

Opportunities and Challenges of SBI *for galaxy clustering*

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what is simulation-based inference?

opportunities for simulation-based inference?

challenges for simulation-based inference?

what is simulation-based inference?

opportunities for simulation-based inference?

challenges for simulation-based inference?

goal: infer the *posterior of cosmological parameters* given observations

$$p(\theta \mid \mathbf{X}) = \frac{p(\mathbf{X} \mid \theta) p(\theta)}{p(\mathbf{X})}$$

goal: infer the *posterior* of cosmological parameters given observations

likelihood prior

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

posterior evidence

goal: infer the *posterior of cosmological parameters* given observations

$$p(\theta \mid \mathbf{X}) \propto p(\mathbf{X} \mid \theta) p(\theta)$$

lets ignore evidence since it's independent of θ

goal: infer the *posterior of cosmological parameters* given observations

$$p(\theta | \mathbf{X}) \propto p(\mathbf{X} | \theta) p(\theta)$$

$$\log p(\mathbf{X} | \theta) = \log \mathcal{L} = [(\mathbf{m}(\theta) - \mathbf{X})^T \mathbf{C}^{-1} (\mathbf{m}(\theta) - \mathbf{X})] + \log(2\pi)^{-k/2} |\mathbf{C}|^{-1/2}$$



m = your favorite theory model for \mathbf{X}



\mathbf{C} = covariance matrix from mocks

standard likelihood in cosmology

what is **simulation-based inference**?

$$\mathbf{X}' \sim F(\theta')$$

what is **simulation-based inference**?

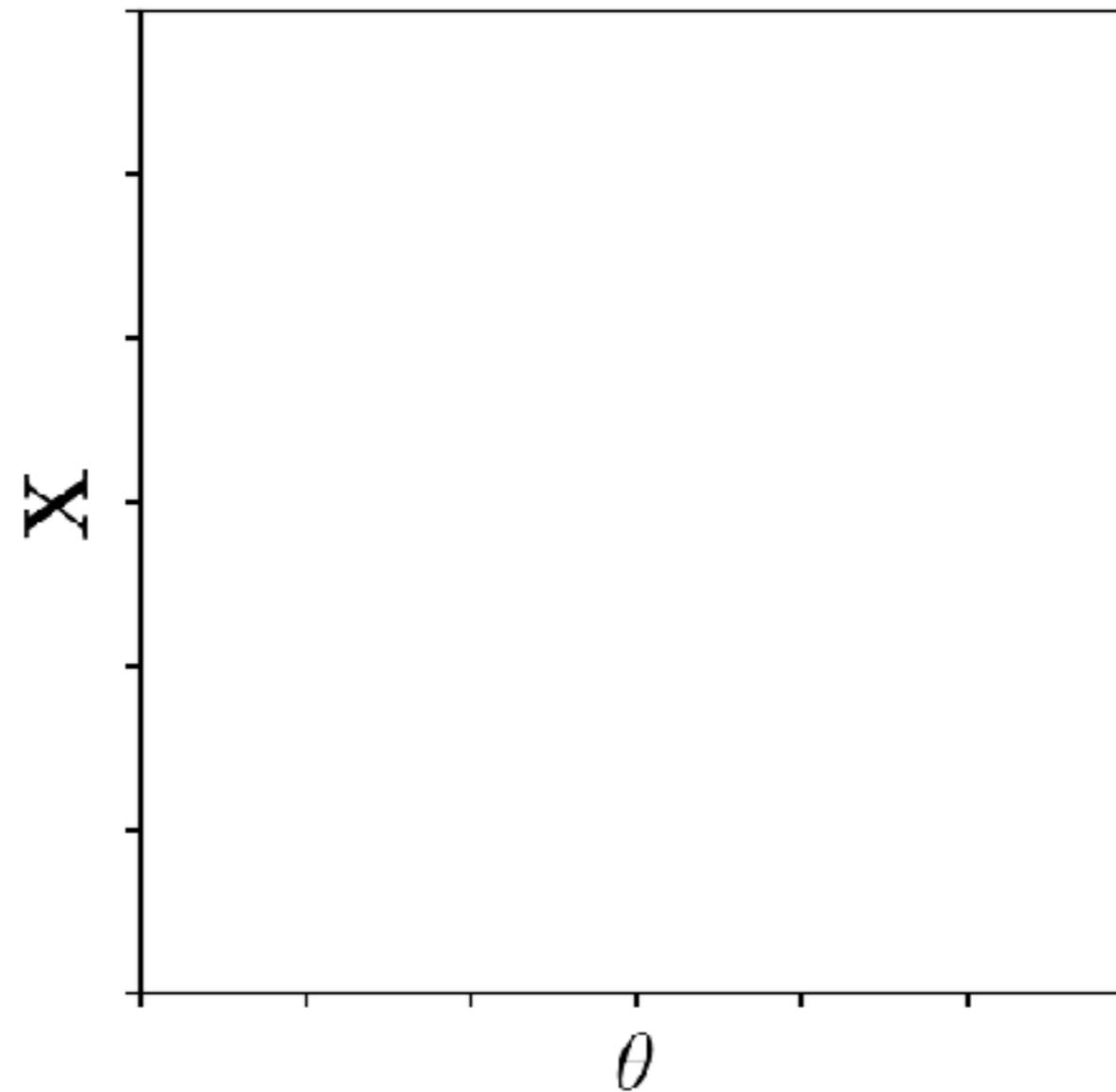
some stochastic forward model/simulator

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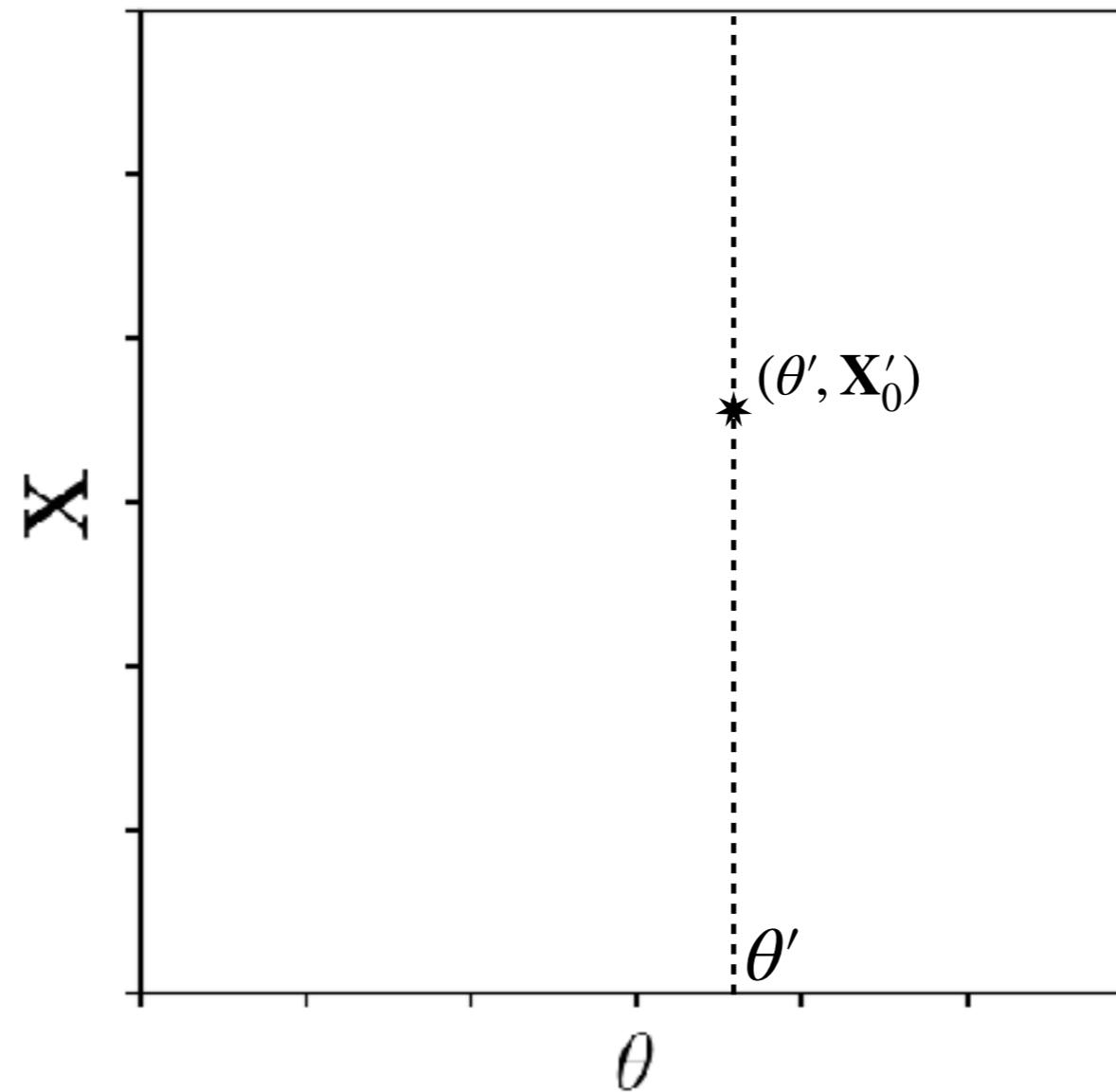
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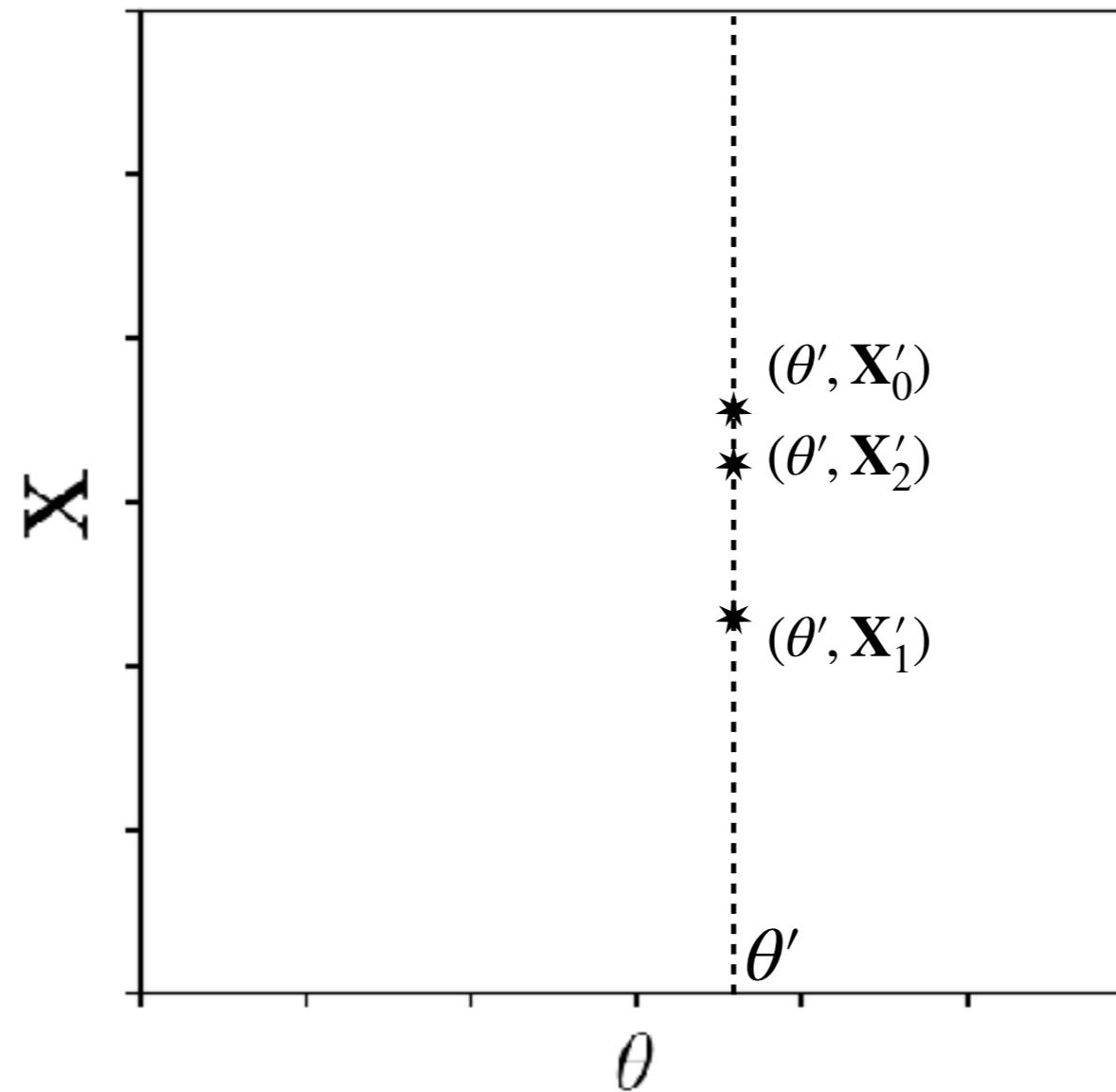
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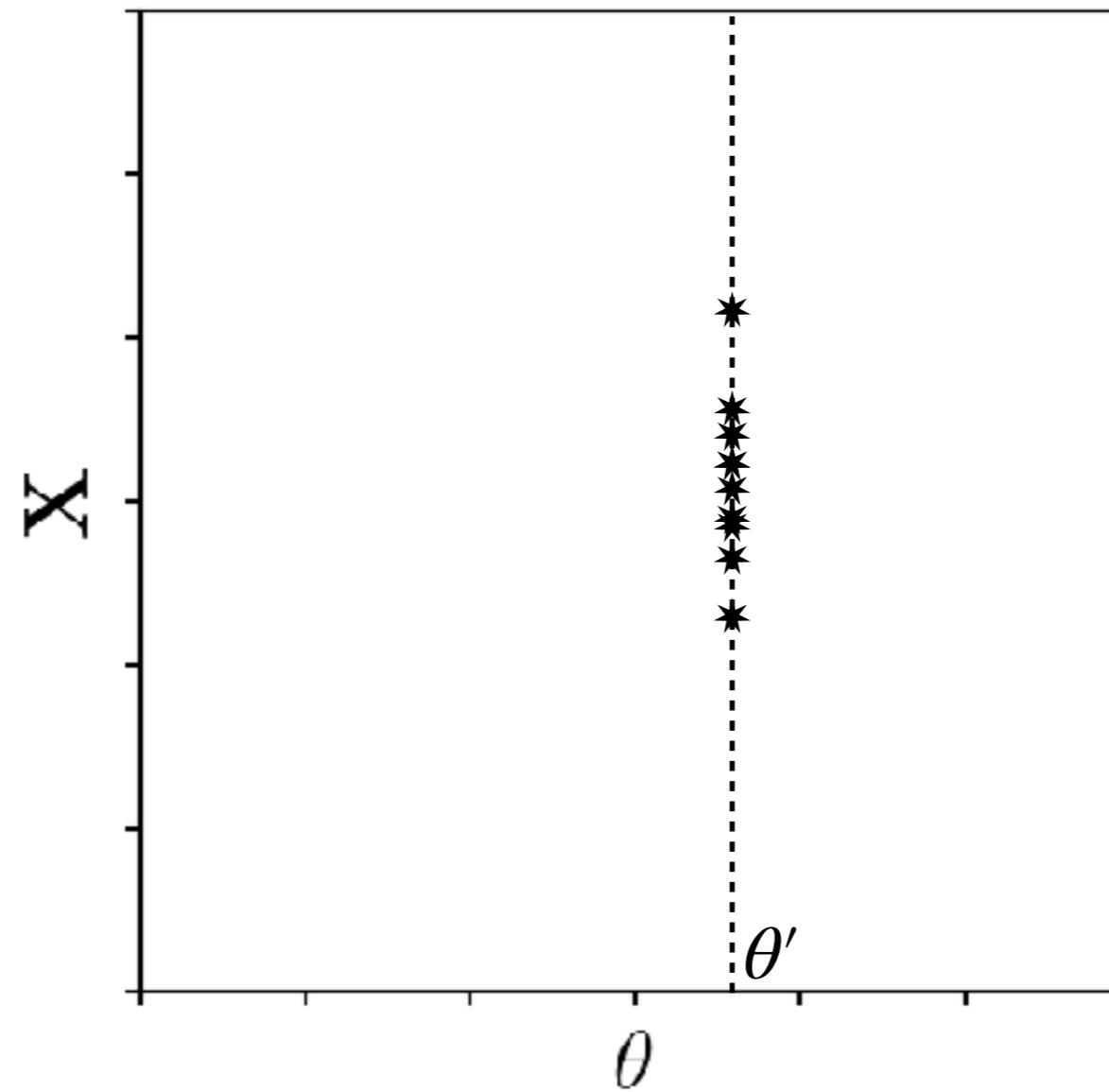
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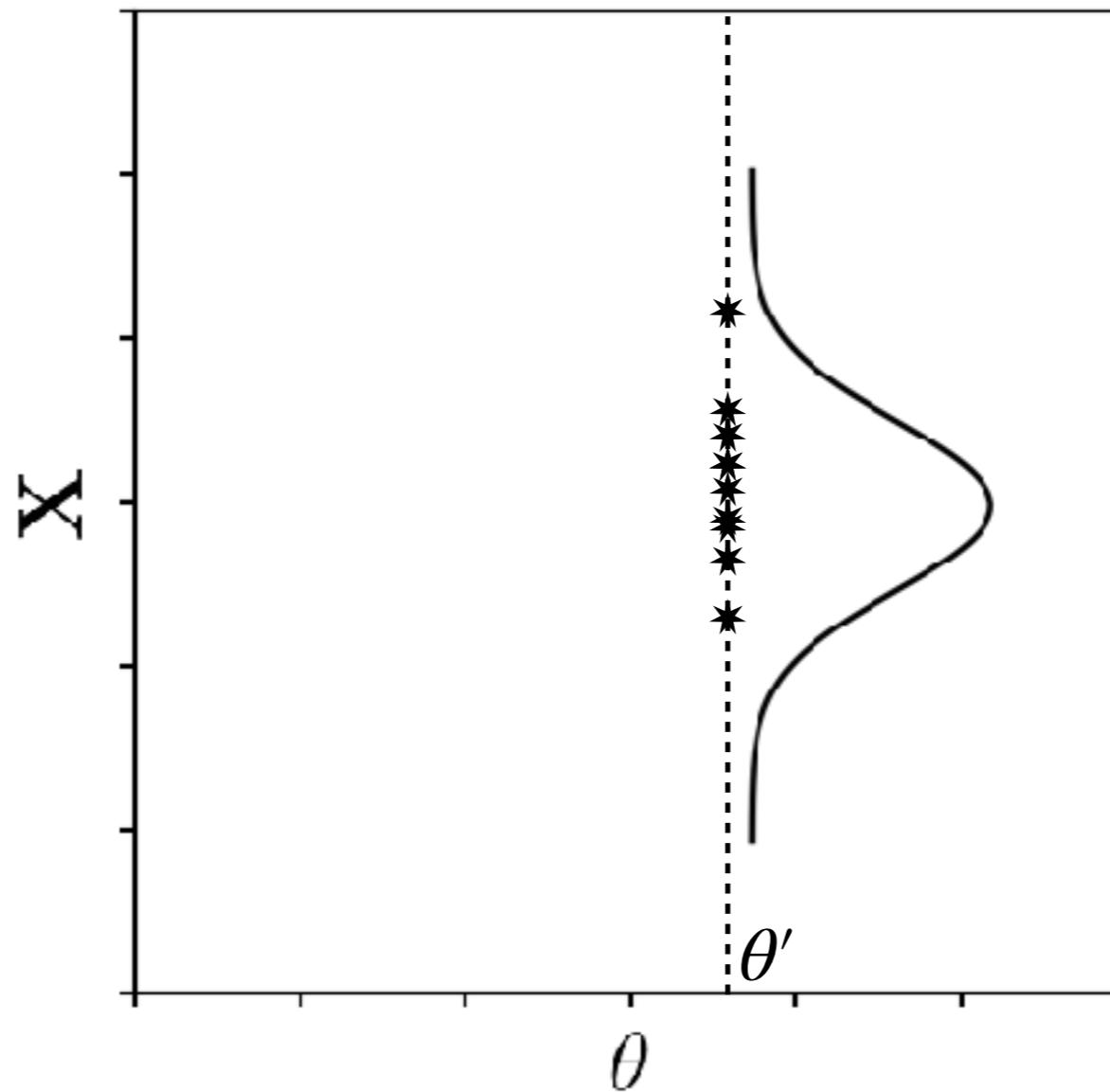
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what is simulation-based inference?

the forward model/simulator implicitly defines our likelihood

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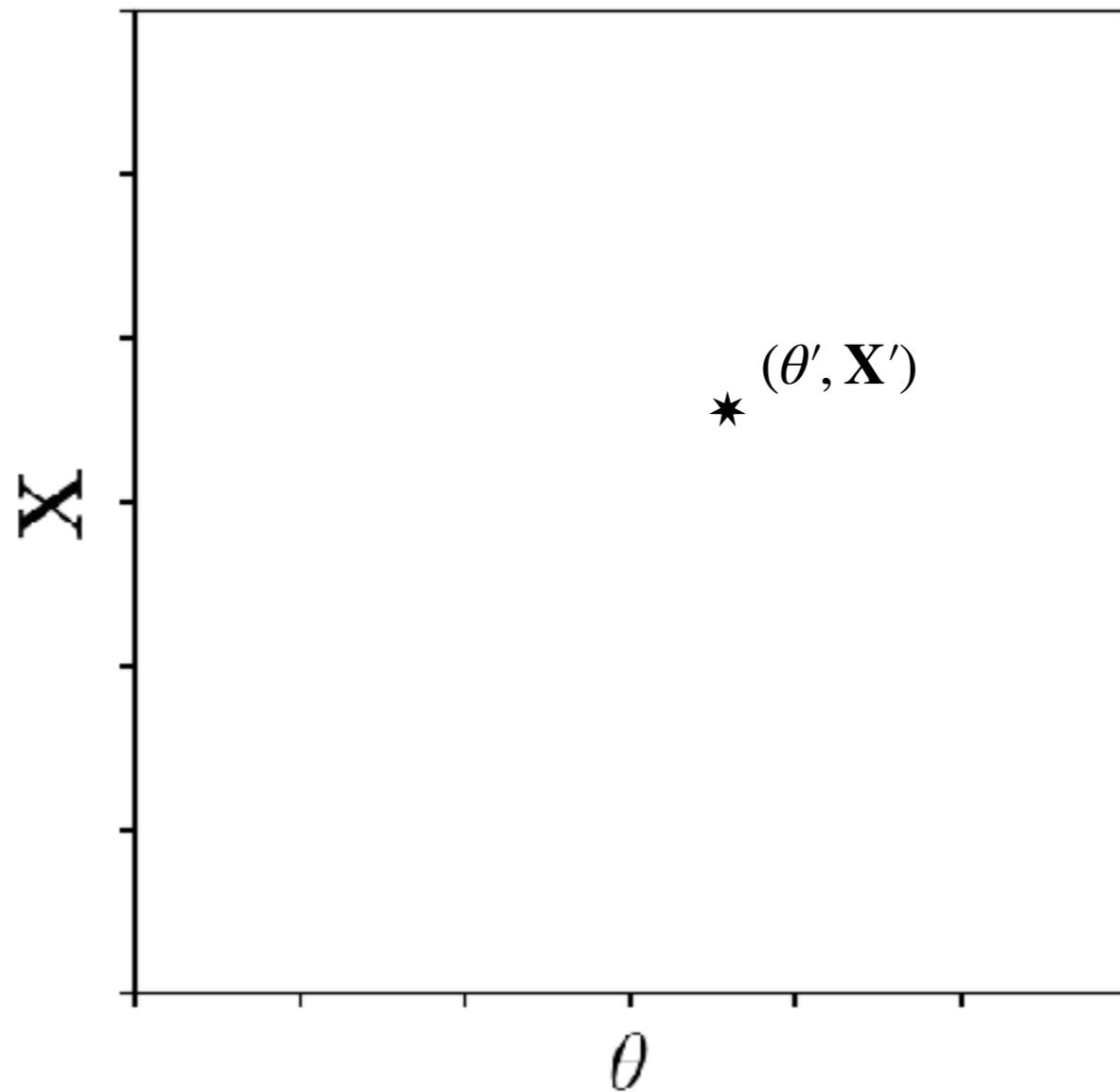
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$$\theta' \sim p(\theta)$$

2. run simulator

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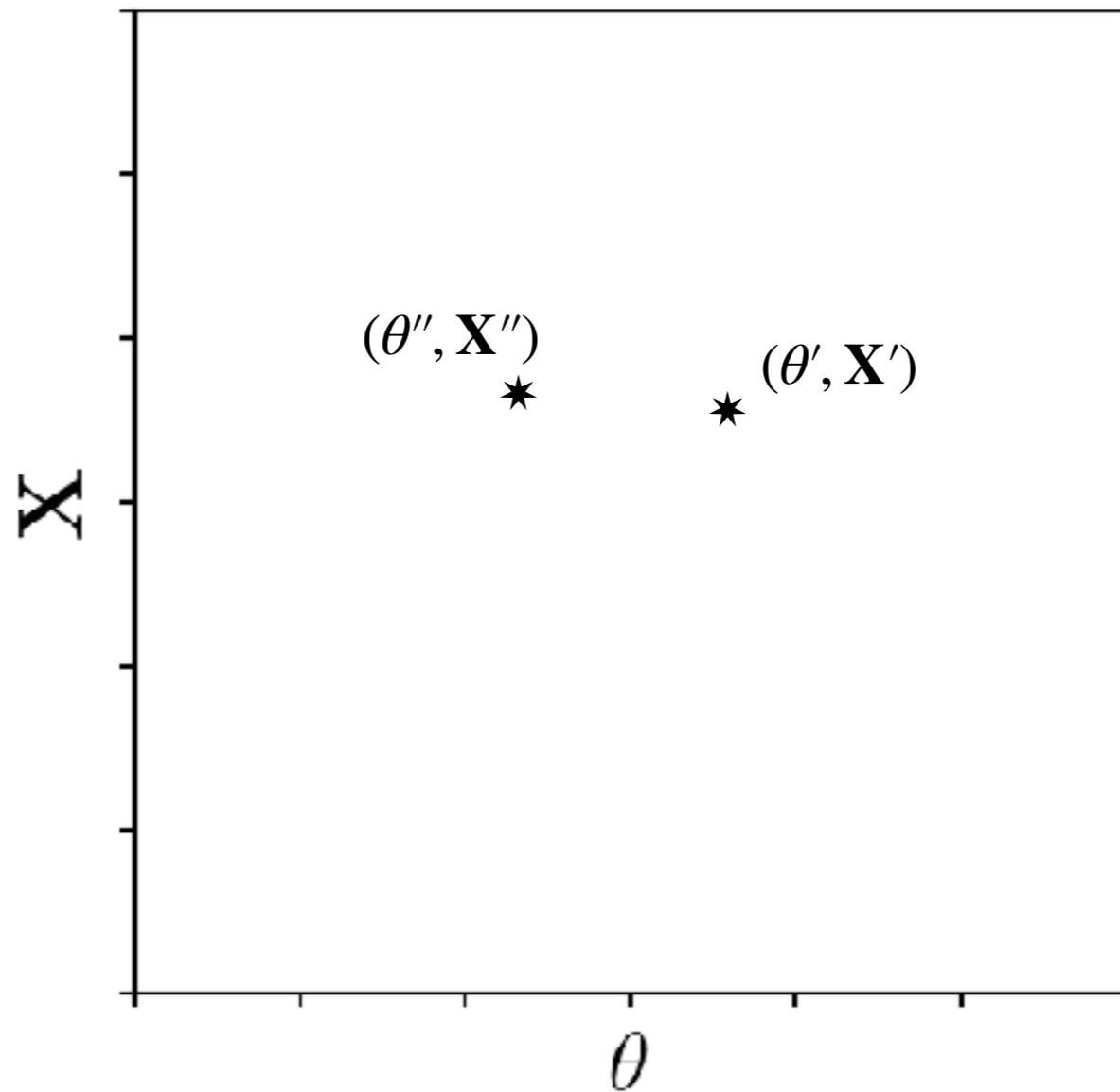
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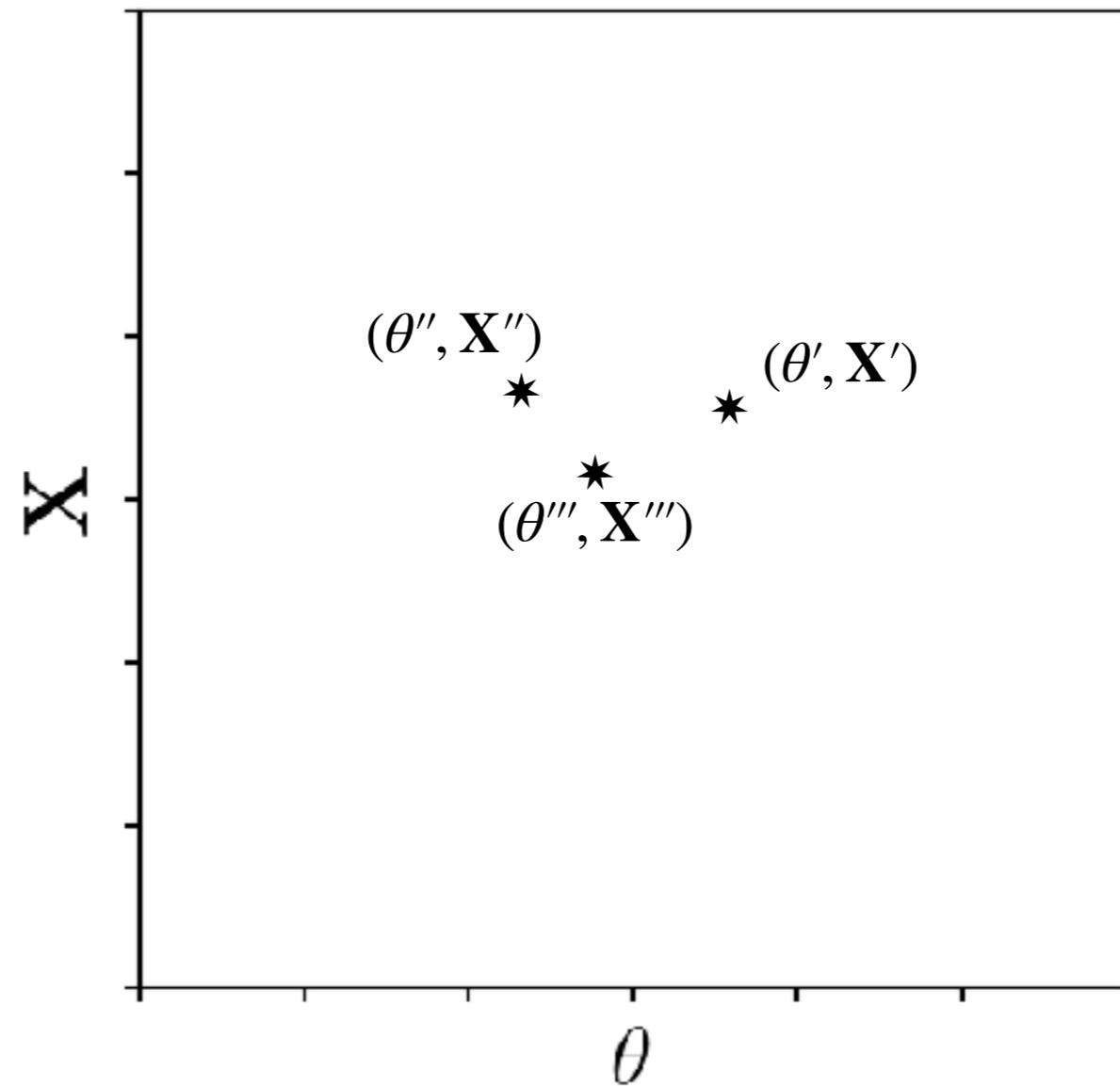
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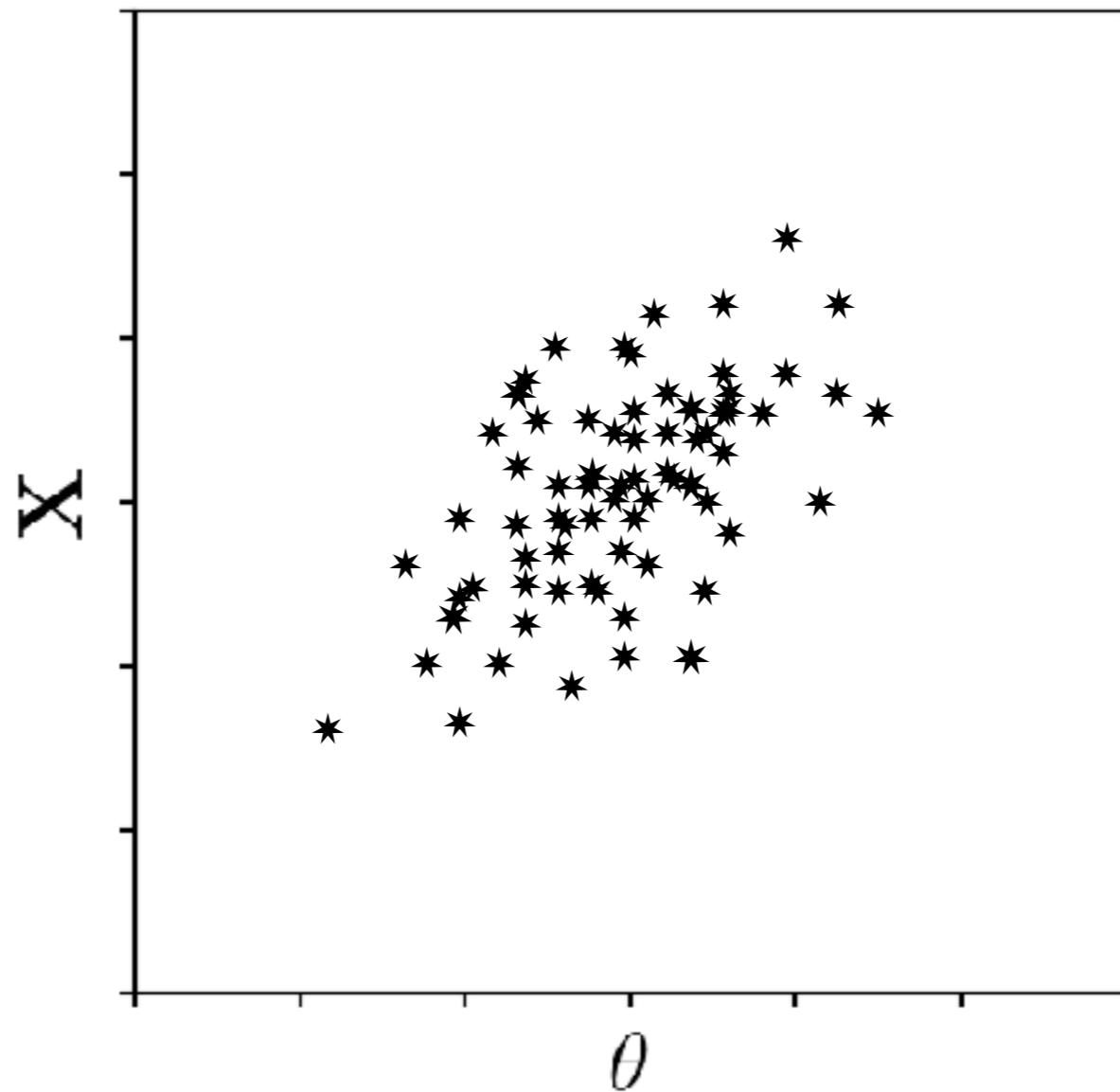
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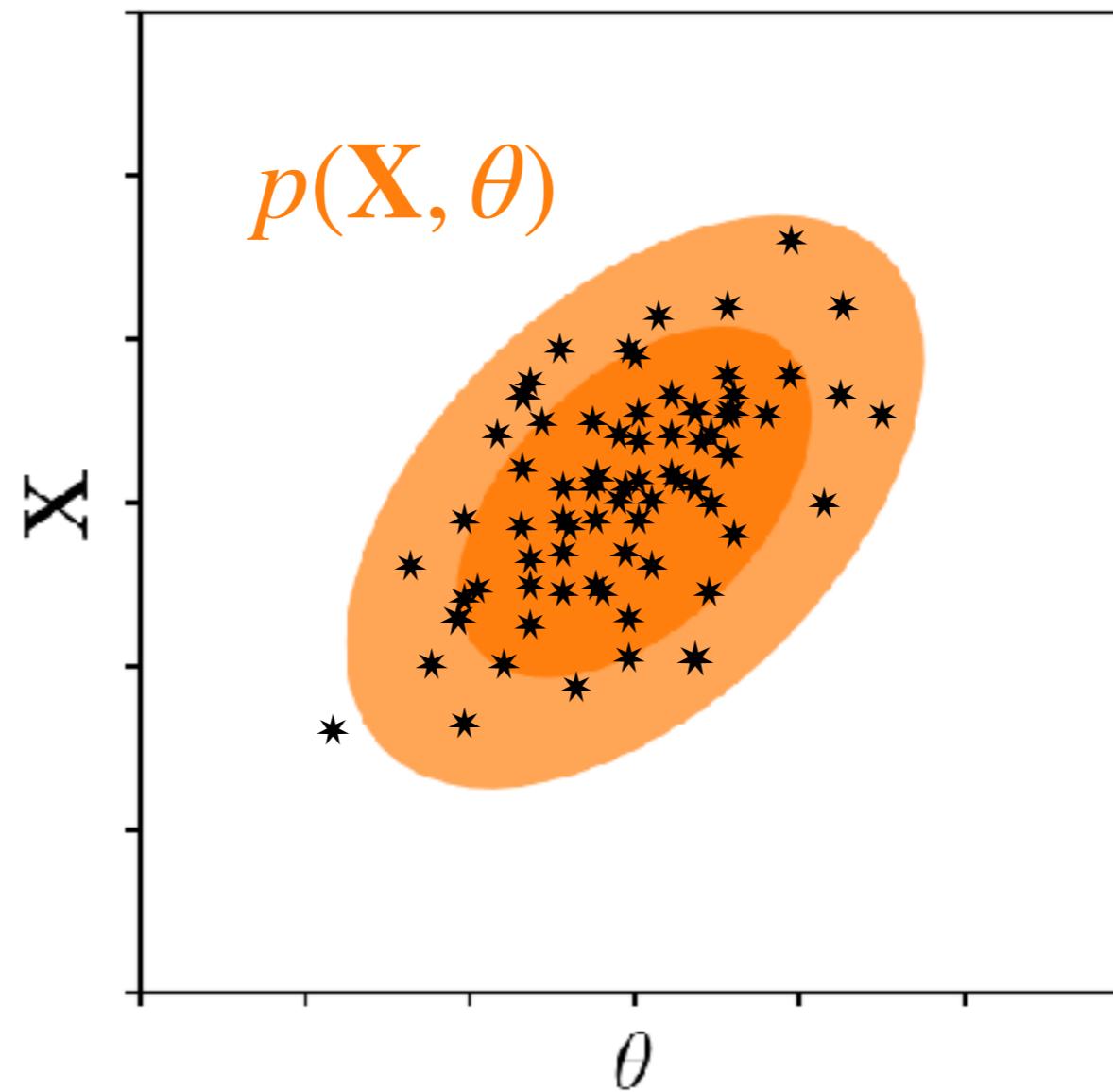
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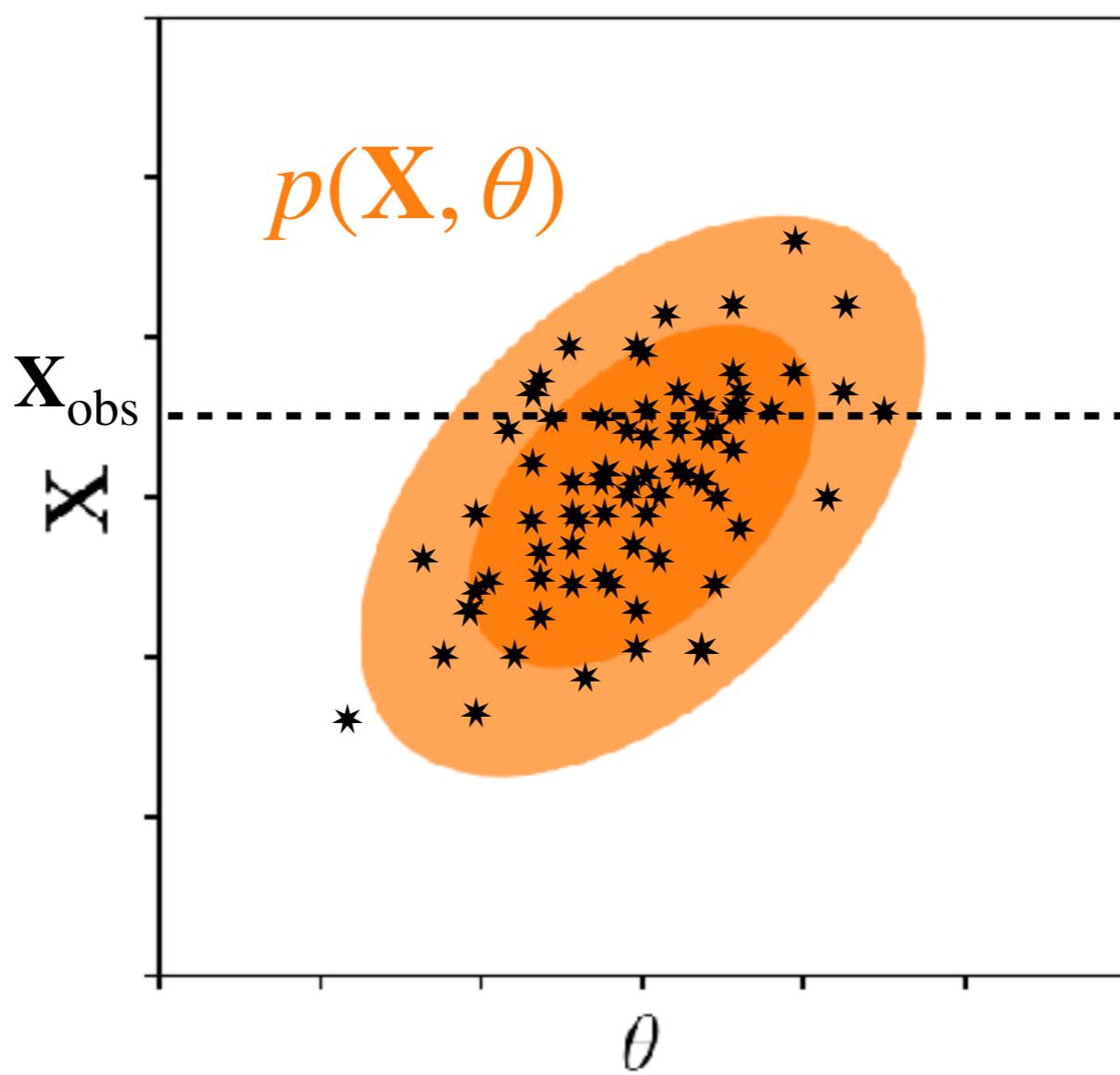
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2. run simulator

