Implicit Likelihood Inference

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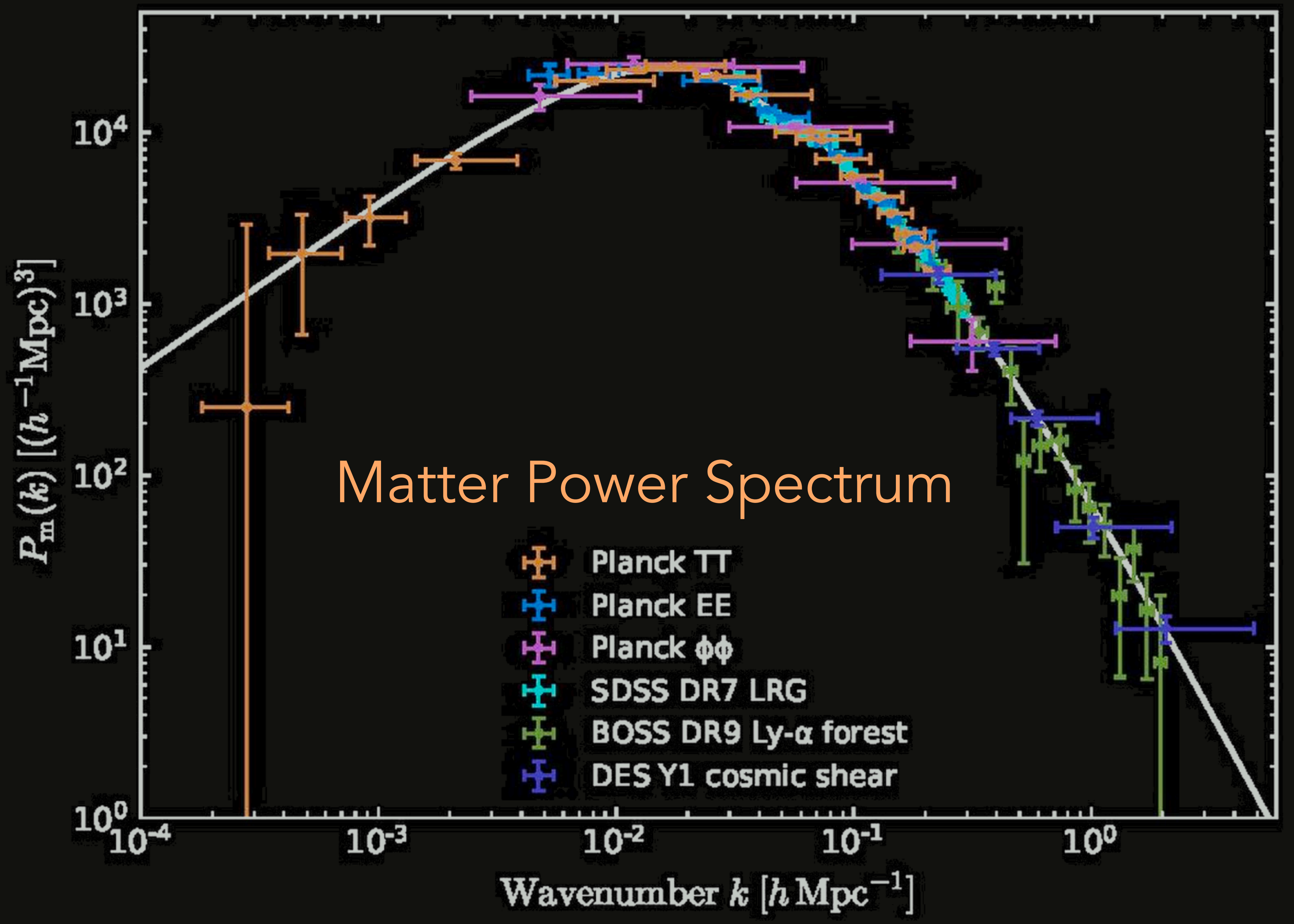
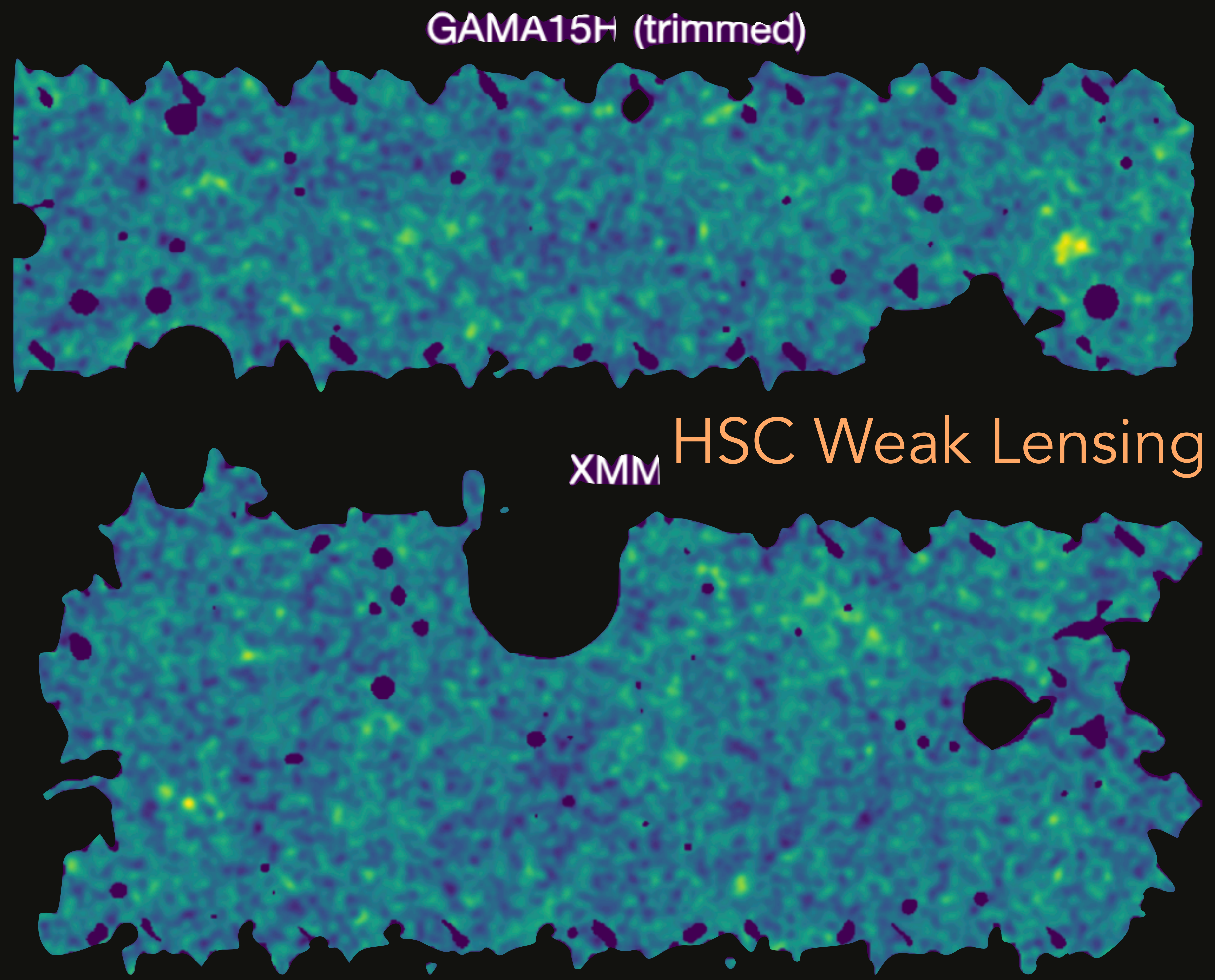
A3Net Seoul, 8/22/2025

Outline

Why should nature have conspired to put all information into the (quasi-)linear modes we happen to be able to describe with perturbation theory?

Accessing the information in non-linear regime typically requires simulation-based methods.





HSC Weak Lensing Mass Maps

Outline

Implicit Likelihood Inference: A tool to solve inverse problems which are implicitly defined through simulations, typically using deep neural networks

1. Motivation & Overview of Methods

2. Example application

3. Challenges & next steps

Bayesian inference

$$\underbrace{\boxed{P(\text{parameters} \mid \text{data})}}_{\text{posterior}} = \frac{\overbrace{\boxed{P(\text{data} \mid \text{parameters})}}^{\text{likelihood}} \; \overbrace{\boxed{P(\text{parameters})}}^{\text{prior}}}{\underbrace{\boxed{P(\text{data})}}_{\text{evidence}}}$$

Bayesian inference

More concretely:

θ=interesting parameters, η=nuisance parameters, ζ=initial conditions,

x=data, m=model:

$$P(x \mid \theta) = \int D\eta\, D\zeta\, \delta[\, x - m(\theta, \eta, \zeta)\,]$$

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initial conditions $\zeta \sim P(\zeta)$,
e.g. quantum fluctuations

nuisance parameters $\eta \sim P(\eta)$,
e.g. star formation model

parameters $\theta \sim P(\theta)$,
e.g. Ω_m

observable data x,
e.g. catalog of galaxies

physical process $m(\theta, \eta, \zeta)$

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Traditional case:

$$P(x \mid \theta) = \int D\eta \; \mathrm{Gaussian}[\, x - \mu(\theta, \eta), \Sigma \,]$$

[do remaining low-dimensional η-integral with Monte Carlo]

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Traditional case:

$$P(x \mid \theta) = \int D\eta\, \mathrm{Gaussian}[\, x - \mu(\theta, \eta), \Sigma\,]$$

But what do we do if the Gaussian approximation doesn't hold?

