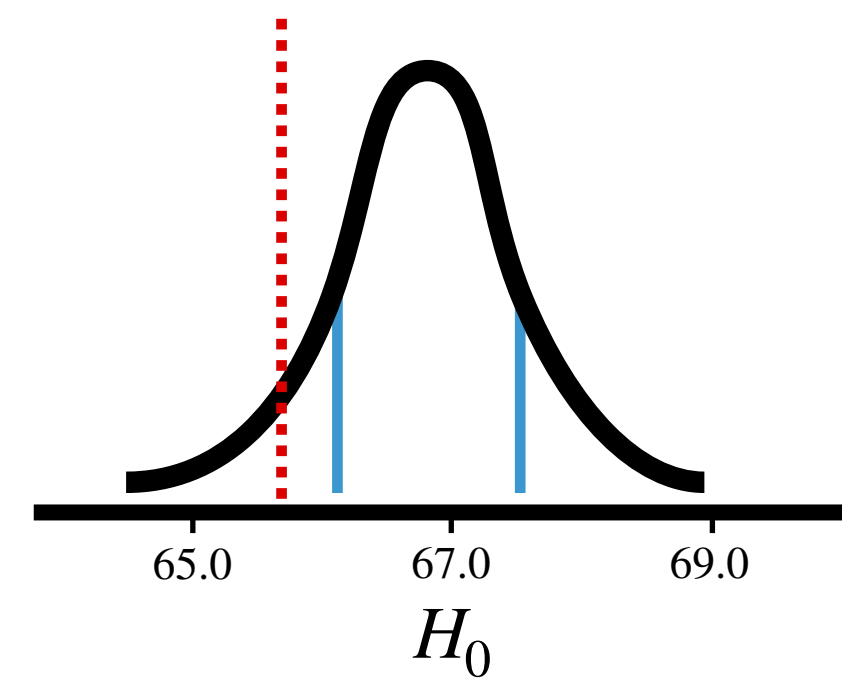
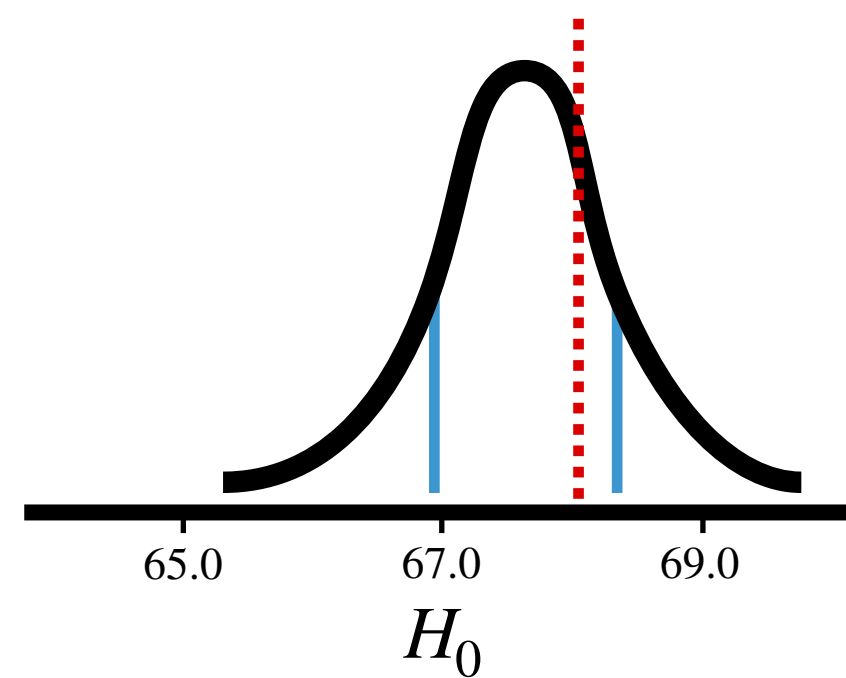
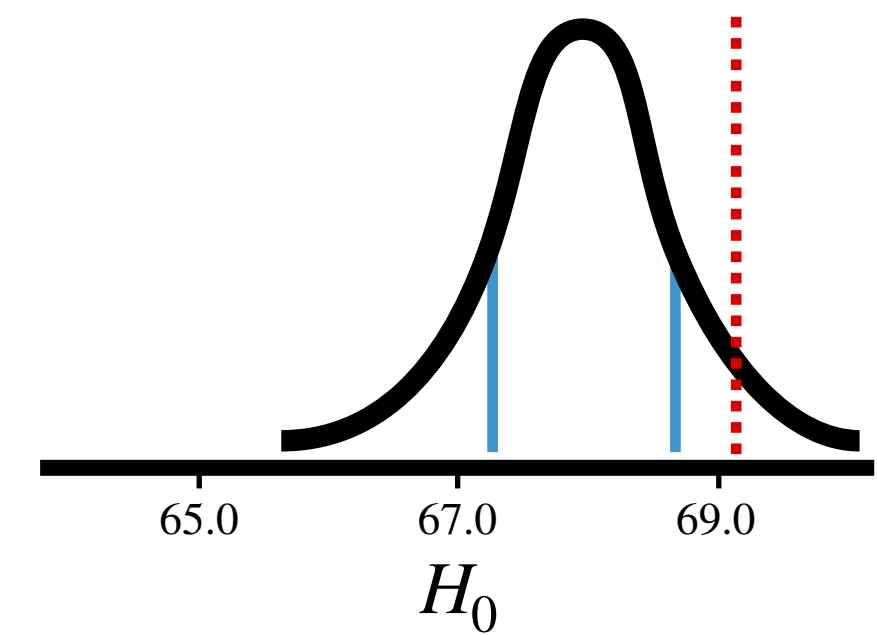
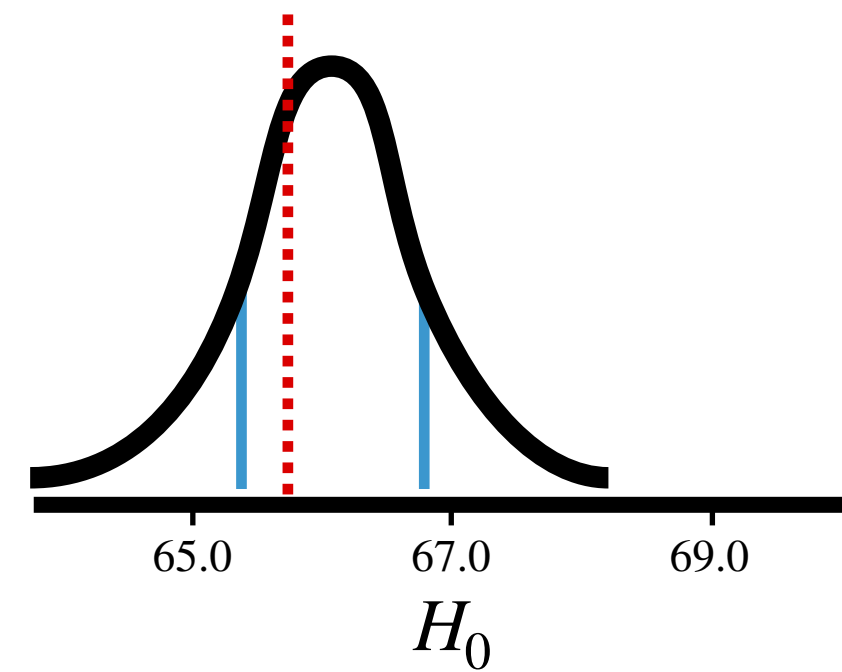