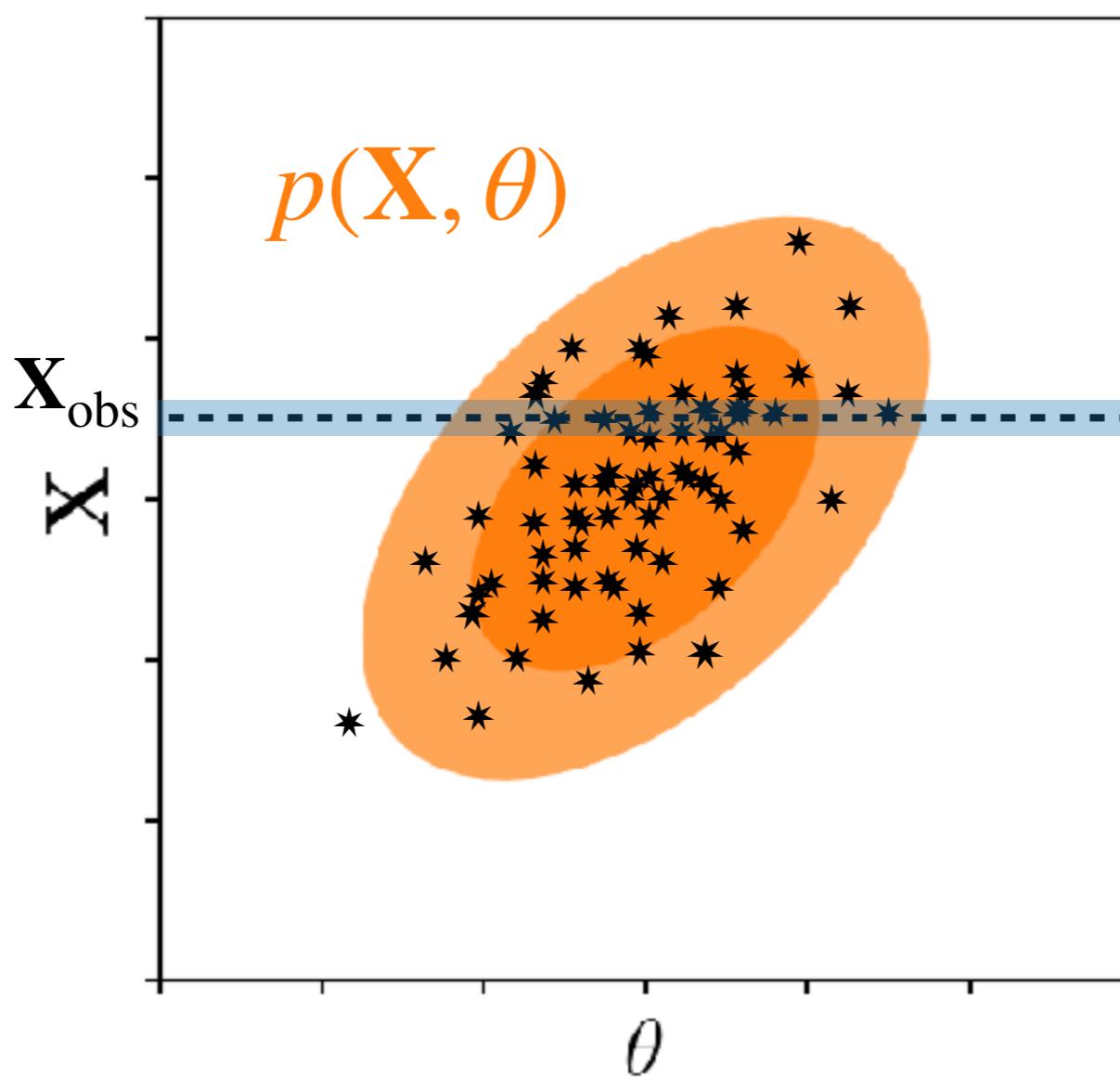
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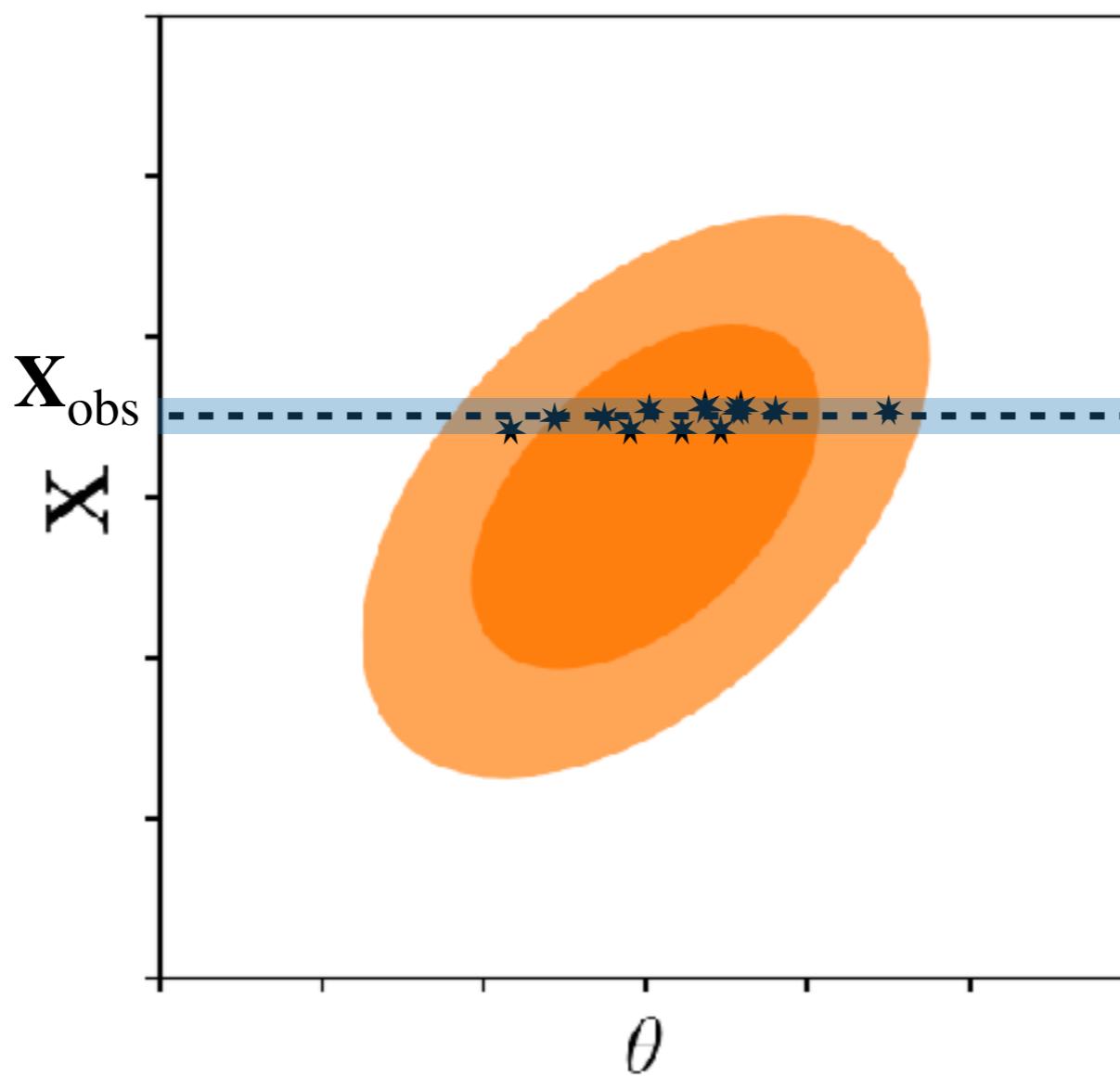
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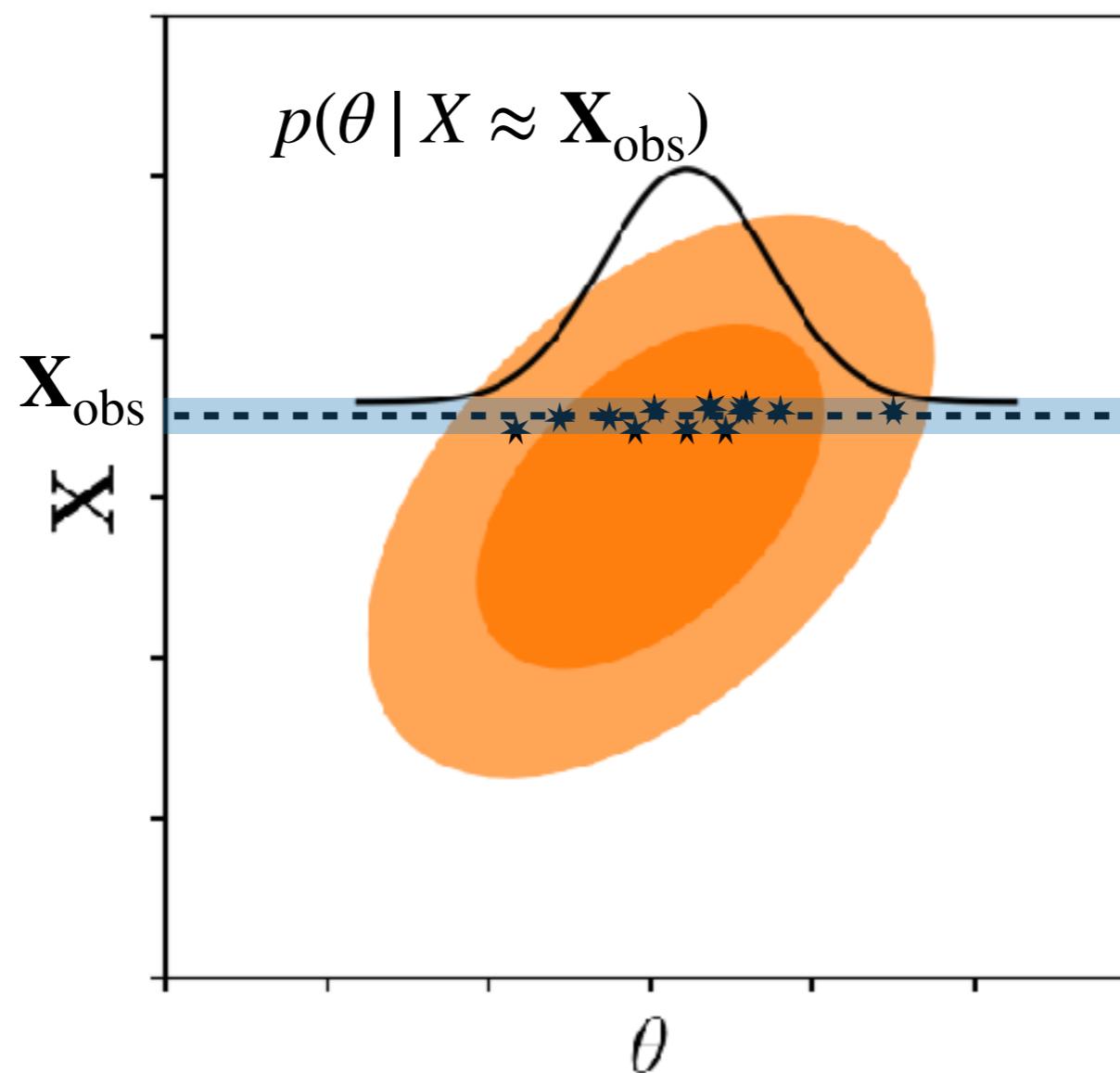


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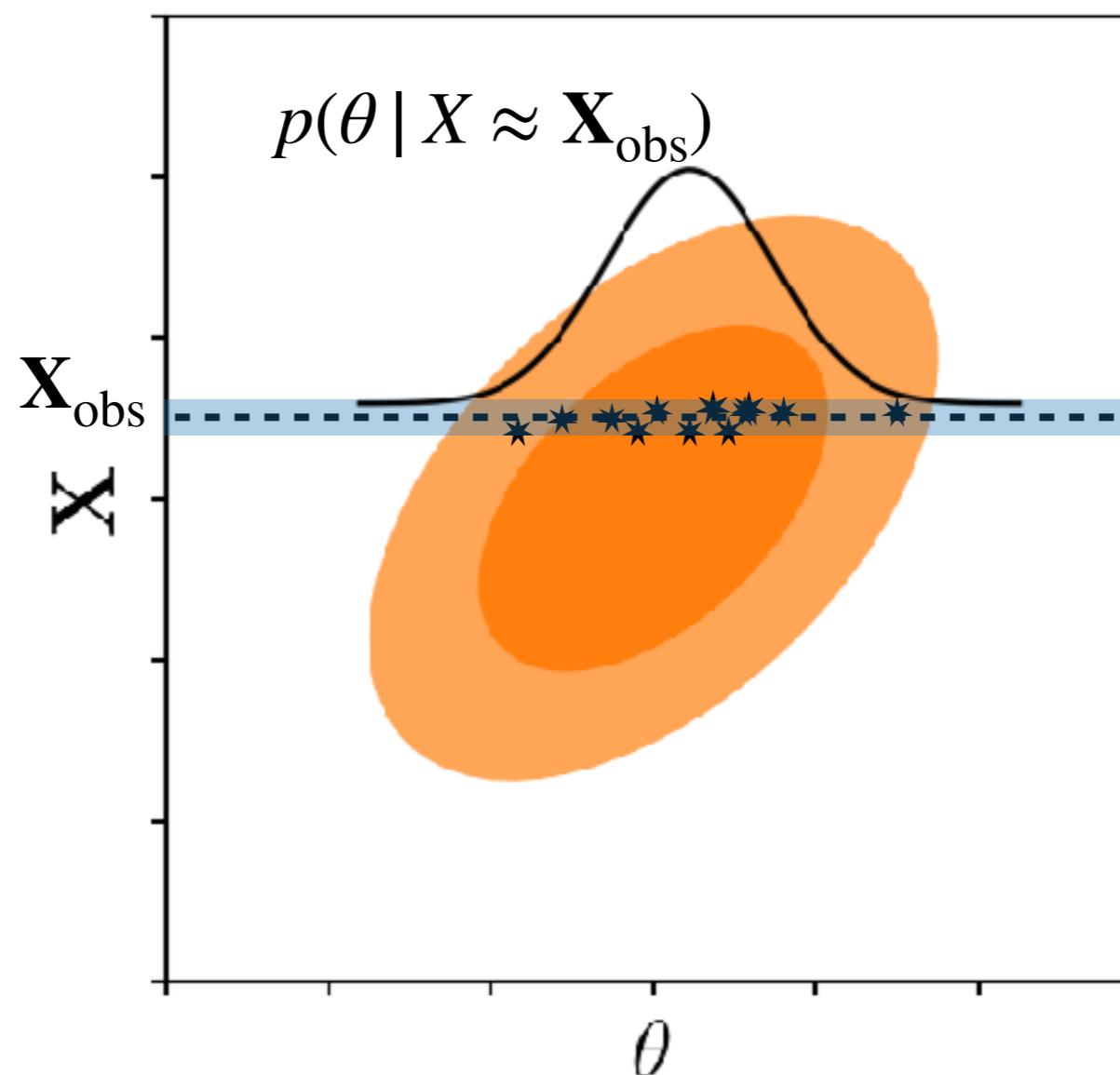
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$$p(\theta | \mathbf{X}_{\text{obs}}) \approx p(\theta | X \approx \mathbf{X}_{\text{obs}})$$

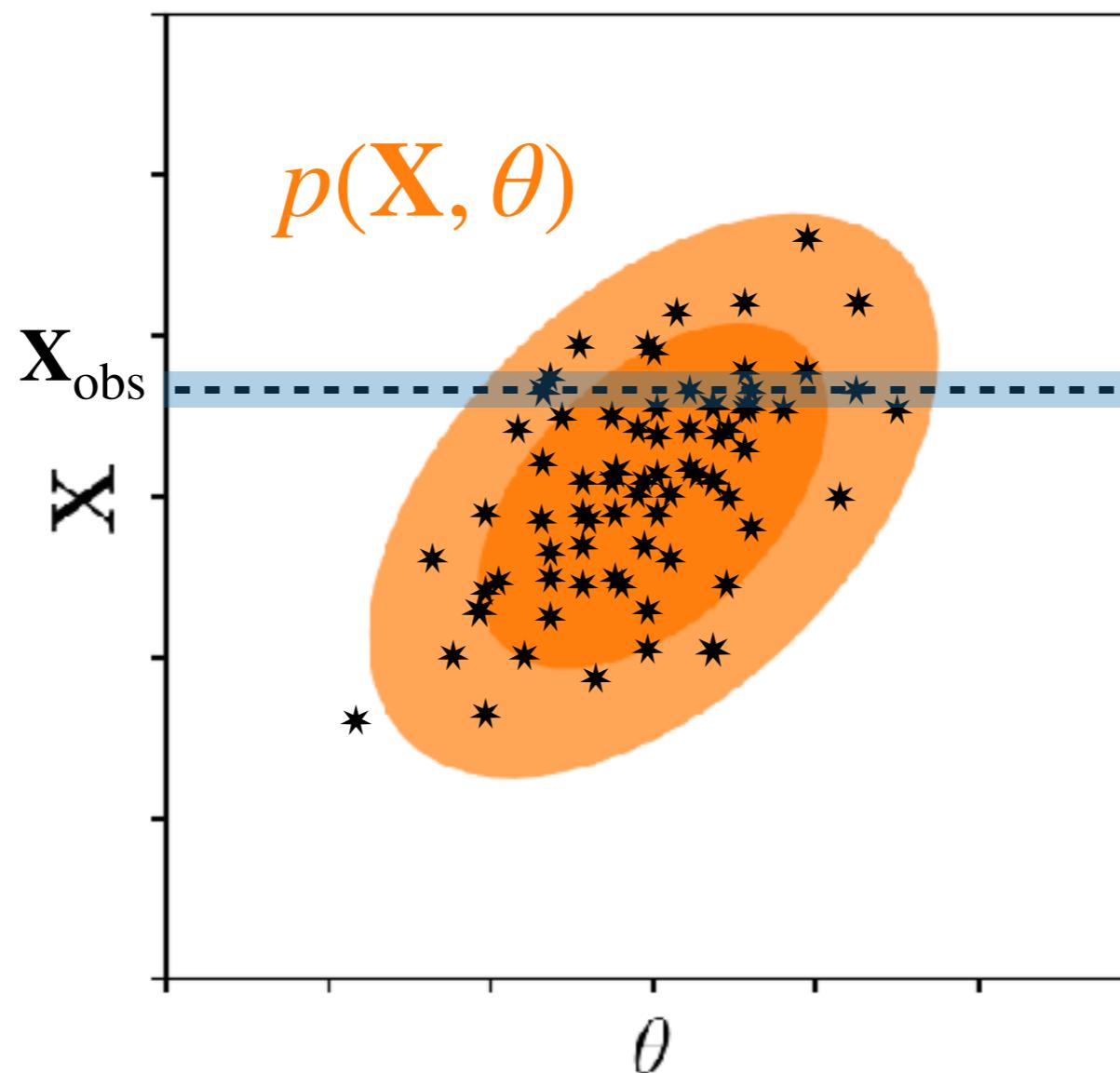


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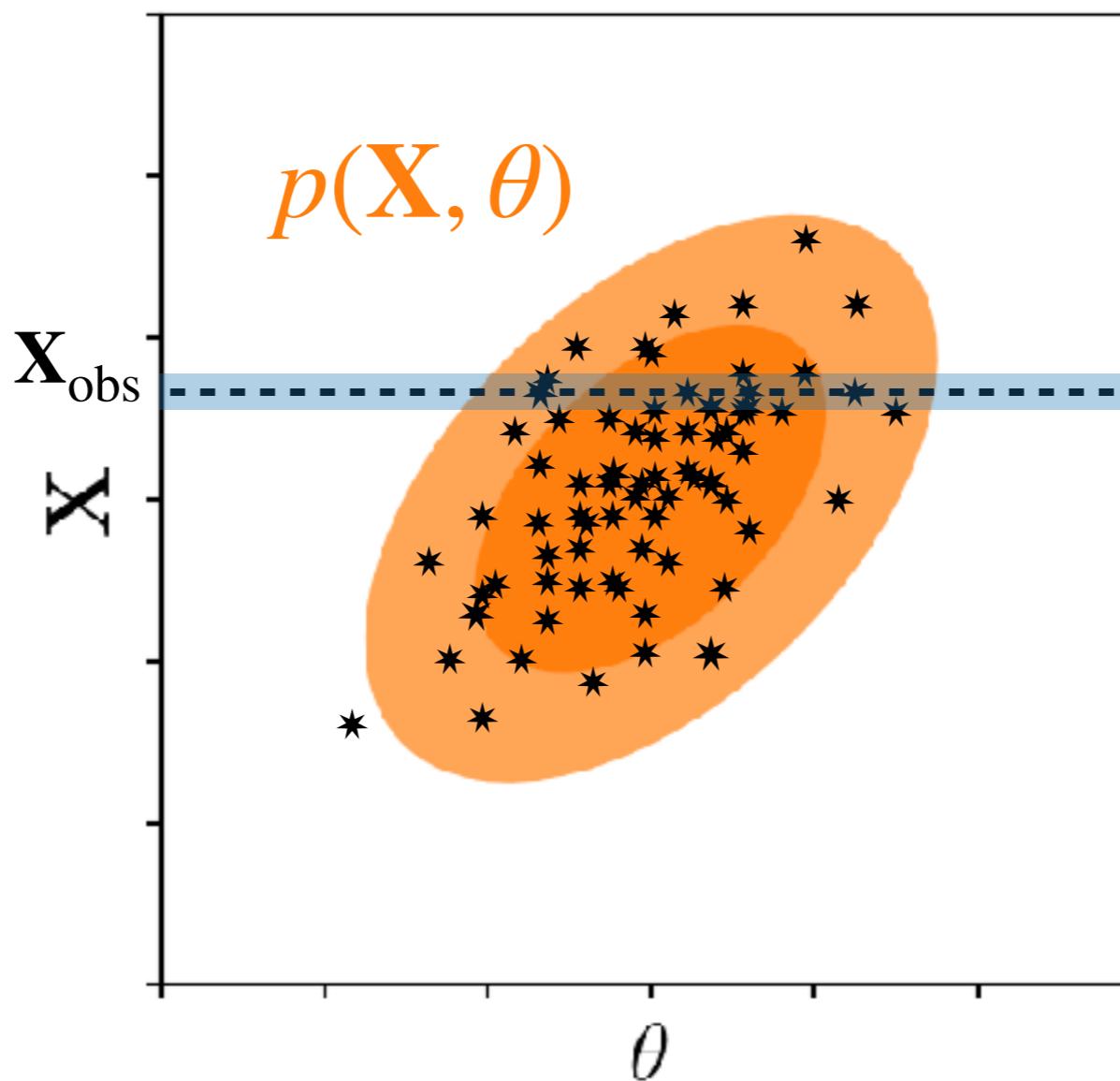
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simulation-based inference *in practice*

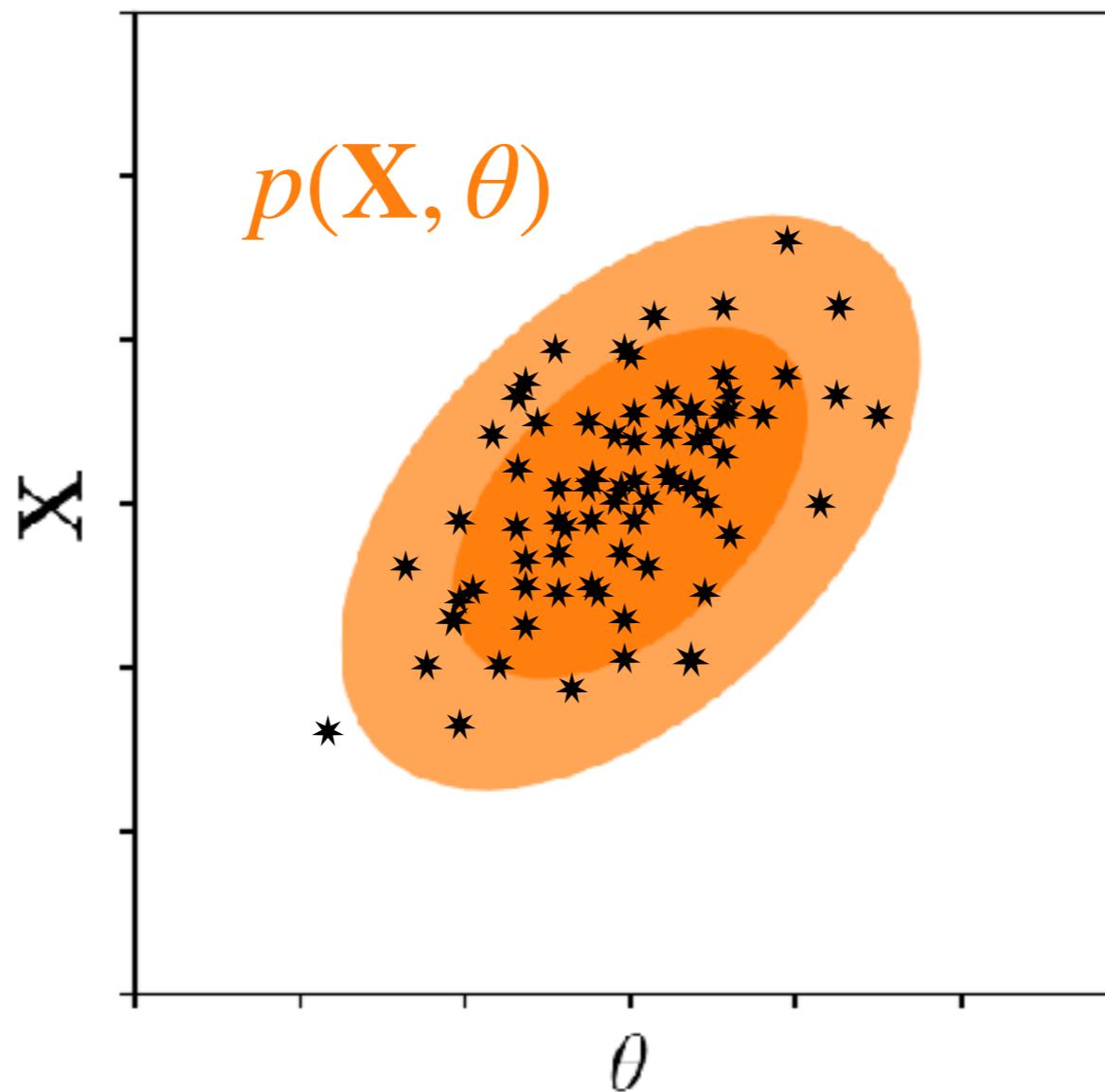


simulation-based inference *in practice*



approximate bayesian computation is often *infeasible*

simulation-based inference *in practice* — density estimation



can we estimate $p(\theta | \mathbf{X})$ from $\mathbf{X}' \sim F(\theta)$?

$$\sim p(\mathbf{X} | \theta)$$

estimate $p(\theta \mid \mathbf{X}) \approx q_\phi(\theta \mid \mathbf{X})$ from $\{(\theta', \mathbf{X}')\} \sim p(\mathbf{X}, \theta)$?

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some model q with free parameters ϕ

**Gaussian Mixture Models,
Independent Component Analysis, neural density estimators...*

estimate $p(\theta | \mathbf{X}) \approx q_\phi(\theta | \mathbf{X})$ from $\{(\theta', \mathbf{X}')\} \sim p(\mathbf{X}, \theta) ?$

we can determine ϕ by

$$\min_{\phi} D_{\text{KL}}(p(\theta | \mathbf{X}) p(\mathbf{X}) \parallel q_\phi(\theta | \mathbf{X}) p(\mathbf{X}))$$

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“it quantifies how much more surprising it would be to observe data from P if you were assuming it was coming from Q ”

“the amount of additional information required to encode samples from P using the distribution Q instead of P ”

estimate $p(\theta | \mathbf{X}) \approx q_\phi(\theta | \mathbf{X})$ from $\{(\theta', \mathbf{X}')\} \sim p(\mathbf{X}, \theta) ?$

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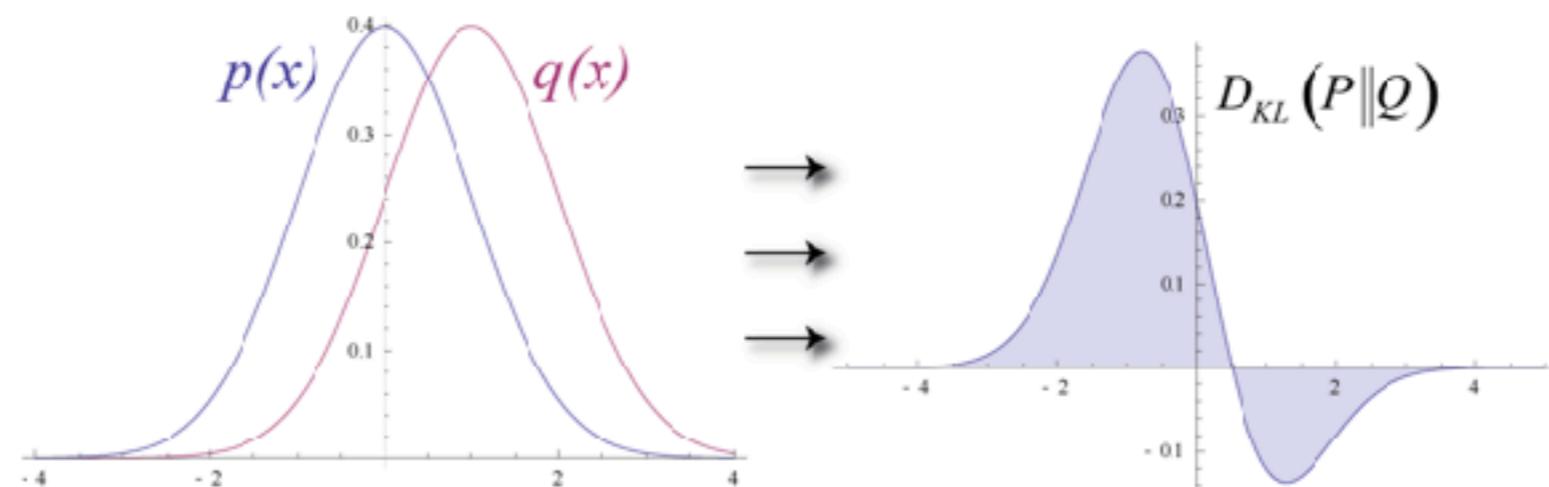


image: wikipedia

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$q_\phi(\theta | \mathbf{X})$ is guaranteed to converge to $p(\theta | \mathbf{X})$ if

q_ϕ is flexibly expressive

$N \rightarrow \infty$ samples from $p(\mathbf{X}, \theta)$

successful optimization

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q_ϕ is flexibly expressive*

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*normalizing flows, diffusion,
(your favorite neural density estimation)

if you've ever trained a neural network, *you've done neural posterior estimation*

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$$\mathbf{X} \xrightarrow{F_\phi} \boldsymbol{\theta}$$

train a neural network F_ϕ to take input \mathbf{X} and predict $\boldsymbol{\theta}$

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$$\mathbf{X} \xrightarrow{F_\phi} \theta$$

train a neural network F_ϕ to take input \mathbf{X} and predict θ by minimizing the mean squared error:

$$\min_{\phi} \sum_{(\mathbf{X}', \theta')} (F_\phi(\mathbf{X}') - \theta')^2$$

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$$= \max_{\phi} \sum_{(\mathbf{X}', \theta')} \log \exp - (F_\phi(\mathbf{X}') - \theta')^2$$

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gaussian $q_\phi(\theta | \mathbf{X})$

see also moment networks (Jeffrey & Wandelt 2020)

if you've ever done Bayesian inference in cosmology, *you've likely done simulation-based inference*

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SBI with Gaussian described by m(θ) and C

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SBI with Gaussian described by m(θ) and C

simulation-based!

what is simulation-based inference?

opportunities for simulation-based inference?

challenges for simulation-based inference?

what is simulation-based inference?

why simulation-based inference* for galaxy clustering?

challenges for simulation-based inference?