→ assume we have simulator that evaluates m(θ, η, ζ) accurately

Neural Implicit Likelihood Inference (ILI)

neural likelihood estimation (NLE)

neural posterior estimation (NPE)

$$P(\text{parameters}\,|\,\text{data}) = \frac{P(\text{data}\,|\,\text{parameters}) \quad P(\text{parameters})}{P(\text{data})}$$

neural ratio estimation (NRE)

We are given parameter vectors θ and simulated data vectors x.

Problem is to approximate one of the above probability distributions.

How can we map these tasks to optimization problems solvable with neural networks?

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neural likelihood estimation (NLE) neural posterior estimation (NPE)

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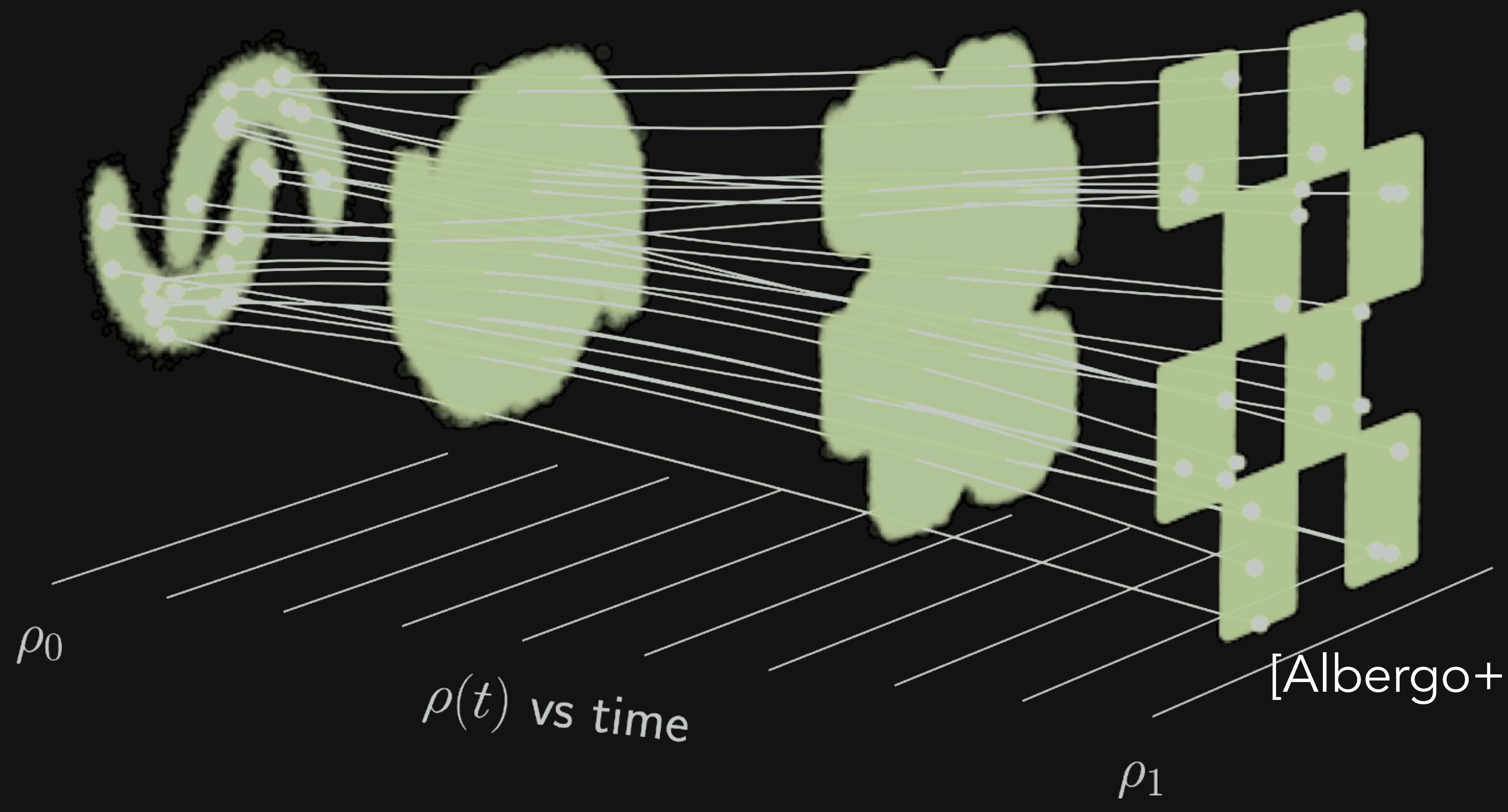
neural ratio estimation (NRE)

neural likelihood estimation (NLE):
conditioned normalizing flow q(x|θ)

neural posterior estimation (NPE):
conditioned normalizing flow q(θ|x)

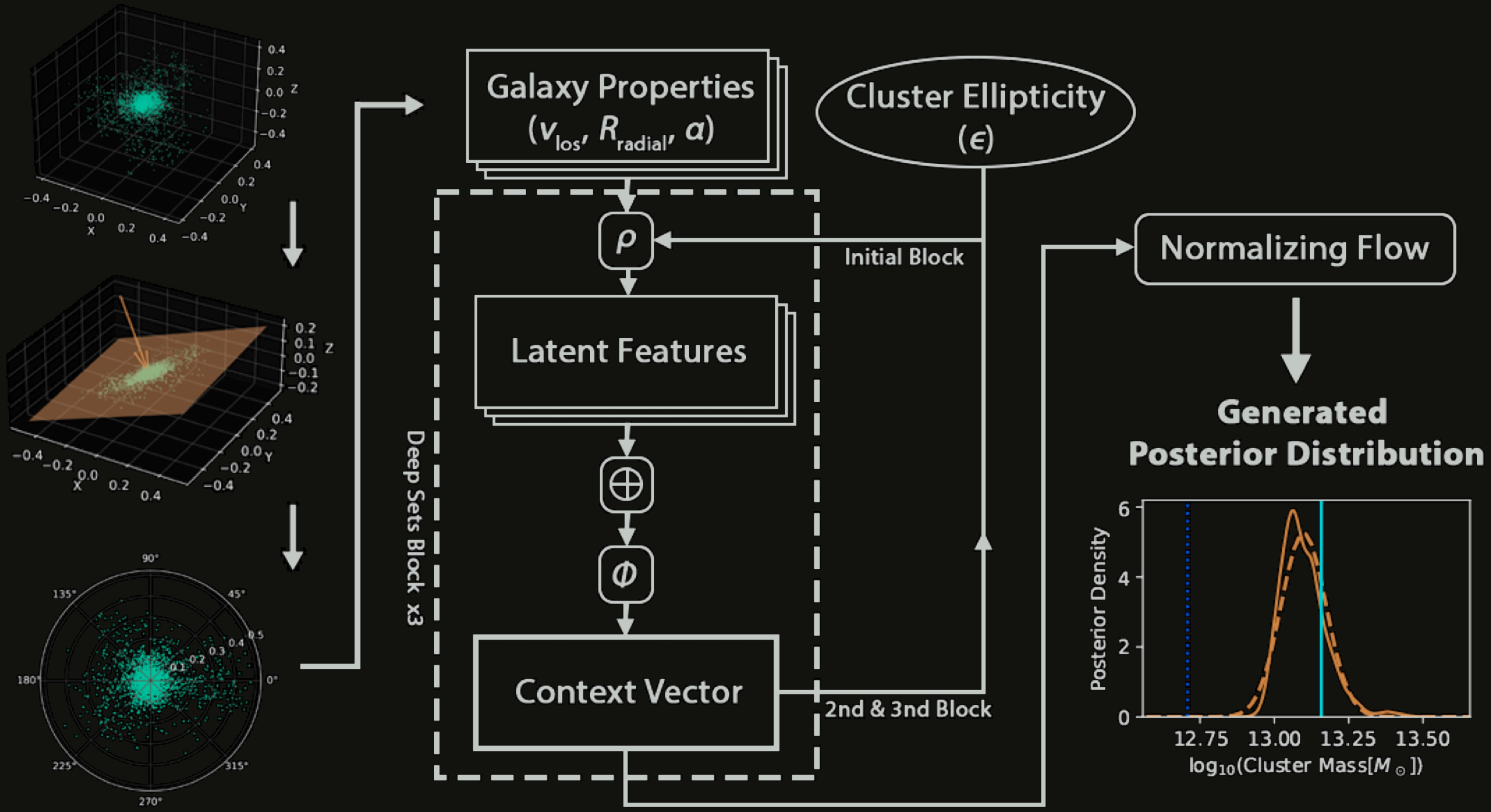
neural ratio estimation (NRE):
classifier between (x, θ) ~p(x, θ) and ~p(x)p(θ)



[Albergo+2023]

Practicality: data size & structure

Usually, data vectors too high dimensional or live in awkward spaces
→ We deal with this by constructing a useful latent representation through *embedding networks*



[B.Y.Wang & LT 2025]

Neural Implicit Likelihood Inference (ILI)

- *in the limit*, any likelihood learnable
- any simulate-able effect can be incorporated
- no formal difference between nuisance parameters and initial conditions
- primary choice at the moment:
  - NPE: empirically good performance, need to deal with flow
  - NRE: classification → super flexible, empirically more tuning required

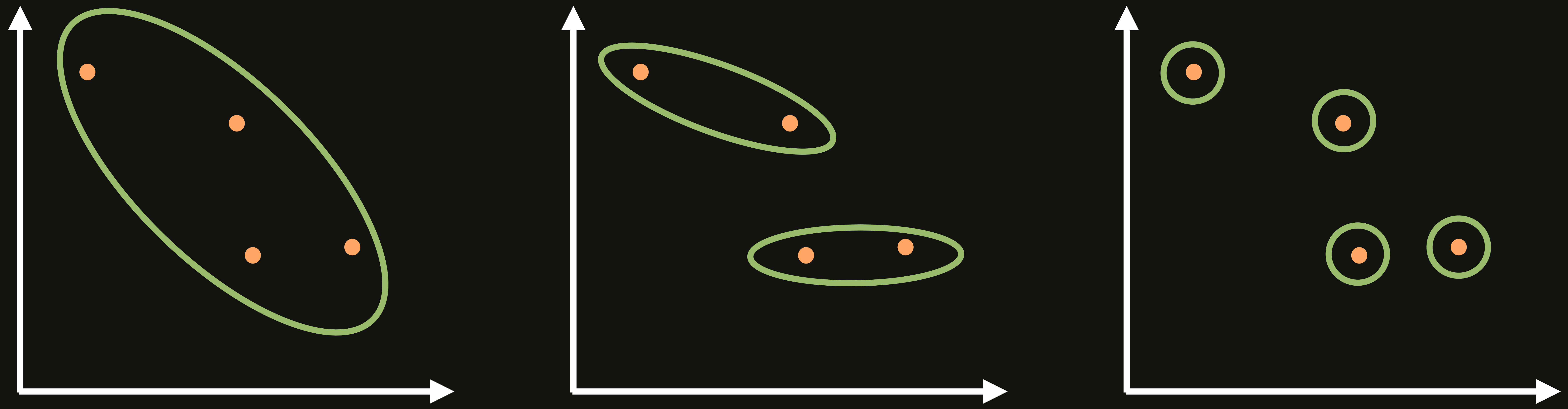
Curse of dimensionality

Let's say: 200,000 simulations, 10 model parameters, 10 data points
→ this is optimistic!