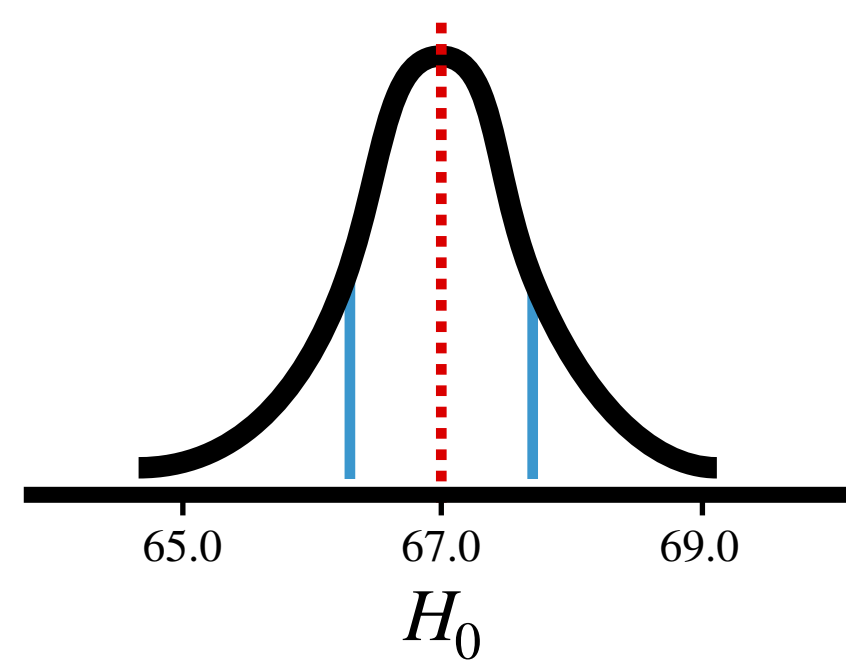
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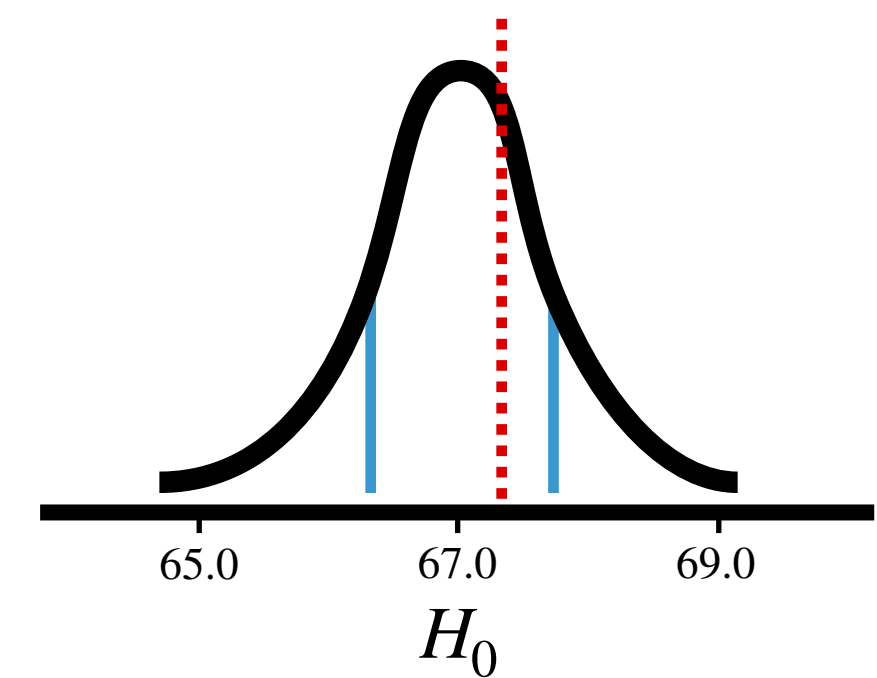