**state-of-the-art SBI (e.g. neural posterior estimation)*

misconception: standard inference is more “rigorous” than SBI

$$\log p(\mathbf{X} | \theta) = \log \mathcal{L} = [(\mathbf{m}(\theta) - \mathbf{X})^T \mathbf{C}^{-1} (\mathbf{m}(\theta) - \mathbf{X})] + \log(2\pi)^{-k/2} |\mathbf{C}|^{-1/2}$$

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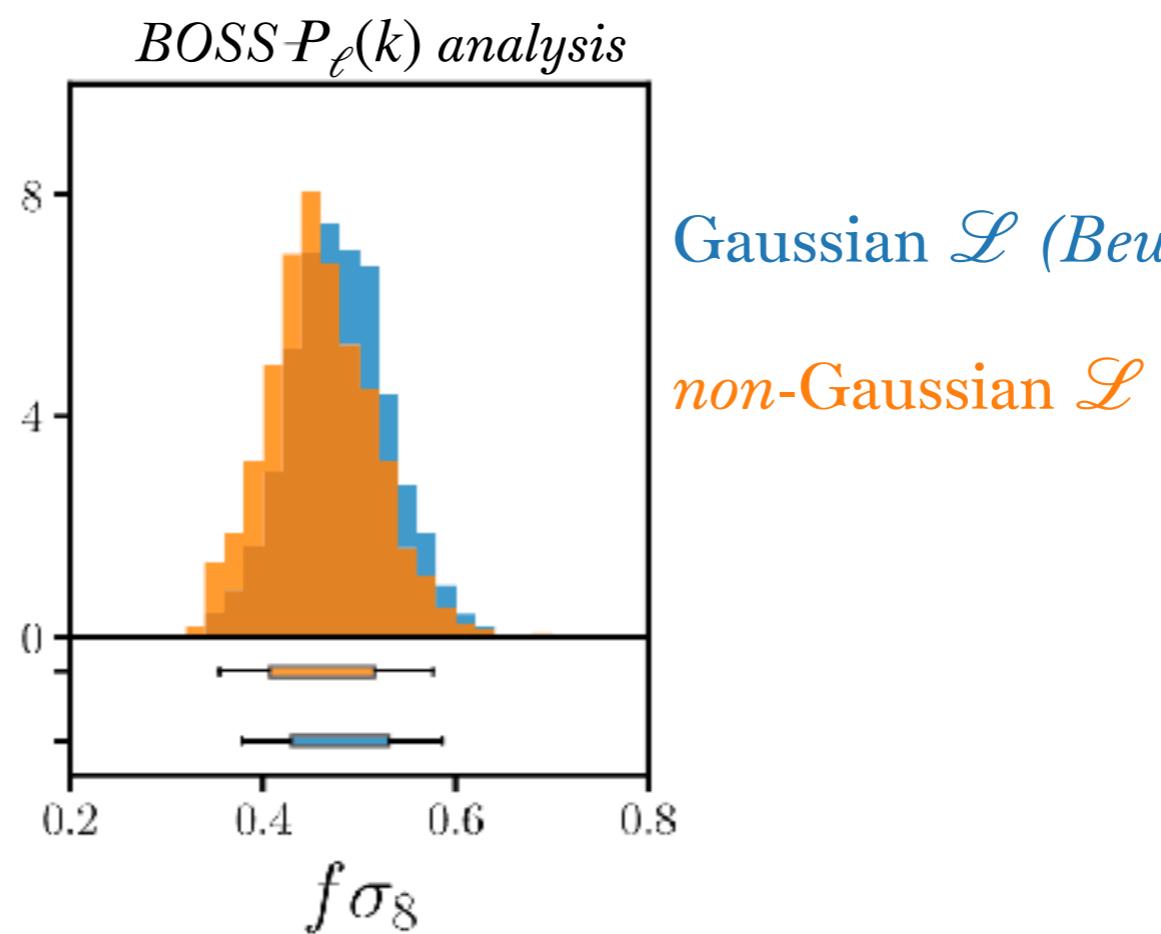
SBI with *Gaussian* described by $\mathbf{m}(\theta)$ and \mathbf{C}

assumptions!

assumptions: Gaussian likelihood with cosmology independent covariance matrix from approximate mocks

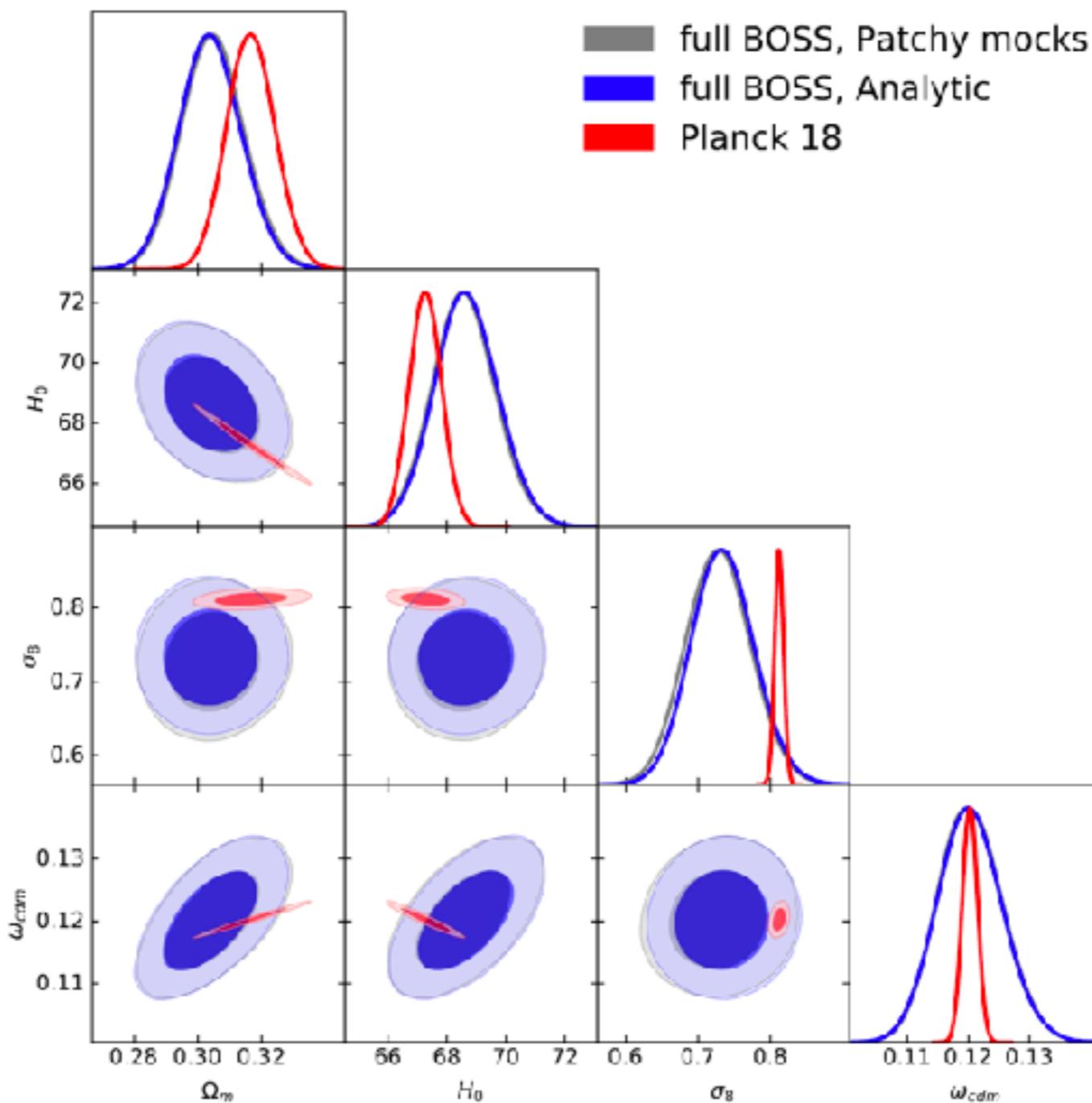
*Hahn et al.(2019);
see also Sellentin & Heavens (2017), Sellentin et al. (2017)*

assumptions: *Gaussian likelihood* with cosmology independent covariance matrix from approximate mocks

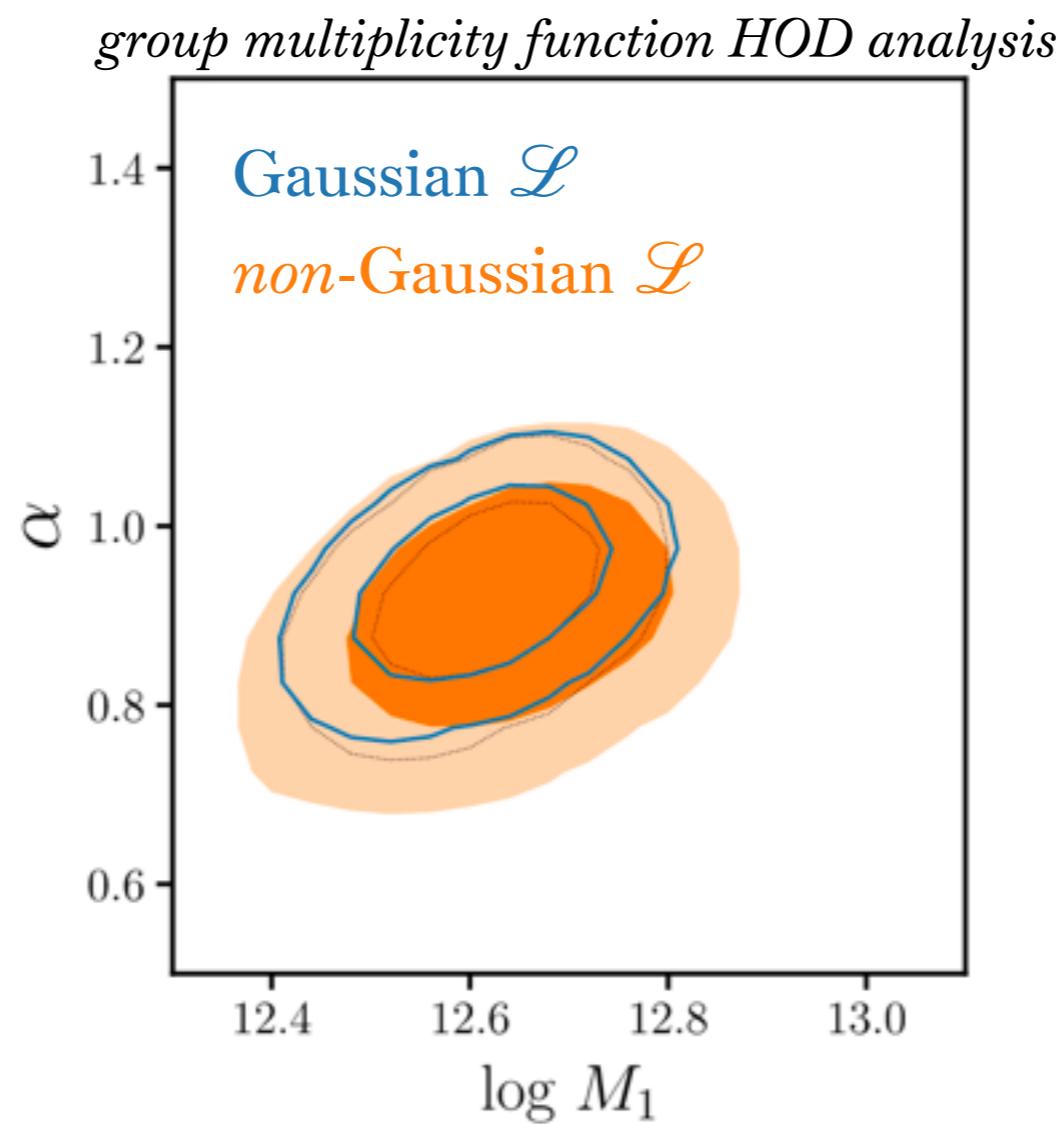


Hahn et al.(2019);
see also Sellentin & Heavens (2017), Sellentin et al. (2017), but **Benedict's talk**

assumptions: Gaussian likelihood with *cosmology independent covariance matrix* from approximate mocks

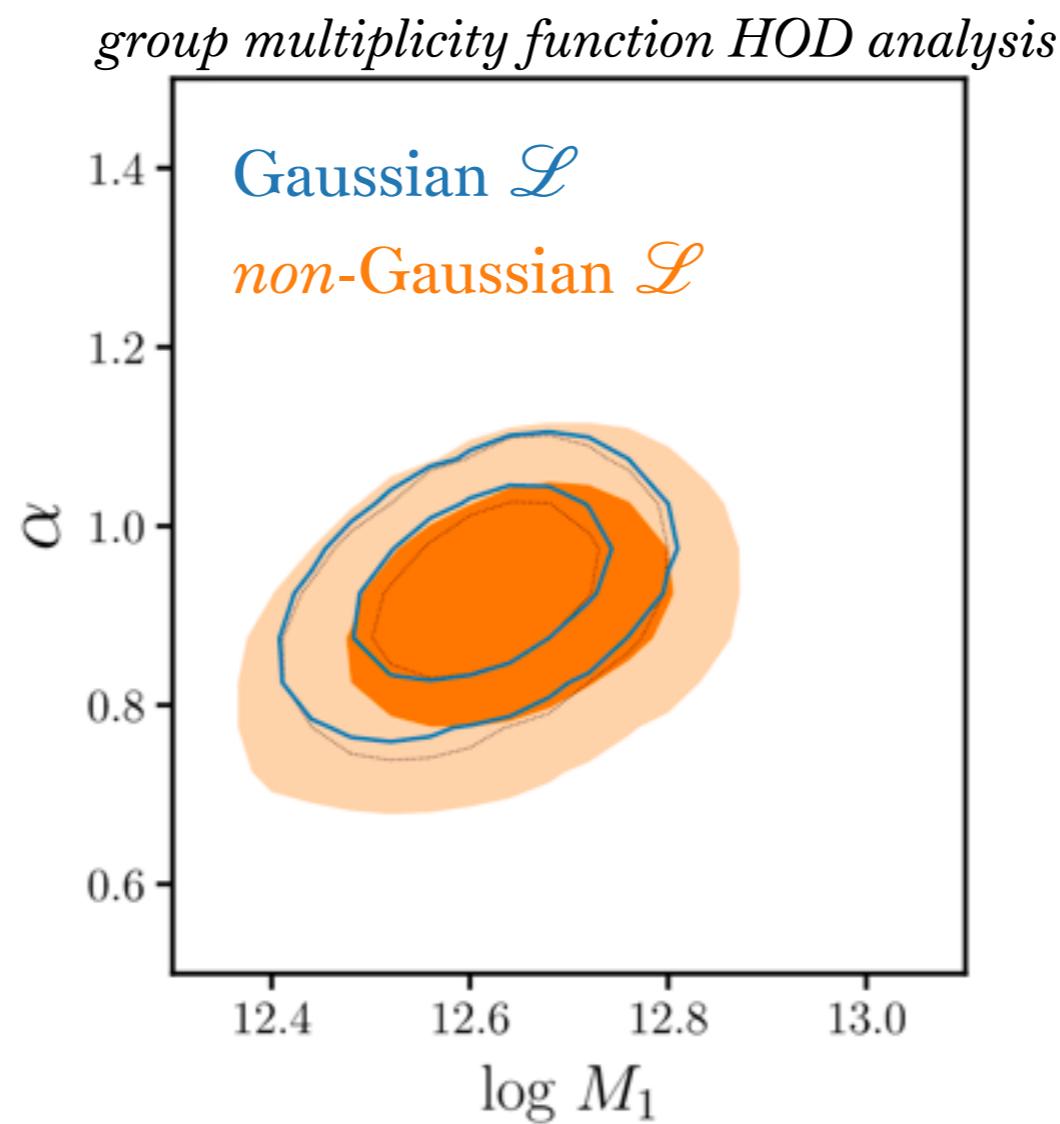


assumptions: Gaussian likelihood with cosmology independent covariance matrix from approximate mocks



fair assumptions for **beyond 2-pt analyses?**

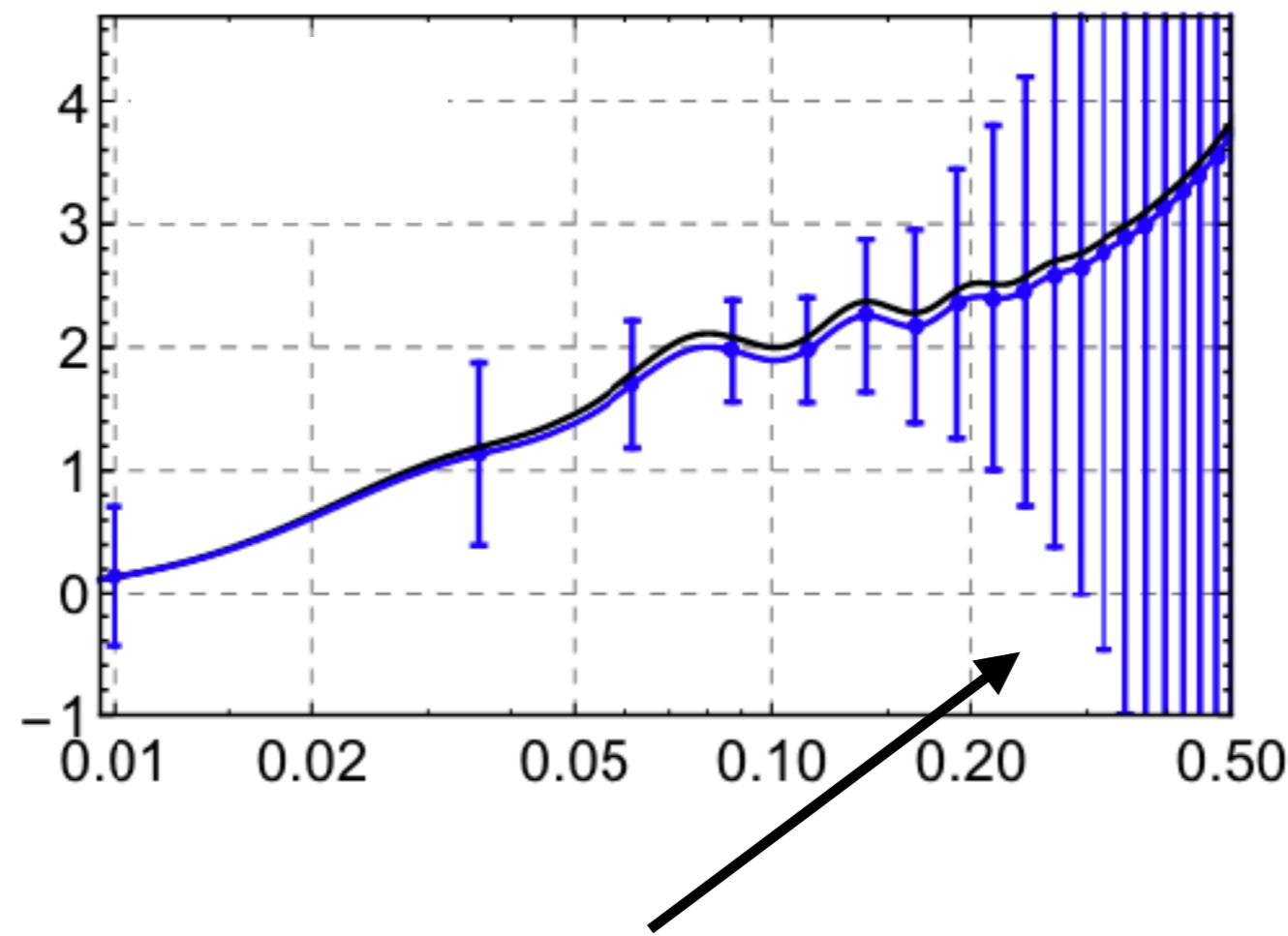
assumptions: Gaussian likelihood with cosmology independent covariance matrix from approximate mocks



SBI can *relax* these assumptions by learning the likelihood from the forward model

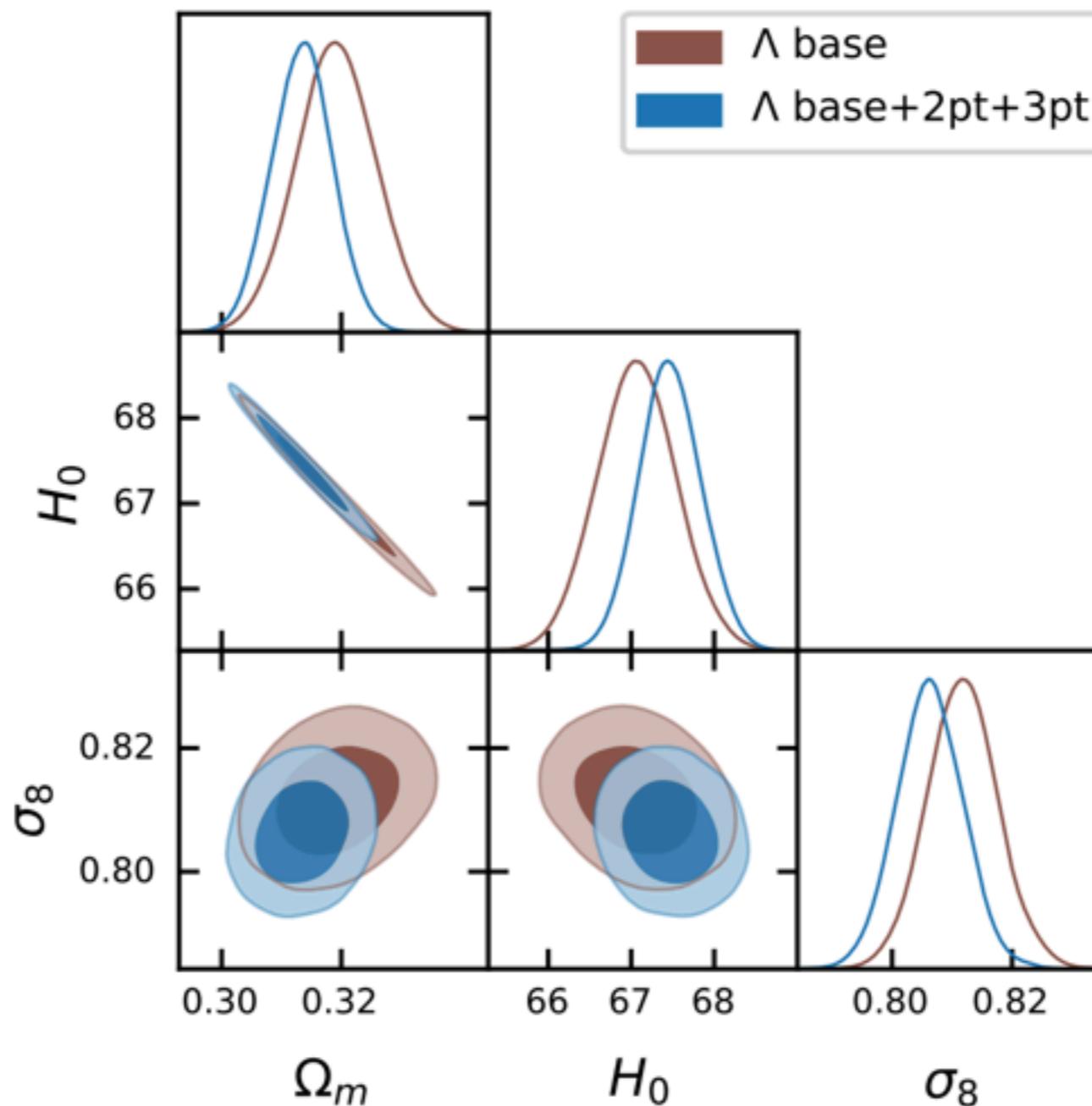
advantages of SBI: leveraging simulations to access *additional cosmological information*

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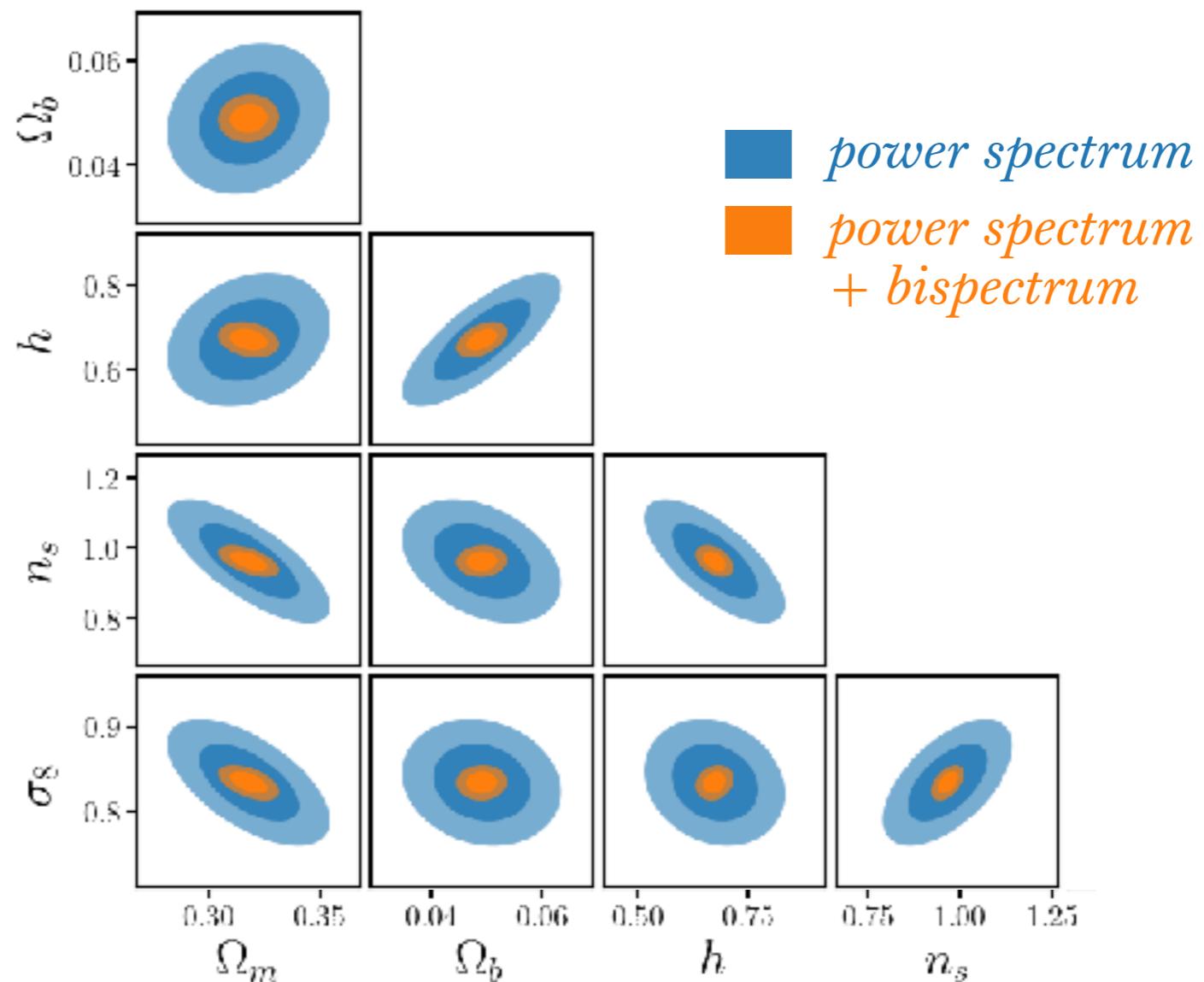
*theoretical uncertainties for
perturbation theory*

advantages of SBI: leveraging simulations to access *additional cosmological information*



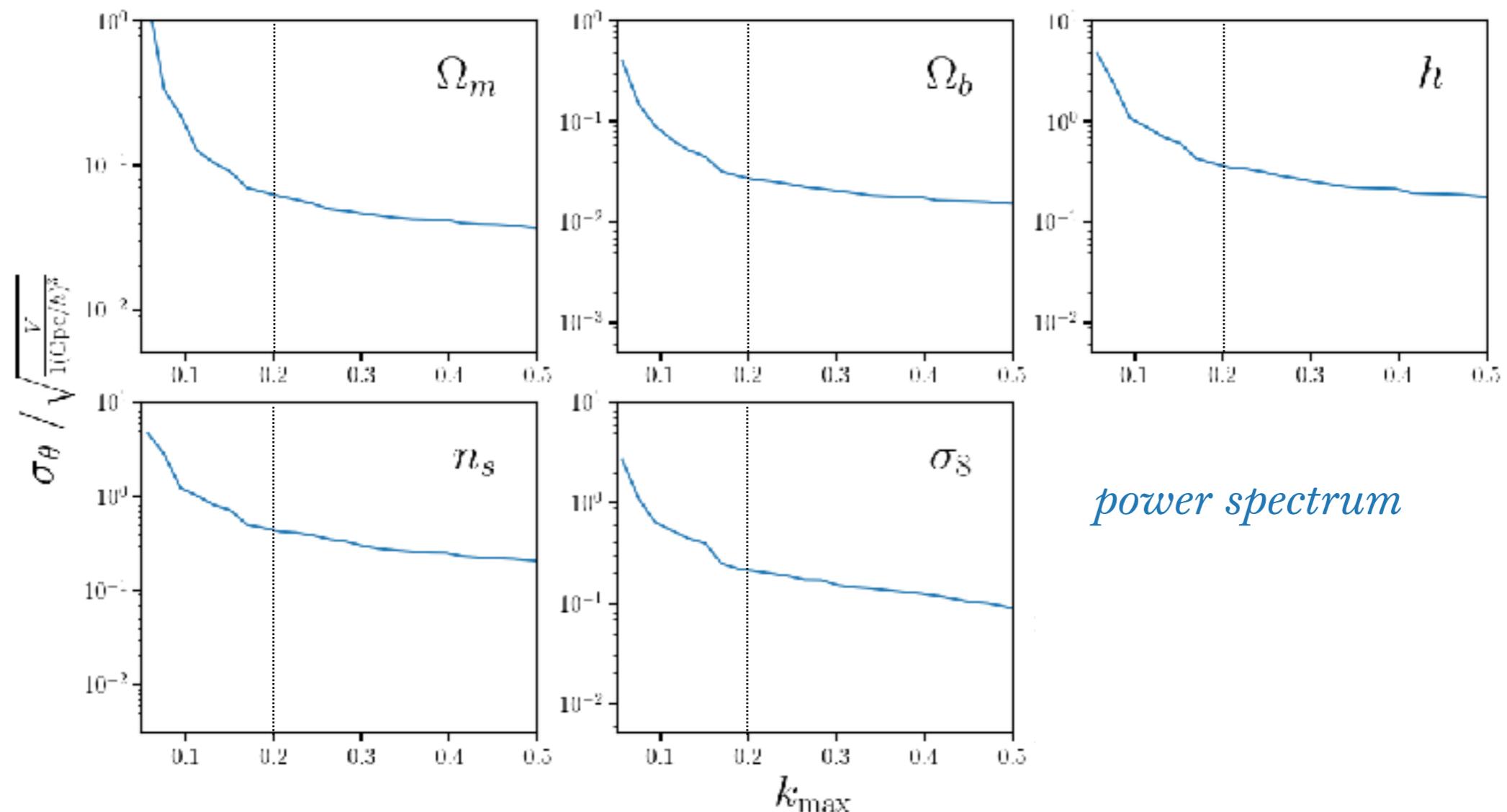
Spaar & Zhang (2023)
see also Scoccimarro *et al.*(2001); Verde *et al.*(2022); Gil-Marin *et al.*(2017);
Philcox & Ivanov (2022); Ivanov *et al.*(2023); D'Amico *et al.*(2024);

advantages of SBI: leveraging simulations to access *additional cosmological information*



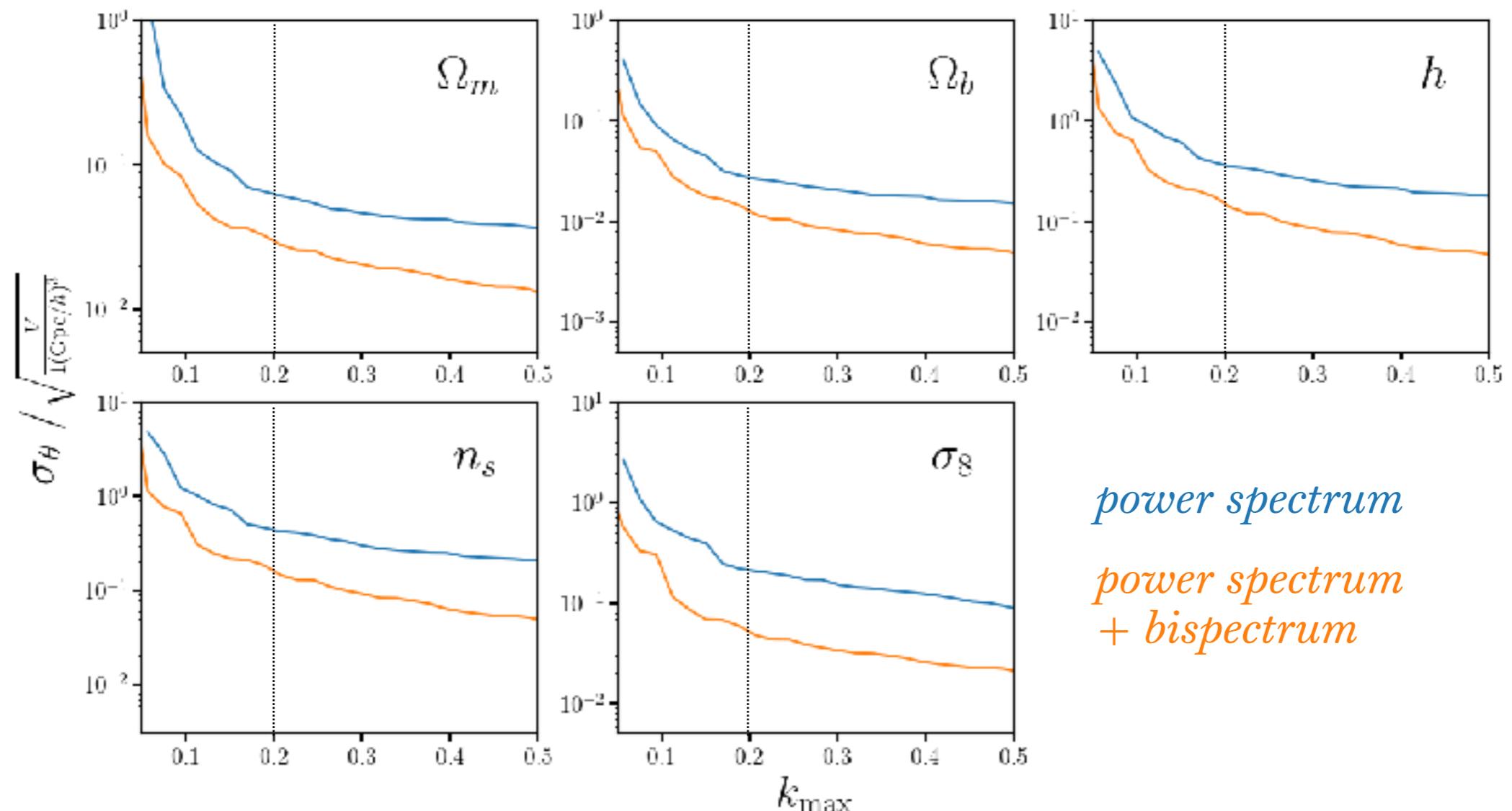
*Quijote and Molino forecasts:
Hahn et al. (2020), Hahn & Villaescusa-Navarro (2021)
see also Lado's talk*

advantages of SBI: leveraging simulations to access *additional cosmological information*

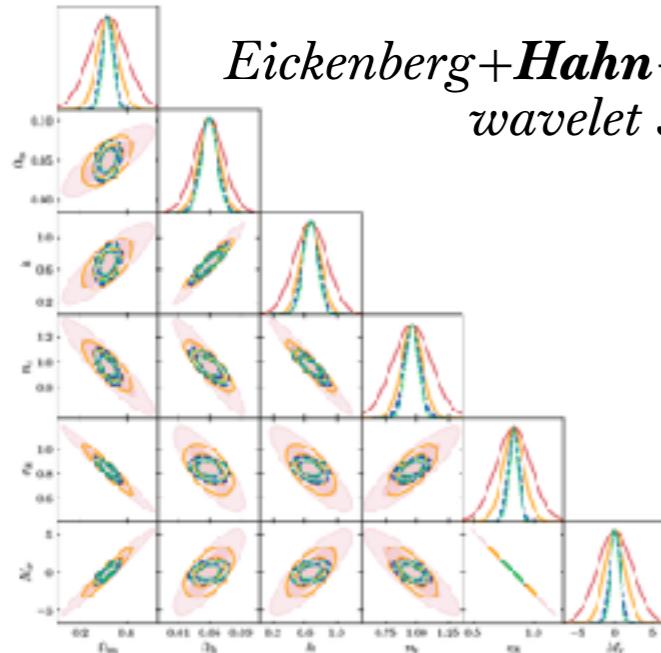


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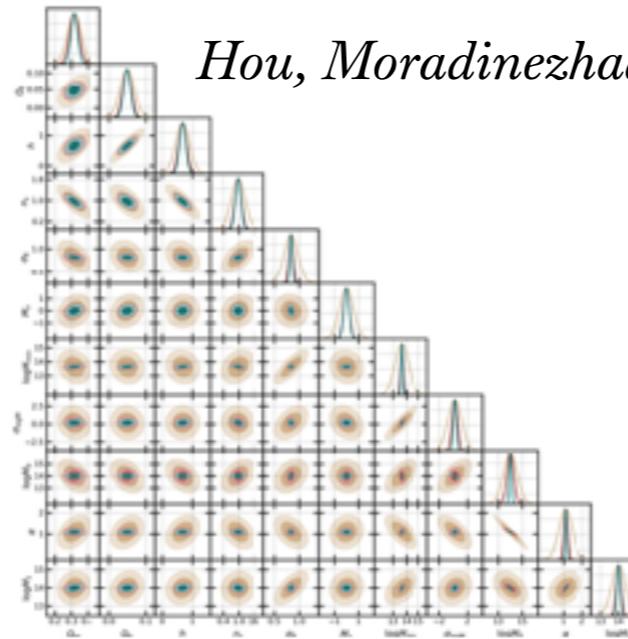
advantages of SBI: leveraging simulations to access *additional cosmological information on non-linear scales*



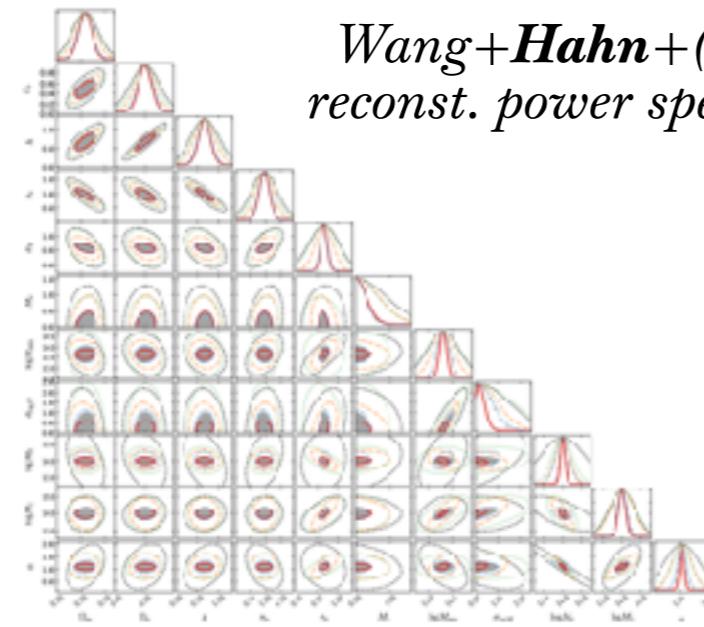
advantages of SBI: leveraging simulations to access *additional cosmological information from beyond standard statistics*



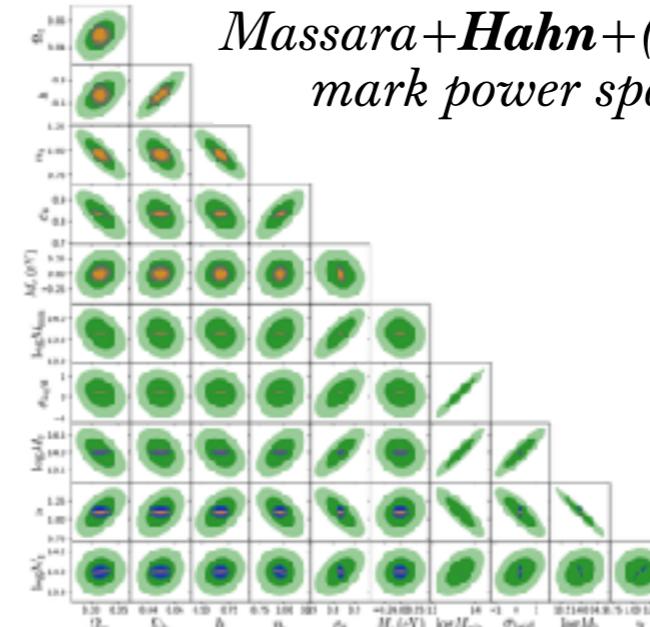
Eickenberg+Hahn+(2022)
wavelet statistics



Hou, Moradinezhad+Hahn+(2022)
skew spectra



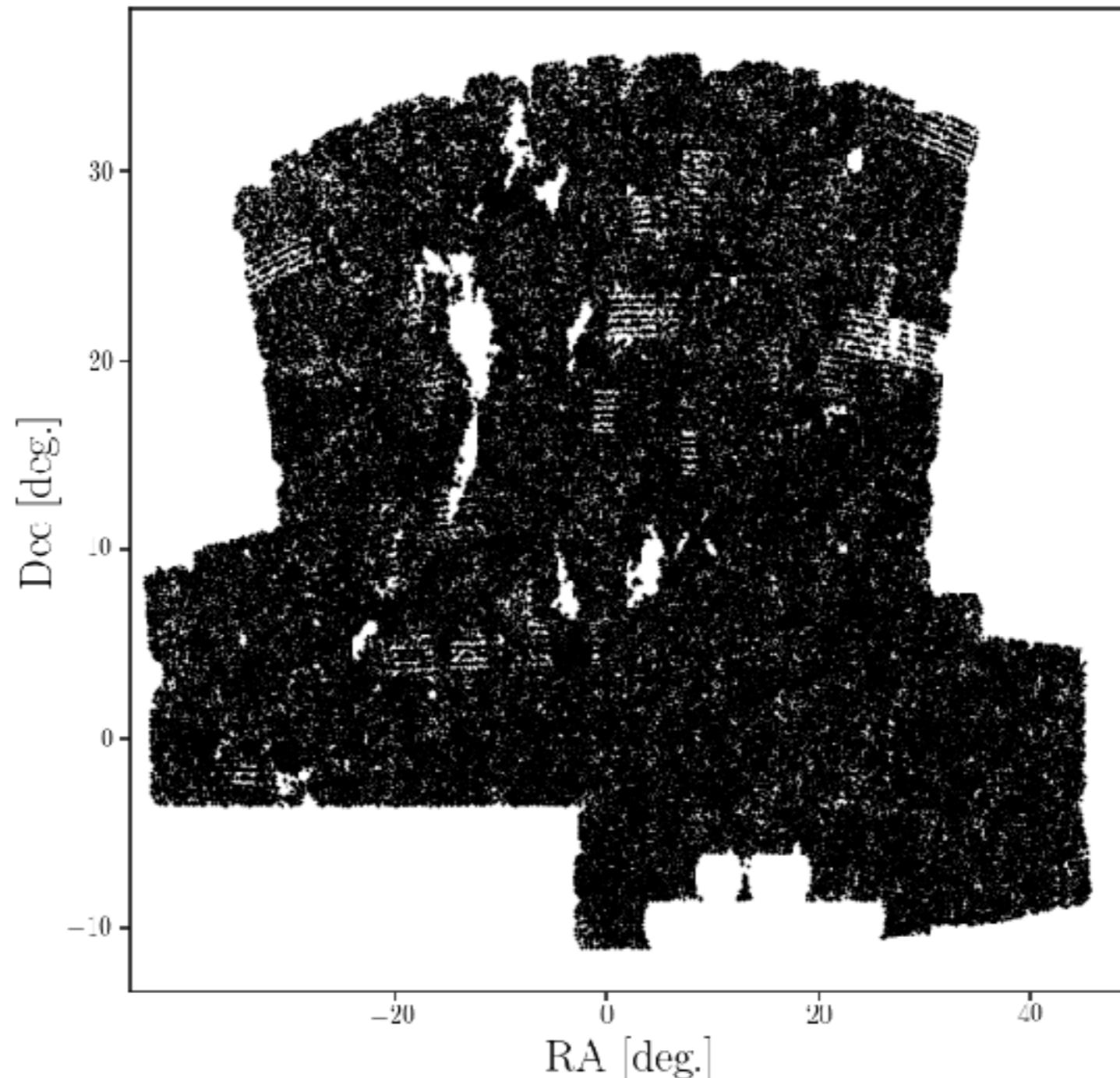
Wang+Hahn+(2024)
reconst. power spectrum