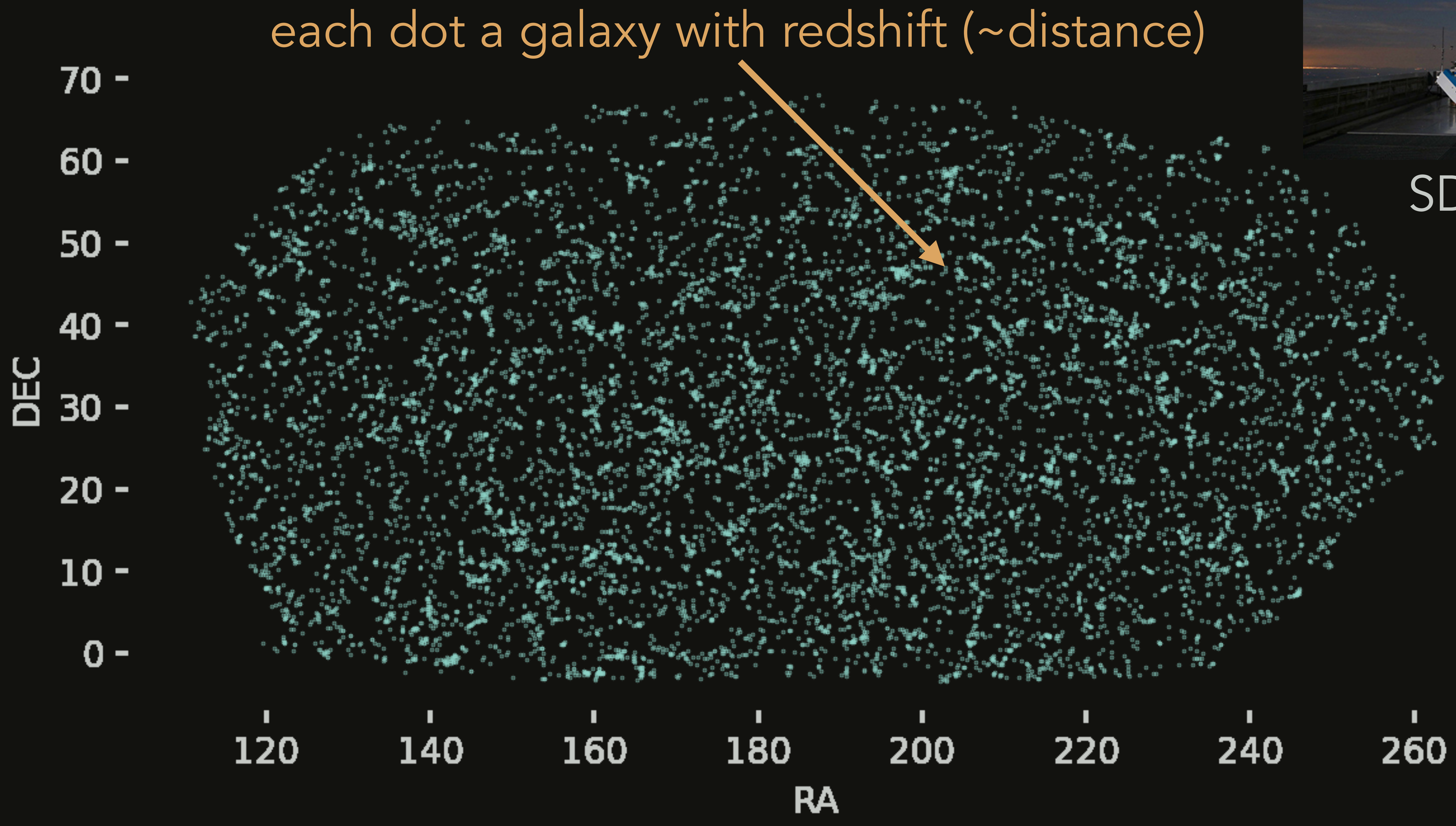
We're trying to learn a density in this 10+10 dimensional space

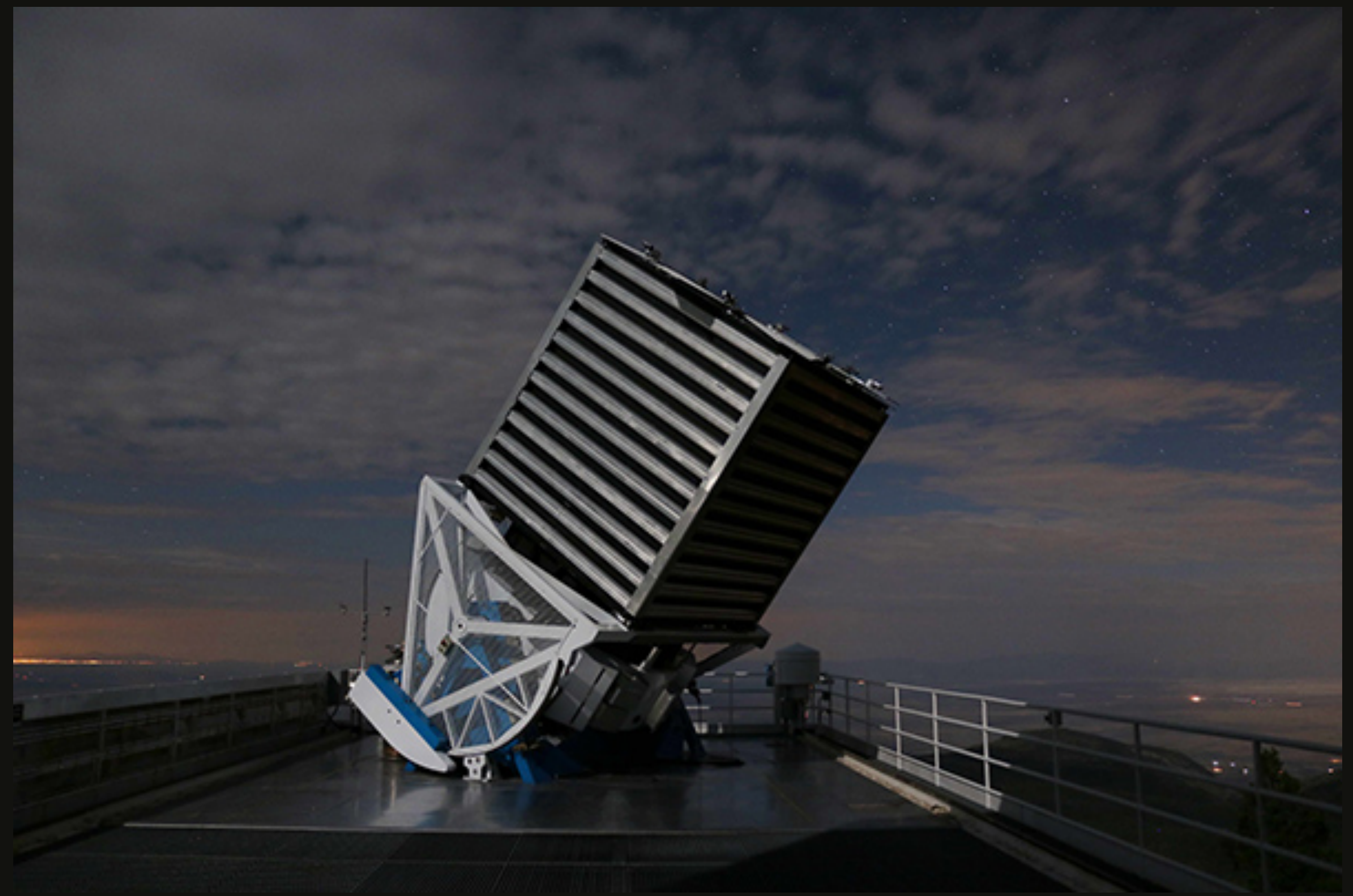
$$(200{,}000)^{1\,/\,(10\,+\,10)} = 1.8, \text{ let's say } 2$$

What is the implicit prior?