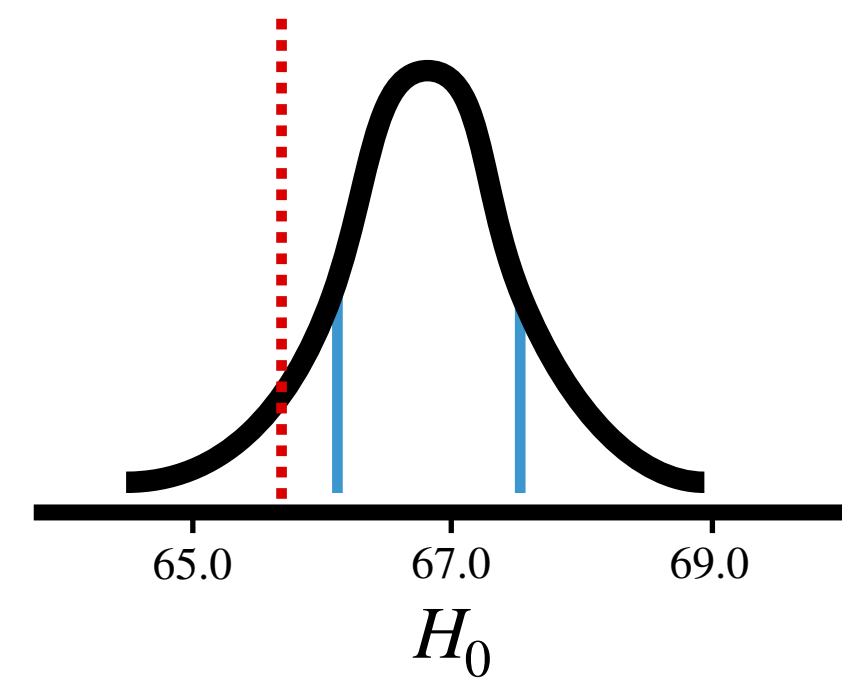
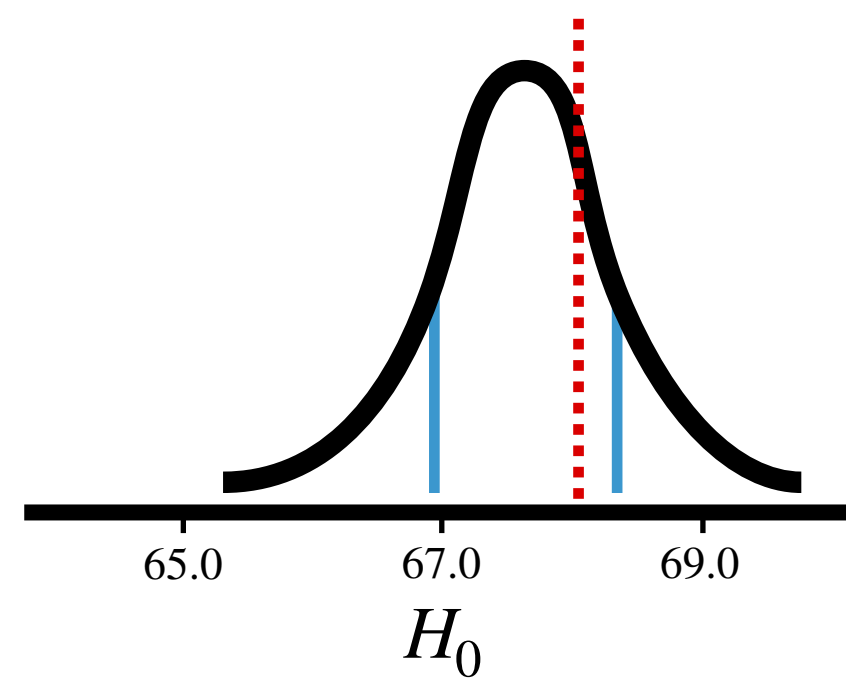
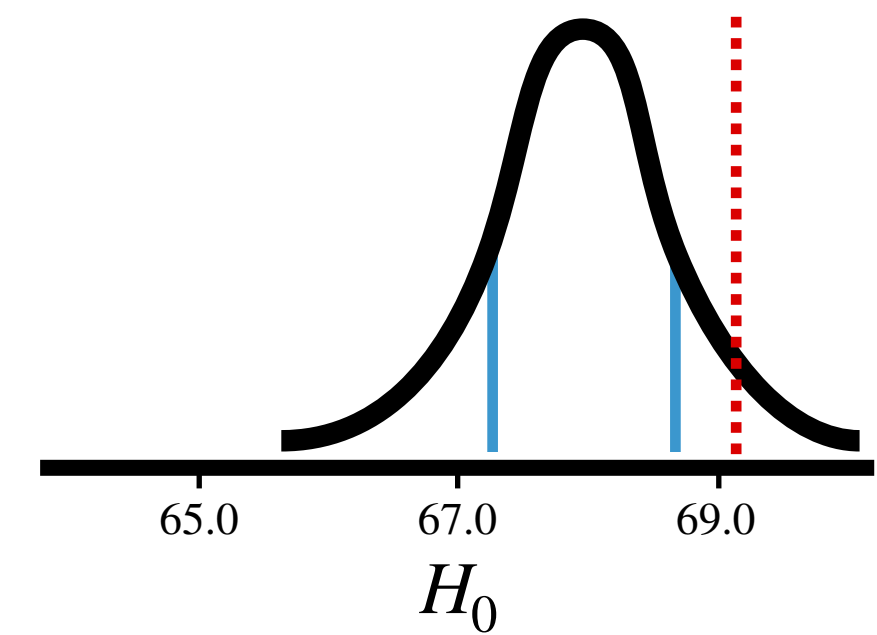