Massara+Hahn+(2022)
mark power spectrum

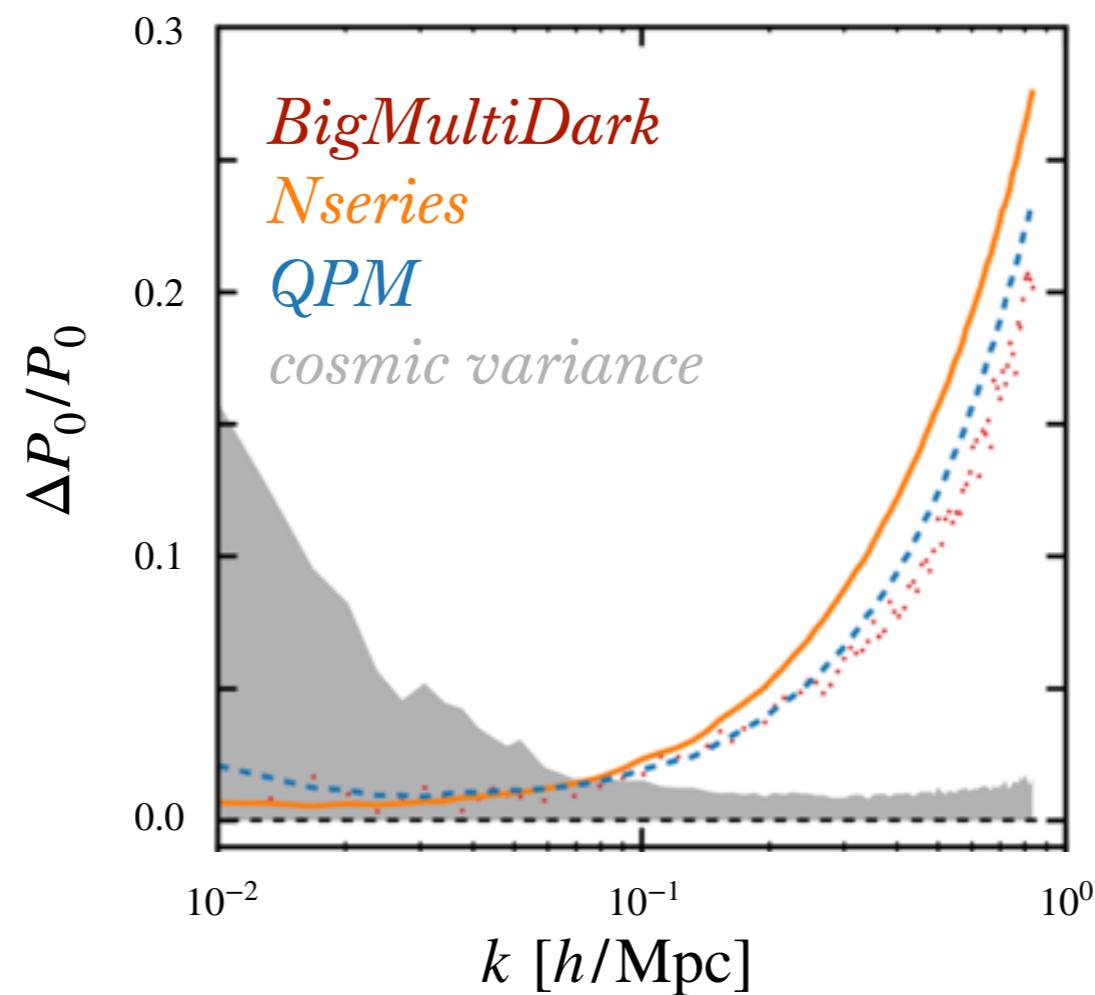
advantages of SBI: leveraging simulations to account for
observational systematics

advantages of SBI: leveraging simulations to account for
observational systematics — complex masks

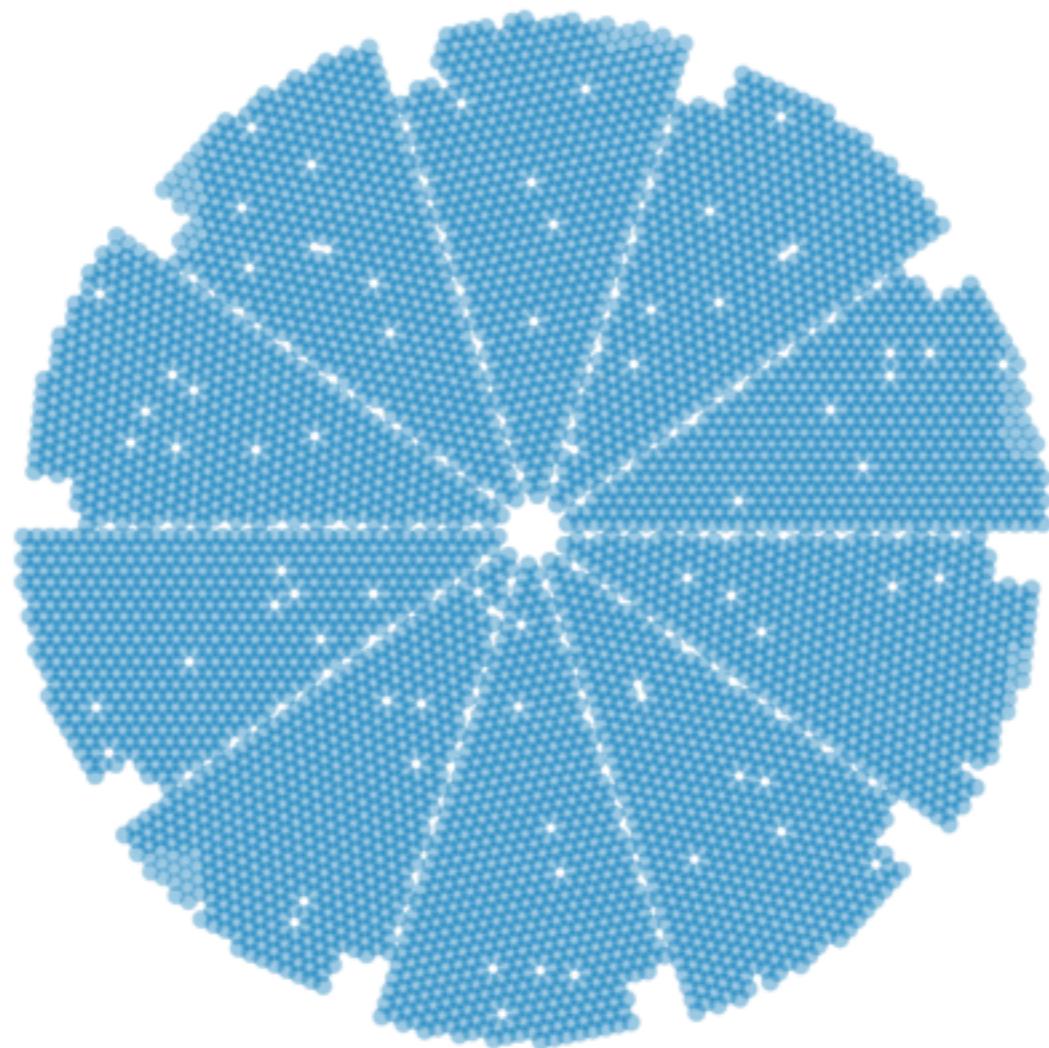


advantages of SBI: leveraging simulations to account for
observational systematics — fiber collisions

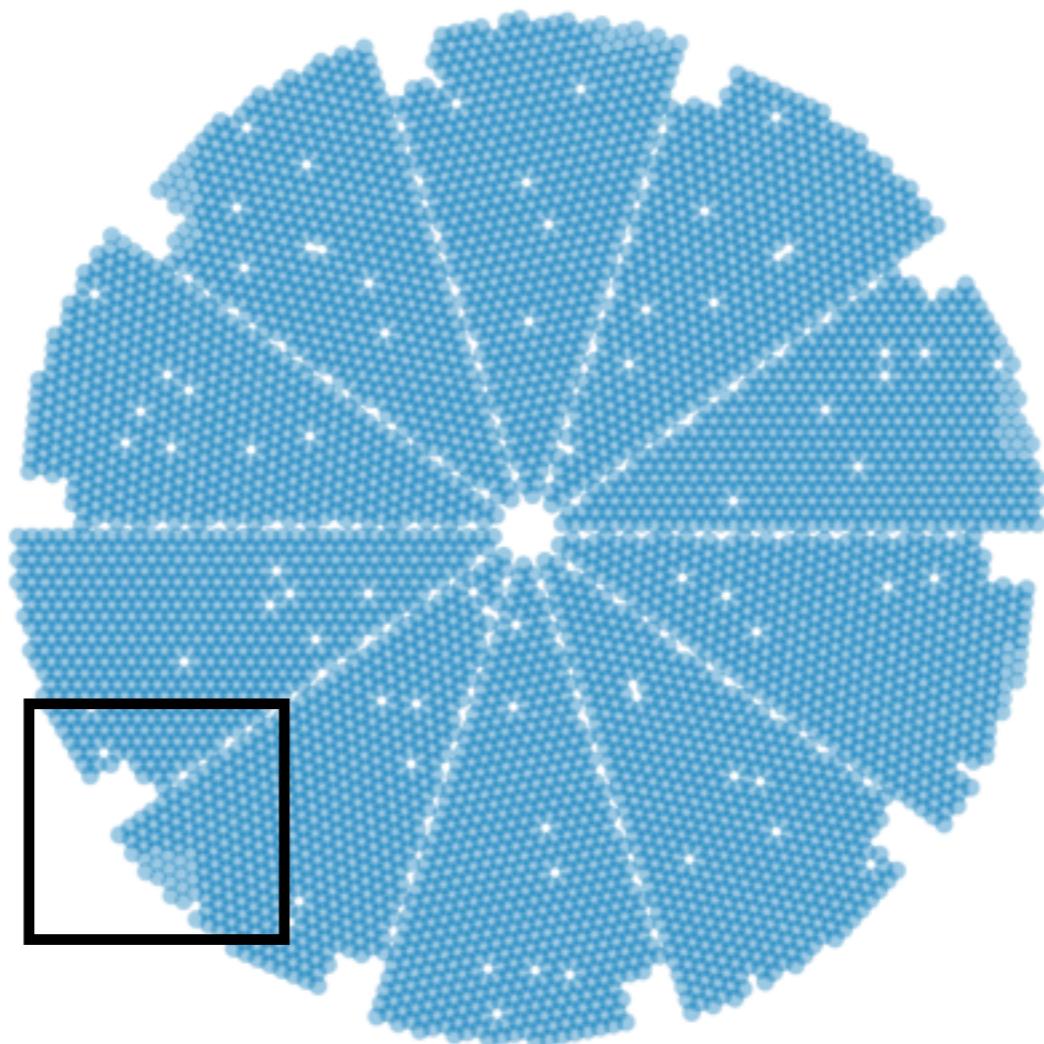
advantages of SBI: leveraging simulations to account for
observational systematics — fiber collisions



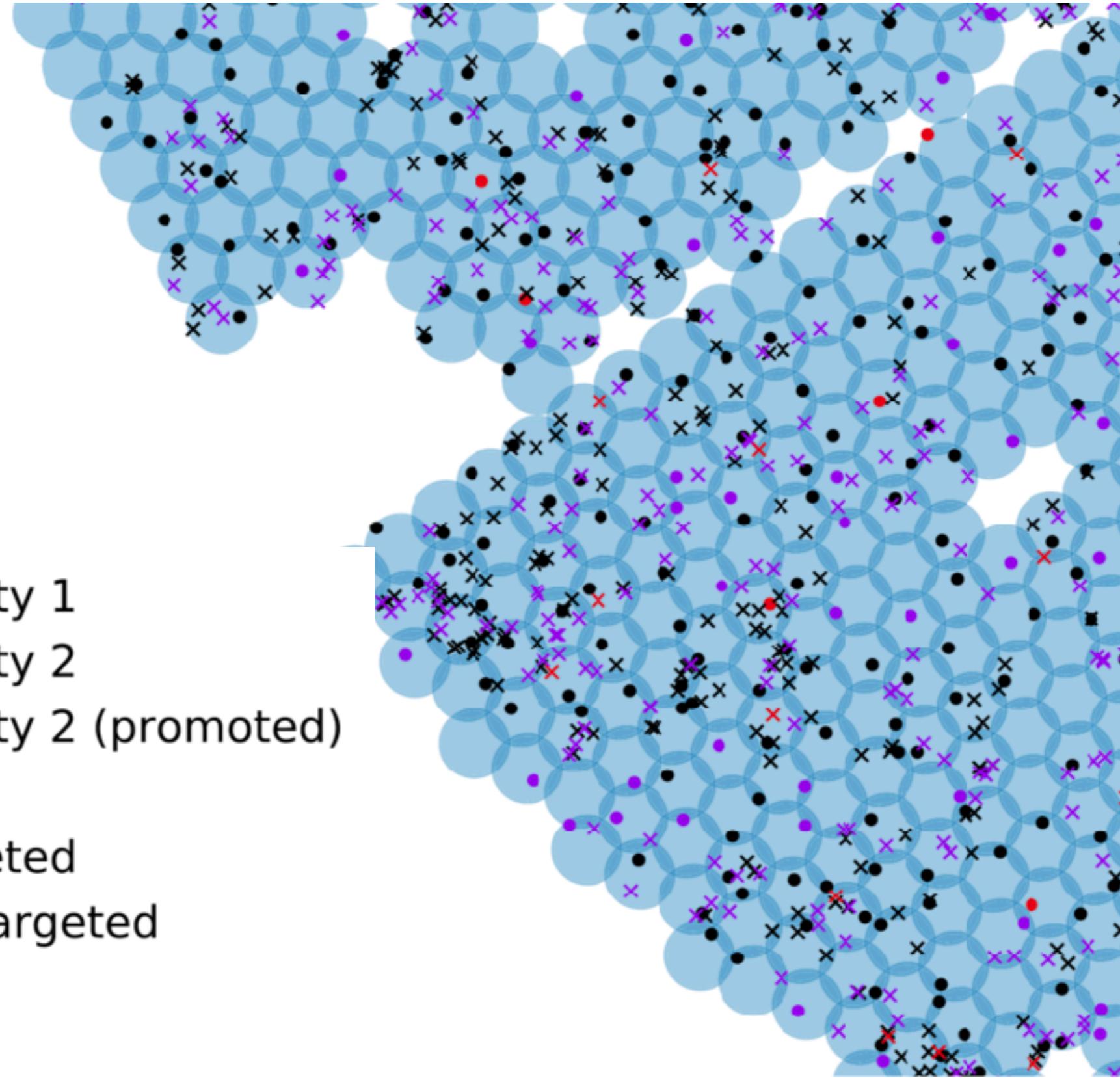
advantages of SBI: leveraging simulations to account for
observational systematics — fiber collisions



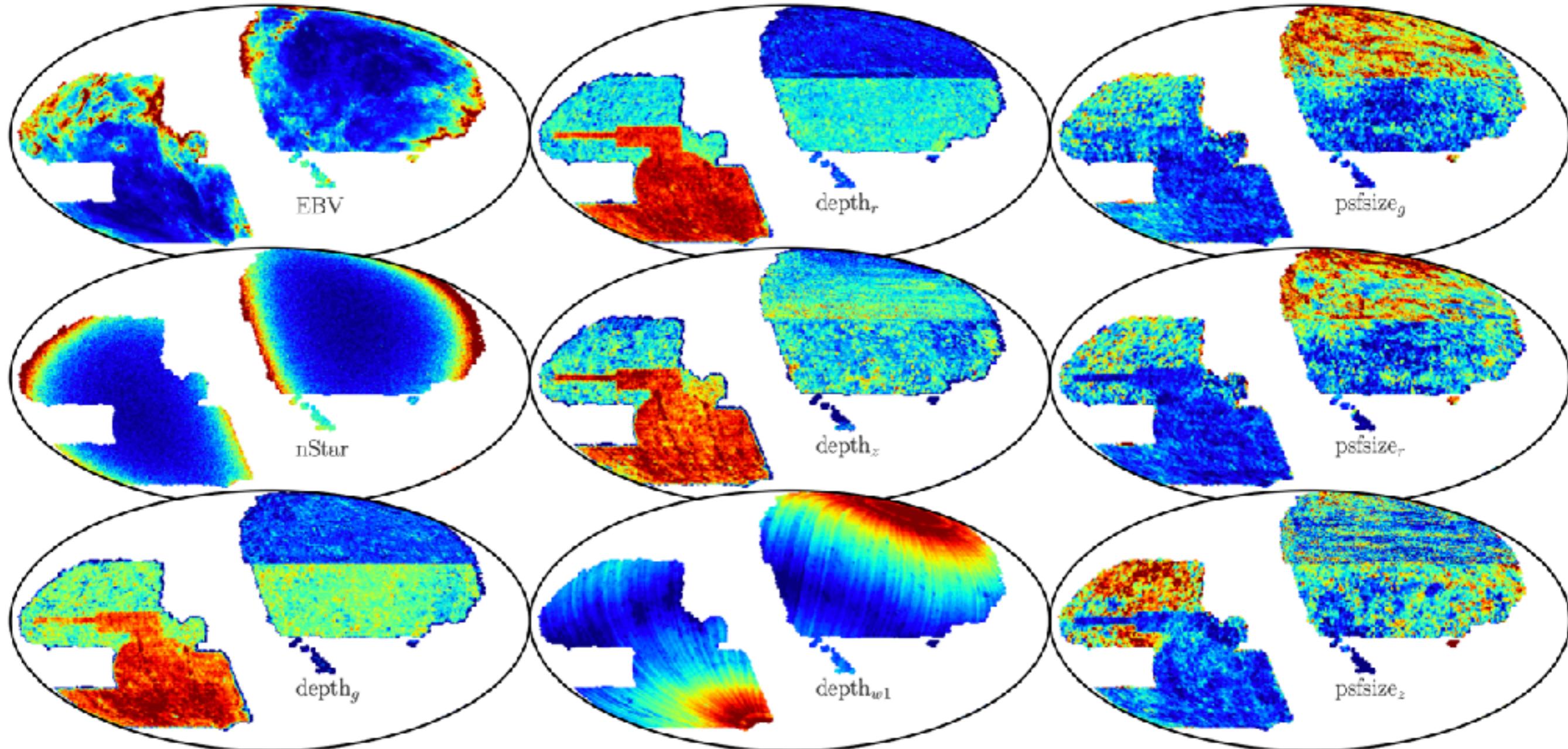
advantages of SBI: leveraging simulations to account for
observational systematics — fiber collisions



- Priority 1
- Priority 2
- Priority 2 (promoted)
- Targeted
- ✗ Not targeted



advantages of SBI: leveraging simulations to account for
observational systematics — imaging systematics



what is simulation-based inference?

simulation-based inference* *in action*

challenges for simulation-based inference?

**state-of-the-art SBI (e.g. neural posterior estimation)*



Simulation-Based Inference of Galaxies



ChangHoon Hahn
Princeton Univ.
(spokesperson)



Michael
Eickenberg
CCM Flatiron



Shirley Ho
CCA Flatiron



Jiamin Hou
Univ. of Florida



Liam Parker
Princeton Univ.



Pablo Lemos
MILA



Elena Massara
UWaterloo



Chirag Modi
CCA CCM
Flatiron

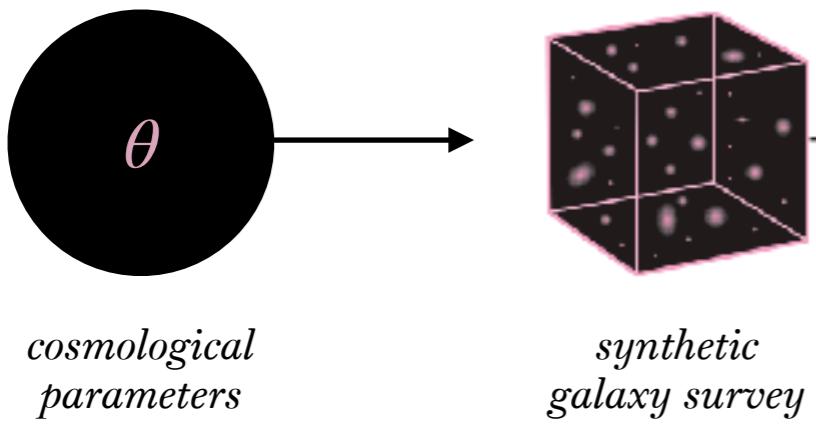


Azadeh
Moradinezhad
Univ. de Genève



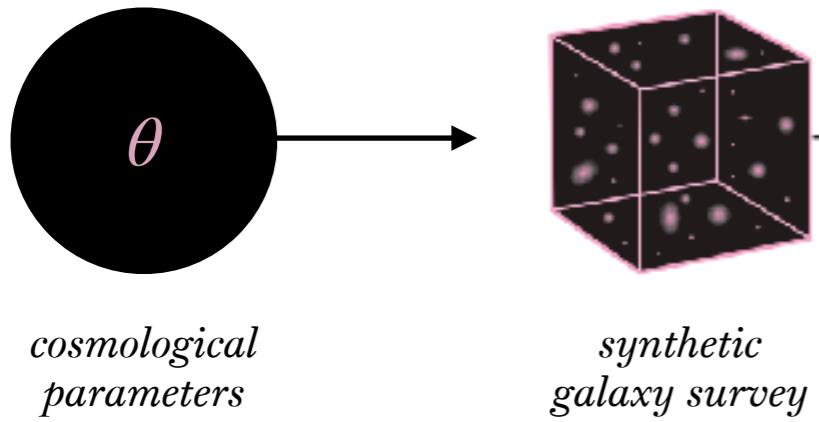
Bruno Régaldo-
Saint Blanchard
CCM Flatiron

SIMBIG — 1. *generating training data of synthetic observations*



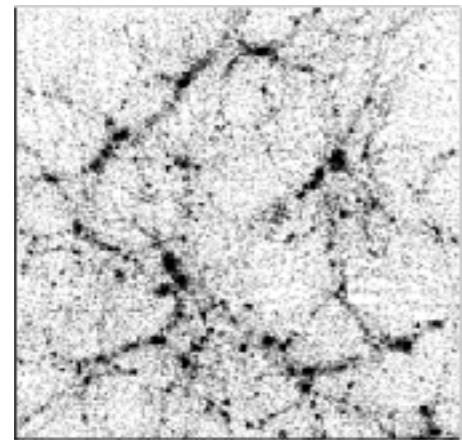
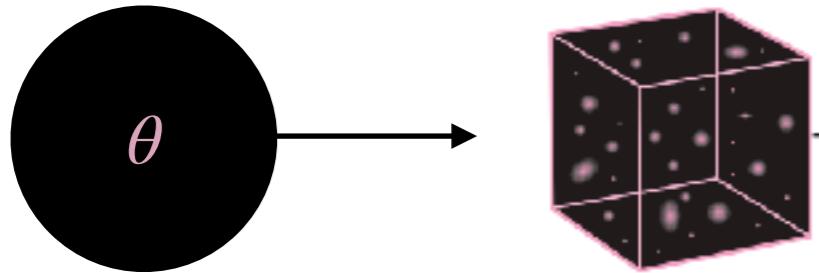
SDSS-III: BOSS

SIMBIG — 1. *generating training data of synthetic observations*



SDSS-III: BOSS

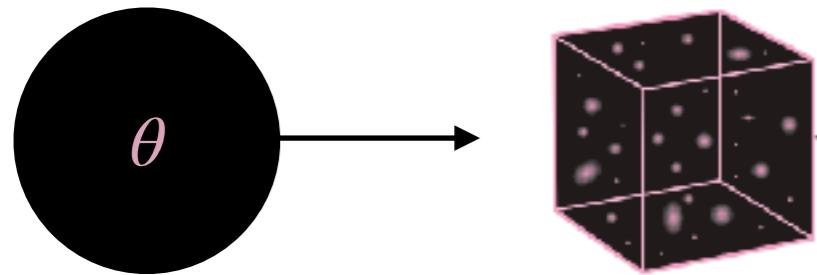
SIMBIG — 1. *generating training data of synthetic observations*



Quijote high-res
 N -body simulations

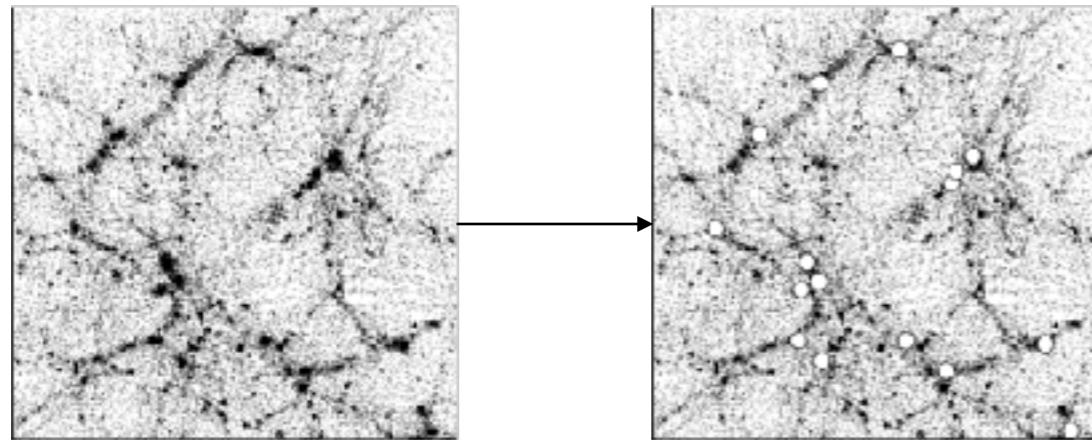
SDSS-III: BOSS

SIMBIG — 1. *generating training data of synthetic observations*



*cosmological
parameters*

*synthetic
galaxy survey*

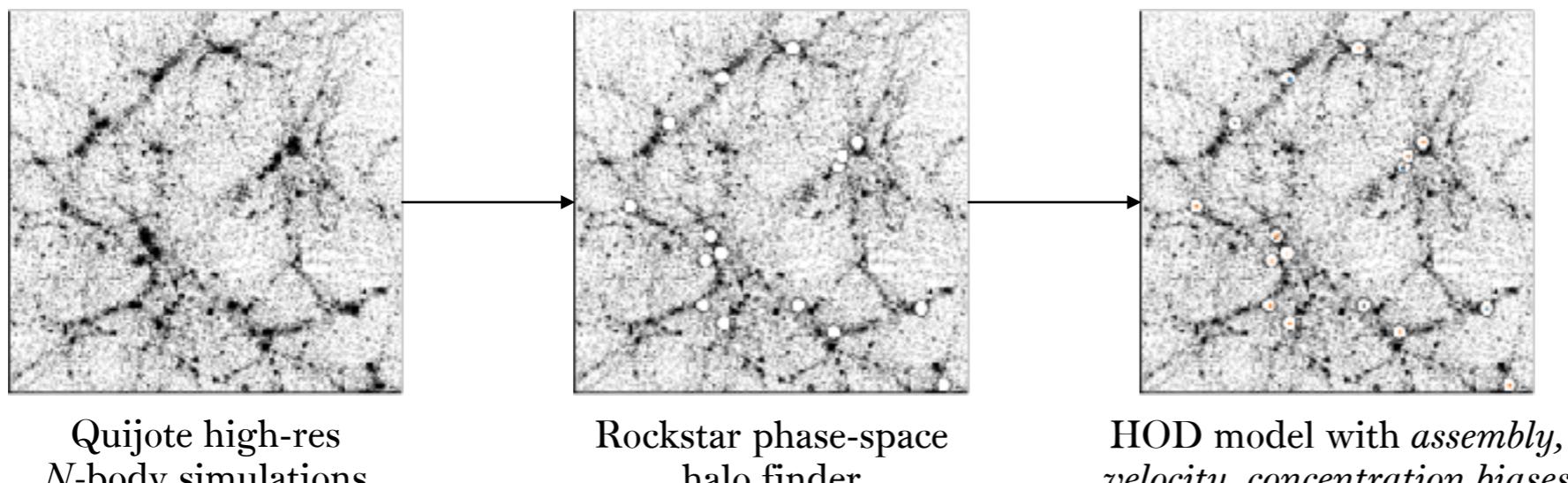
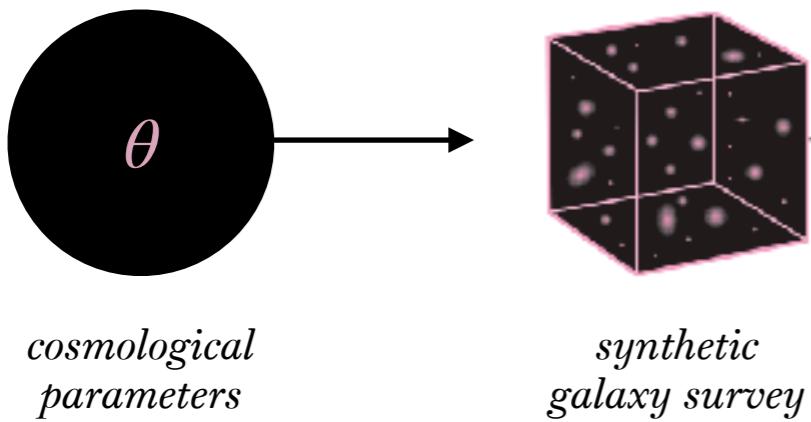


Quijote high-res
 N -body simulations

Rockstar phase-space
halo finder

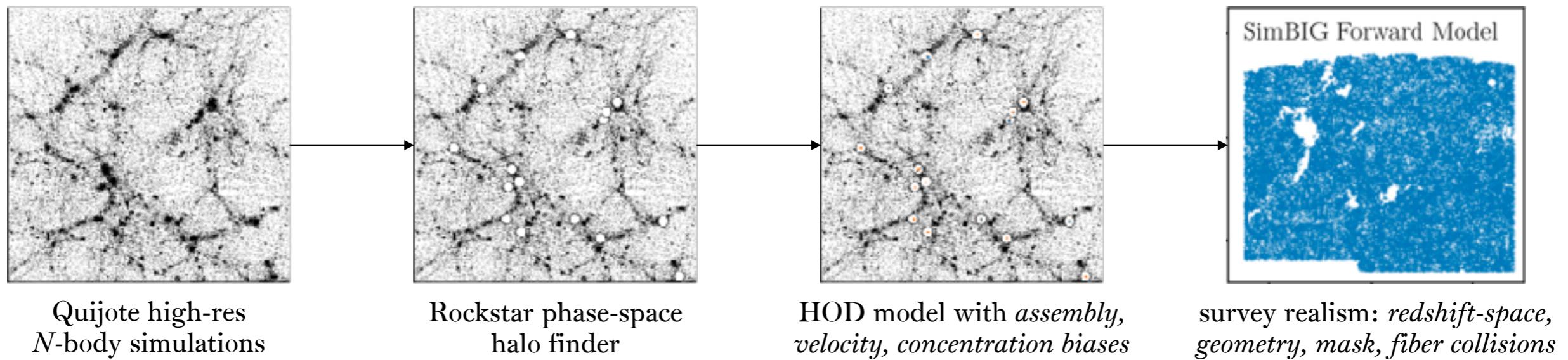
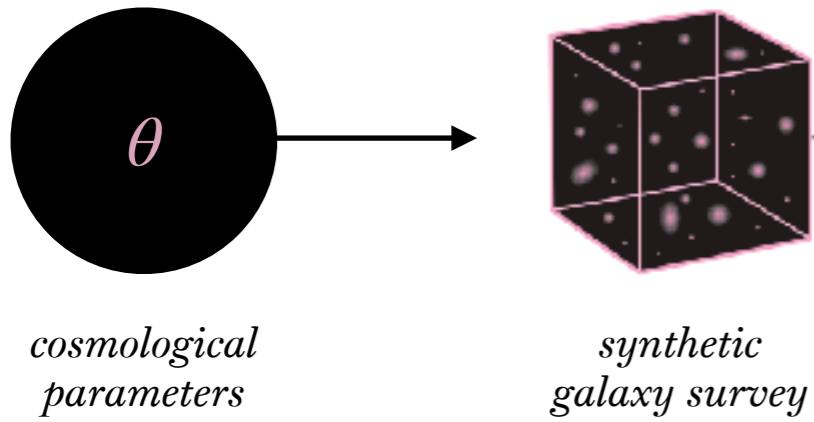
SDSS-III: BOSS

SIMBIG — 1. *generating training data of synthetic observations*



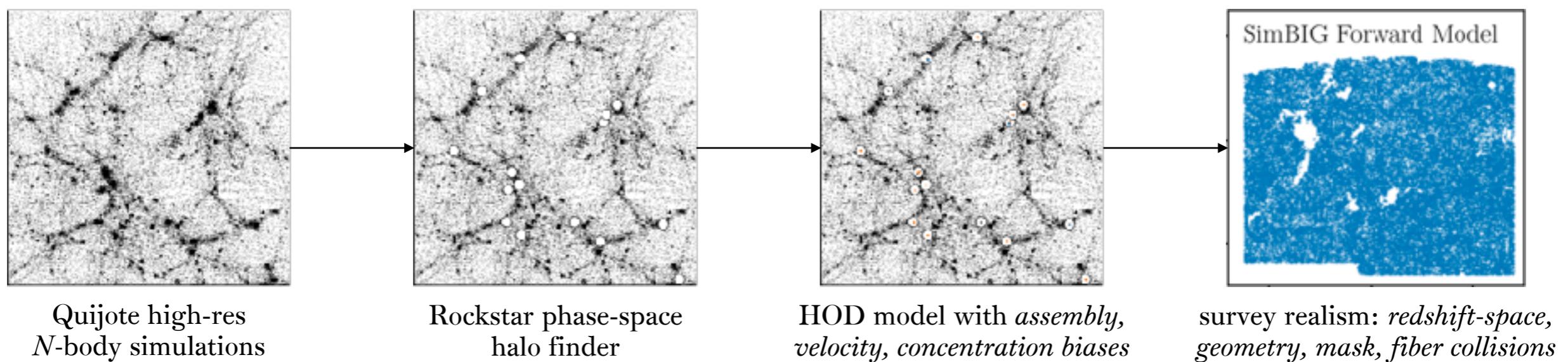
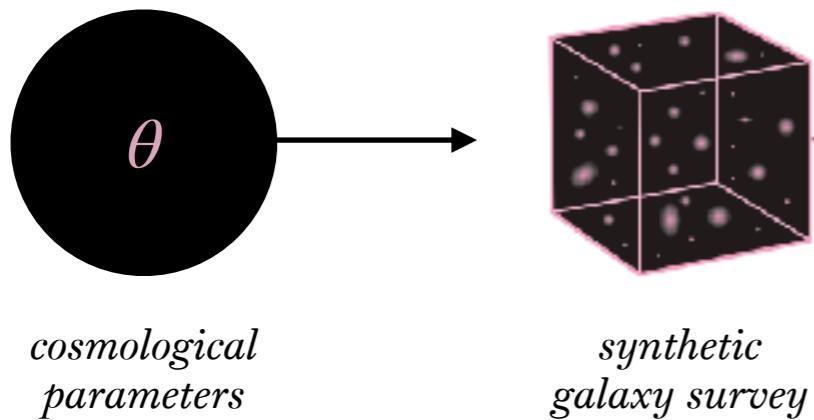
SDSS-III: BOSS