A 3-D Map of the Universe





SDSS/BOSS survey

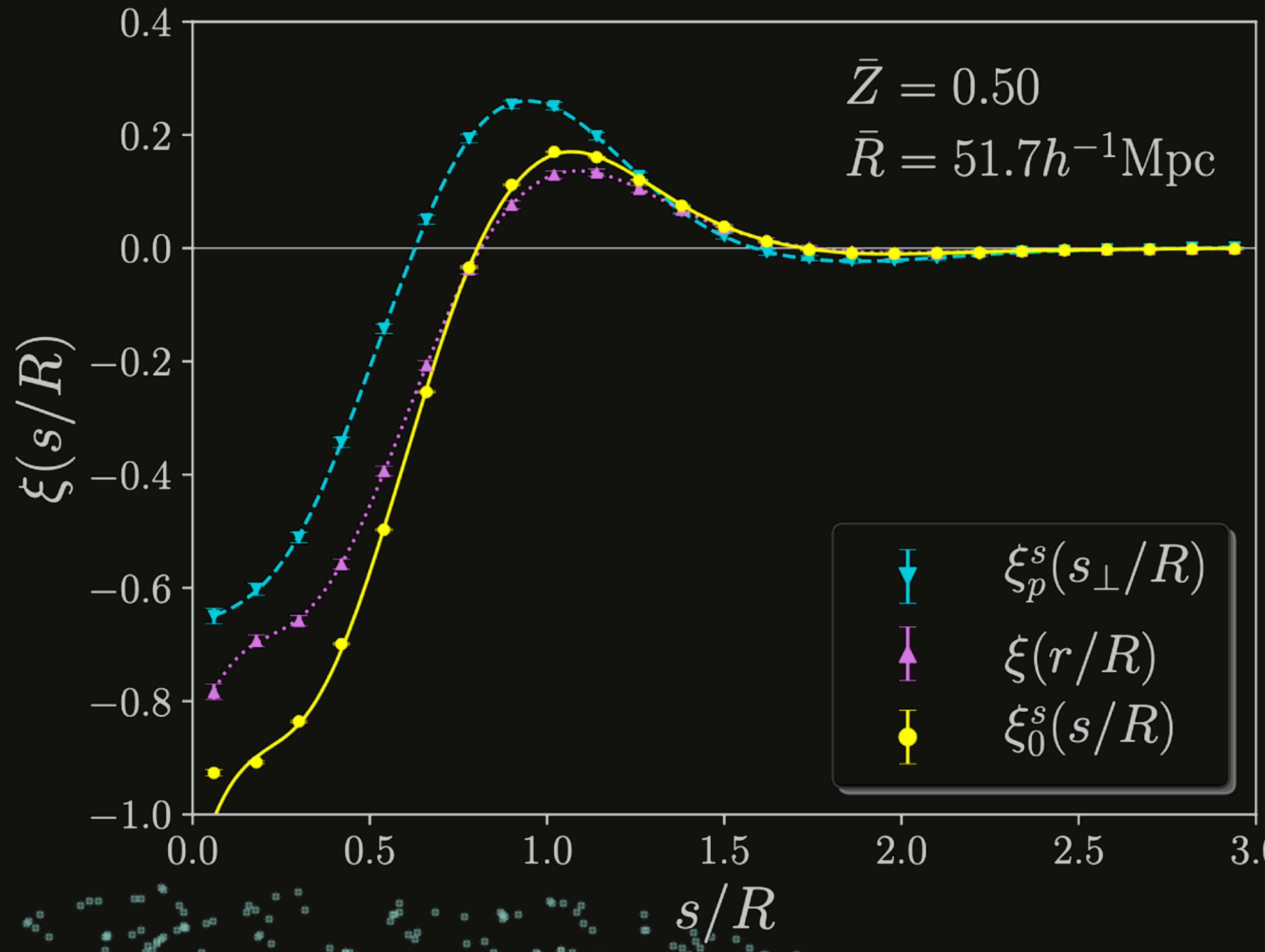
How to summarize this map?

1) pairs of galaxies (power spectrum)

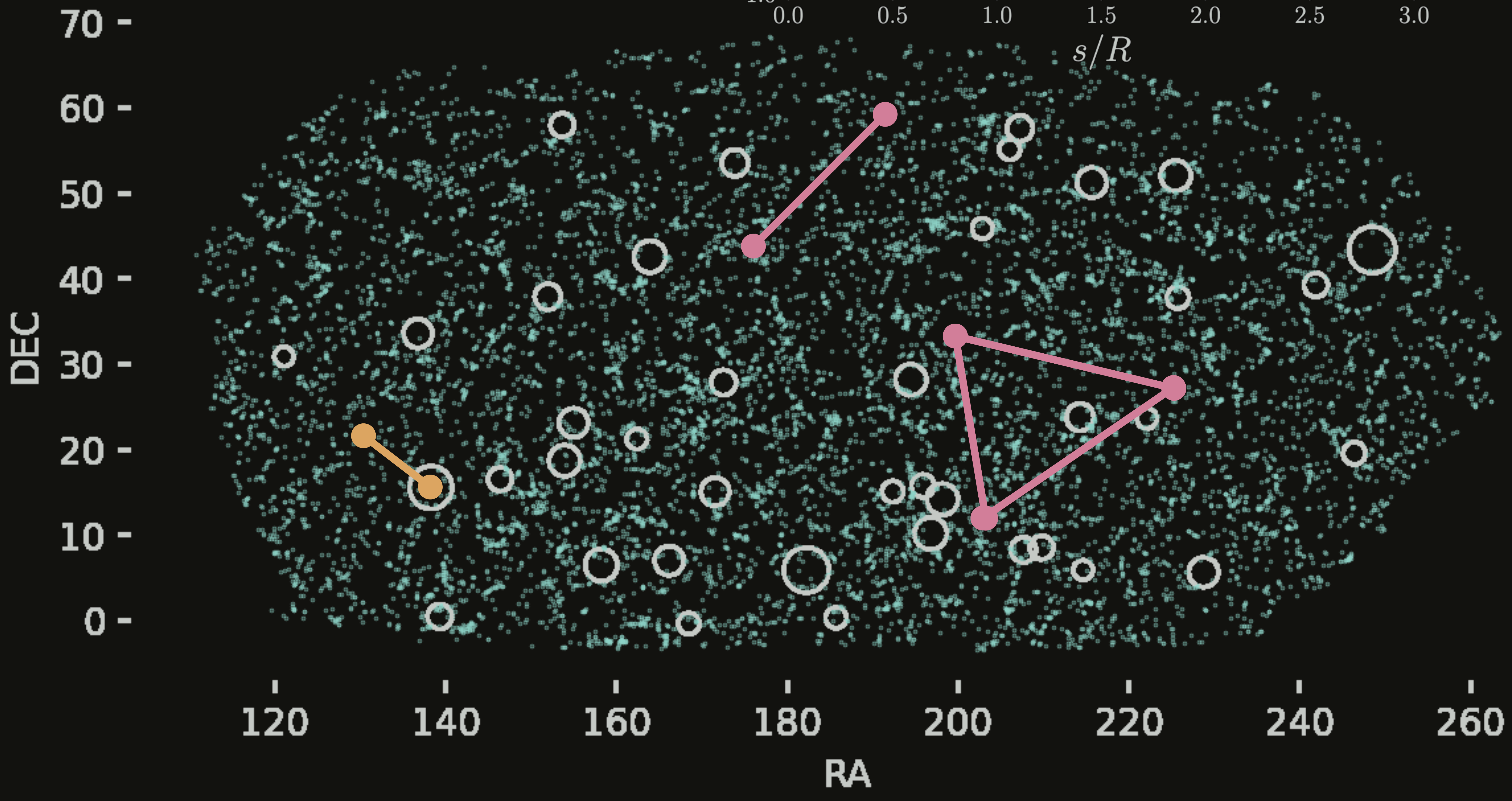
2) triangles of galaxies (bispectrum)

3) …

4) "empty regions": *cosmic voids*
   - size distribution
   - void-galaxy pairs
   - …



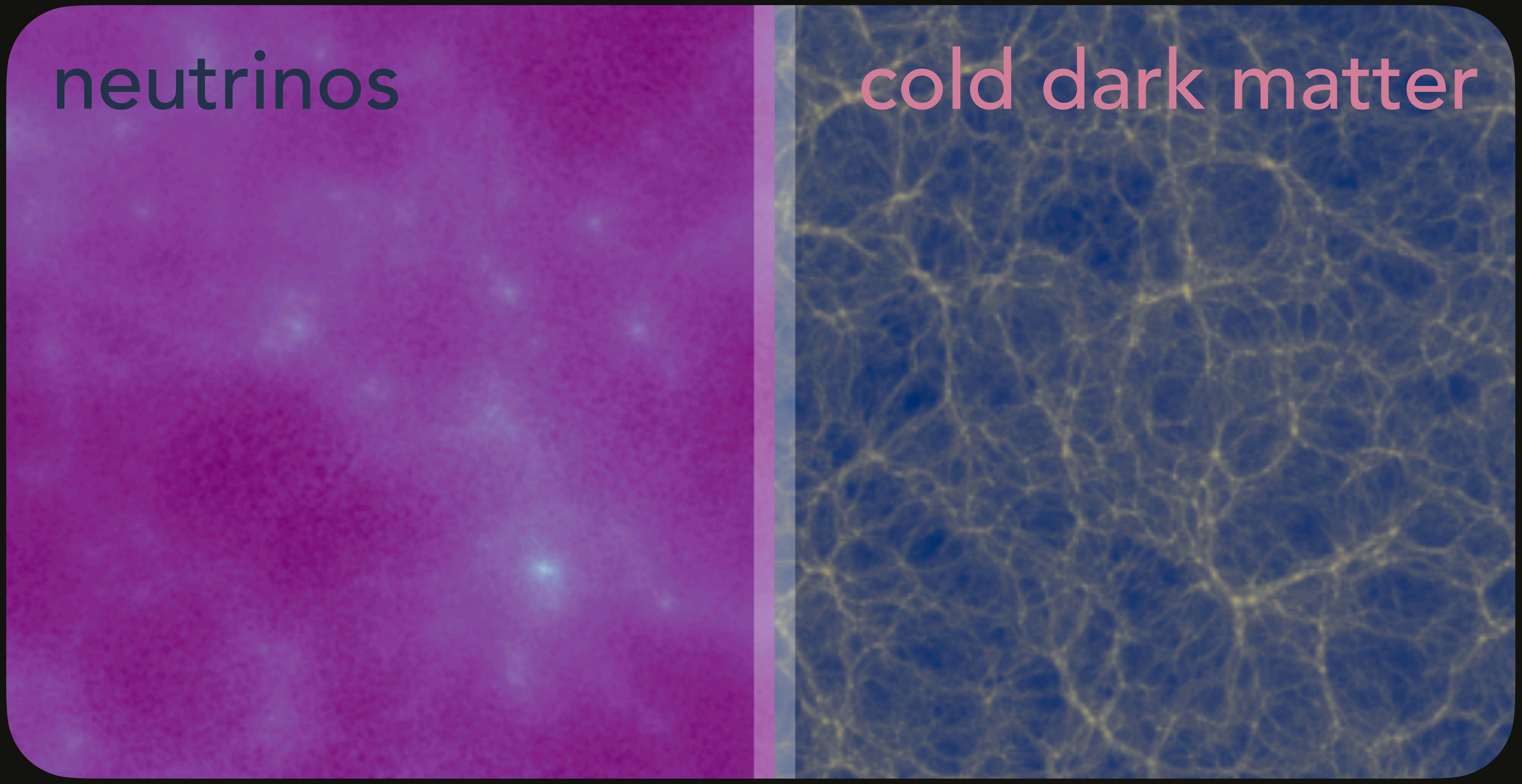
[Hamaus+2020]