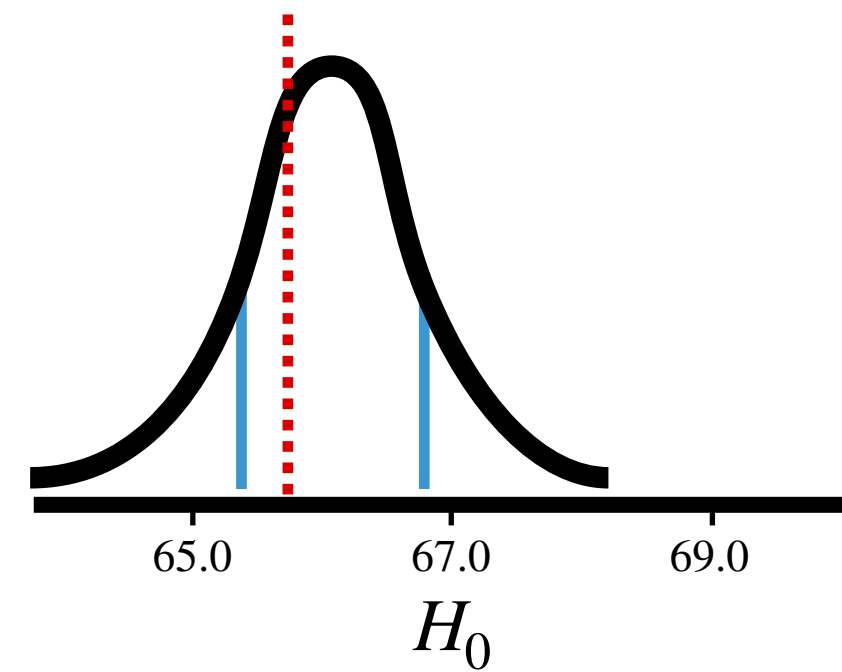
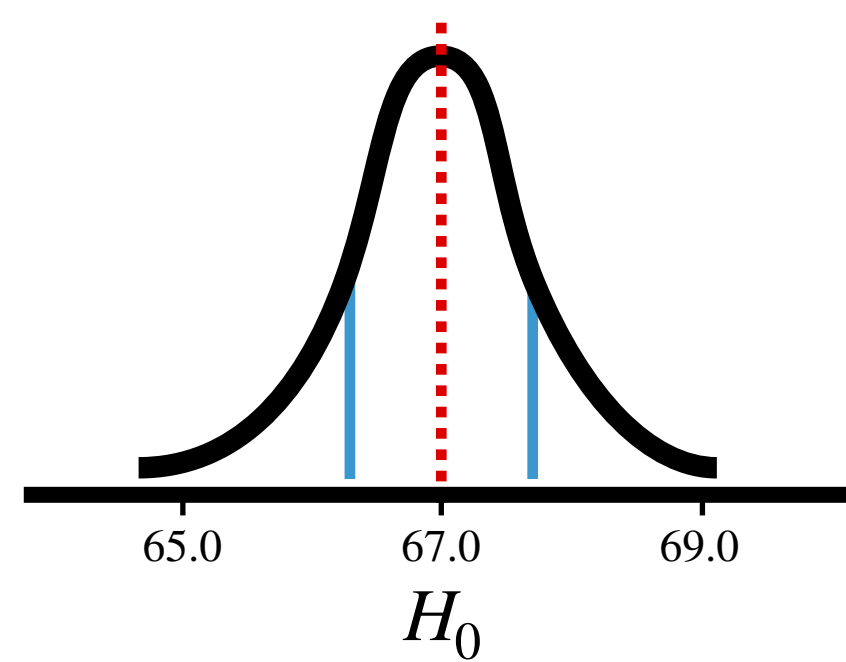
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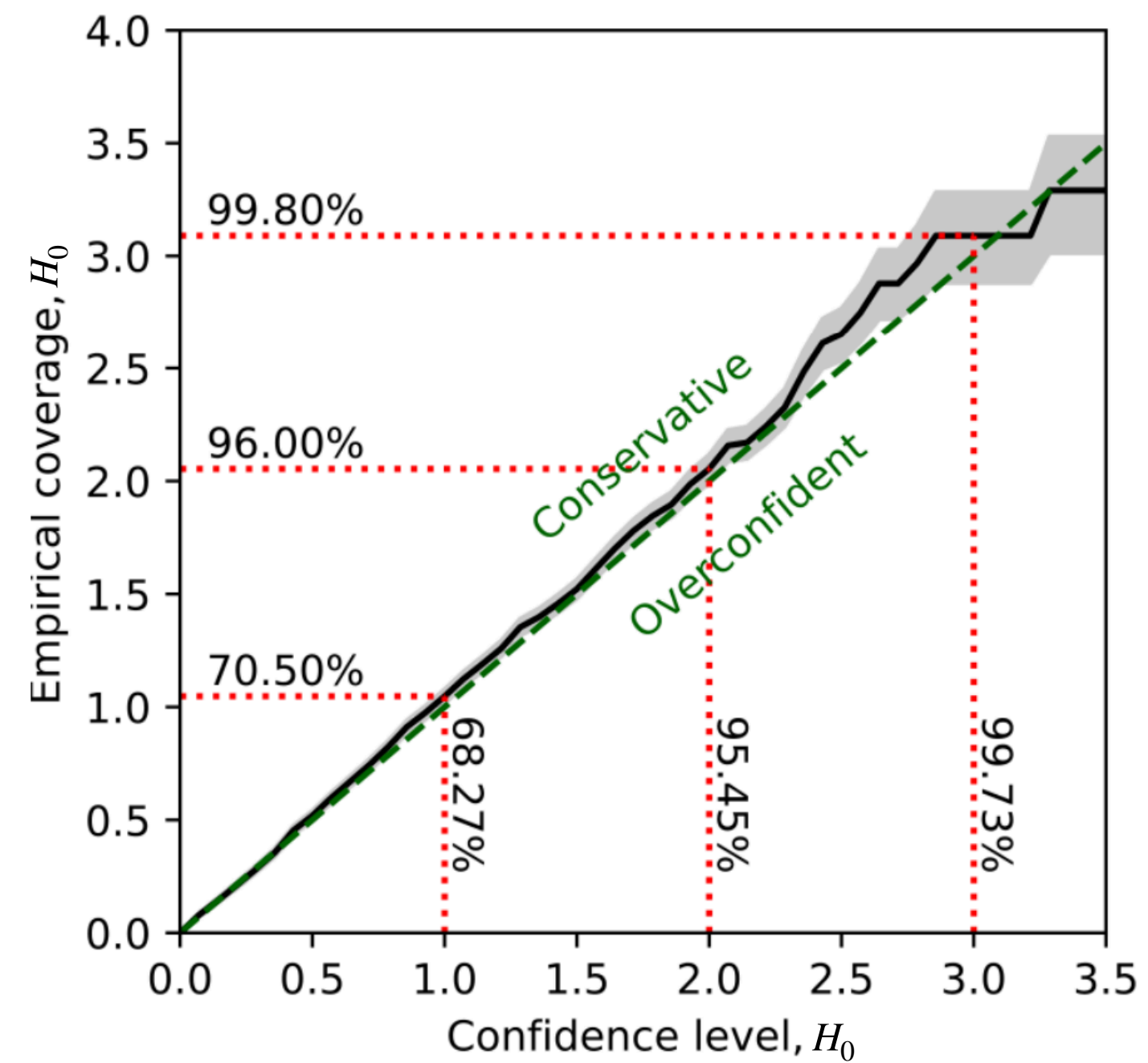