SIMBIG — 1. generating training data of synthetic observations

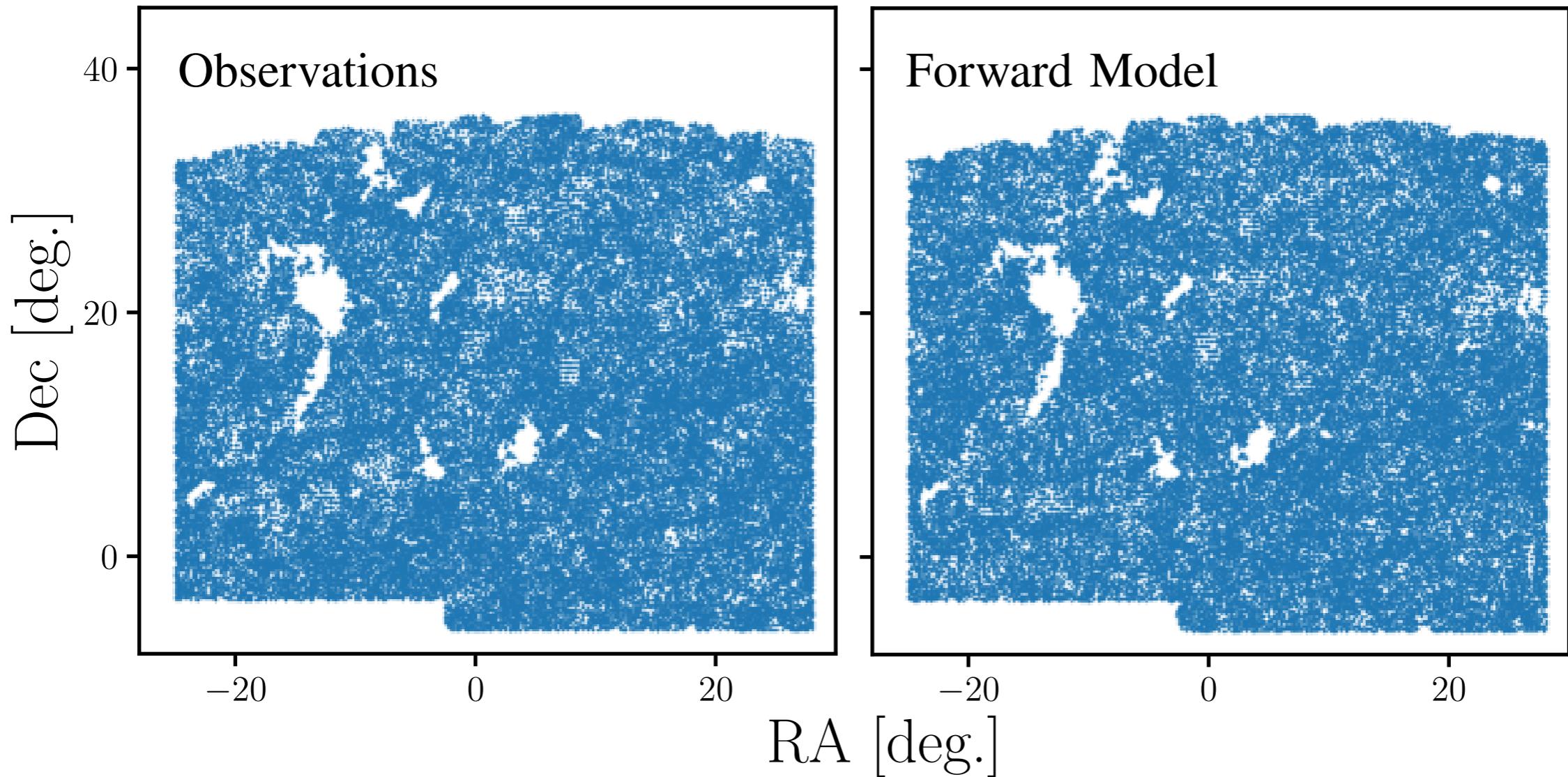


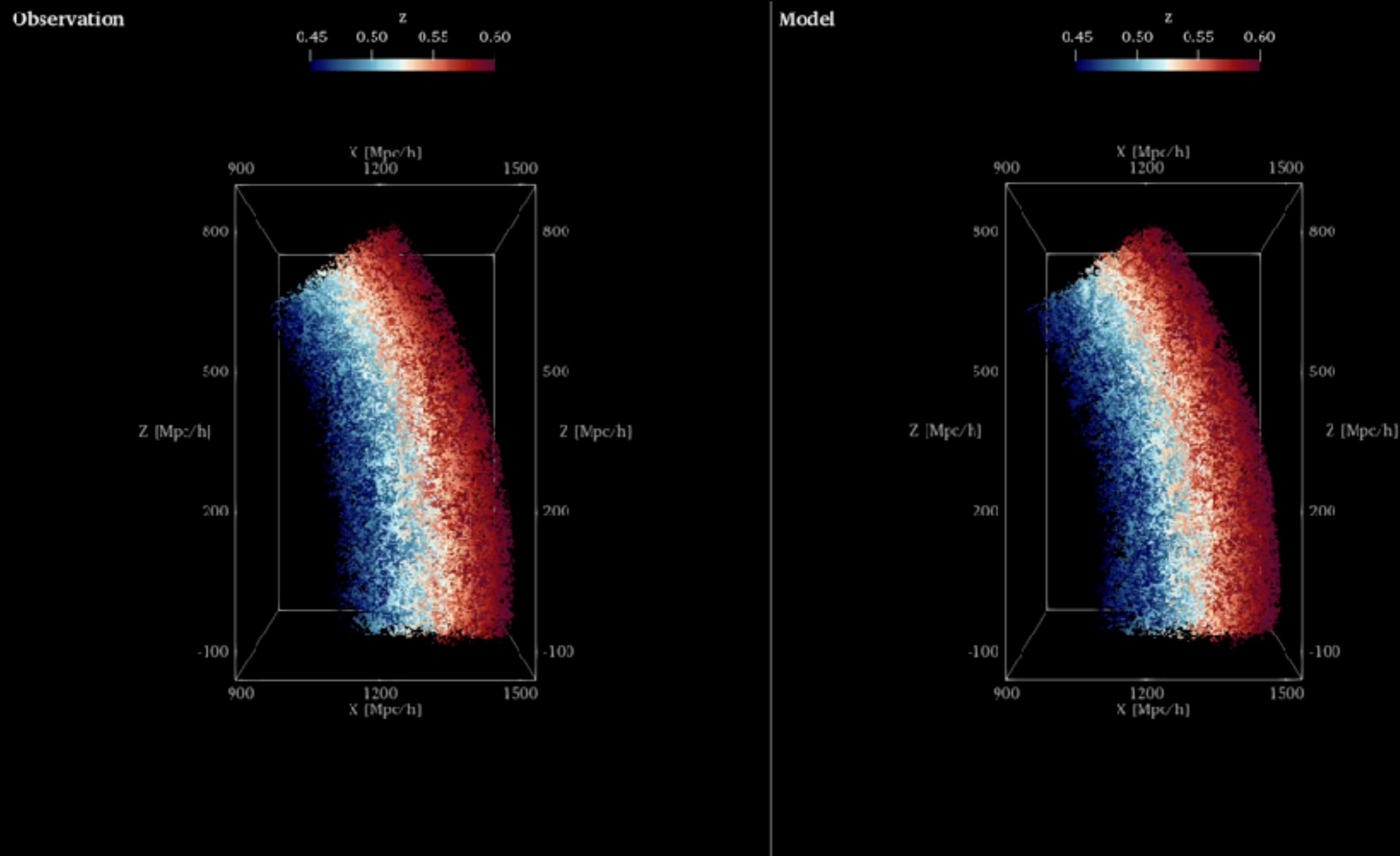
SDSS-III: BOSS

SIMBIG — 1. generating training data of synthetic observations

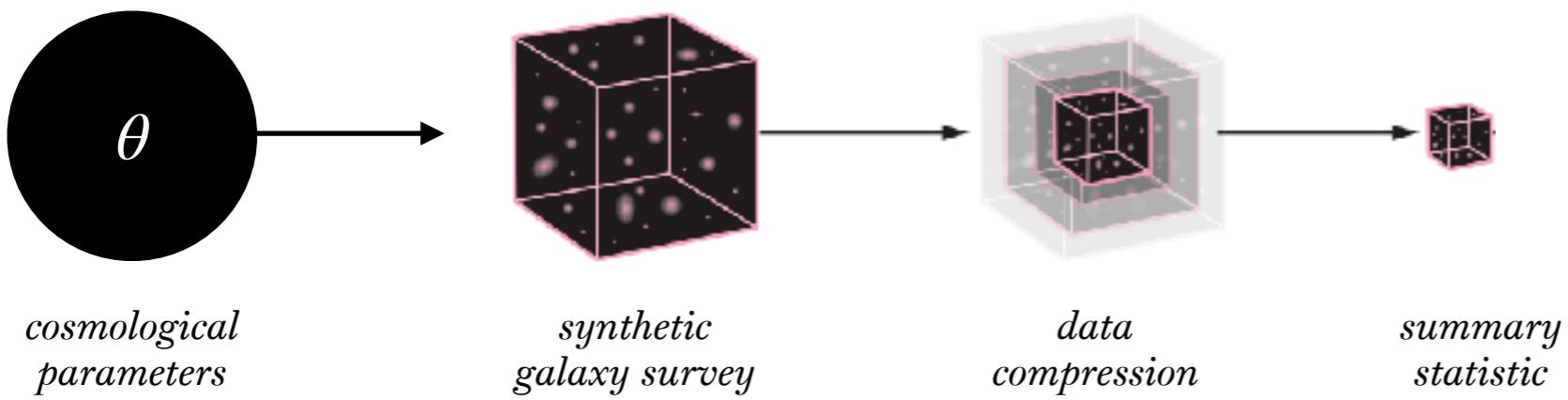


20,000 training simulations spanning broad range of cosmologies and HOD parameters

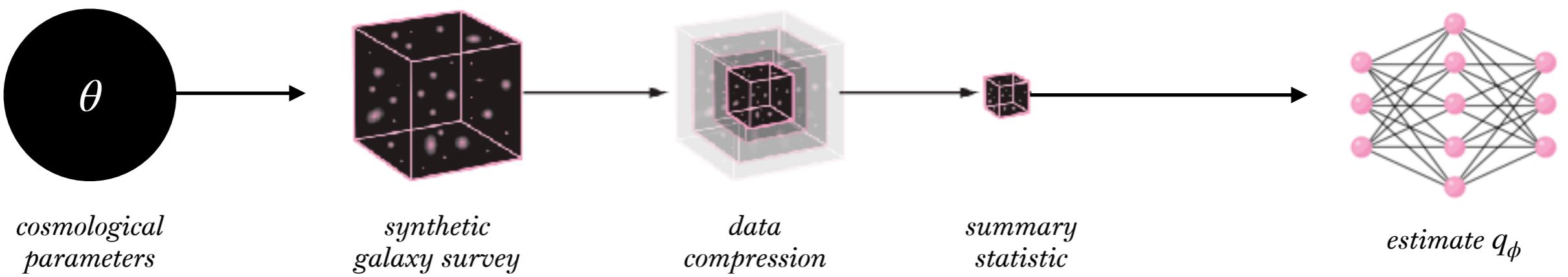




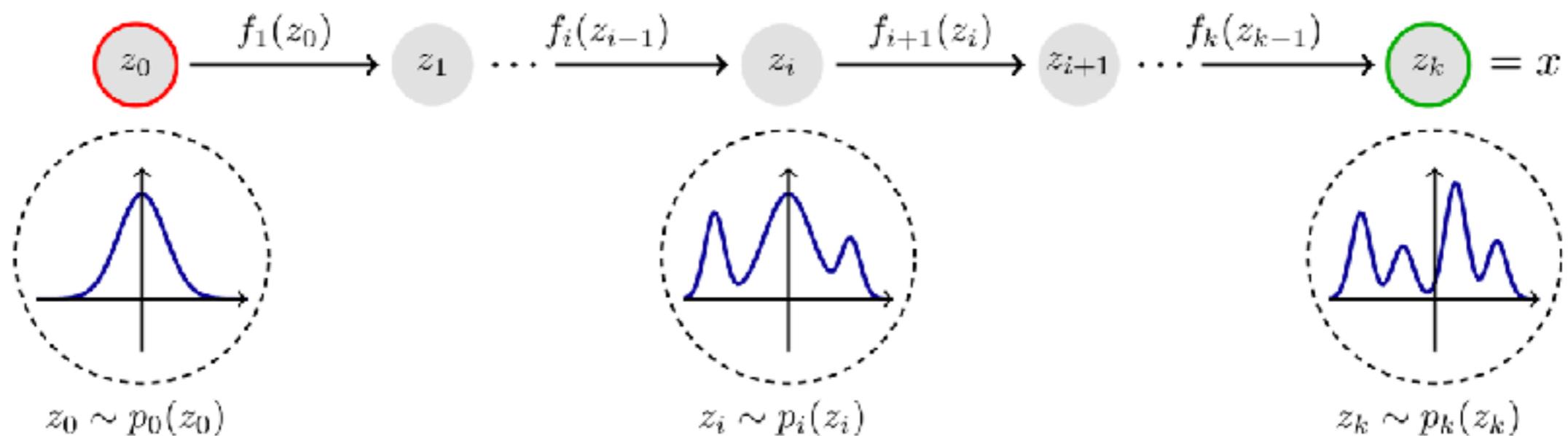
SIMBIG — 1. *generating training data of synthetic observations*



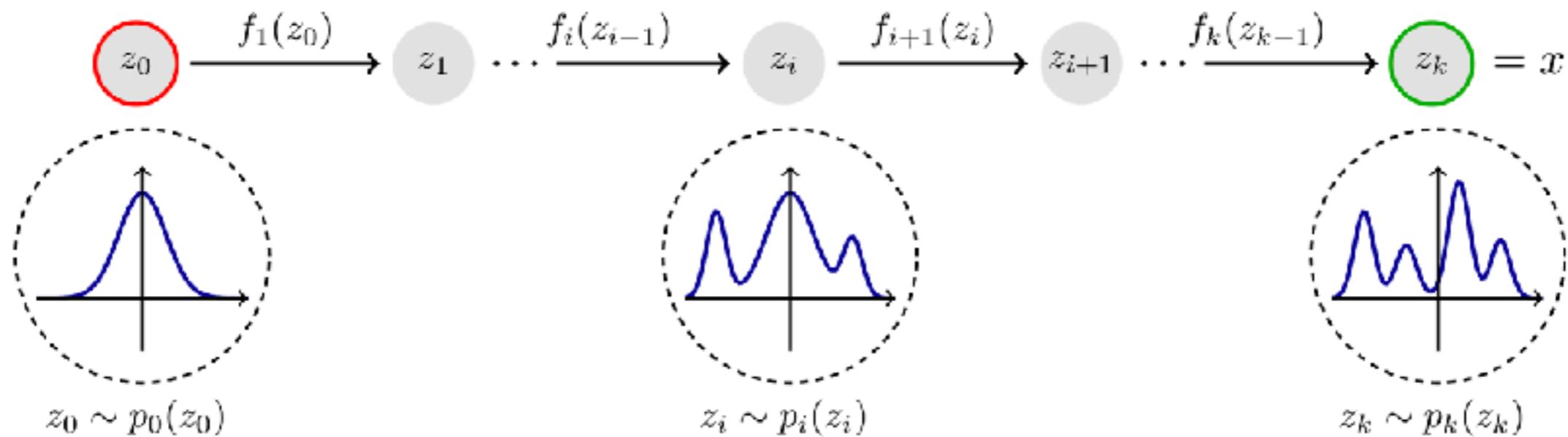
SIMBIG – 2. estimating the neural posterior estimator q_ϕ



normalizing flows: generative models that are easy to evaluate and flexibly expressive



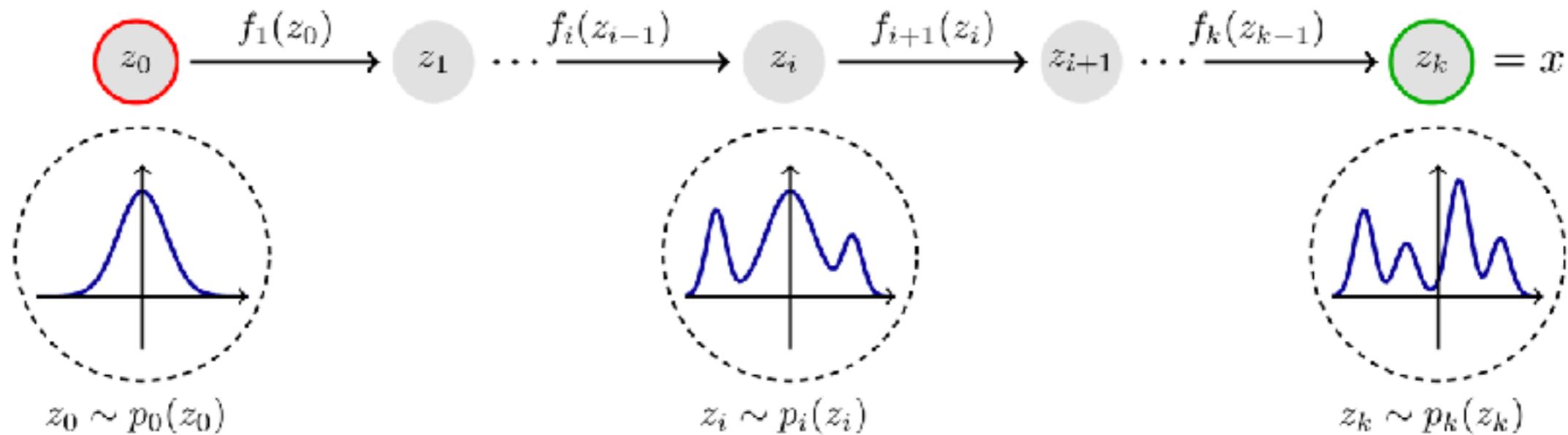
normalizing flows: generative models that are easy to evaluate and flexibly expressive



$z_i = f_i(z_{i-1})$ are invertible and differentiable transformations

$$p(z_i) = p(z_{i-1}) \left| \det \left(\frac{\partial f_i^{-1}}{\partial z_i} \right) \right|$$

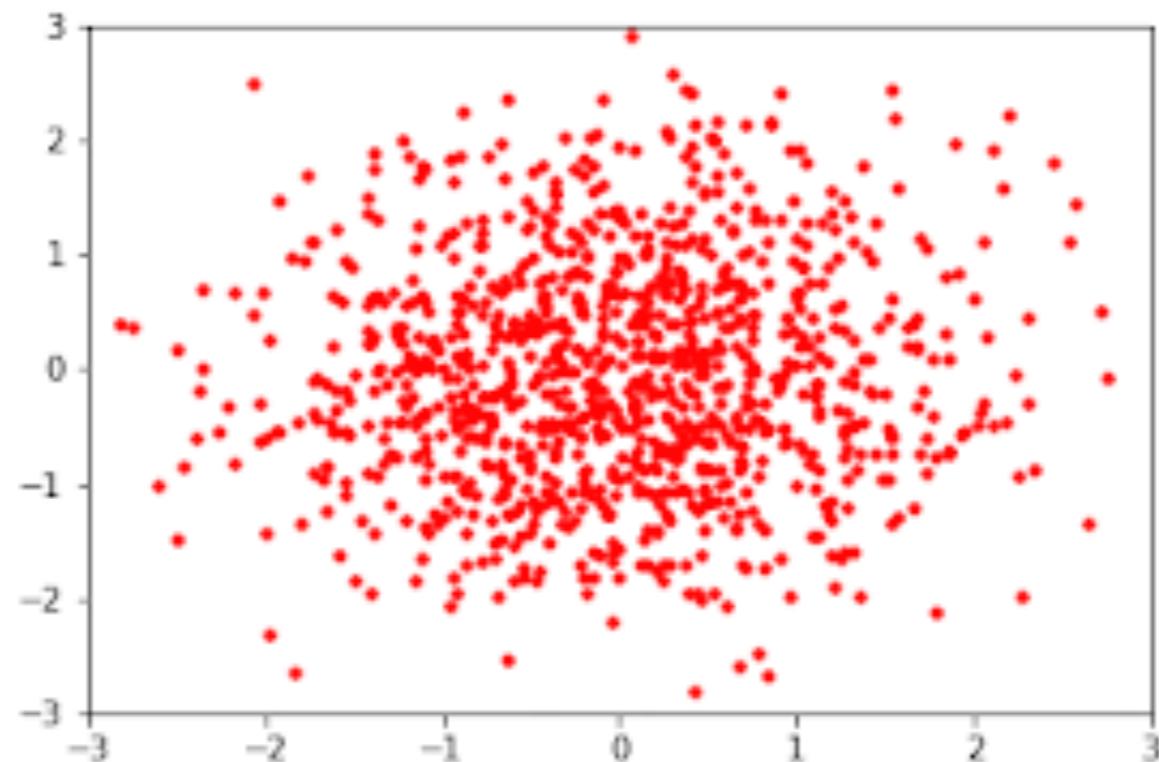
normalizing flows: generative models that are easy to evaluate and flexibly expressive



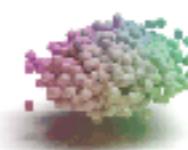
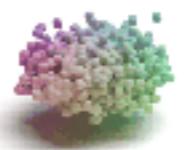
$z_i = f_i(z_{i-1})$ are invertible and differentiable transformations

$f = f_1 \circ f_2 \dots \circ f_{k-1} \circ f_k$ is also invertible and differentiable

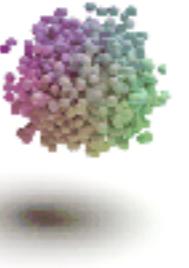
normalizing flows: generative models that are easy to evaluate and flexibly expressive



normalizing flows: generative models that are easy to evaluate and flexibly expressive



$p(\text{plane})$

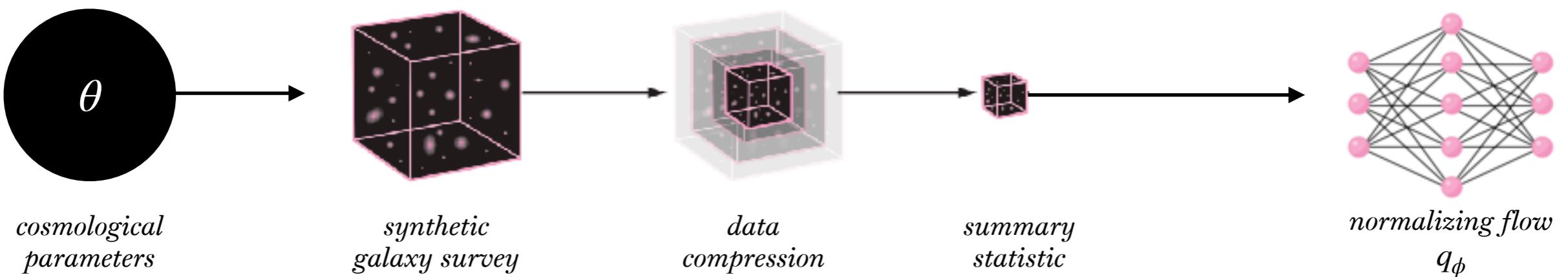


$p(\text{chair})$

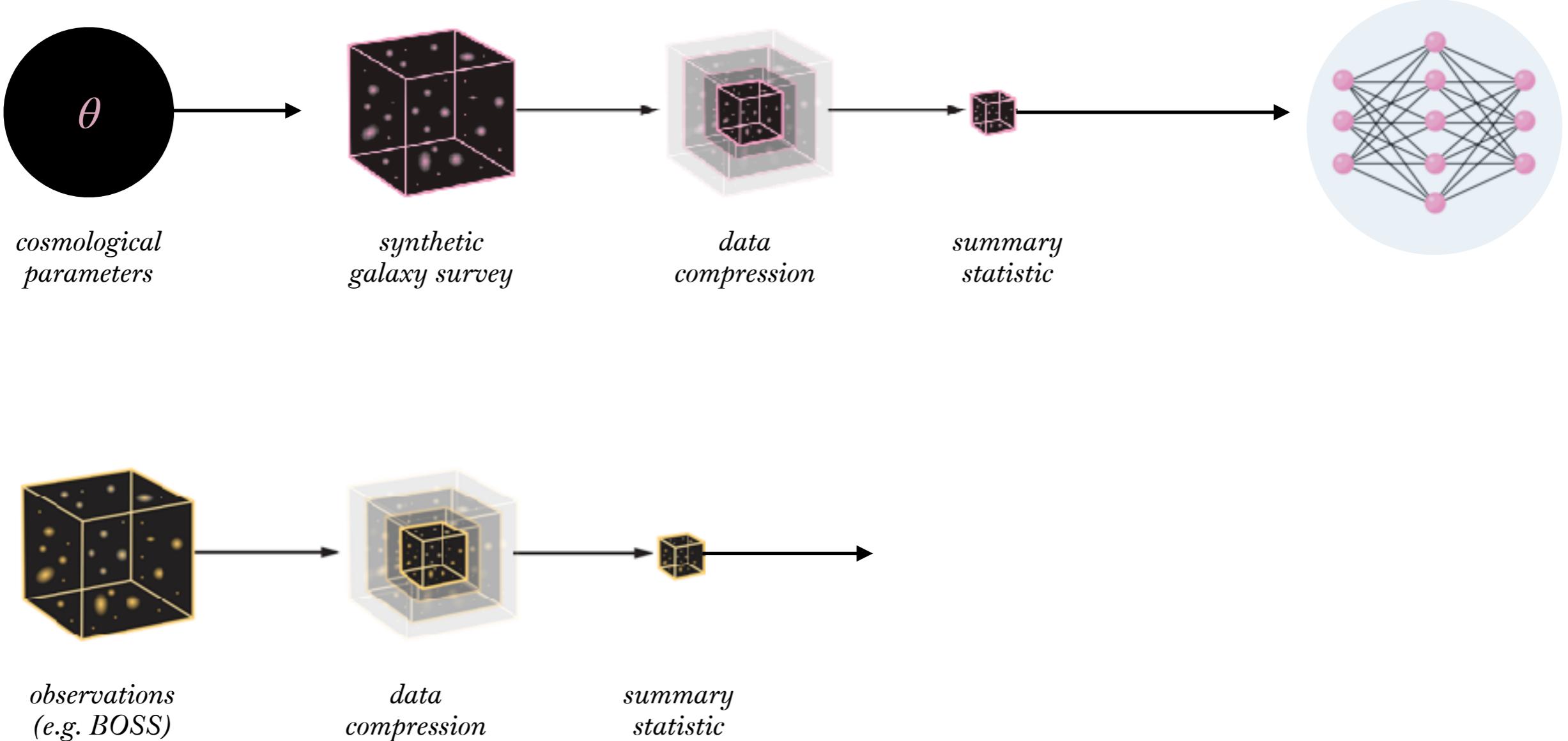


$p(\text{car})$

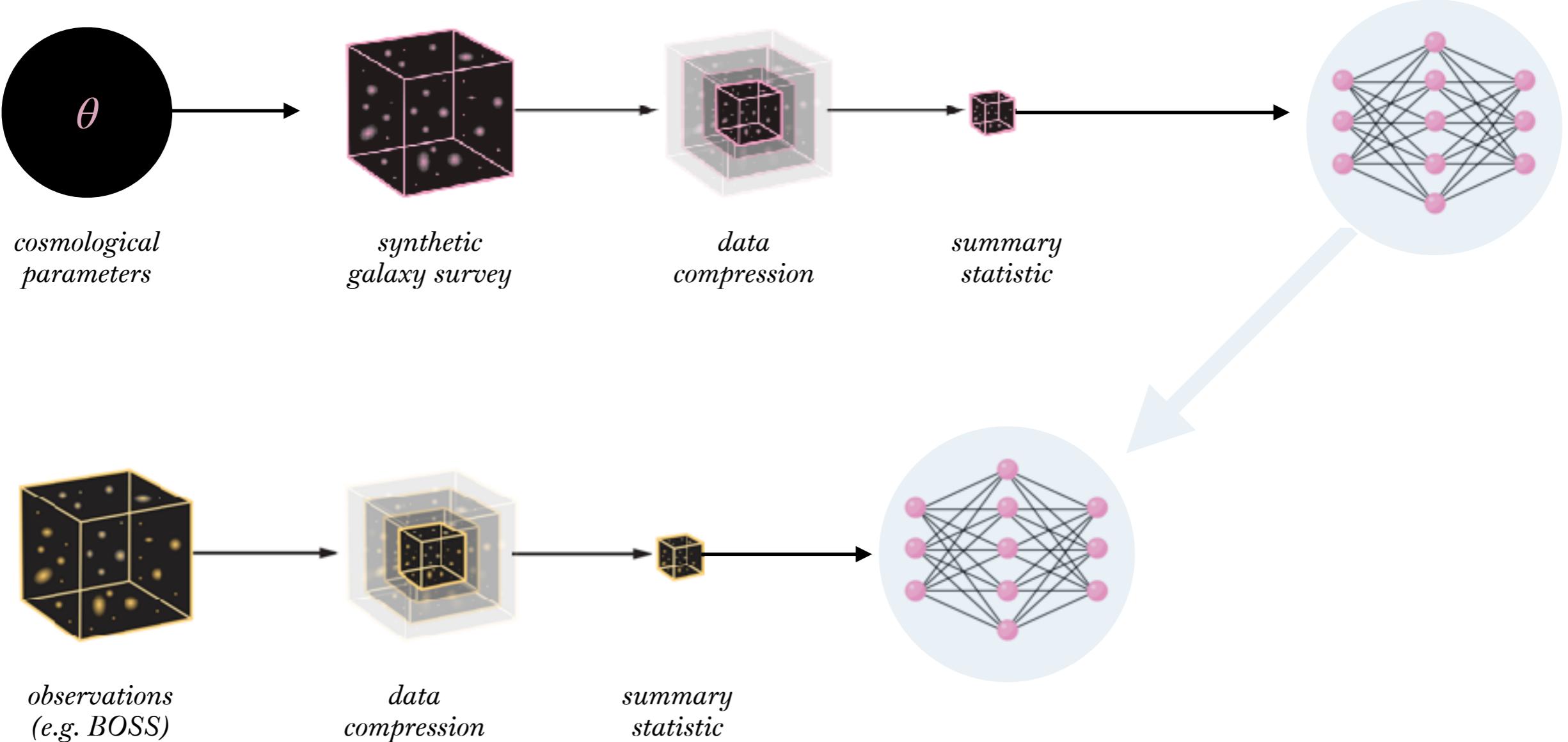
SIMBIG – 2. *training the normalizing flow*



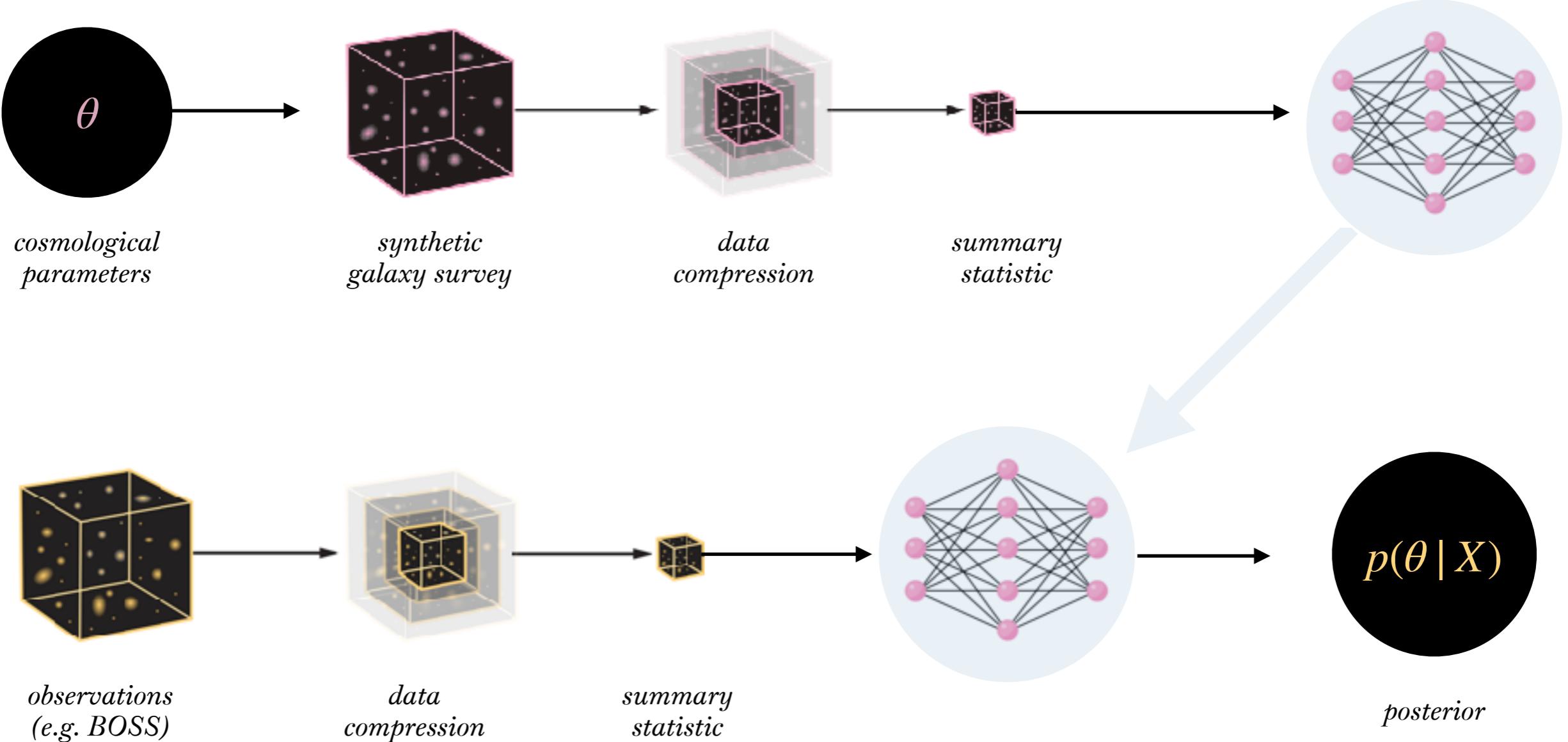
SIMBIG — 3. inference using real observations



SIMBIG — 3. inference using real observations

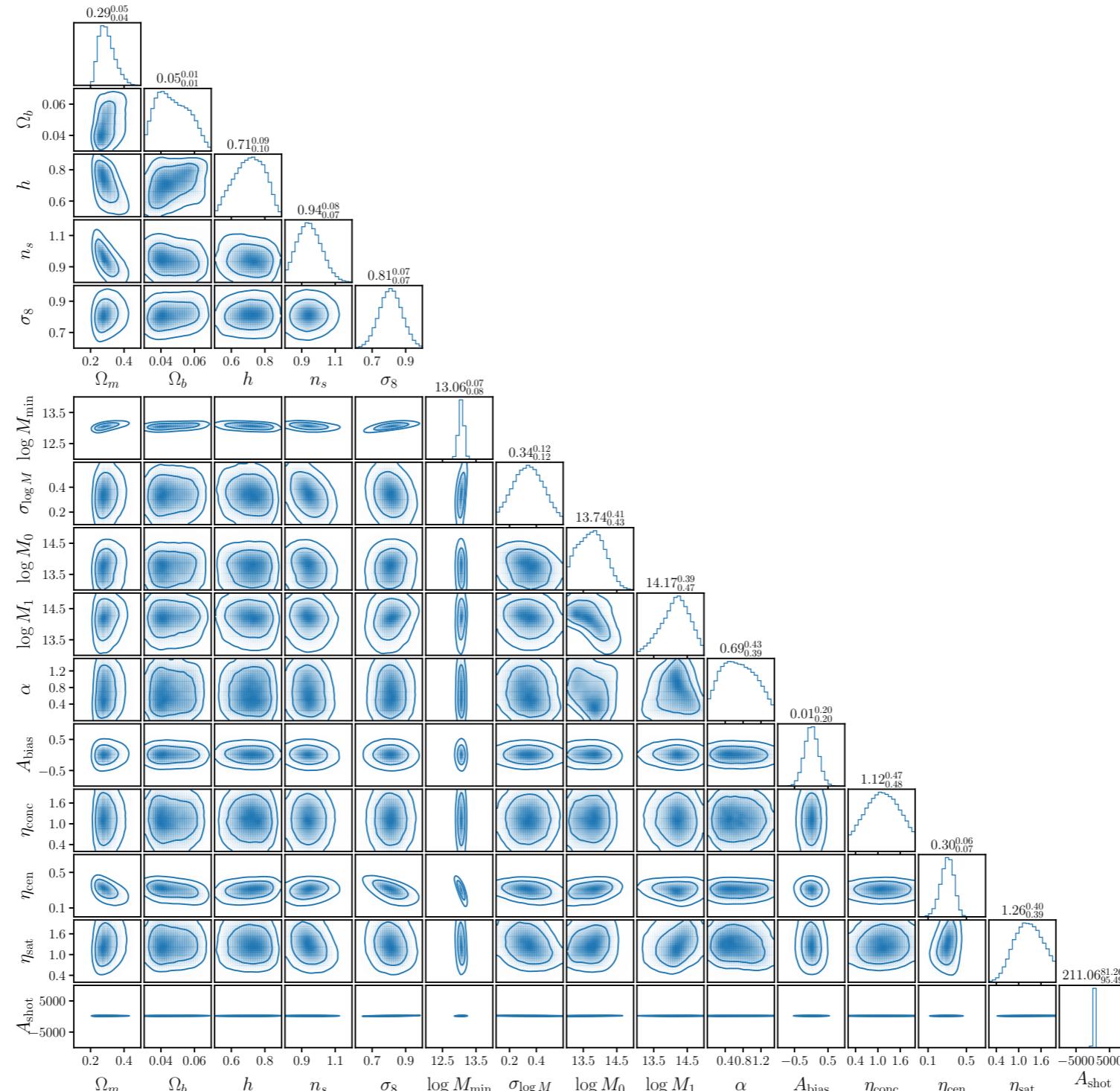


SIMBIG — 3. inference using real observations

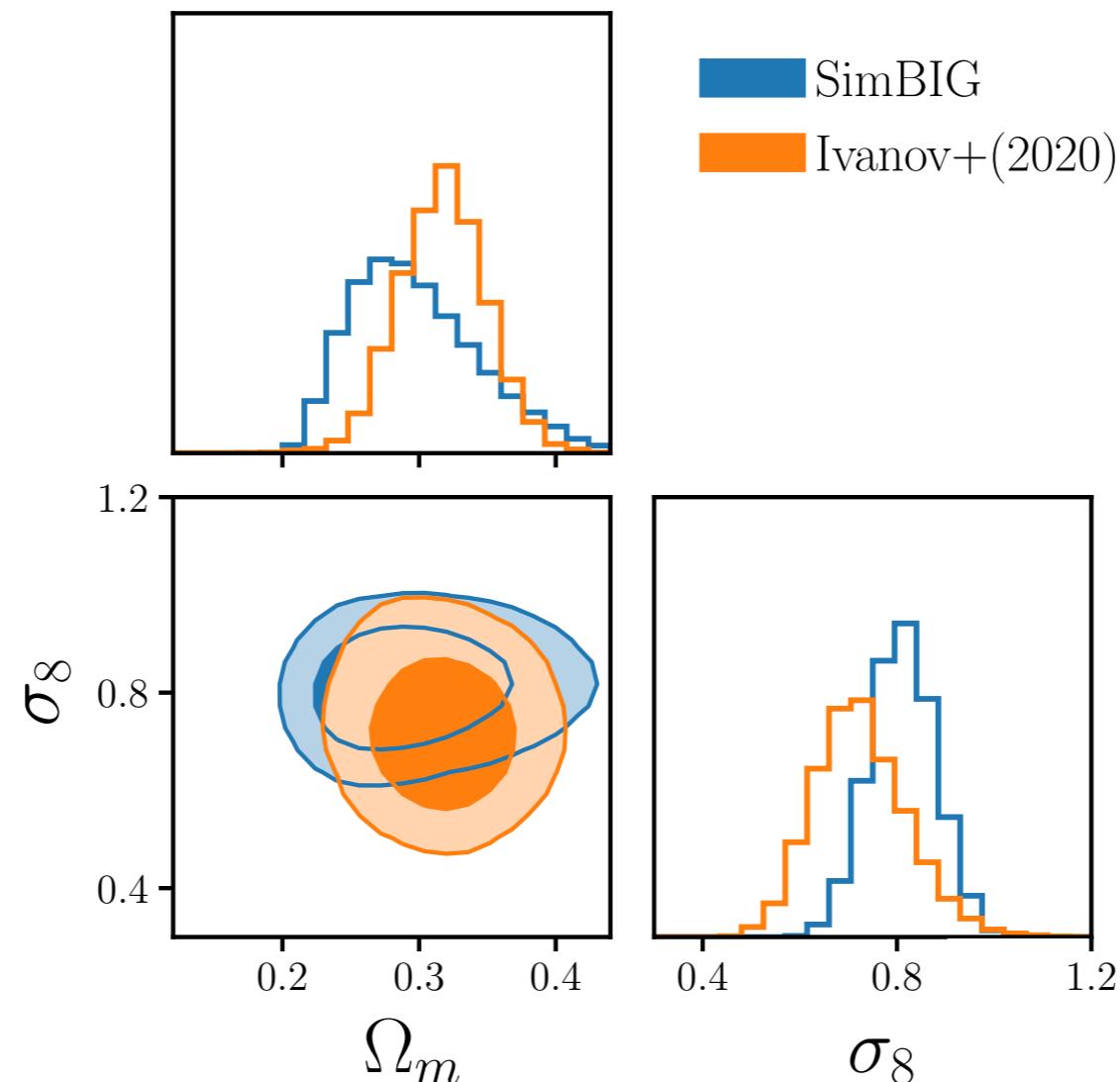


SIMBIG: non-linear galaxy power spectrum $P_\ell(k < 0.5 h/\text{Mpc})$

SIMBIG: non-linear galaxy power spectrum $P_\ell(k < 0.5 h/\text{Mpc})$



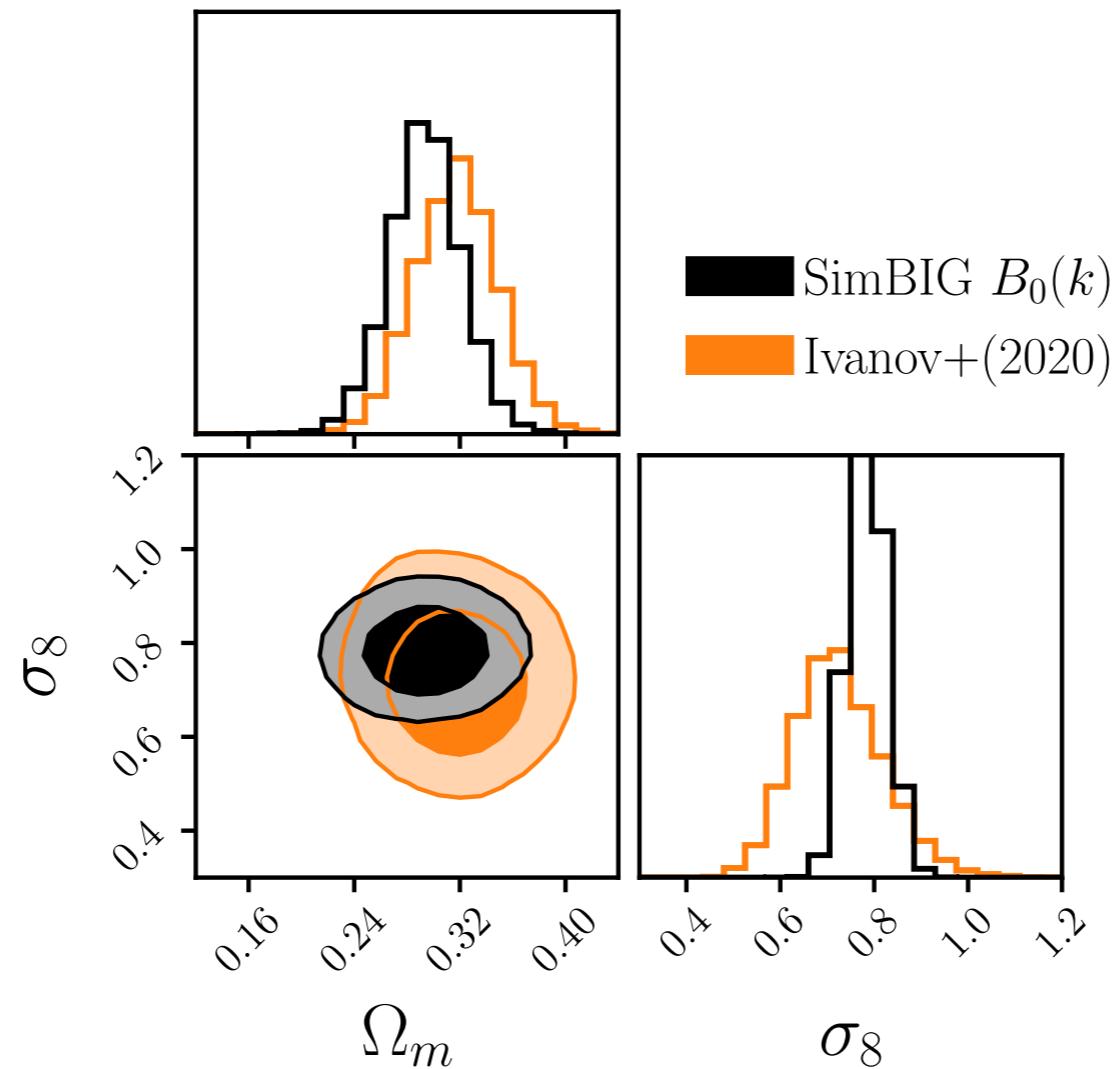
SIMBIG: non-linear galaxy power spectrum $P_\ell(k < 0.5 h/\text{Mpc})$



$1.4 \times$ tighter σ_8 from non-linear scales

SIMBIG: non-linear galaxy bispectrum $B_0(k_1, k_2, k_3 < 0.5 h/\text{Mpc})$

SIMBIG: non-linear galaxy bispectrum $B_0(k_1, k_2, k_3 < 0.5 h/\text{Mpc})$



1.2 and 2.4 \times tighter Ω_m and σ_8 from **non-linear + higher-order** clustering

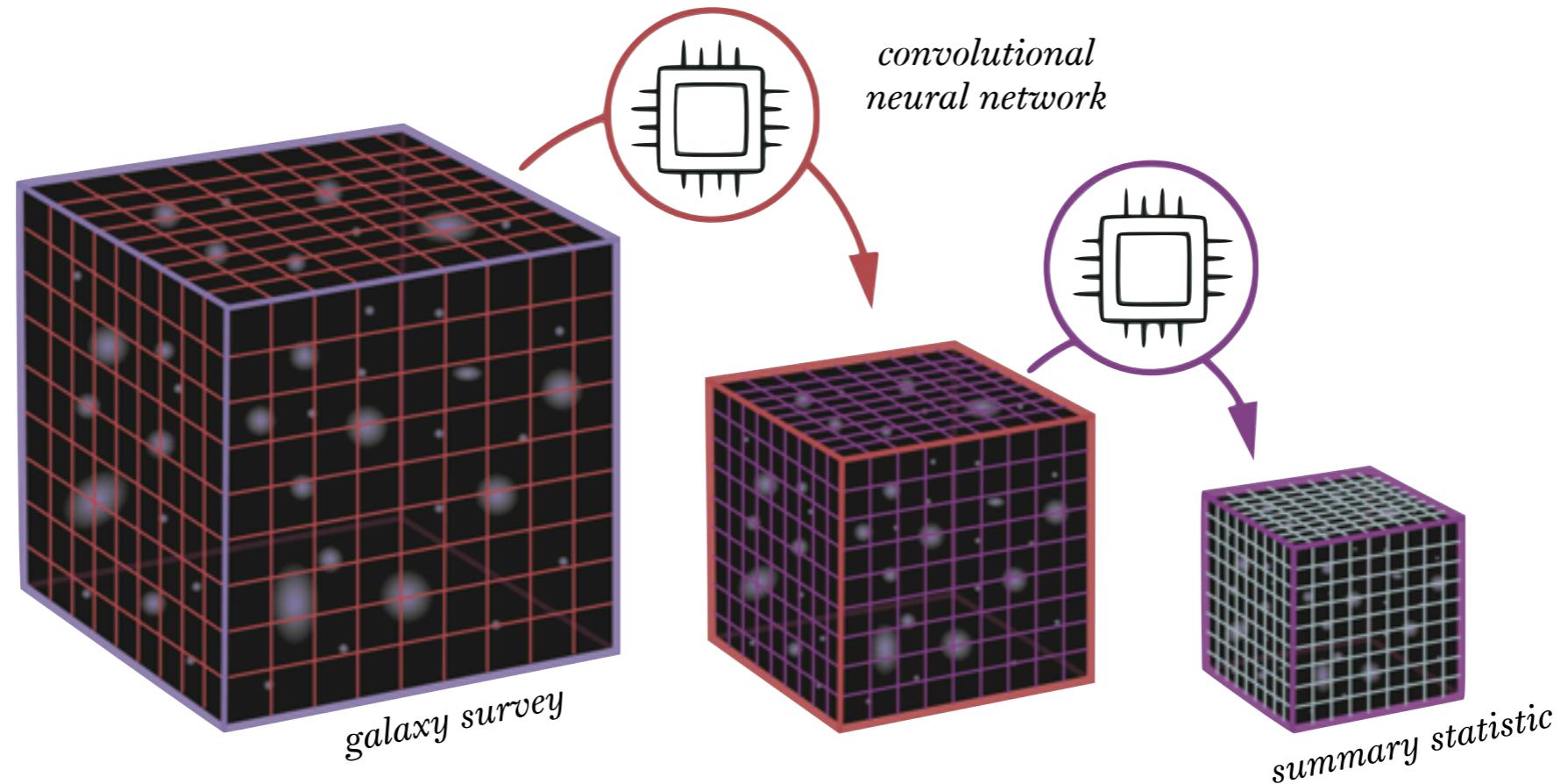


Liam Parker
Princeton Univ.