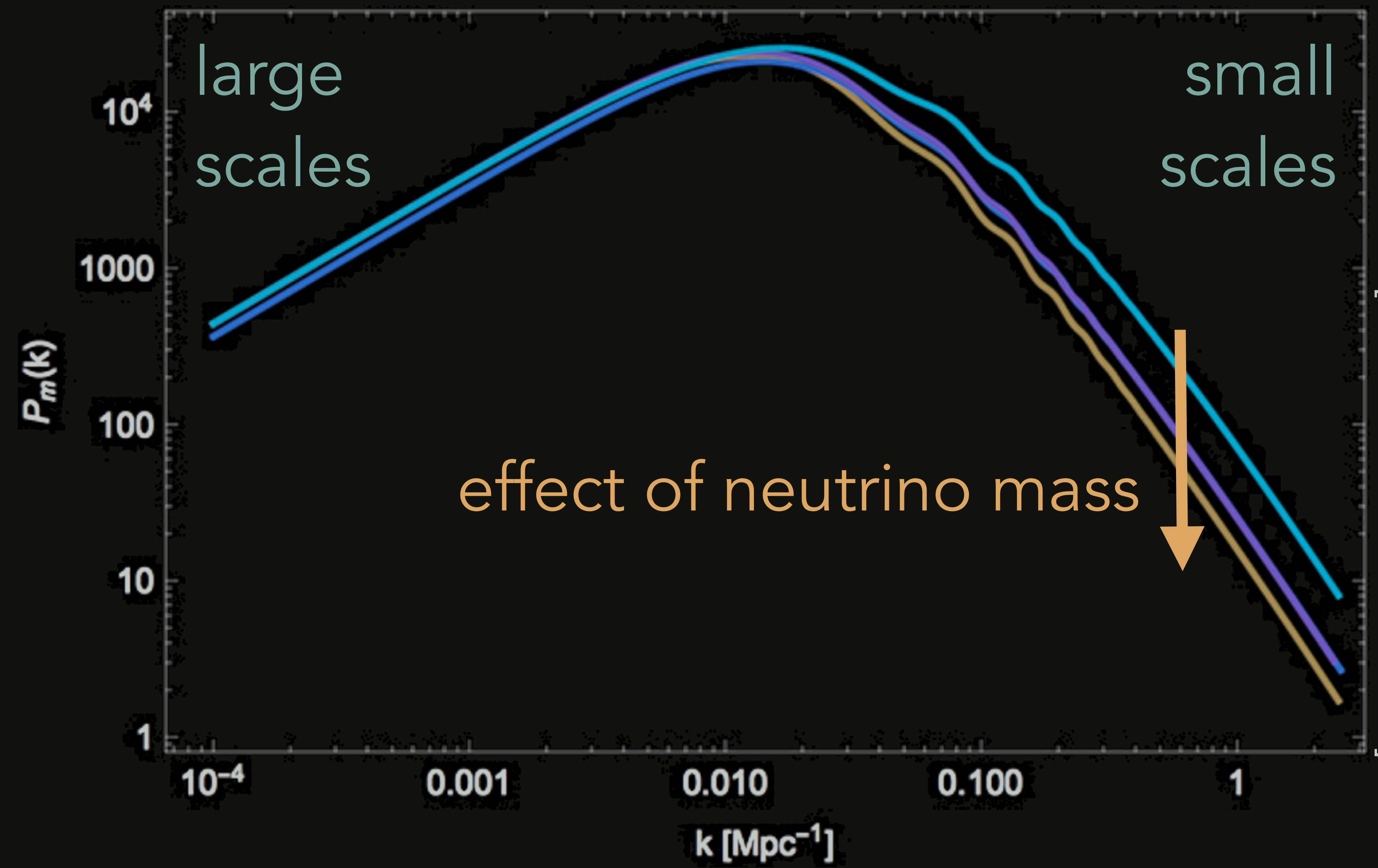


What can voids do for us?

- upweight underdensities → complementary to correlation functions
  - corrections to general relativity
  - dark energy
  - neutrino mass

[FLAMINGO]

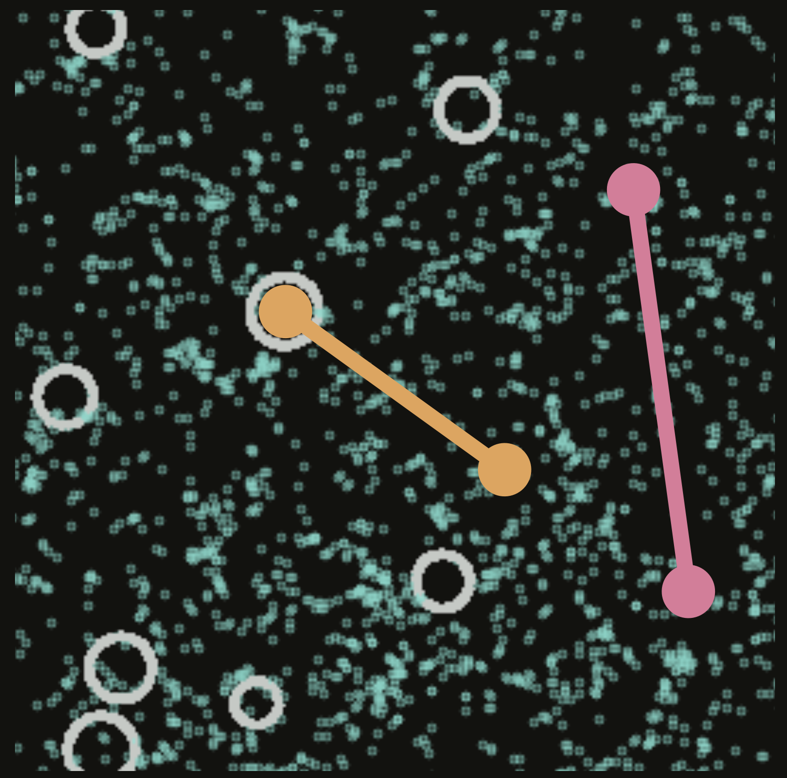




[Gerbino&Lattanzi2018]

Simulation-based inference

- Want to constrain neutrino mass sum, $\sum m_\nu$, with BOSS data:
  - galaxy auto power spectrum
  - void size function (histogram of void sizes)
  - void galaxy cross power spectrum (void profile)