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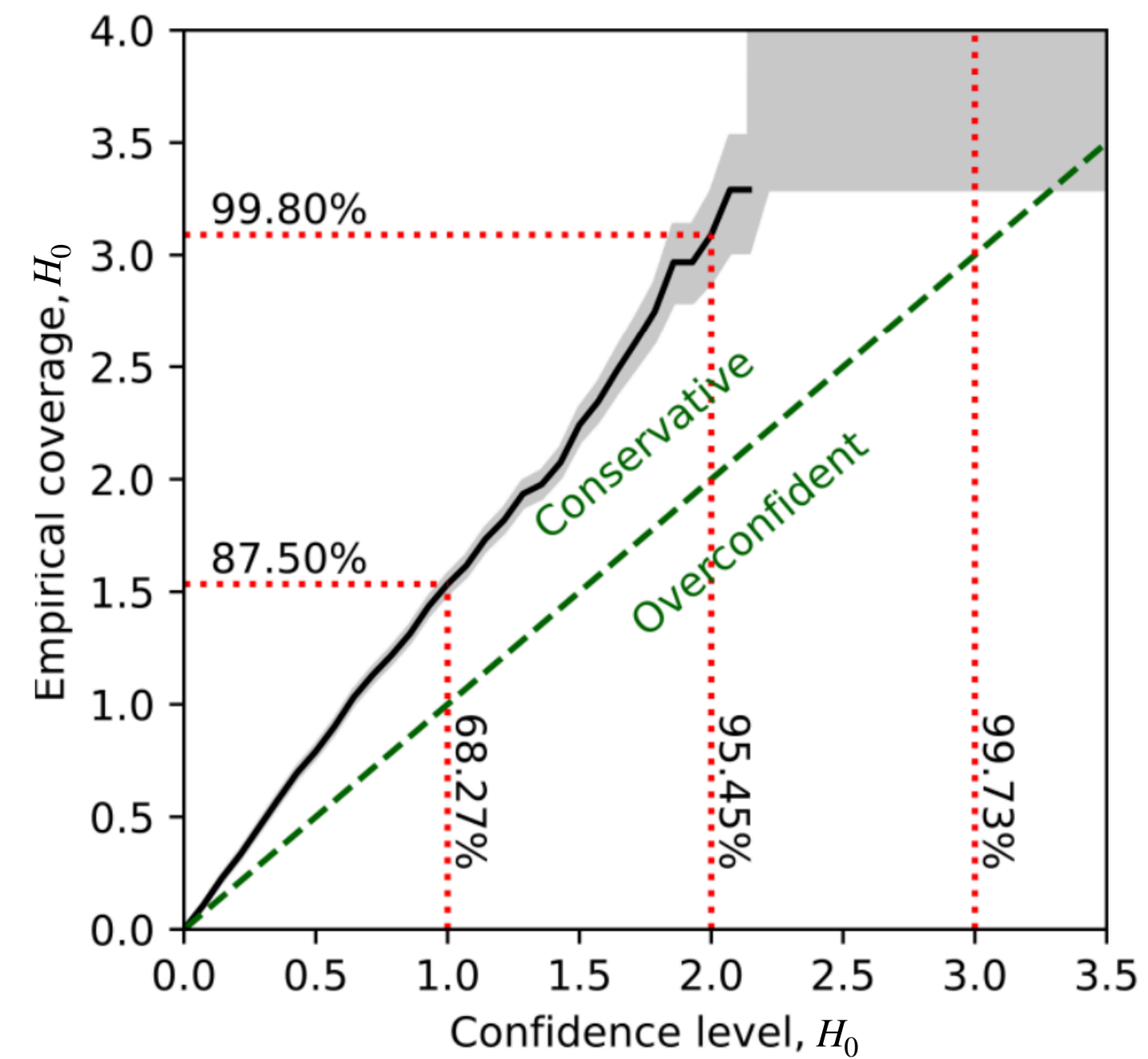


We can empirically estimate the Bayesian coverage