Pablo Lemos
MILA

SIMBIG: convolutional neural network field-level summary



extracting *all* relevant cosmological information in N -pt functions

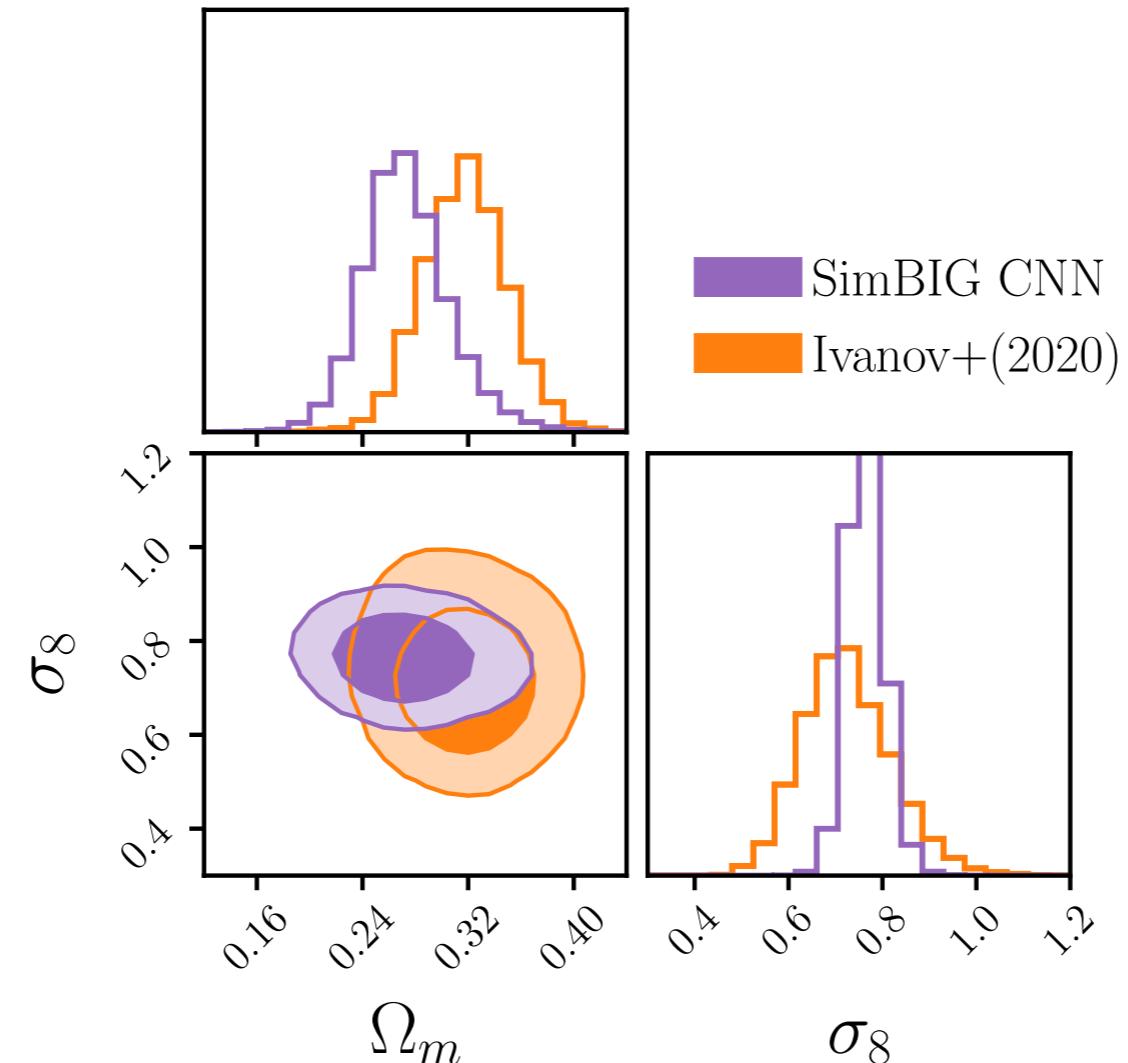


Liam Parker
Princeton Univ.



Pablo Lemos
MILA

SIMBIG: convolutional neural network field-level summary



extracting *all* relevant cosmological information in N -pt functions



wavelet scattering transforms

Régaldo-Saint Blancard, Hahn et al. (2023)



Bruno Régaldo-Saint Blancard
CCM Flatiron

skew spectra

Hou, Moradinezhad Dizgah, Hahn et al. (2024)



Jiamin Hou
Univ. of Florida

marked powerspectrum

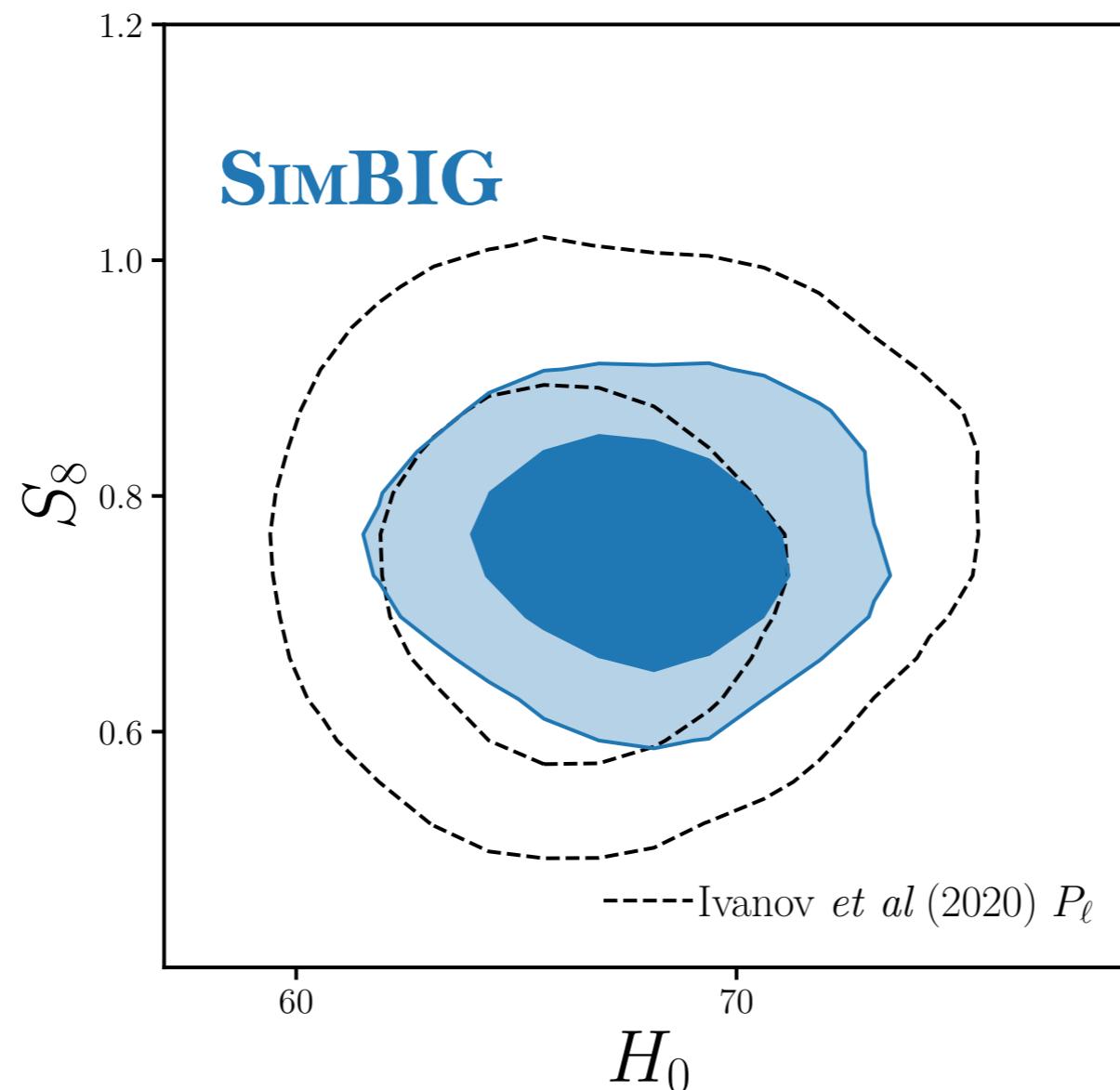
Massara, Hahn et al. (2024)



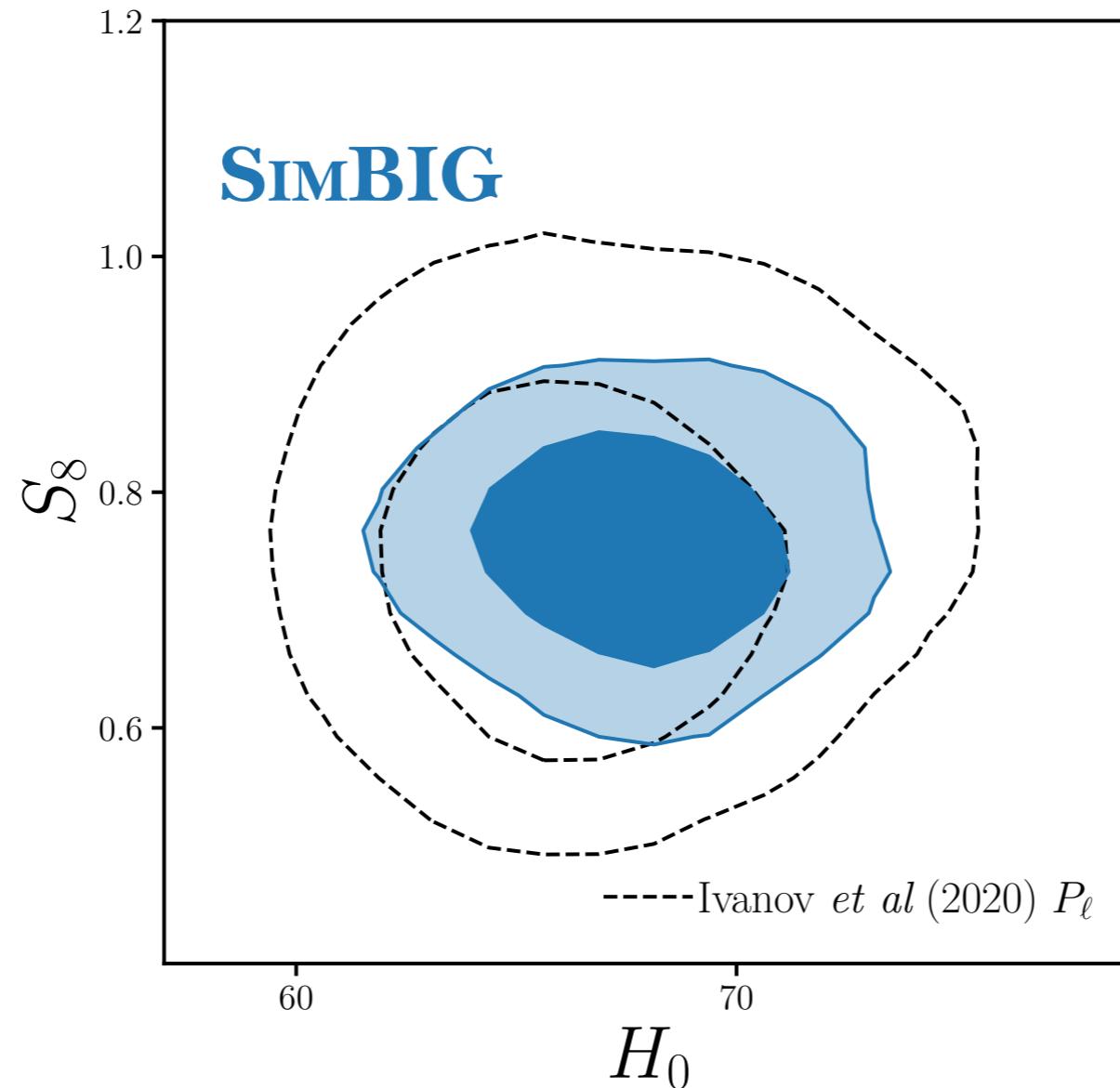
Elena Massara
UWaterloo

voids, clusters, (*your favorite summary statistic*)

SIMBIG: ~ 1.9 and $1.5 \times$ tighter S_8 and H_0



SIMBIG: ~ 1.9 and $1.5 \times$ tighter S_8 and H_0



S_8 improvement is equivalent to analyzing a *survey of $\sim 4 \times$ larger volume*

simulation-based inference* *in action*

see also many other cosmological SBI analyses: *Jeffrey et al.(2021)*, *Fluri et al.(2022)*,
Gatti et al.(2024), *Moser et al.(2024)*, *von Wietersheim-Kramsta et al. (2024)++*

**state-of-the-art SBI (e.g. neural posterior estimation)*

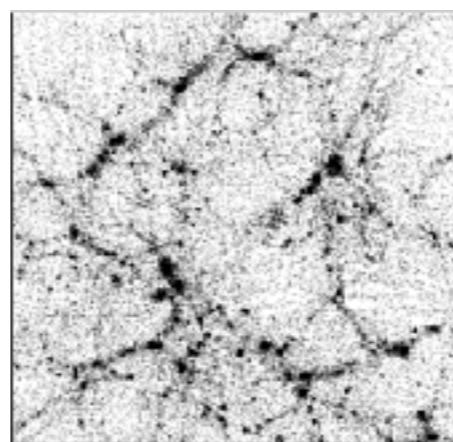
what is simulation-based inference?

opportunities for simulation-based inference?

challenges for simulation-based inference?

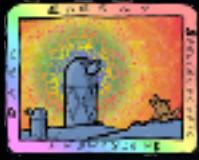
challenges for SBI: can forward models *scale* to the next-generation galaxy surveys?

challenges for SBI: can forward models *scale* to the next-generation galaxy surveys?



Quijote high-res
N-body simulations

1 Gpc/ h box with $\sim 10^{12} M_\odot$ halo mass limit



DARK ENERGY
SPECTROSCOPIC
INSTRUMENT

U.S. Department of Energy Office of Science

DESI will observe >40 million galaxies

15 million bright galaxies

$z < 0.6$

8 million Luminous Red Galaxies

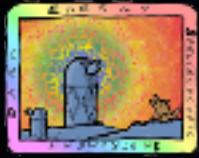
$0.4 < z < 1.0$

16 million Emission Line Galaxies

$0.6 < z < 1.6$

3 million Quasars

$0.9 < z < 2.1$



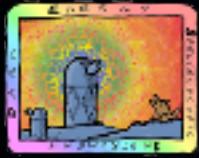
DARK ENERGY
SPECTROSCOPIC
INSTRUMENT

U.S. Department of Energy Office of Science

DESI will observe >40 million galaxies



see Hector's talk; DESI Year 1 papers



DARK ENERGY
SPECTROSCOPIC
INSTRUMENT

U.S. Department of Energy Office of Science

DESI will observe >40 million galaxies

15 million bright galaxies

$$\frac{V_{\text{eff}}}{1 \text{ Gpc}^3}$$

8 million Luminous Red Galaxies

$$12 \text{ Gpc}^3$$

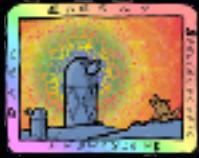
16 million Emission Line Galaxies

$$5 \text{ Gpc}^3$$

3 million Quasars

$$1.5 \text{ Gpc}^3$$

for year 1!



U.S. Department of Energy Office of Science

DESI will observe >40 million galaxies

15 million bright galaxies

$$\frac{M_{h,\min}}{< 10^{11} M_\odot}$$

8 million Luminous Red Galaxies

$$\sim 10^{12} M_\odot$$

16 million Emission Line Galaxies

$$> 10^{11} M_\odot$$

3 million Quasars

$$\sim 10^{12} M_\odot$$



Prime Focus
Spectrograph

the SuMIRe Prime Focus Spectrograph (PFS) Cosmology Survey
will observe on the **8.2m** Subaru telescope *next year*

5 million *emission line galaxy*

$0.6 < z < 2.4$



Yuka Yamada
Univ. of Tokyo
PFS Cosmology target selection



Prime Focus
Spectrograph

the SuMIRe Prime Focus Spectrograph (PFS) Cosmology Survey will observe on the **8.2m** Subaru telescope *next year*

5 million *emission line galaxy*

$$\frac{V_{\text{eff}}}{\sim 10 \text{ Gpc}^3}$$





Prime Focus
Spectrograph

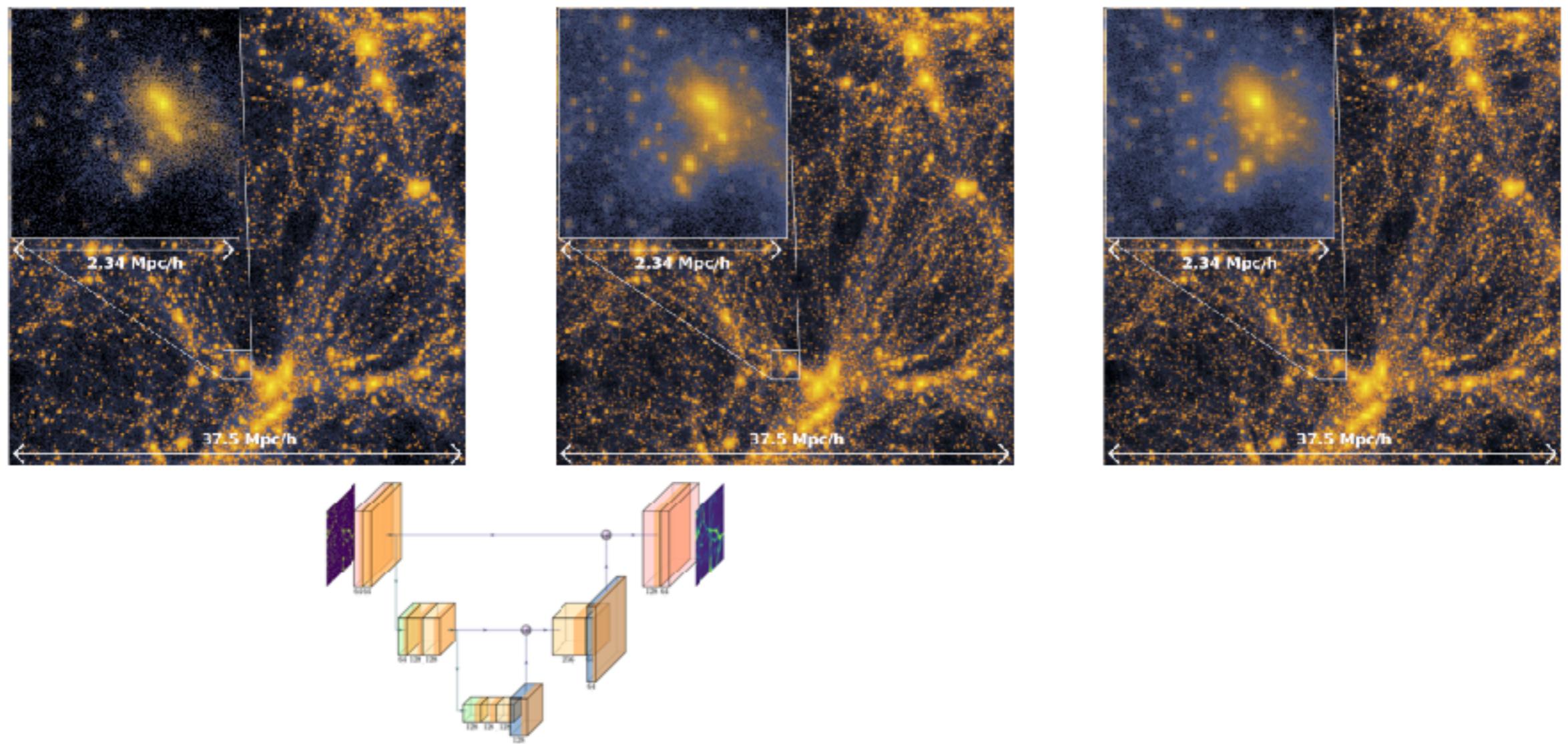
the SuMIRe Prime Focus Spectrograph (PFS) Cosmology Survey will observe on the **8.2m** Subaru telescope *next year*

5 million *emission line galaxy*

$$\frac{M_{h,\min}}{> 10^{11} M_\odot}$$

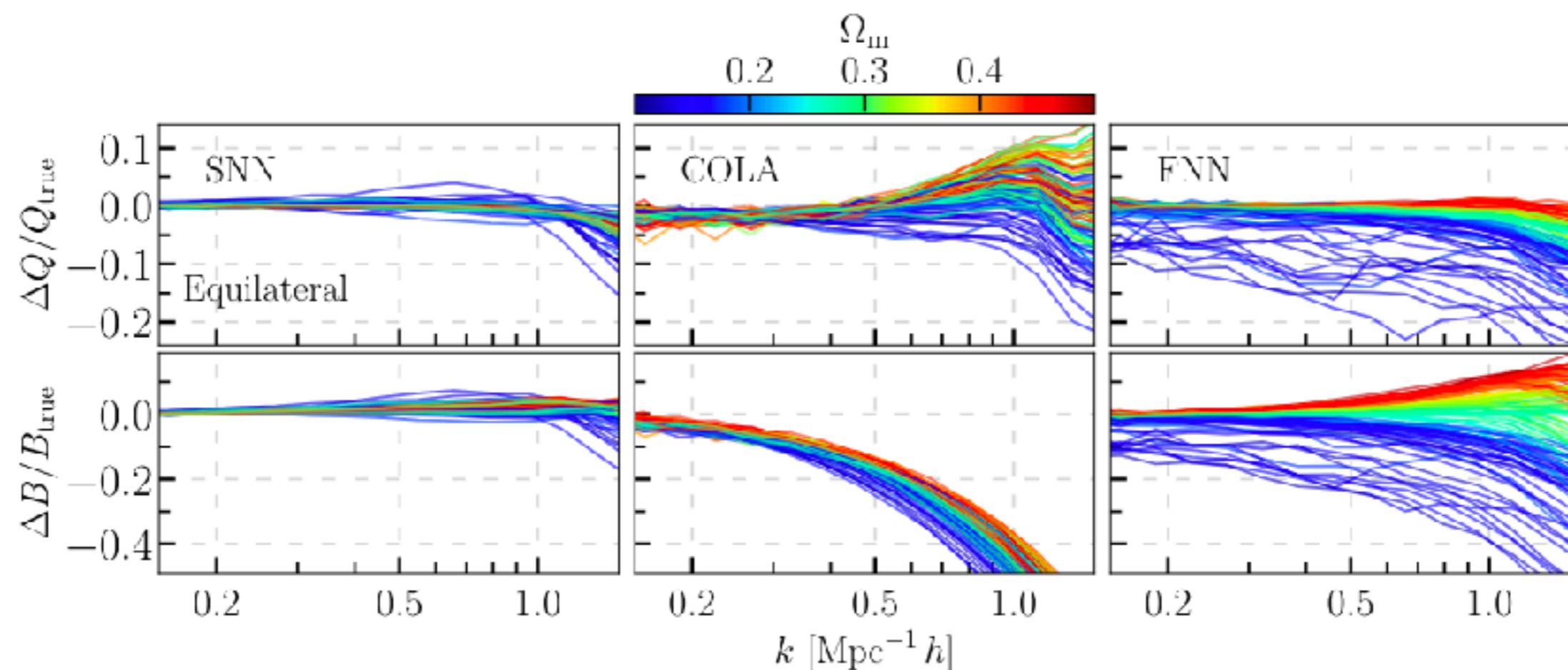
SIMBIGGER – we need larger volumes, higher resolution

SIMBIGGER – we need larger volumes, higher resolution *emulation*



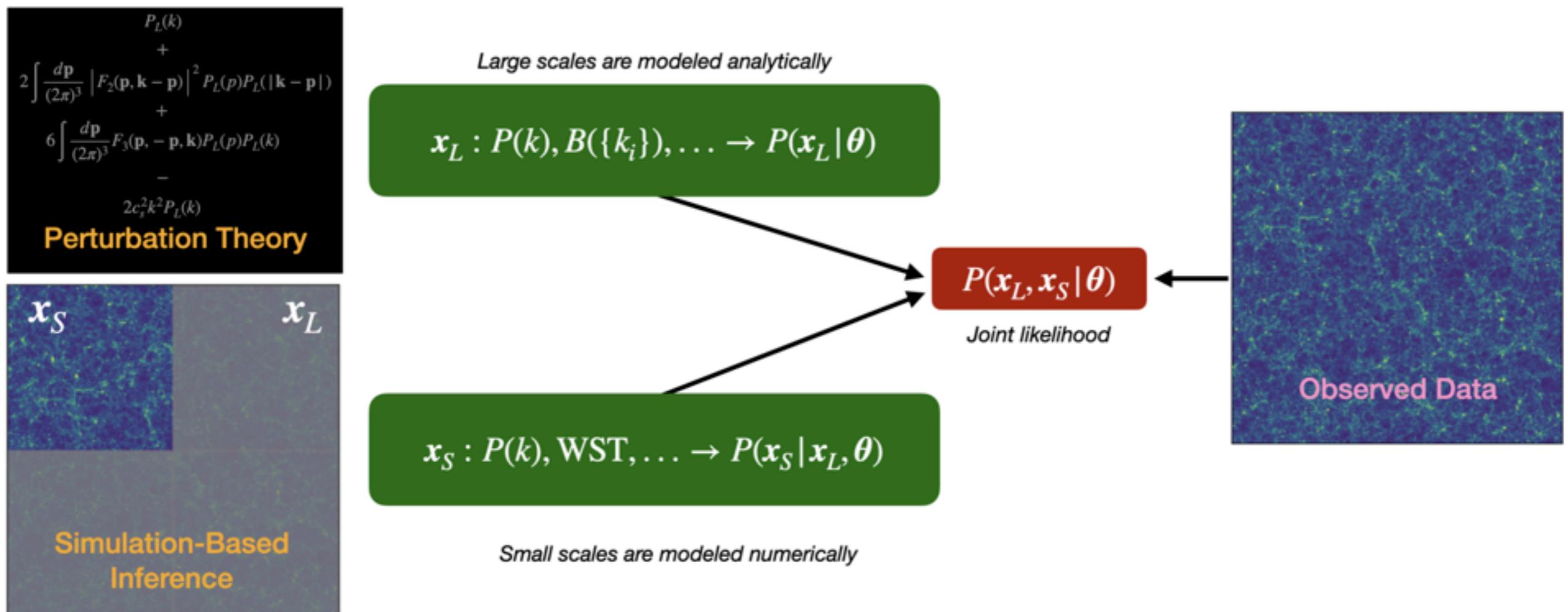
e.g. Alves de Oliveira et al.(2020), Li et al. (2021), Schaurecker et al.(2022),
Jamieson et al.(2022), Giusarma et al.(2023), Zhang et al.(2023), **Ariel's emulator**

SIMBIGGER – we need larger volumes, higher resolution
emulation



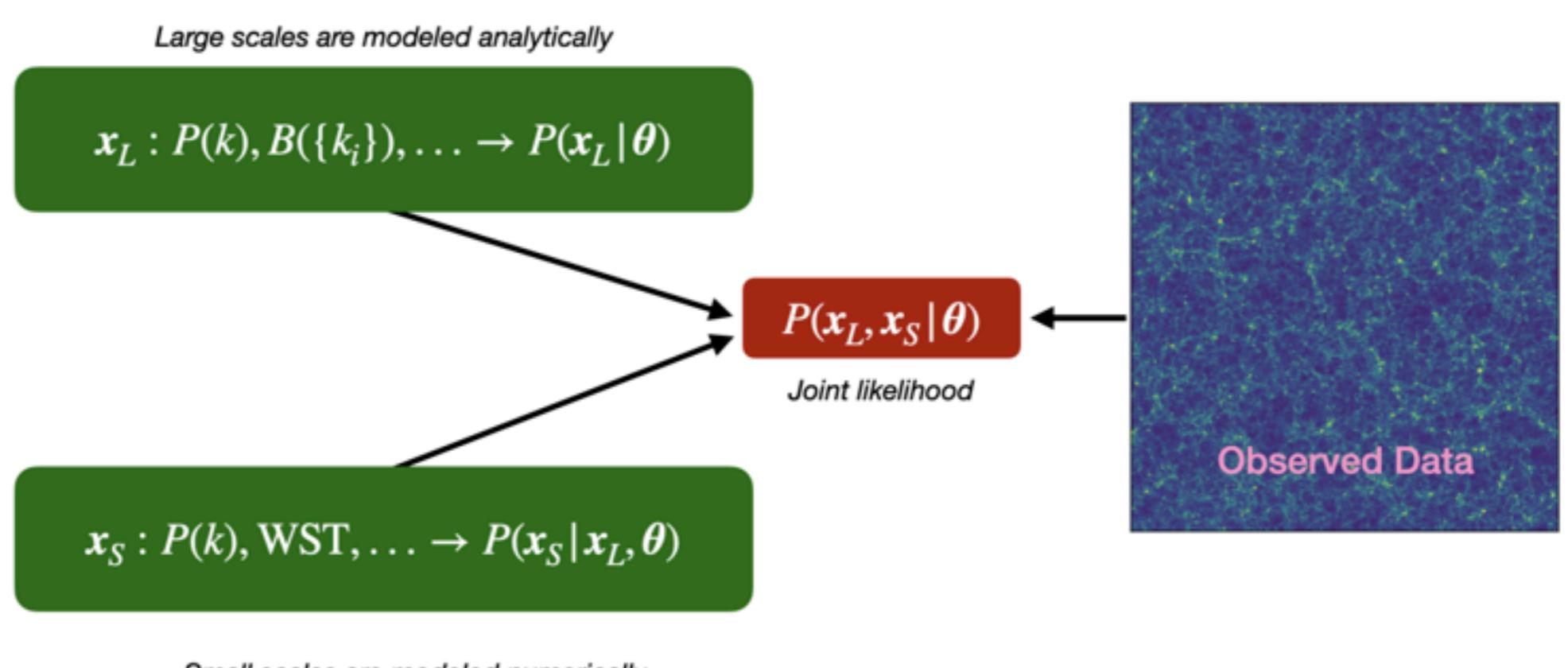
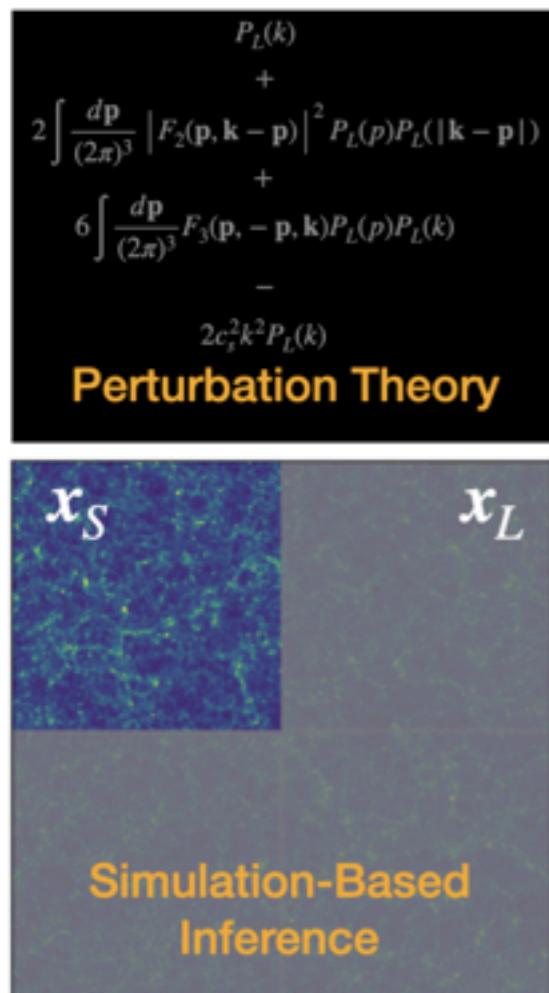
SIMBIGGER – we need larger volumes, higher resolution

hybrid SBI



SIMBIGGER – we need larger volumes, higher resolution

hybrid SBI



$$p(\mathbf{X} | \boldsymbol{\theta}) = p(\mathbf{X}_L | \boldsymbol{\theta}) p(\mathbf{X}_S | \mathbf{X}_L, \boldsymbol{\theta})$$

challenges for SBI: how can we trust SBI results?