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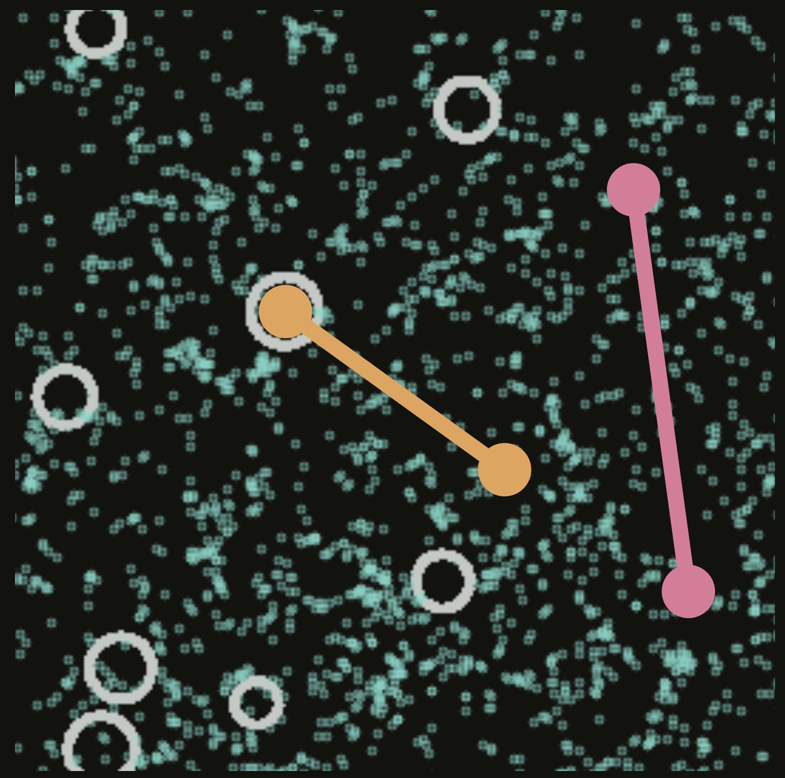
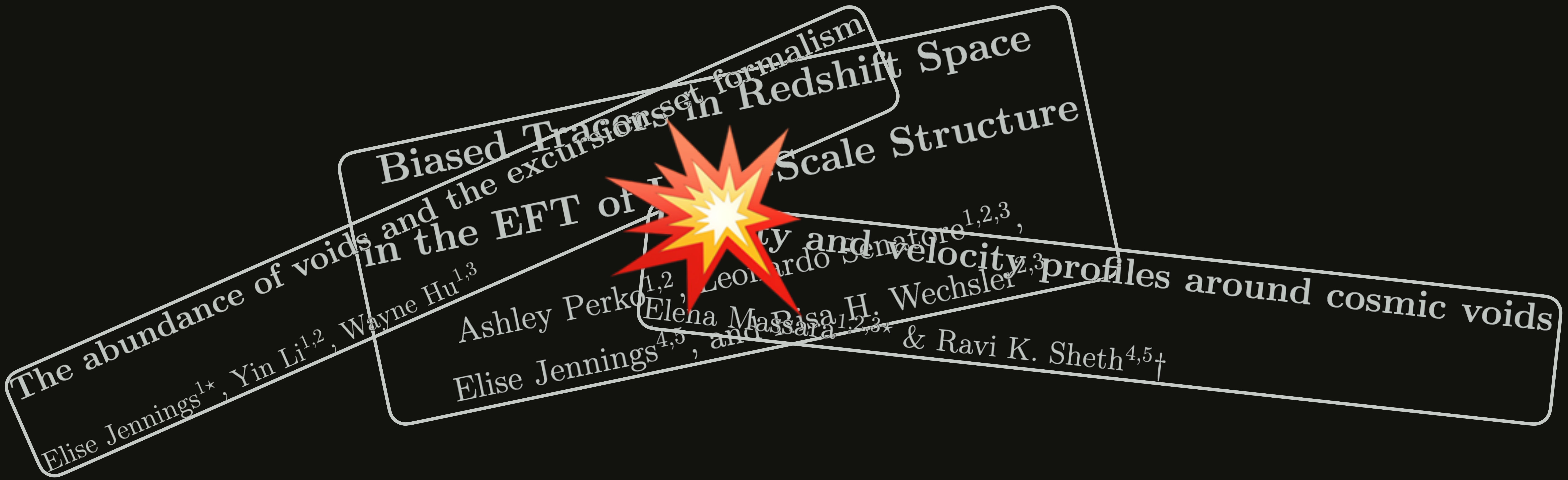


- Joint modeling of these statistics difficult with analytic methods



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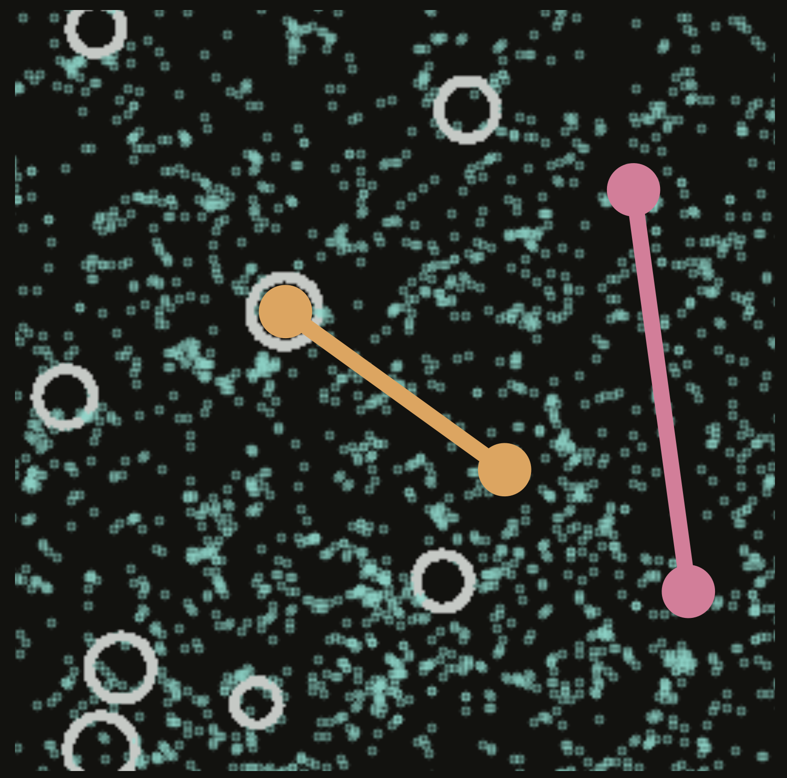
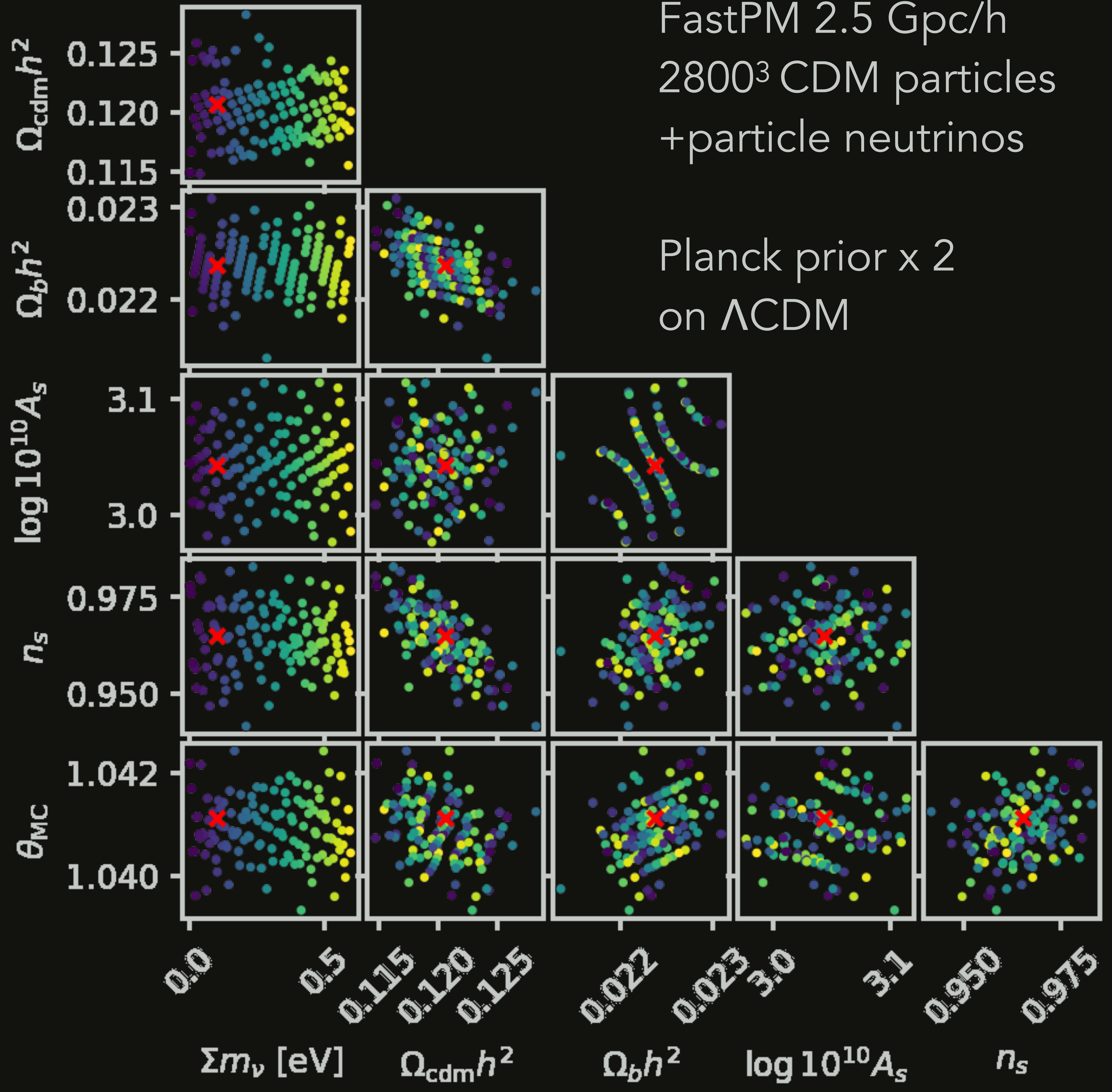


- Joint modeling of these statistics difficult with analytic methods
- Thus, resort to simulations (PM + HOD)
- Likelihood unknown → Implicit-Likelihood Inference