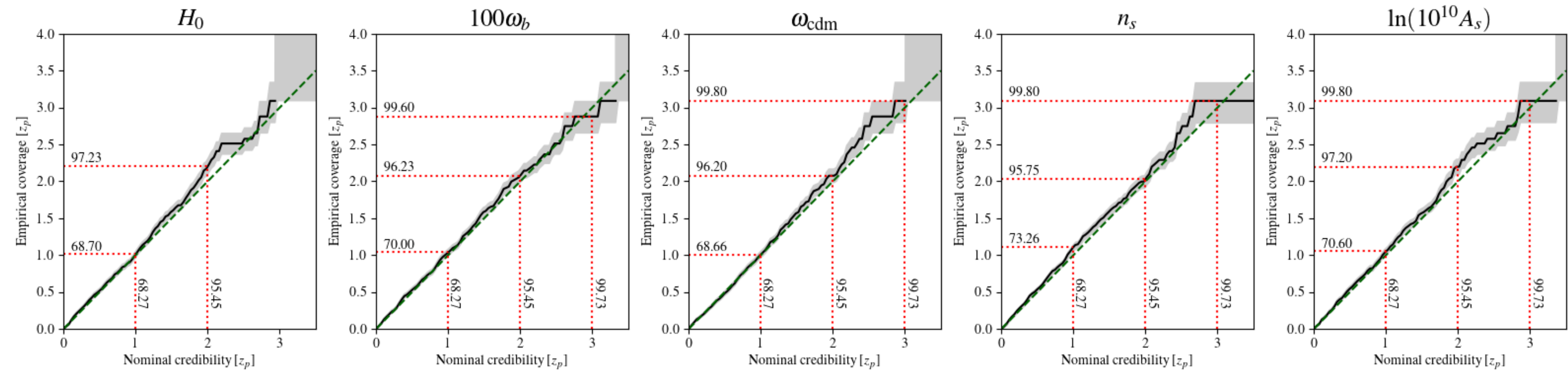
**Converged network**



**Non-converged network**

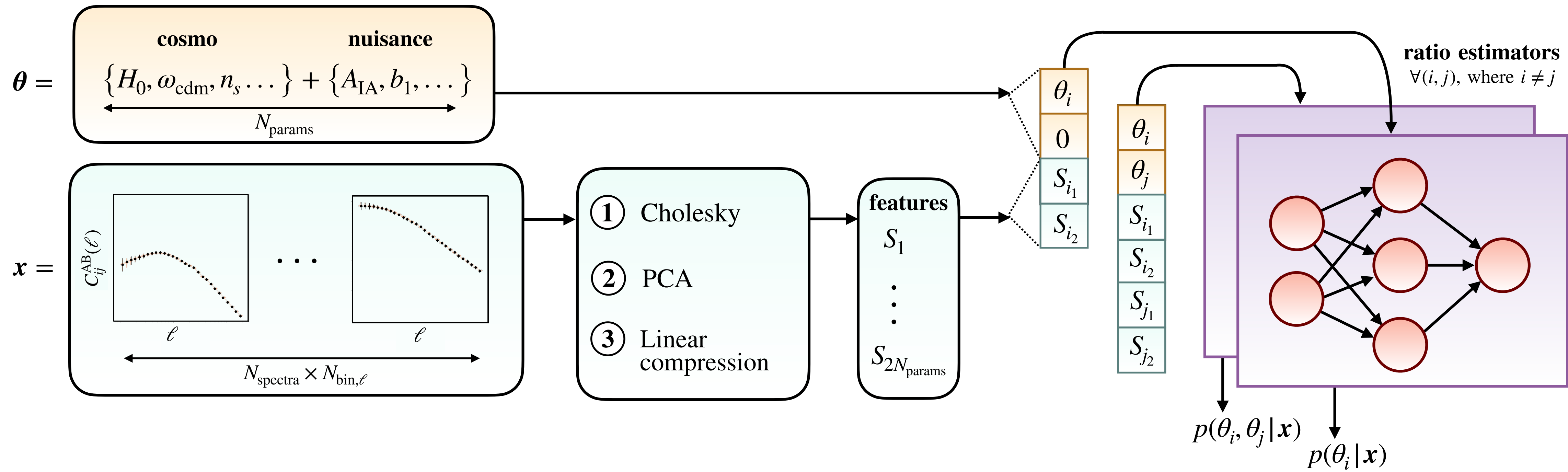