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posterior validation

$q_\phi(\theta | \mathbf{X})$ is guaranteed to converge to $p(\theta | \mathbf{X})$ if

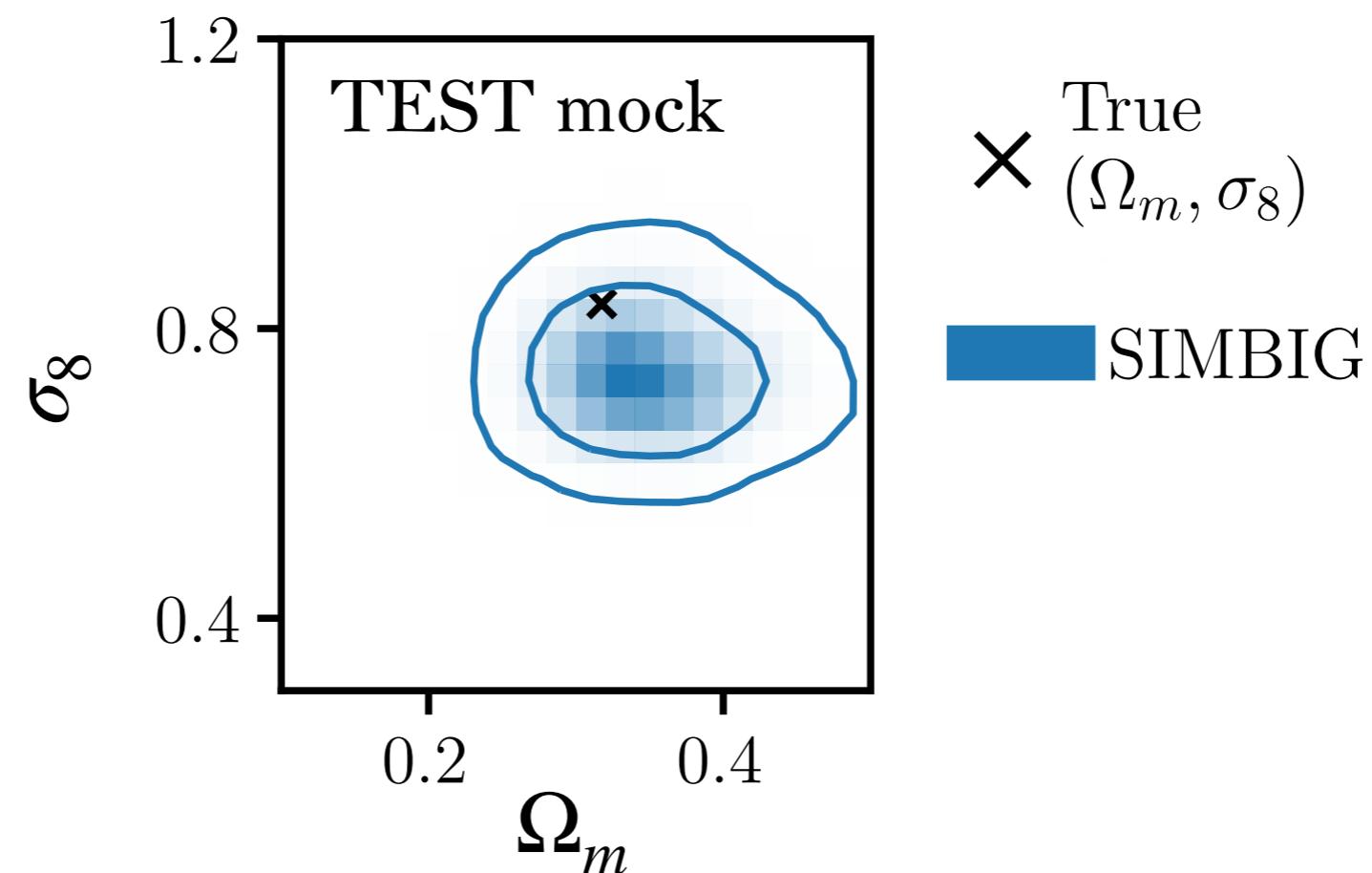
q_ϕ is flexibly expressive

$N \rightarrow \infty$ samples from $p(\mathbf{X}, \theta)$

successful optimization

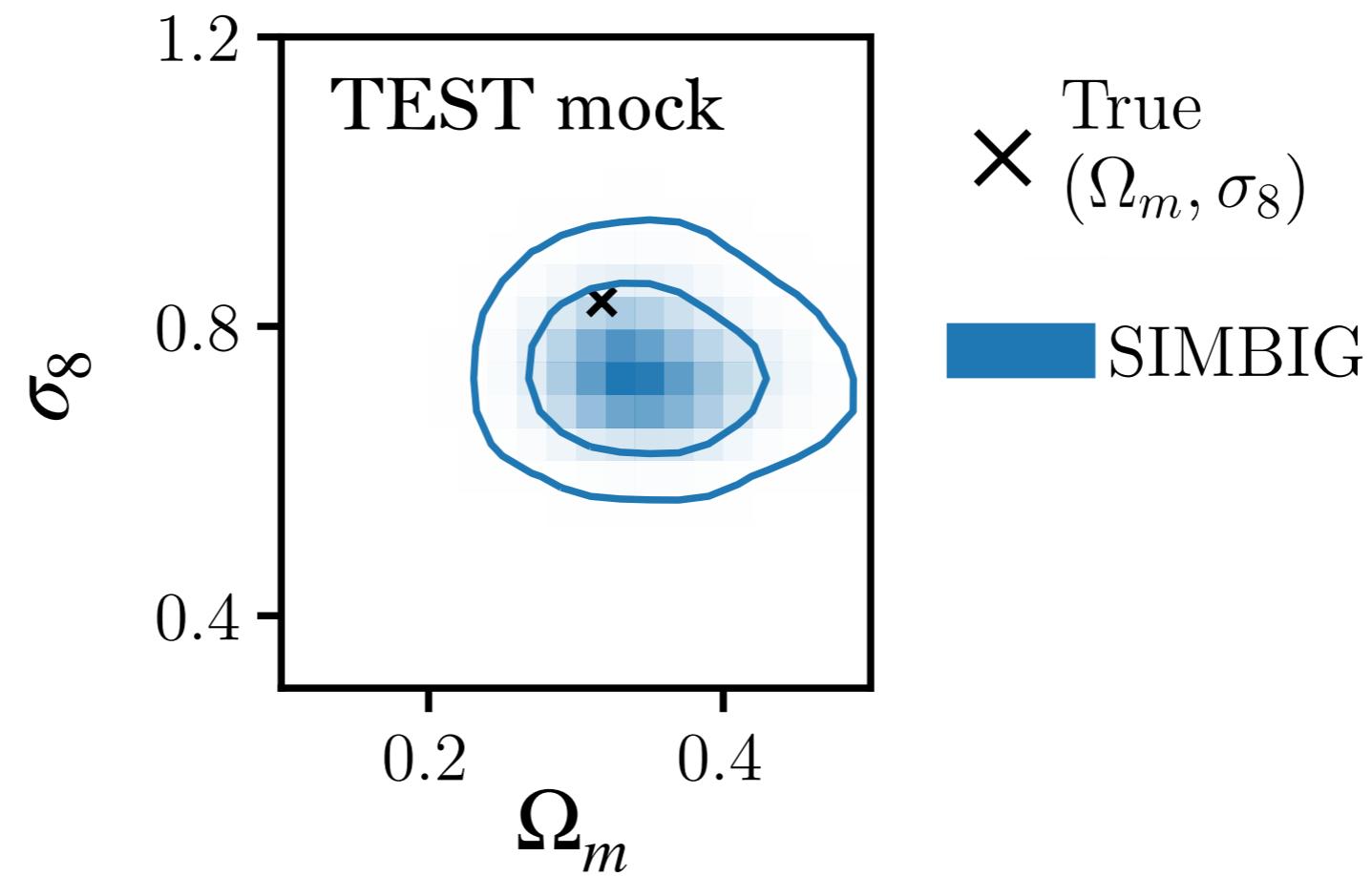
challenges for SBI: how can we trust SBI results?

posterior validation



challenges for SBI: how can we trust SBI results?

posterior validation

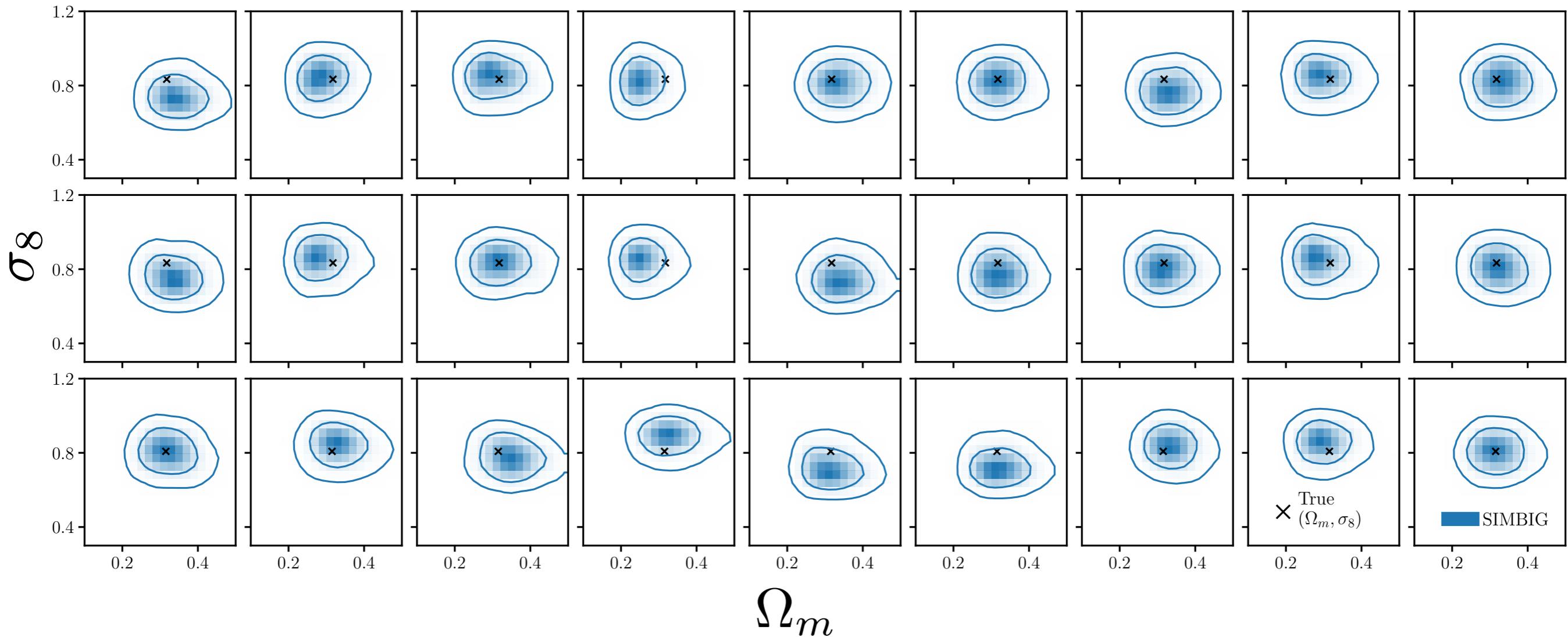


we need to validate *both* accuracy and precision

challenges for SBI: how can we trust SBI results?

posterior validation

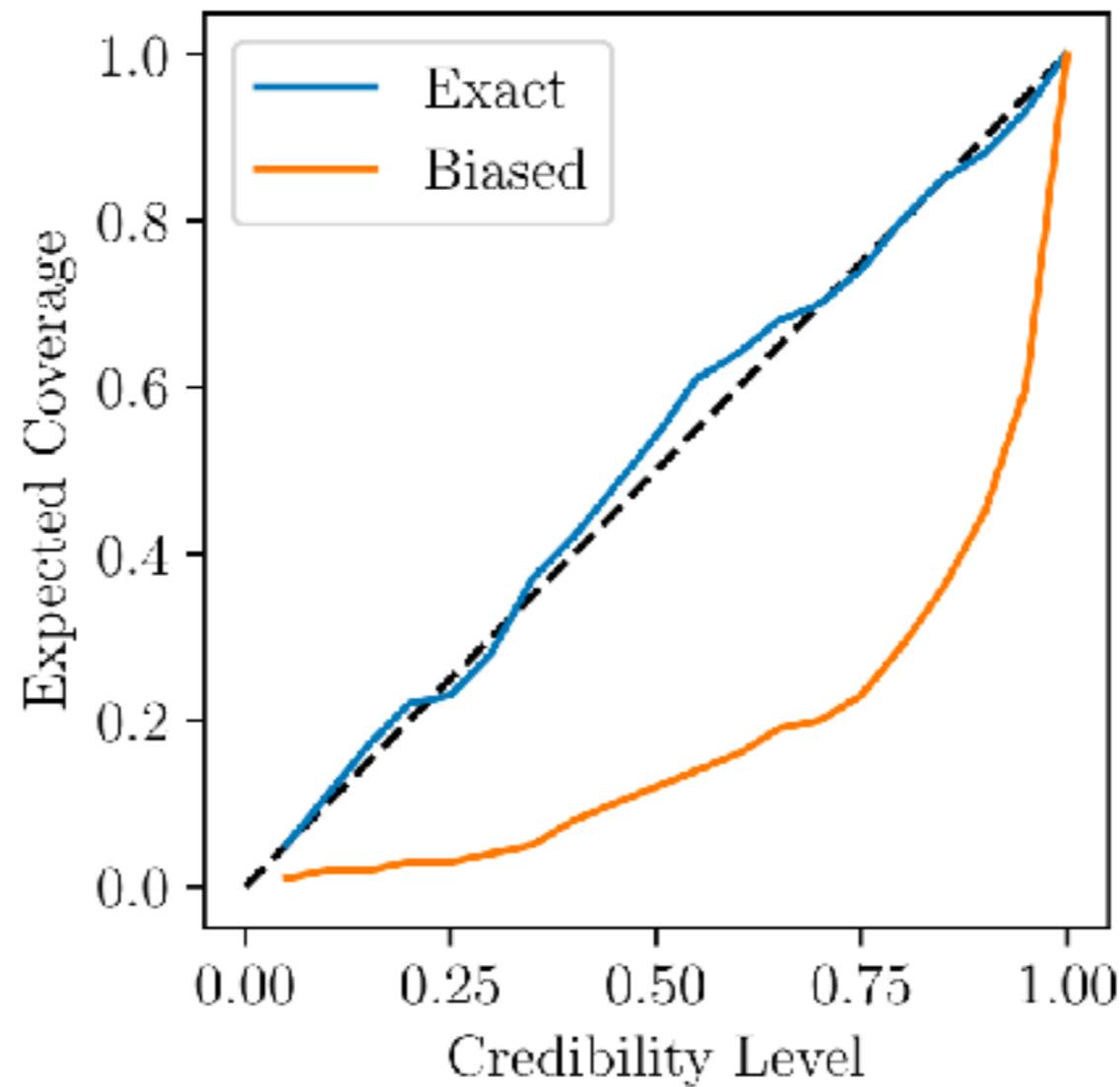
TEST mocks



a single validation mock is not sufficient!

challenges for SBI: how can we trust SBI results?

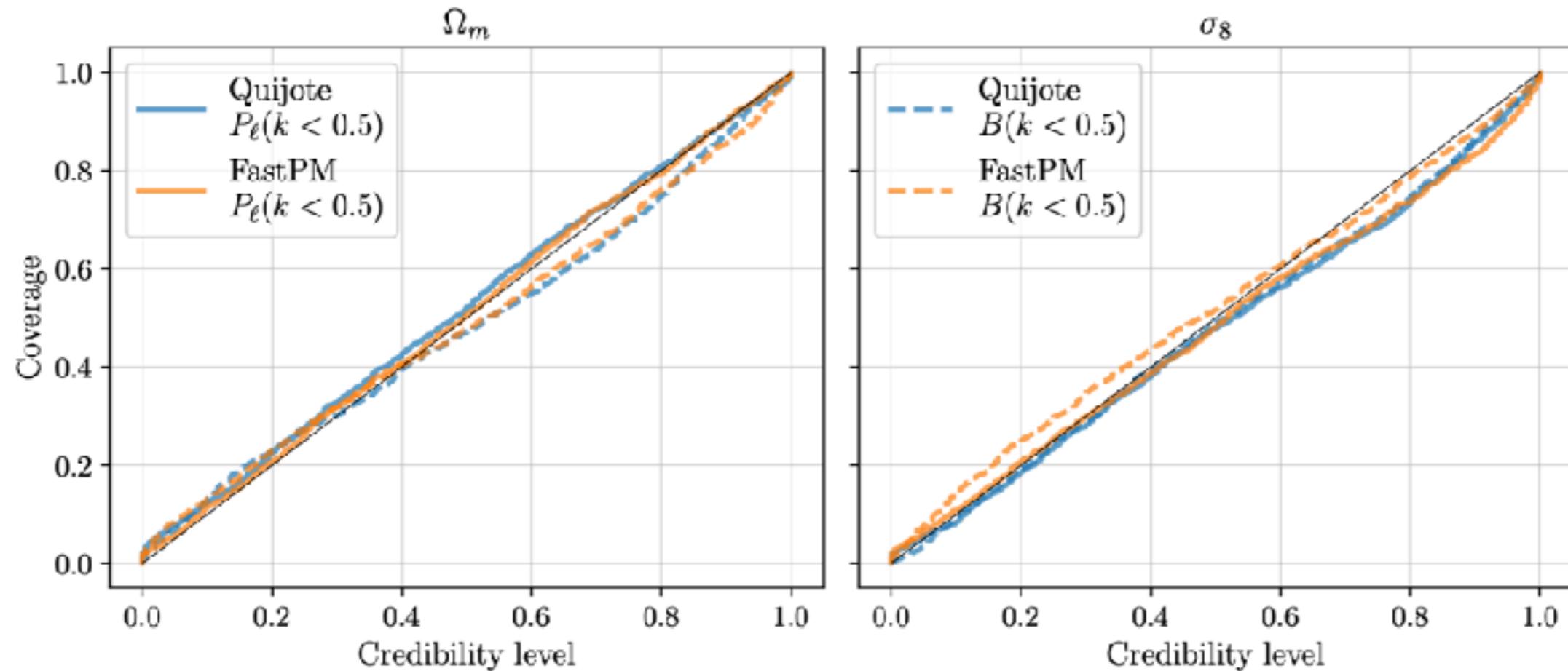
posterior validation



coverage tests — e.g. Lemos et al.(2023); see also Talts et al. (2020)

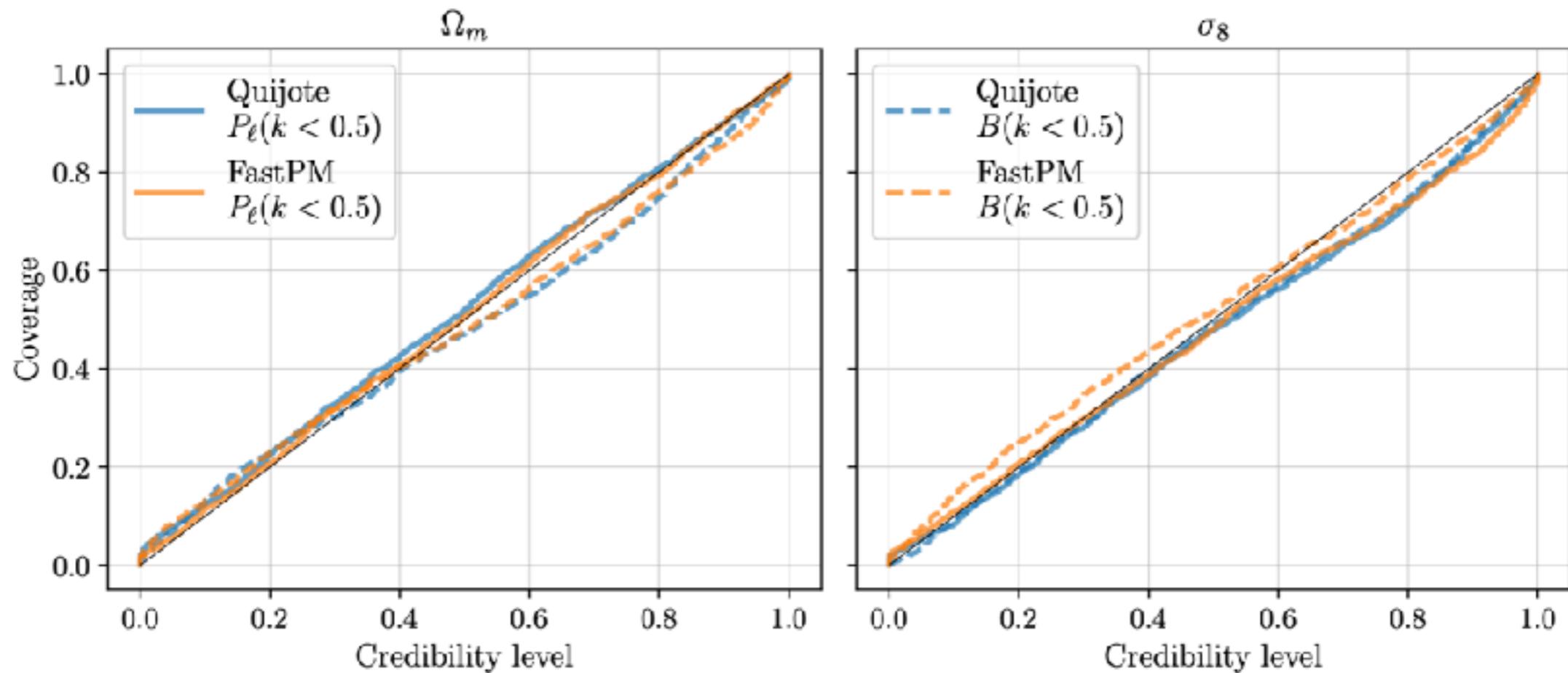
challenges for SBI: how can we trust SBI results?

posterior validation



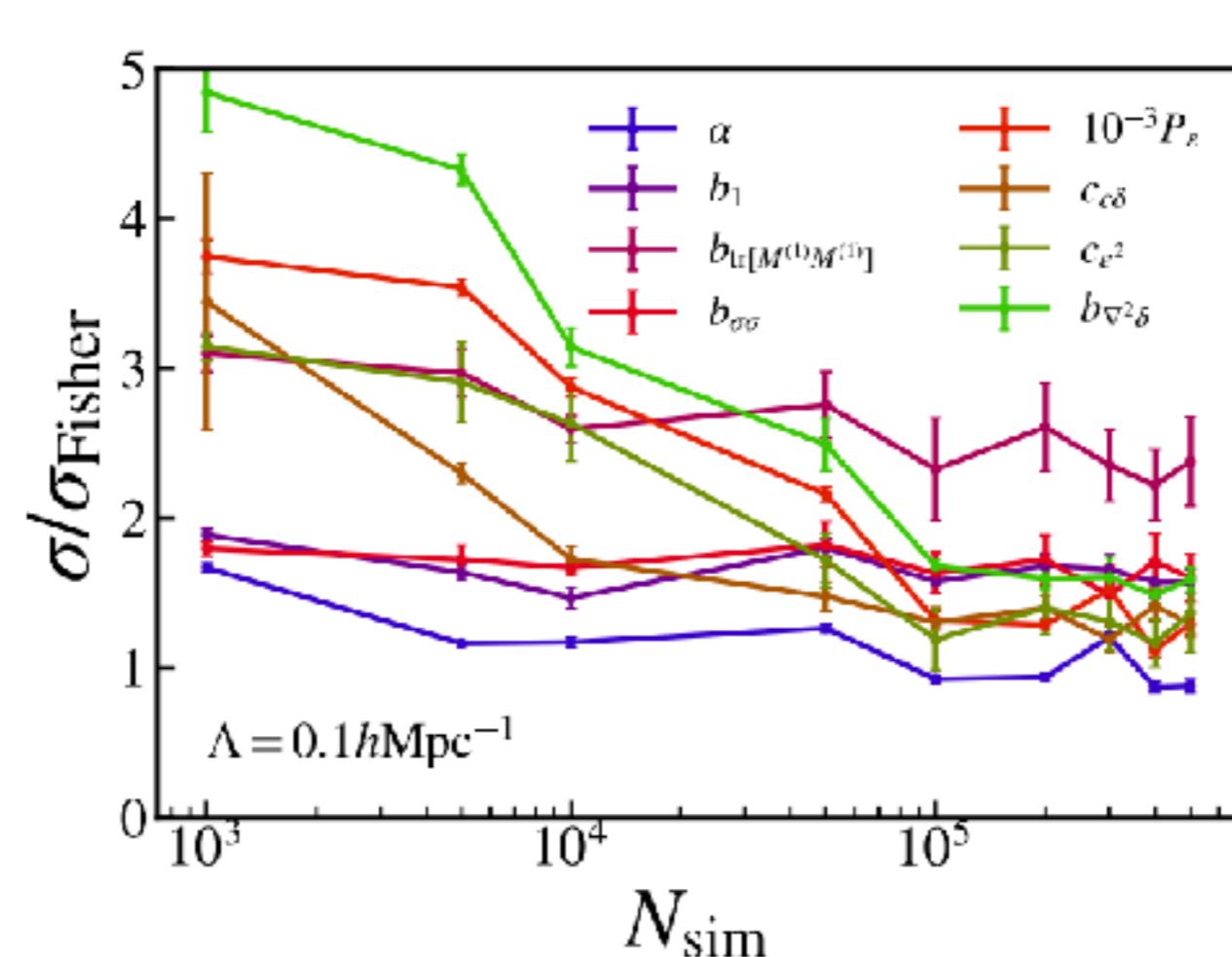
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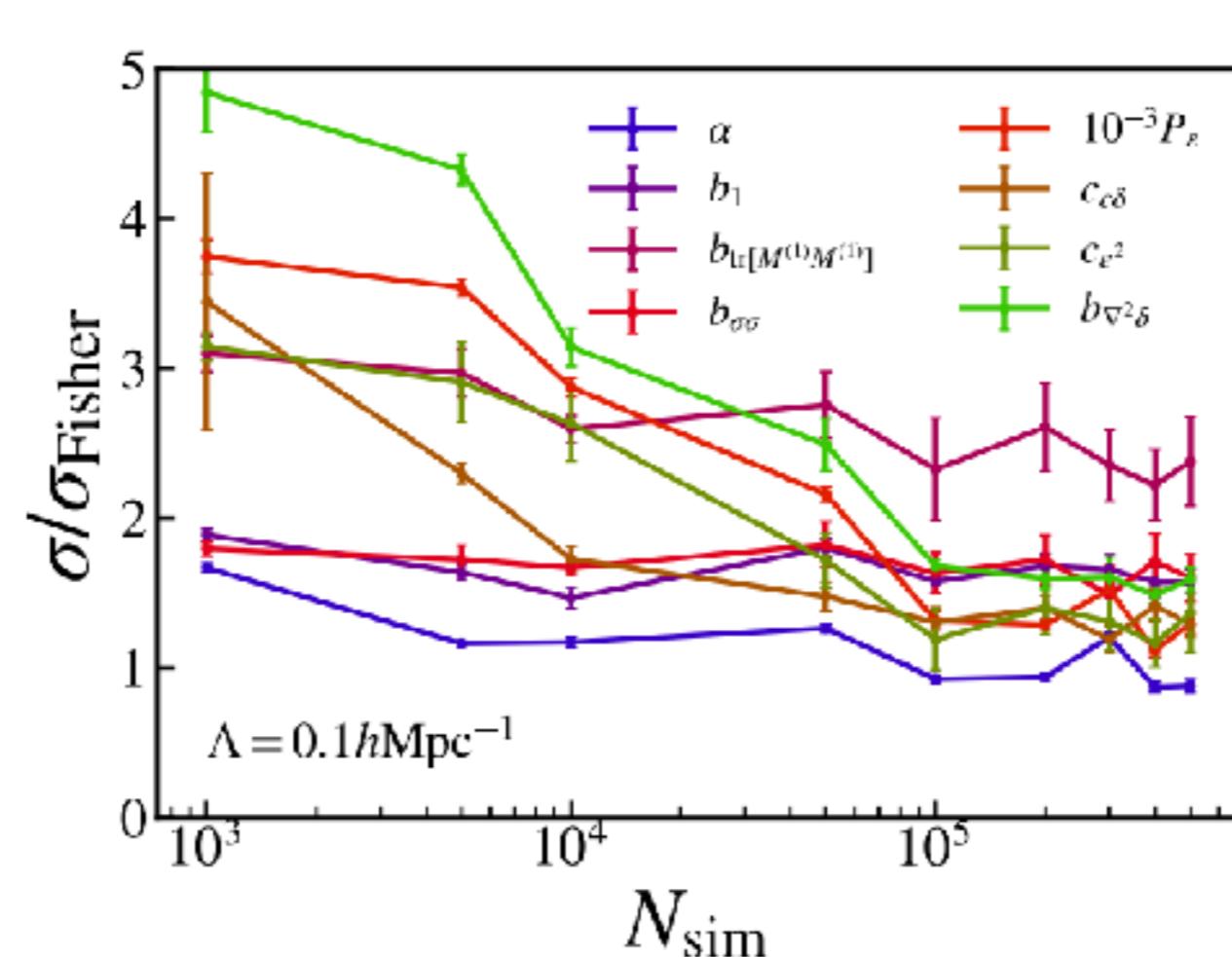


SBI for galaxy clustering is possible with *just* $\sim 2,000$ simulations

caution: “good” coverage doesn’t guarantee “optimal”

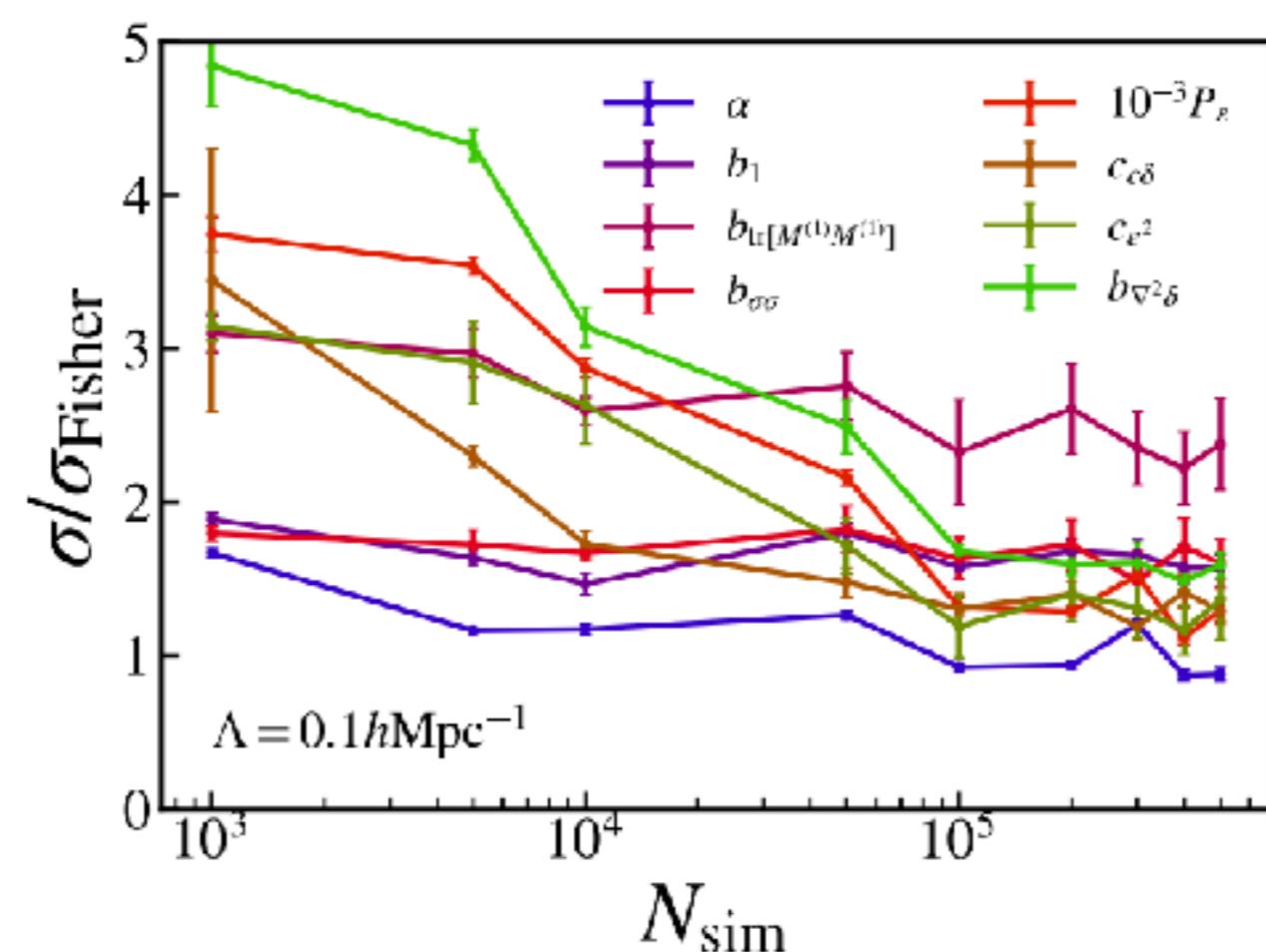


caution: “good” coverage doesn’t guarantee “optimal”



“Il meglio è l'inimico del bene”
“perfect is the enemy of good”

caution: “good” coverage doesn’t guarantee “optimal”

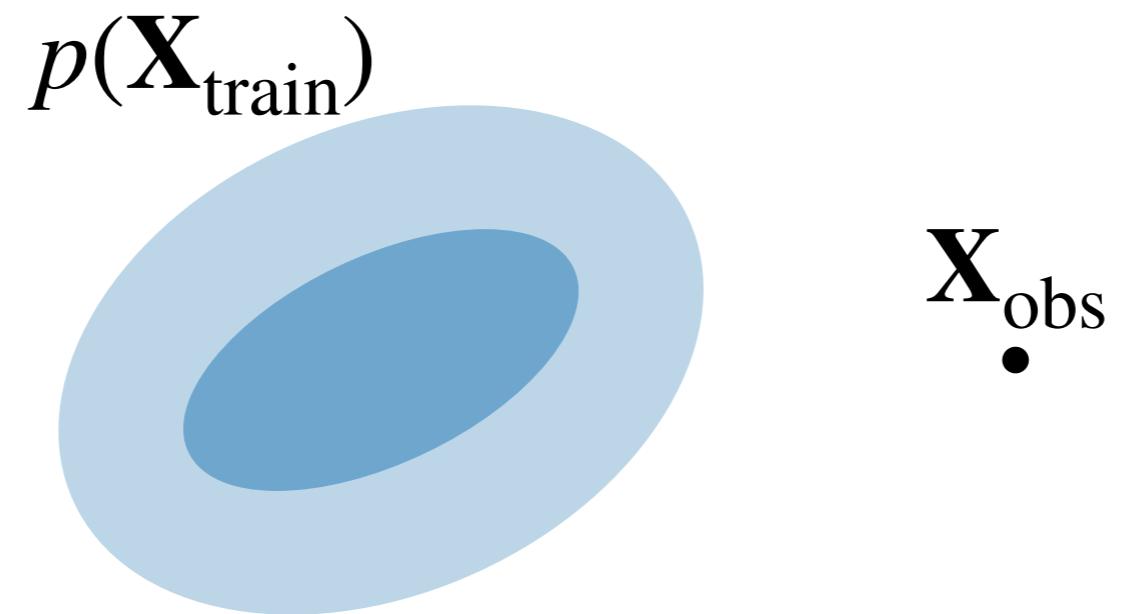


“Il meglio è l'inimico del bene”
“perfect is the enemy of good”
Friday discussion: **Field-level vs Summaries**

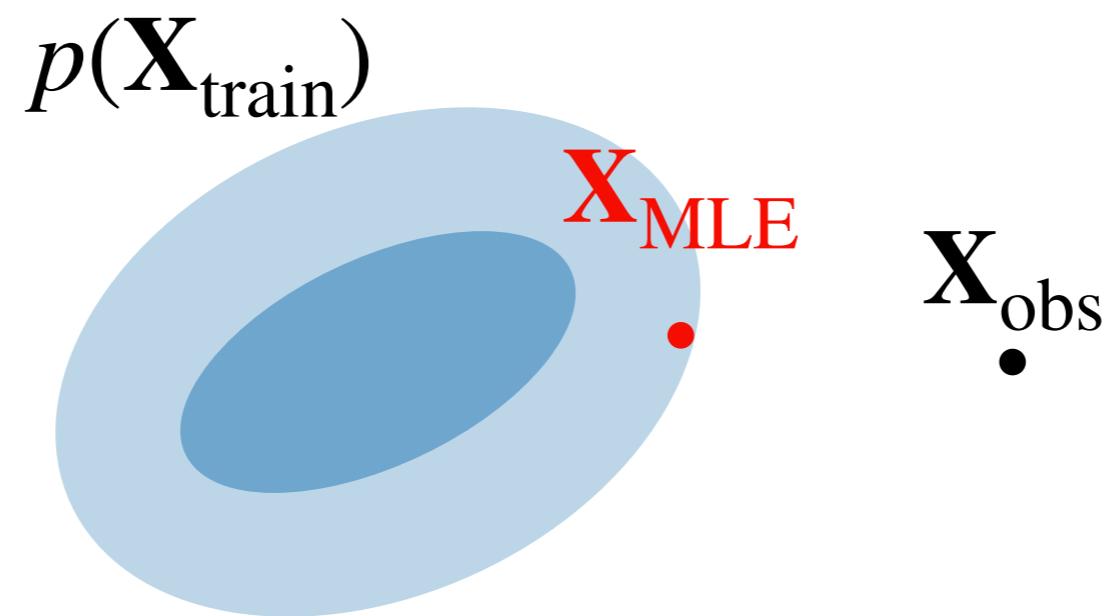
challenges for SBI: how can we trust SBI results?