Simulations



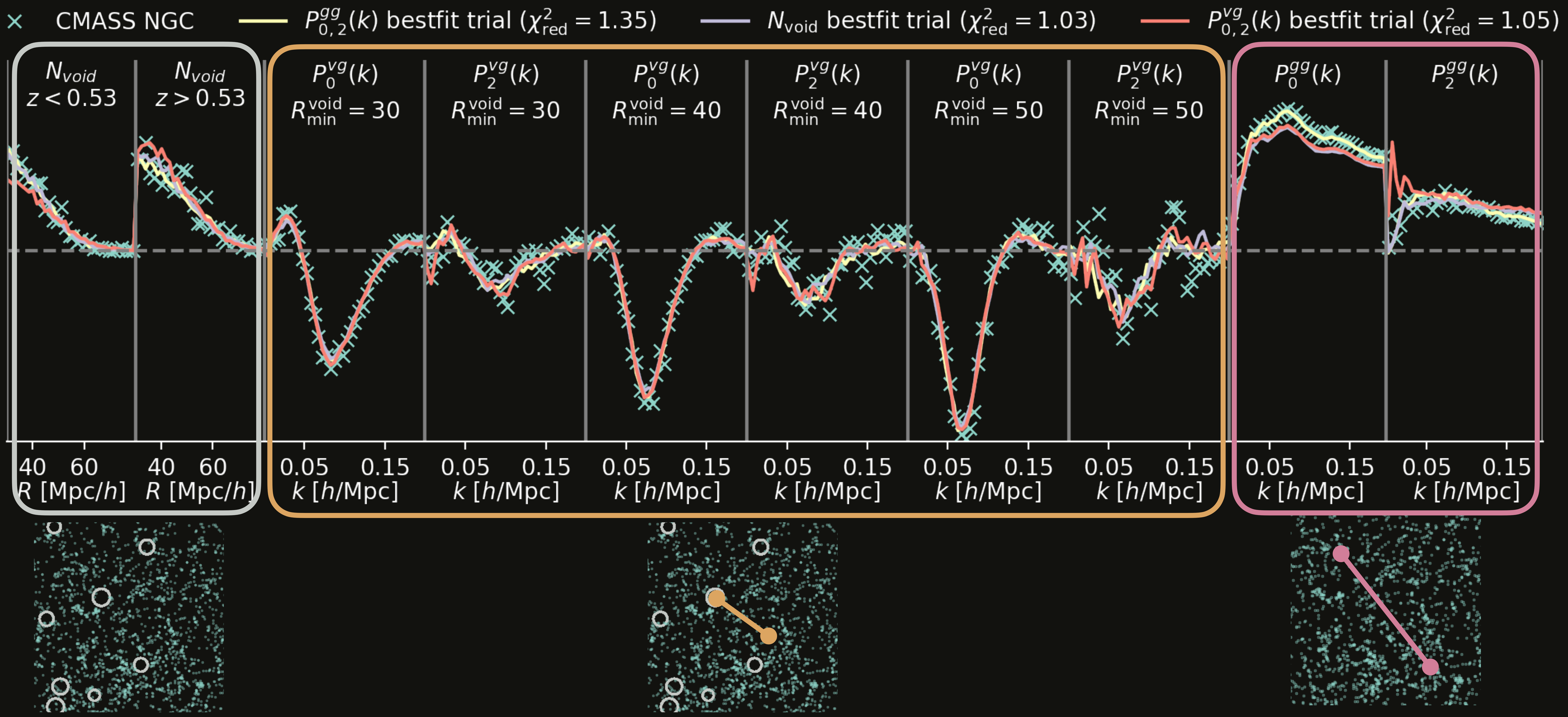
FastPM 2.5 Gpc/h
2800^3 CDM particles
+particle neutrinos

Planck prior x 2
on ΛCDM

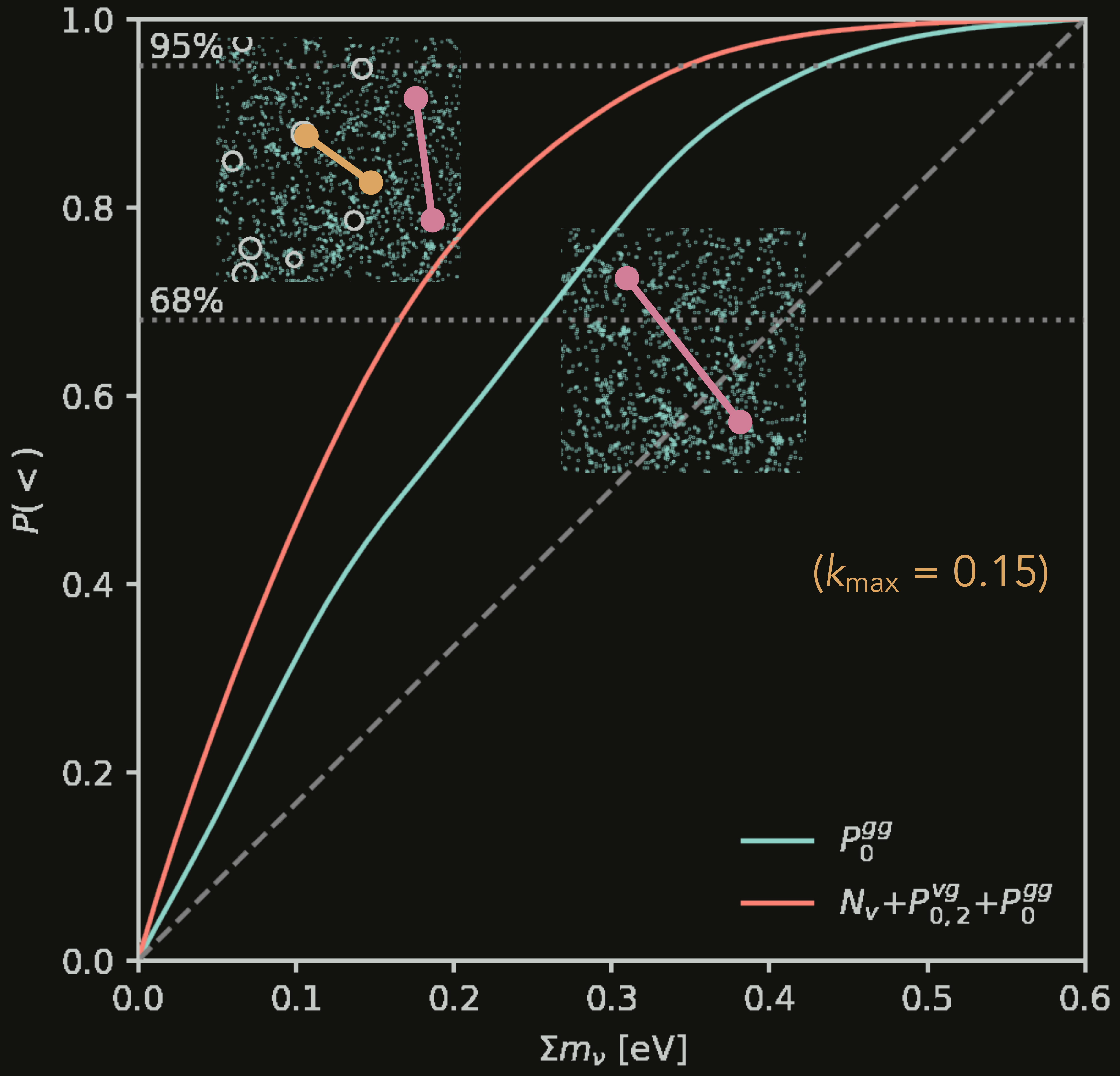
- populate gravity-only simulations with galaxies using HOD
- project on lightcone and add survey realism

Data Vector

Use MOPED compression to reduce dimensionality.



Main posterior



With conservative scale cut of k_{max}=0.15 hMpc^{-1}, voids tighten upper bound on neutrino mass.

Issues away from the limit

- *in the limit*, any likelihood learnable
- what is the limit?
    - infinite model expressivity (usually ok in astro & cosmology)
    - ability to find good global optimum (usually ok)
    - infinite training set size / fast & accurate simulation codes

$$L = \int_{p(x,\theta)} \mathscr{L} \approx \sum_{\text{training set}} \mathscr{L}_{\text{approx}}$$

Implicit Likelihood Inference in Crisis?

A Trust Crisis In Simulation-Based Inference? Your Posterior Approximations Can Be Unfaithful

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Arnaud Delaunoy*
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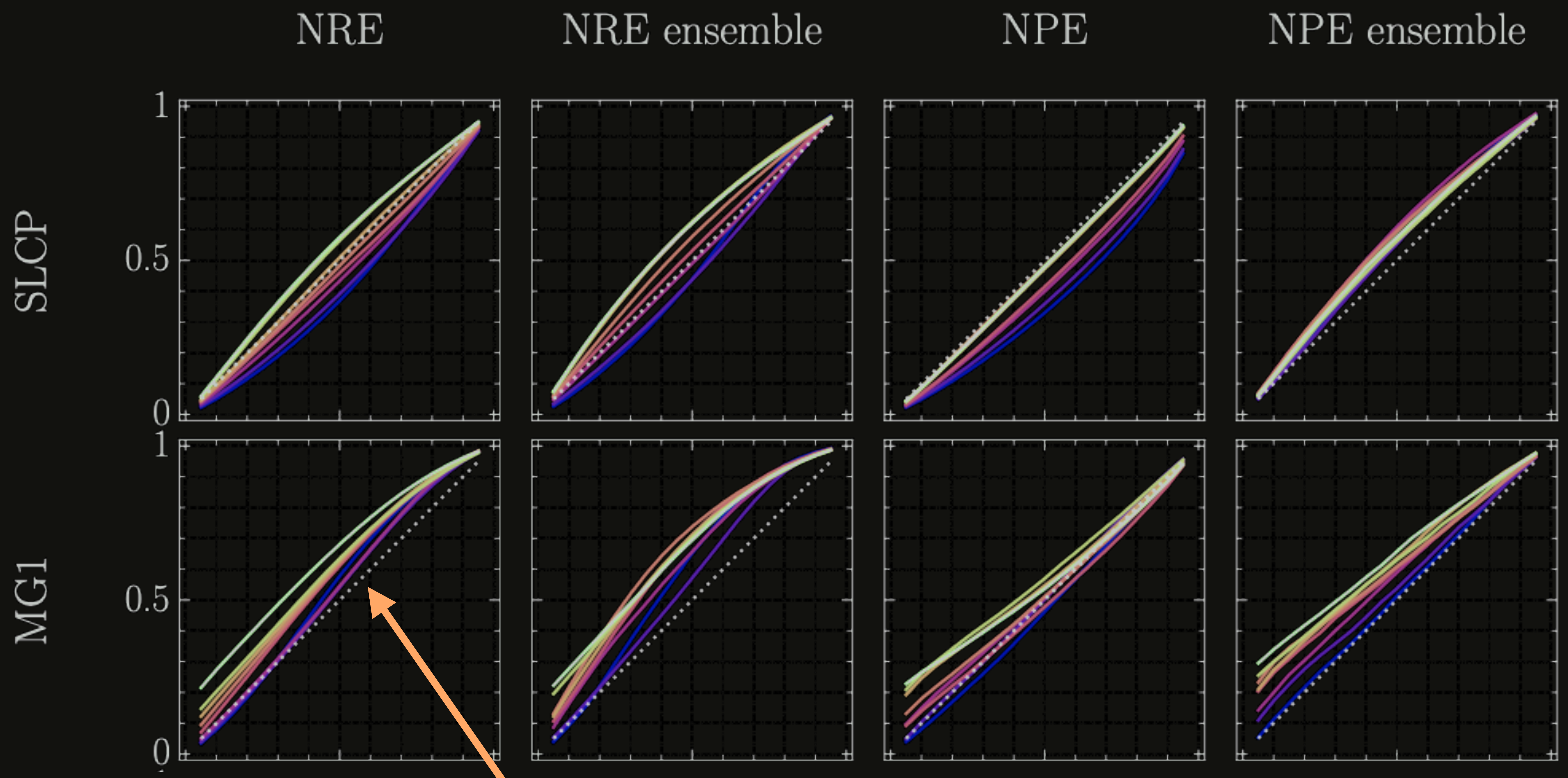
François Rozet
University of Liège