# Coverage test for Euclid 3x2pt



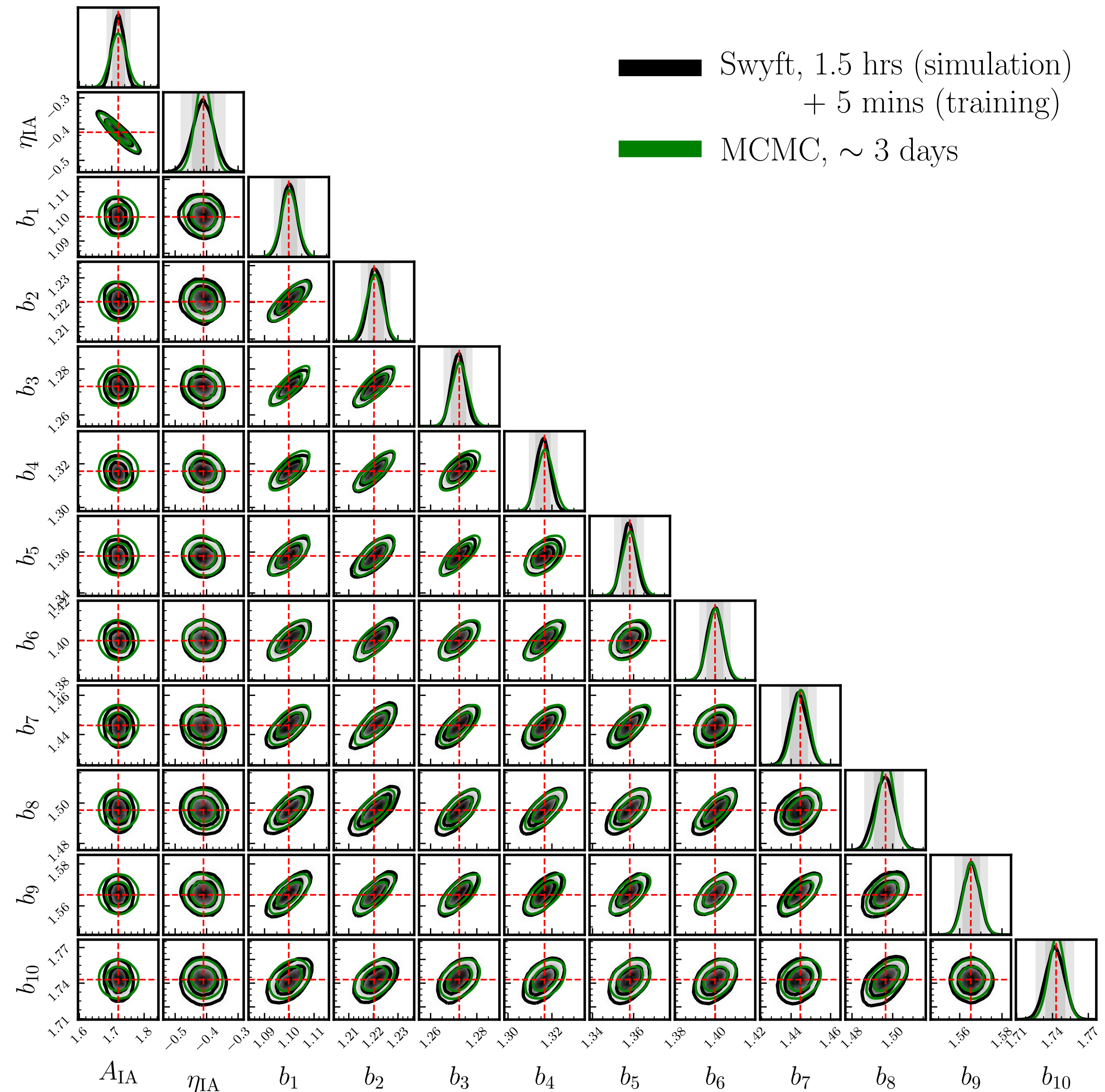
Empirical coverage and confidence level match to excellent precision!