model misspecification

model misspecification is a *concern for everyone* not just SBI



model misspecification is a *concern for everyone* not just SBI



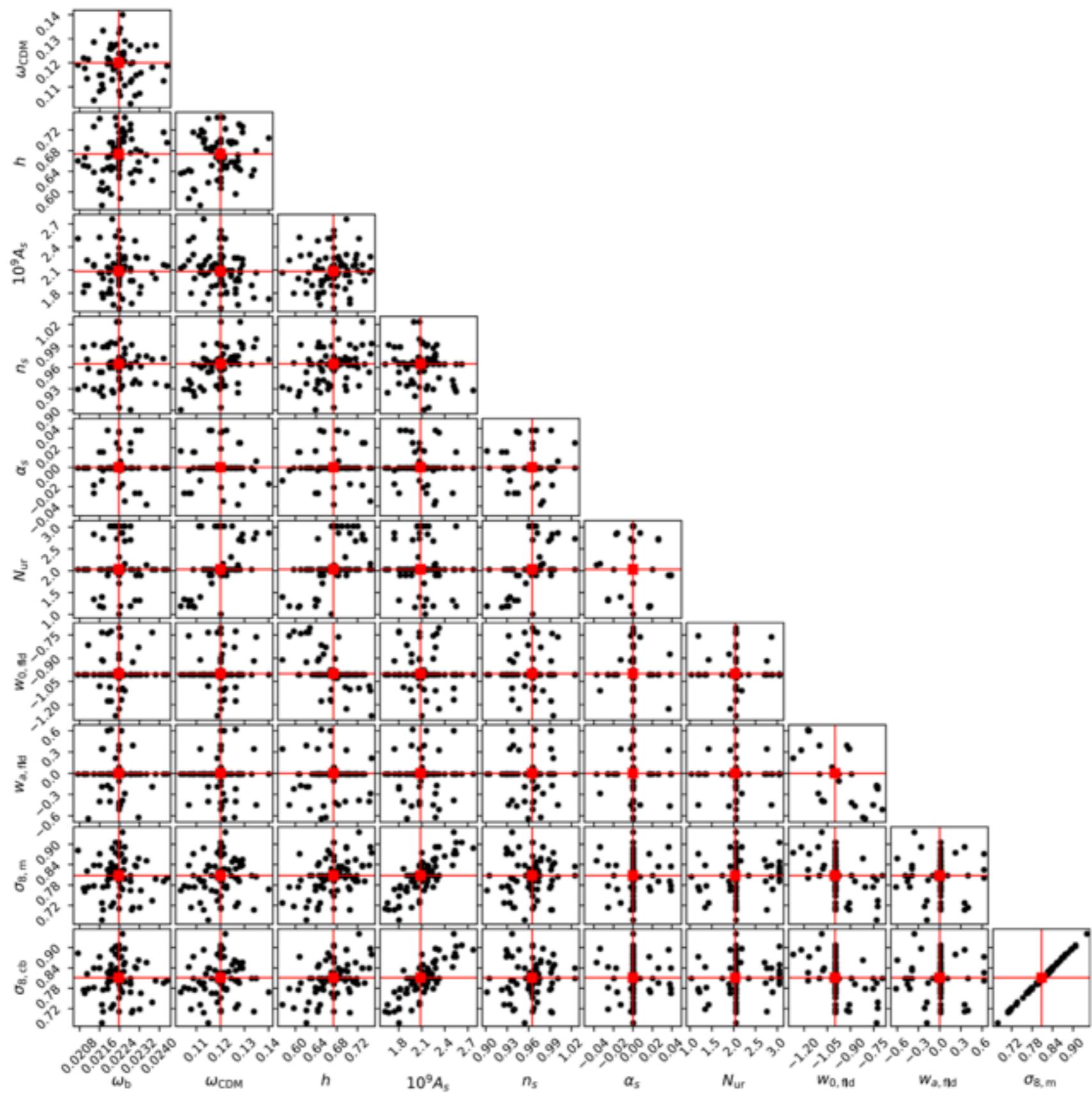
model misspecification concerns for “standard” analyses

$$\mathbf{X}' \sim F(\theta') = \mathcal{N}(m(\theta'), \mathbf{C})$$

*lets say the true likelihood is Gaussian

model misspecification concerns for “standard” analyses

$$\mathbf{X}' \sim F(\theta') = \mathcal{N}(m(\theta'), \mathbf{C})$$

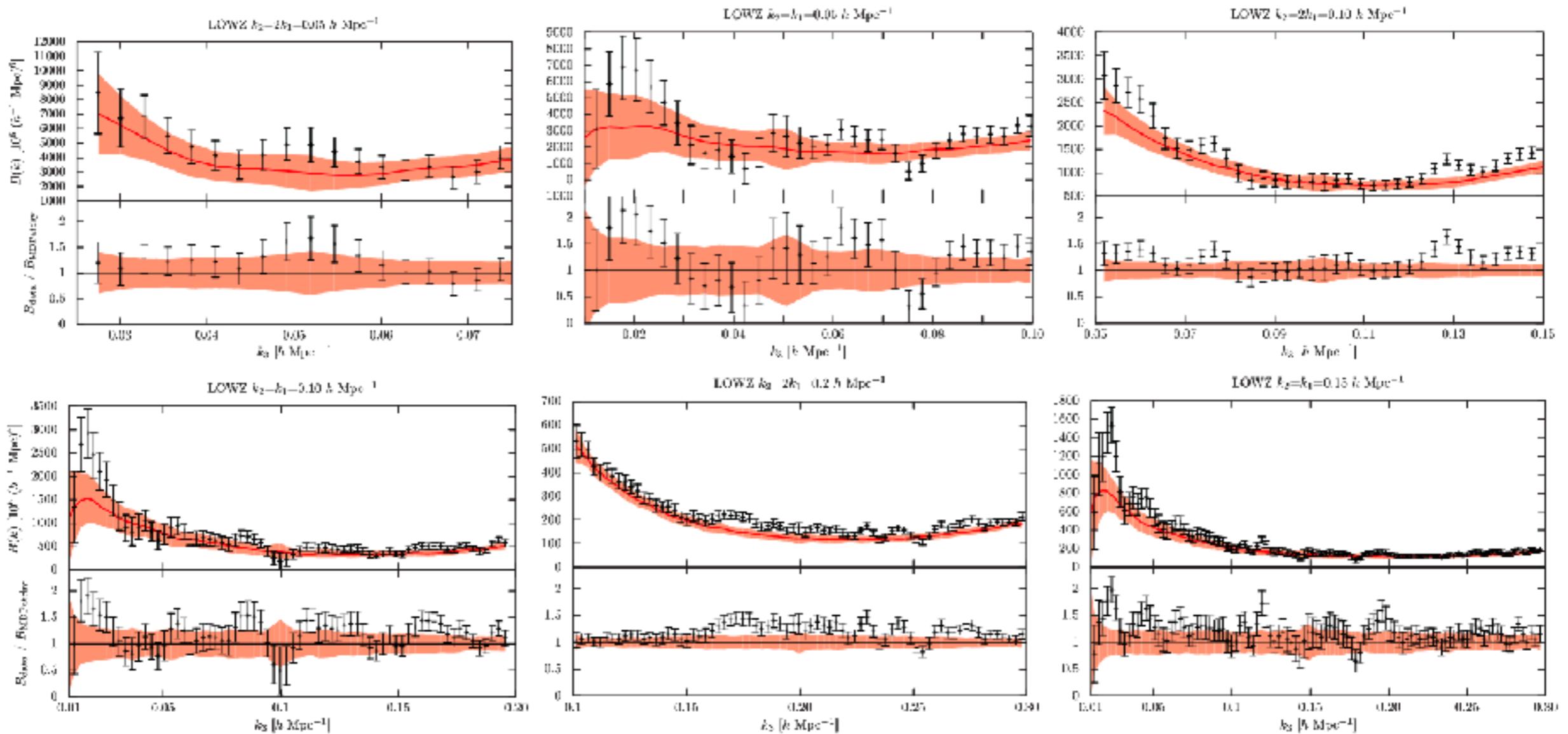


Maksimova et al.(2021); Hector's comment

model misspecification concerns for “standard” analyses

$$\mathbf{X}' \sim F(\theta') = \mathcal{N}(m(\theta'), \mathbf{C})$$

model misspecification concerns for “standard” analyses

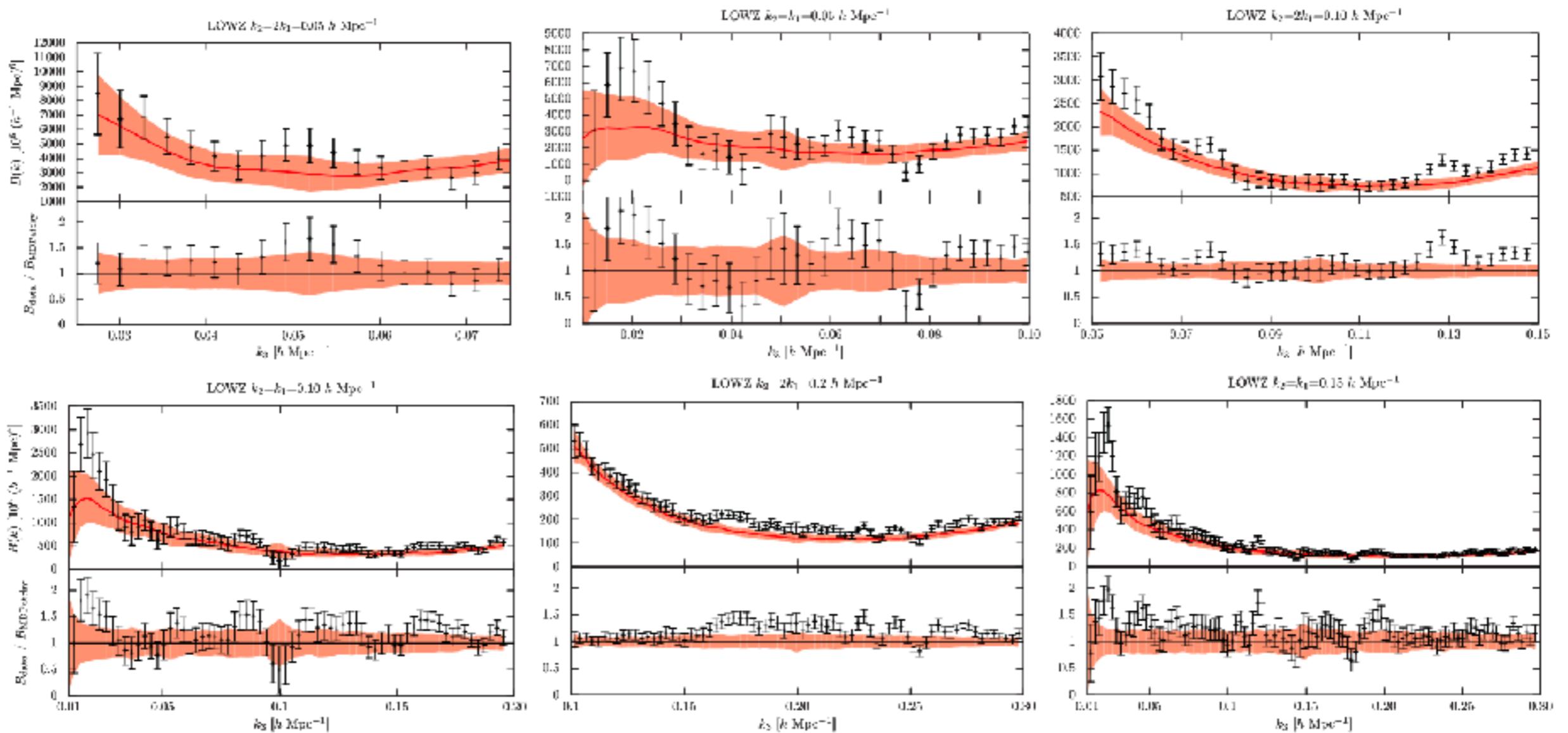


100 PATCHY mocks

BOSS

bispectrum; Kitaura et al. (2016)

model misspecification concerns for “standard” analyses — can we use approximate mocks *designed for 2pt analyses* for beyond 2pt?



model misspecification concerns for “standard” analyses

$$\mathbf{X}' \sim F(\theta') = \mathcal{N}(m(\theta'), \mathbf{C})$$

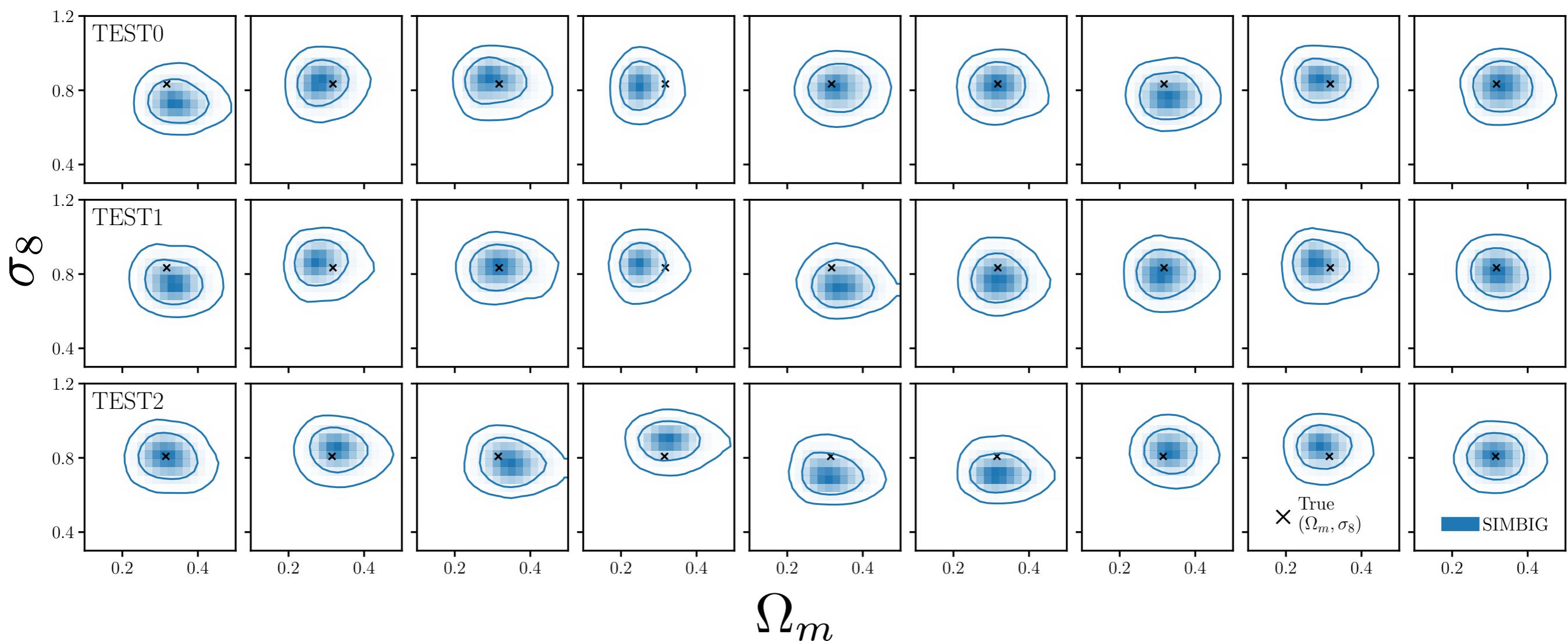
would you trust an SBI analysis with forward model $F(\theta') = \mathcal{N}(m(\theta'), \mathbf{C})$?

tackling model misspecification with *cross-validation*

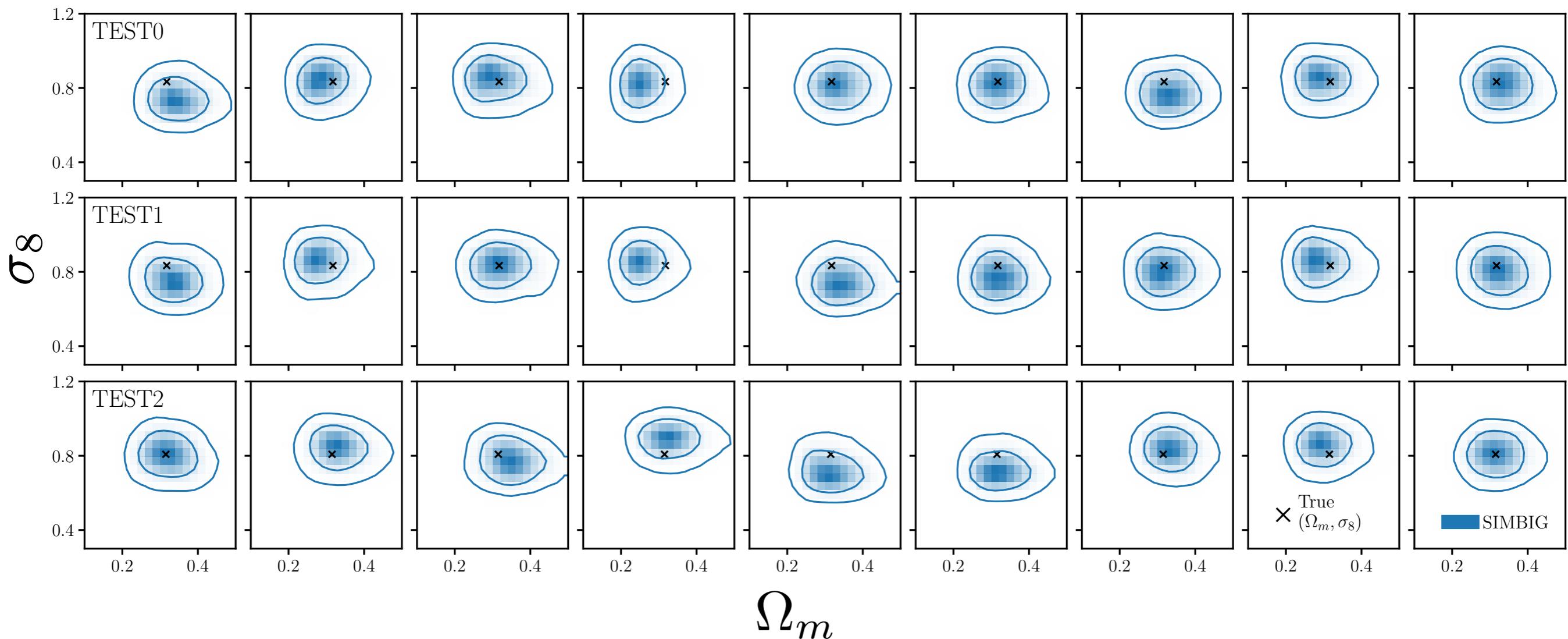
tackling model misspecification with *cross-validation* — SIMBIG:
2,000 simulations with three set of different forward models

	<i>N-body</i>	<i>halo finder</i>	<i>HOD</i>	<i>N_{sim}</i>
<i>TEST0</i>	Quijote	Rockstar	fiducial	500
<i>TEST1</i>	Quijote	FoF	<i>Zheng+</i> (2007)	500
<i>TEST2</i>	AbacusSummit	CompaSO	fiducial	1000

tackling model misspecification with *cross-validation* — SIMBIG:
2,000 simulations with three set of different forward models

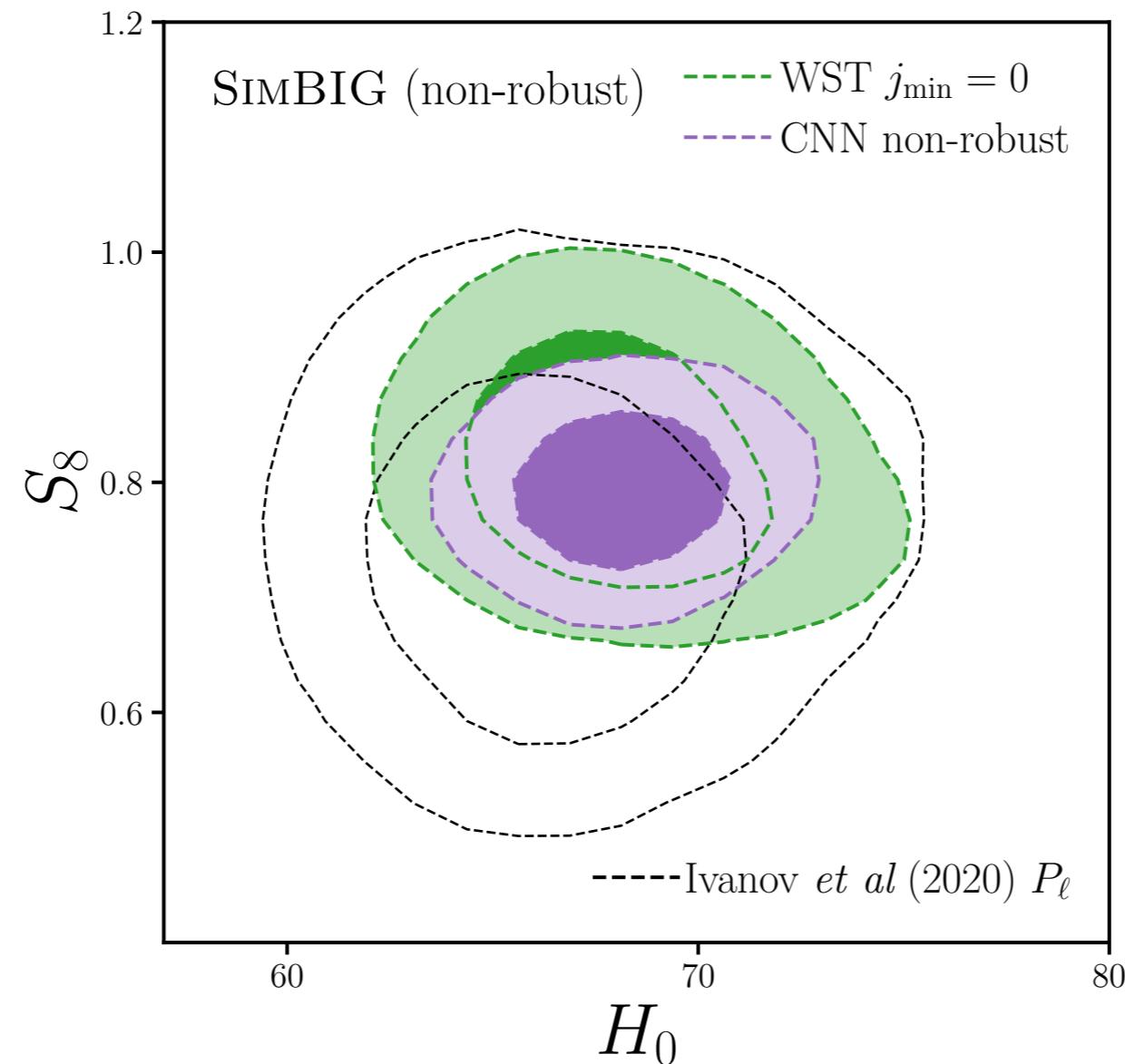


tackling model misspecification with *cross-validation* — SIMBIG:
2,000 simulations with three set of different forward models

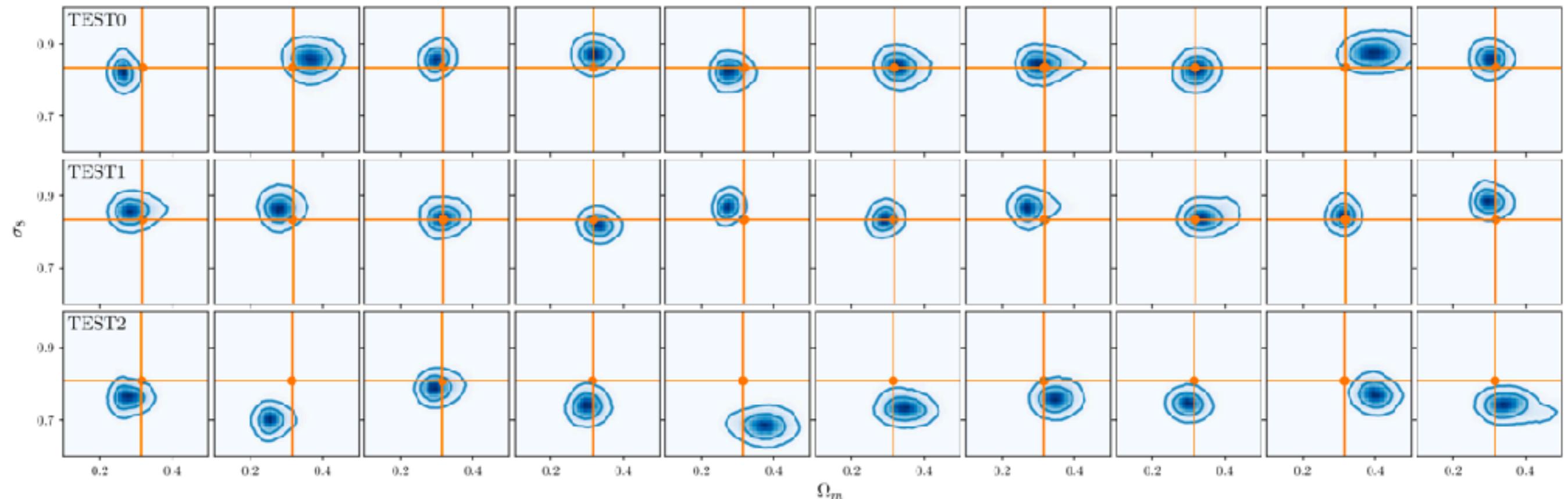


cosmological analyses are only as good as their validation

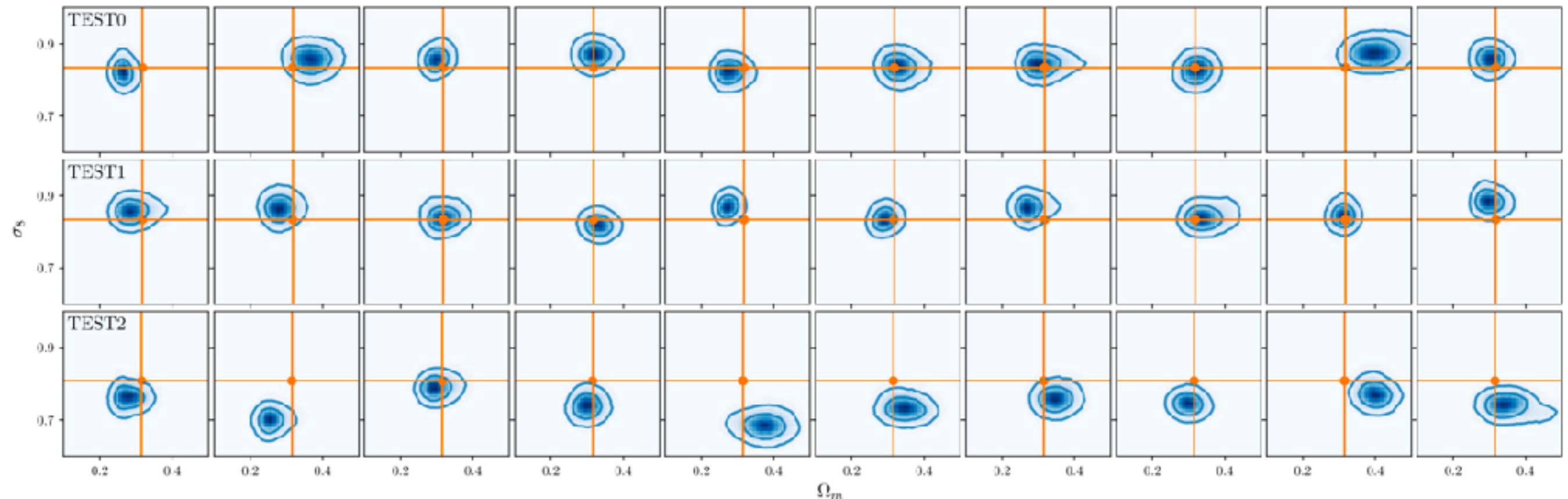
cautionary tale on “optimal observables” — consistency \neq robustness



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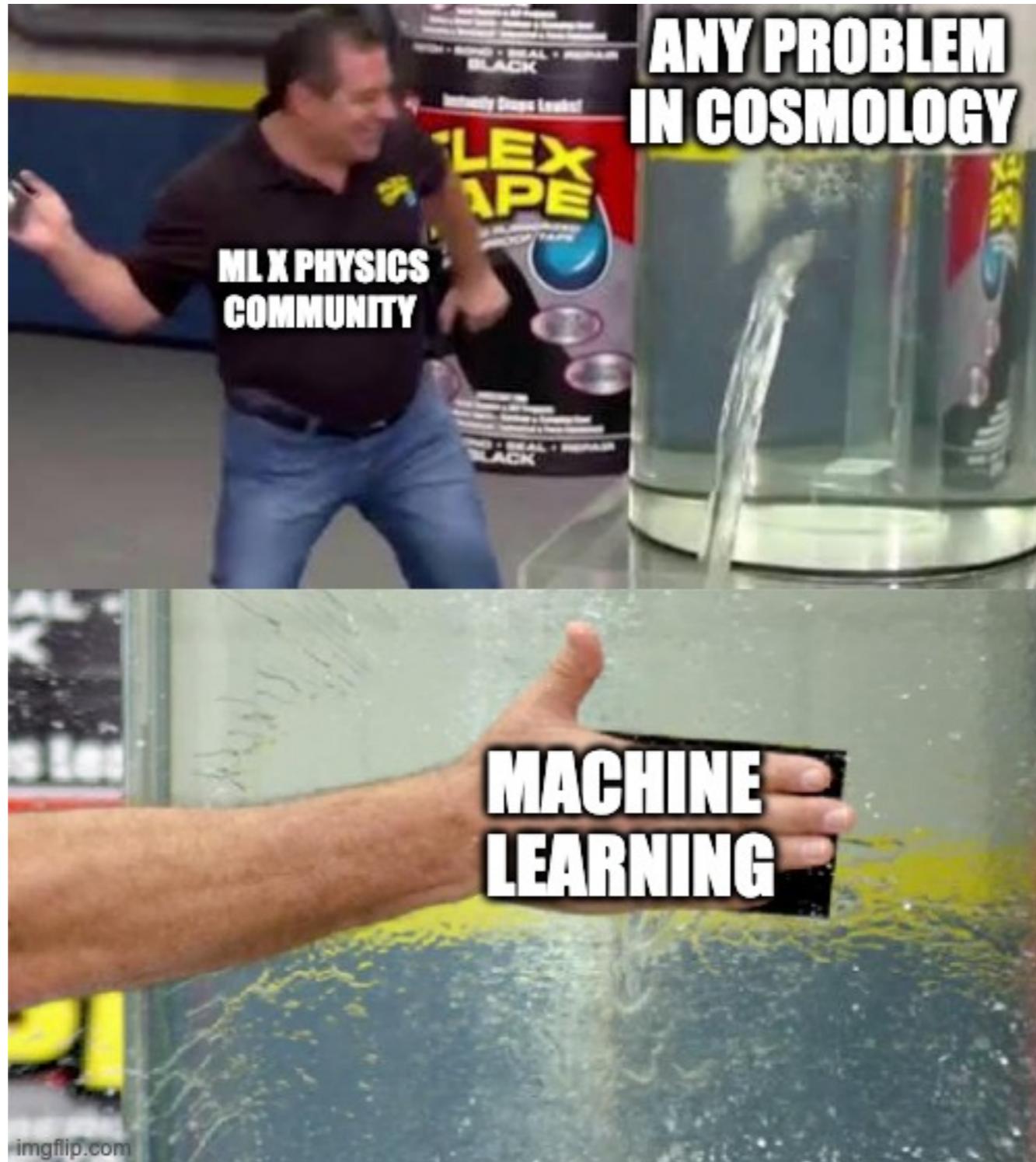
our goal should be optimal **robust** observables

challenges for SBI: how can we trust SBI results?

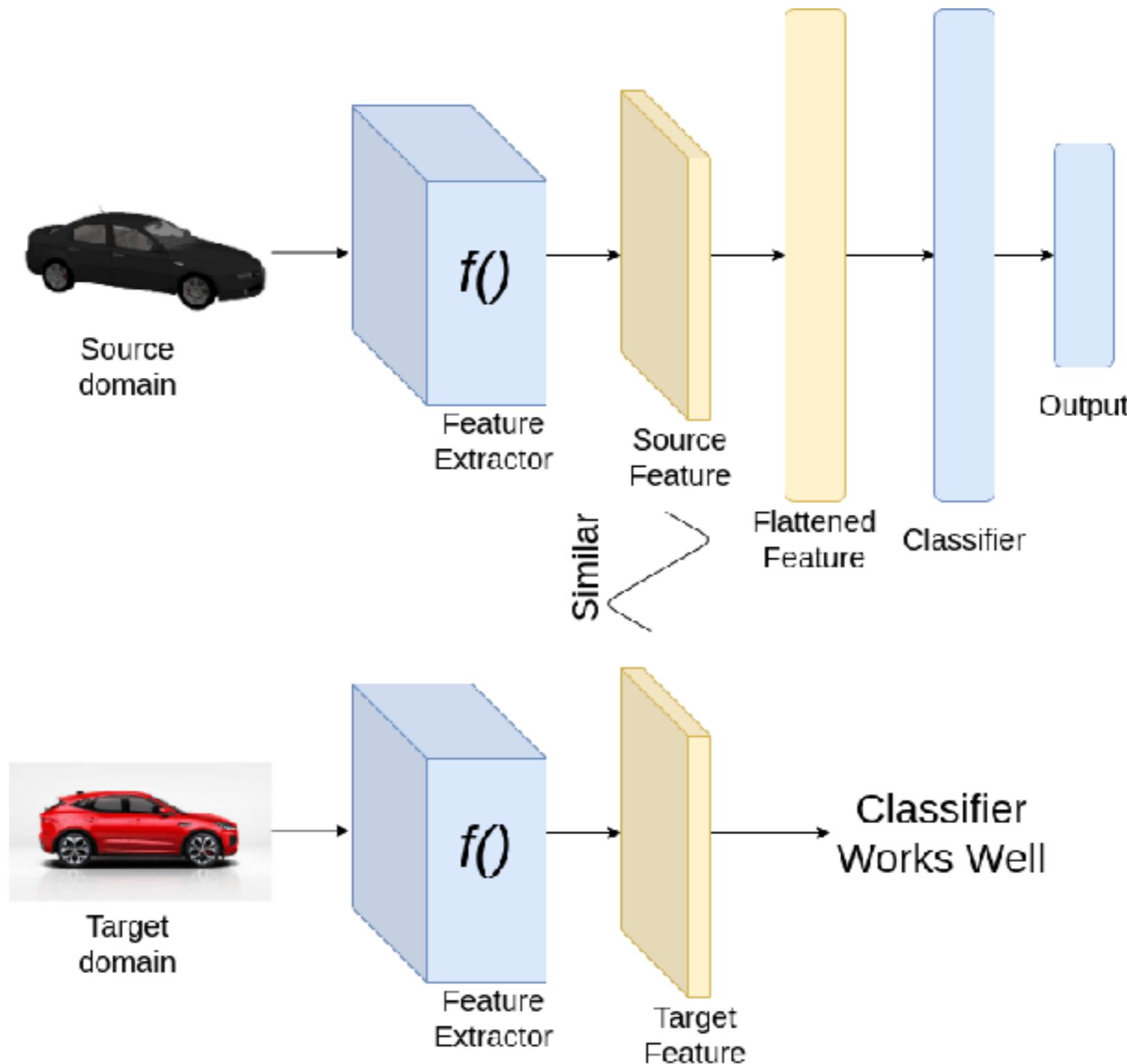
model misspecification

challenges for SBI: how can we trust SBI results?

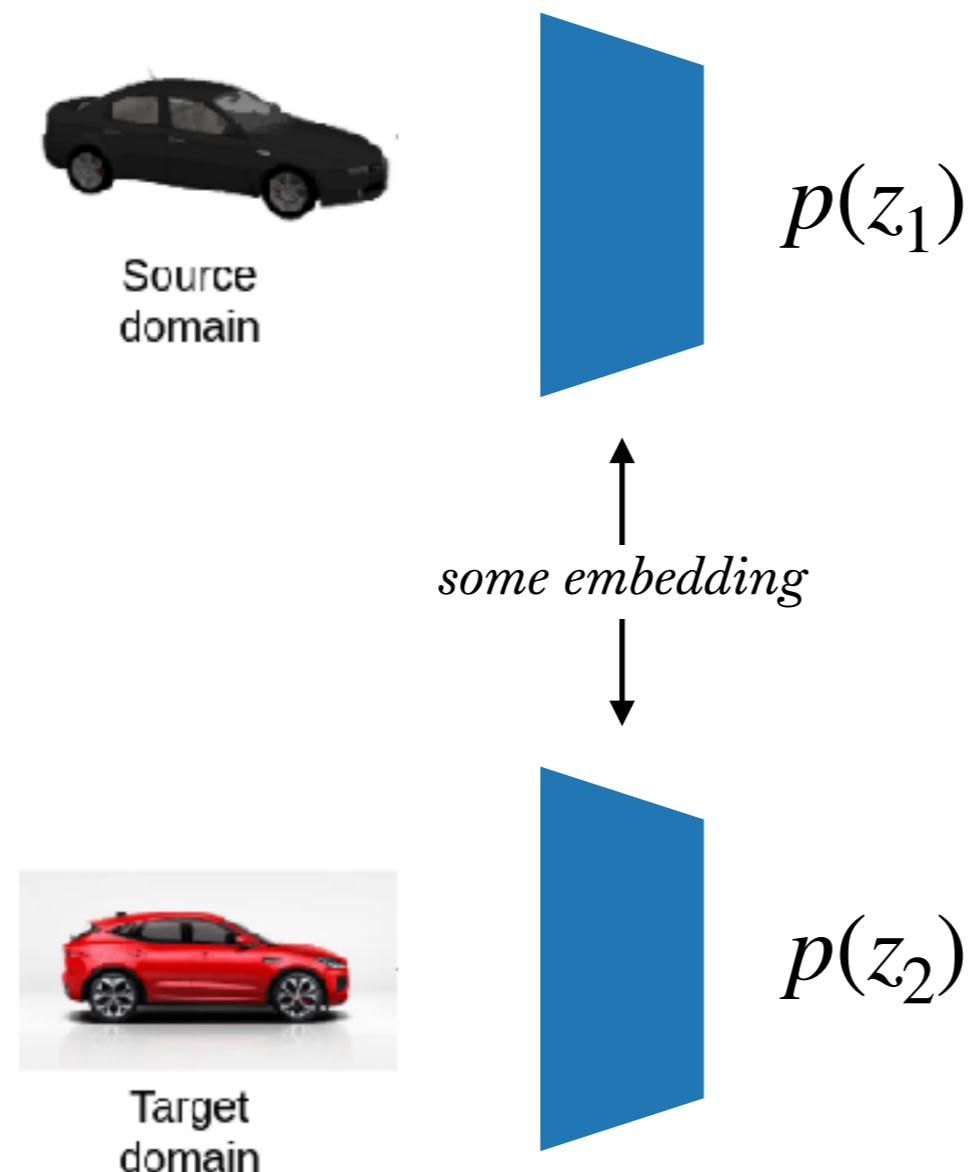
model misspecification



can domain adaptation help us with model misspecification?

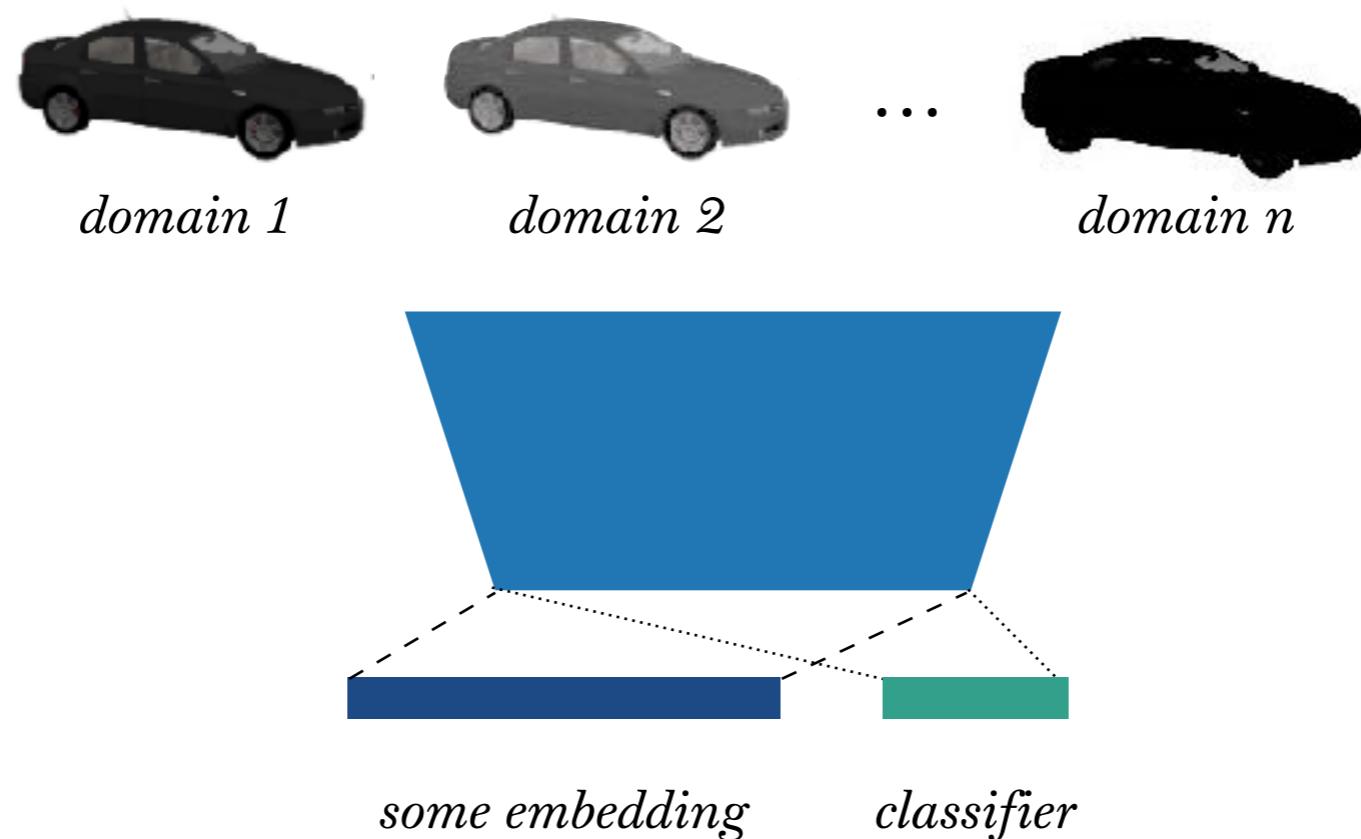


can domain adaptation help us with model misspecification?



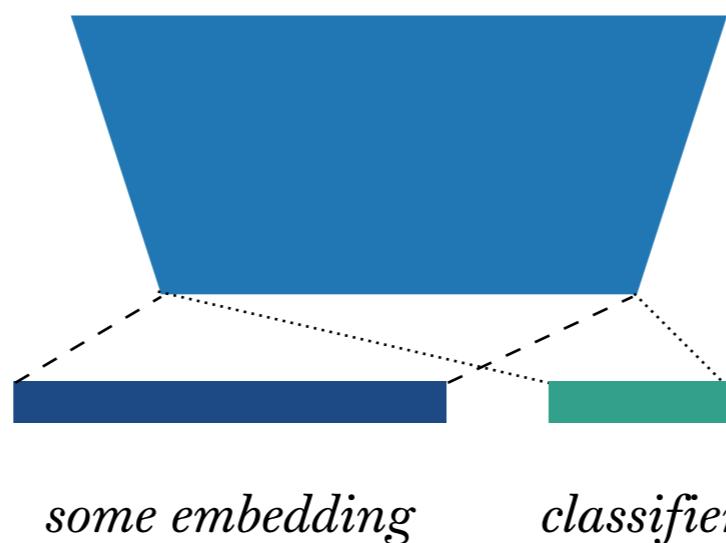
loss penalizes difference between
 $p(z_1)$ and $p(z_2)$ (e.g. MMD)

can **domain adaptation** help us with model misspecification?



$$\text{loss} = \text{MSE} + \text{classifier penalty}$$

can **domain adaptation** help us with model misspecification?



$$\text{loss} = \text{MSE} + \text{classifier penalty}$$

we are all SBI! – just with different assumptions

state-of-the-art SBI provide opportunities to extract information in higher-order and non-linear galaxy clustering — *e.g.* SIMBIG: $1.9 \times$ improvement in S_8

still many challenges:

- scaling up to next-generation surveys (*emulation, hybrid SBI?*)
- posterior validation — accuracy and precision (*coverage plots?*)
- model misspecification (*cross-validation, domain adaptation?*)