Antoine Wehenkel
University of Liège

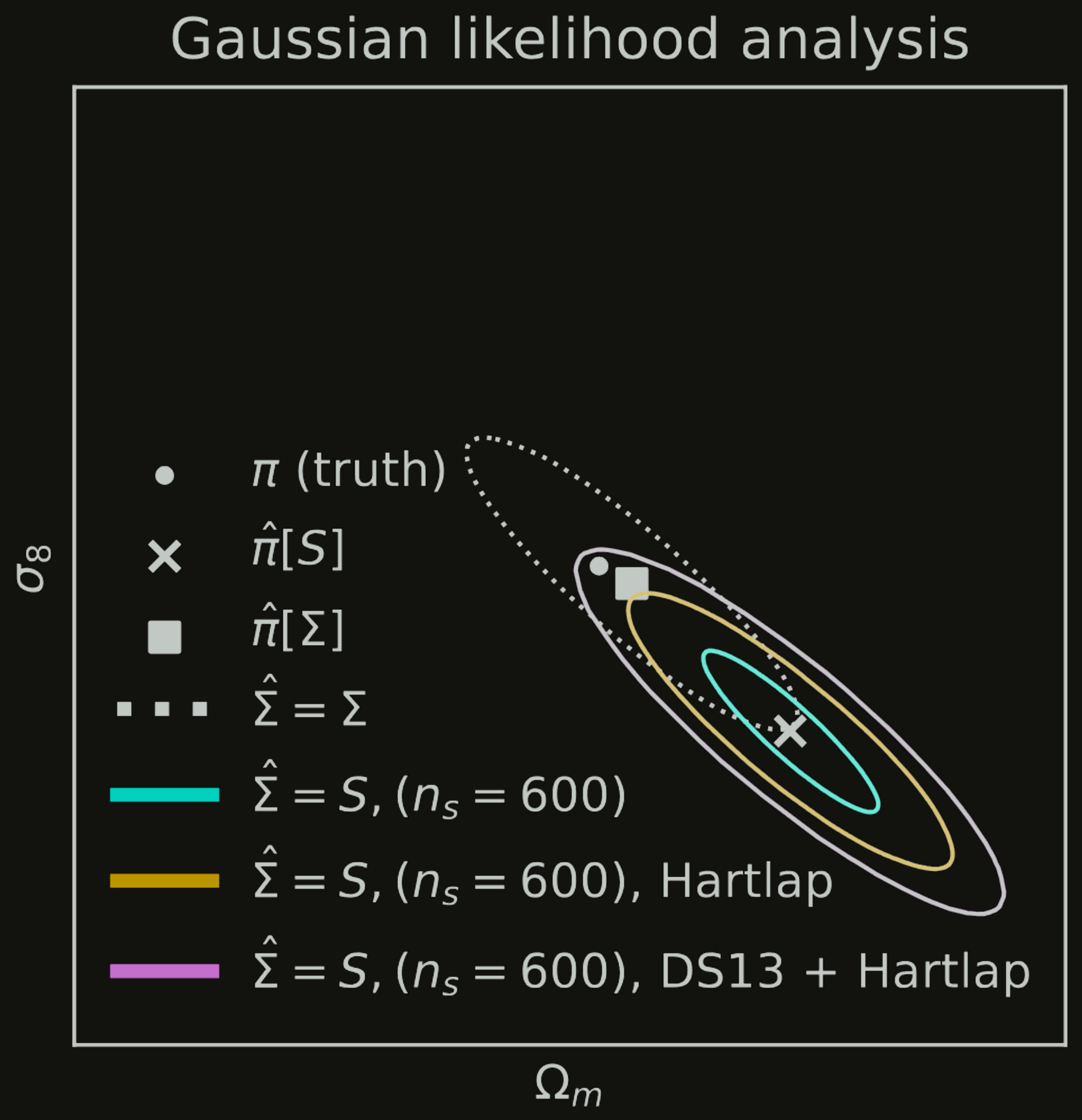
Volodimir Begy
University of Vienna

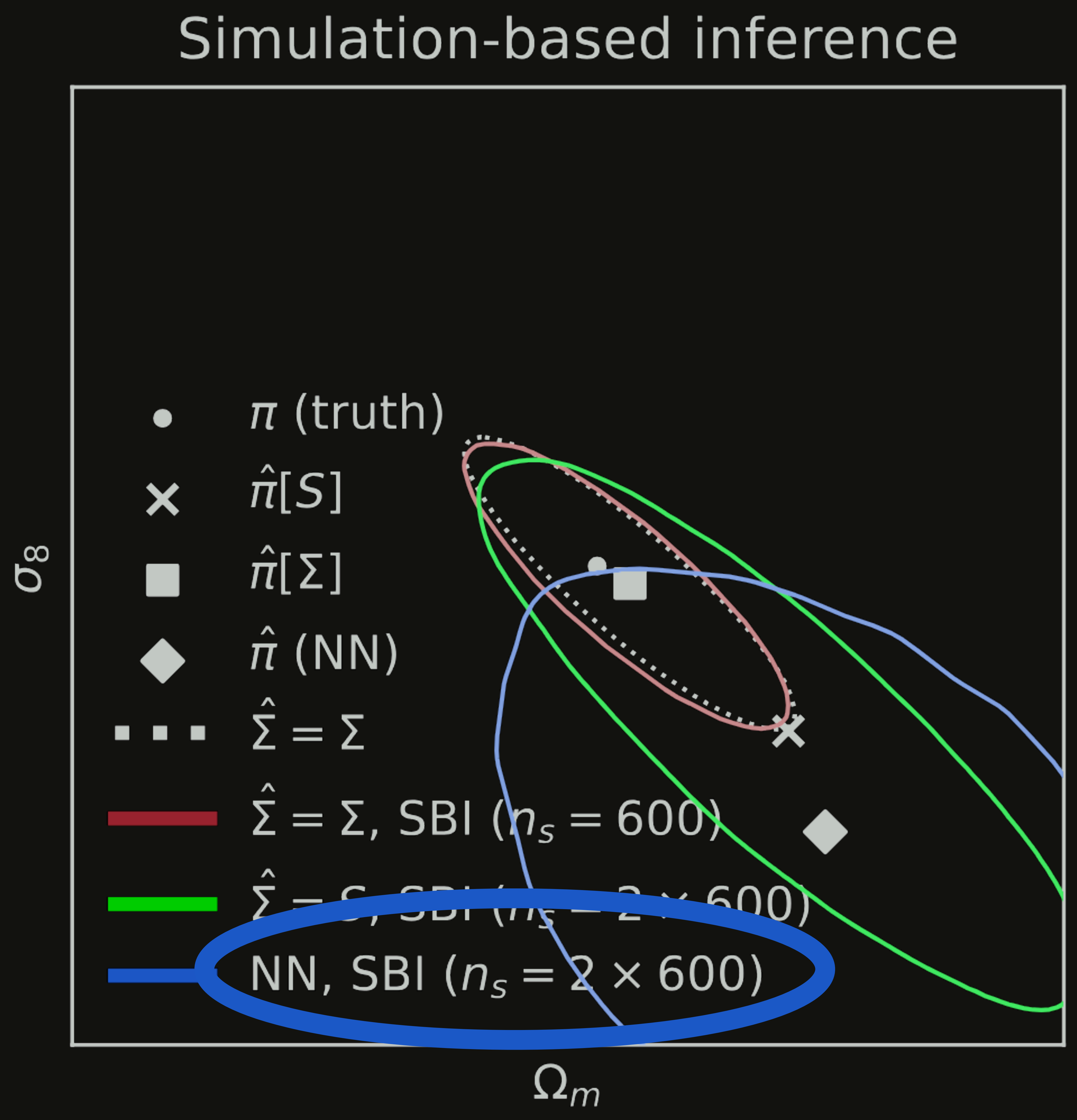
Gilles Louppe
University of Liège



Want to be along diagonal

Implicit Likelihood Inference in Crisis?





[Homer, Friedrich, Gruen 2024]

Implicit Likelihood Inference: Way Forward

The ultimate goal: accurate inferences on physical parameters for analytically intractable inverse problems

Standing in the way: high cost of numerical simulations, limiting training set size and thus accuracy

Progress is being made in several directions:
- bring simulation cost down (hardware, software, ML enhancement)
- improve sample efficiency of ILI
- incorporate information from cheaper simulations (multi-fidelity learning)