# Network architecture



# Posteriors for nuisance parameters

MNRE & MCMC are again in good agreement



**Another big advantage  
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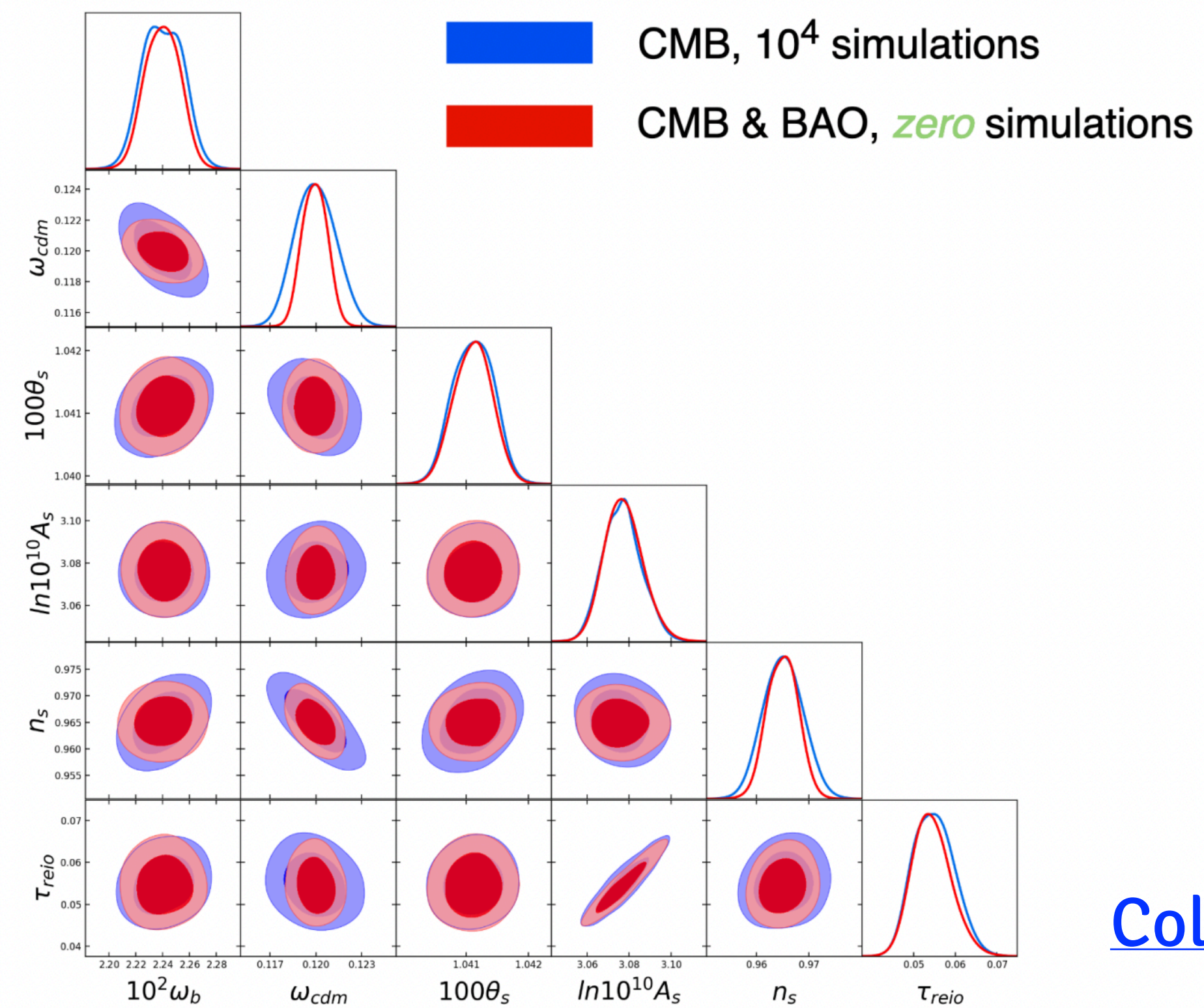
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In MNRE it is possible to **re-use simulations** for different data combinations

The idea is to **simulate all the data** at once, and then **train different inference networks** for different data combinations

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**Ex: Planck+BAO**



[Cole+ 22](#)