Flow-based likelihoods for non-Gaussian inference

Physics ∩ ML

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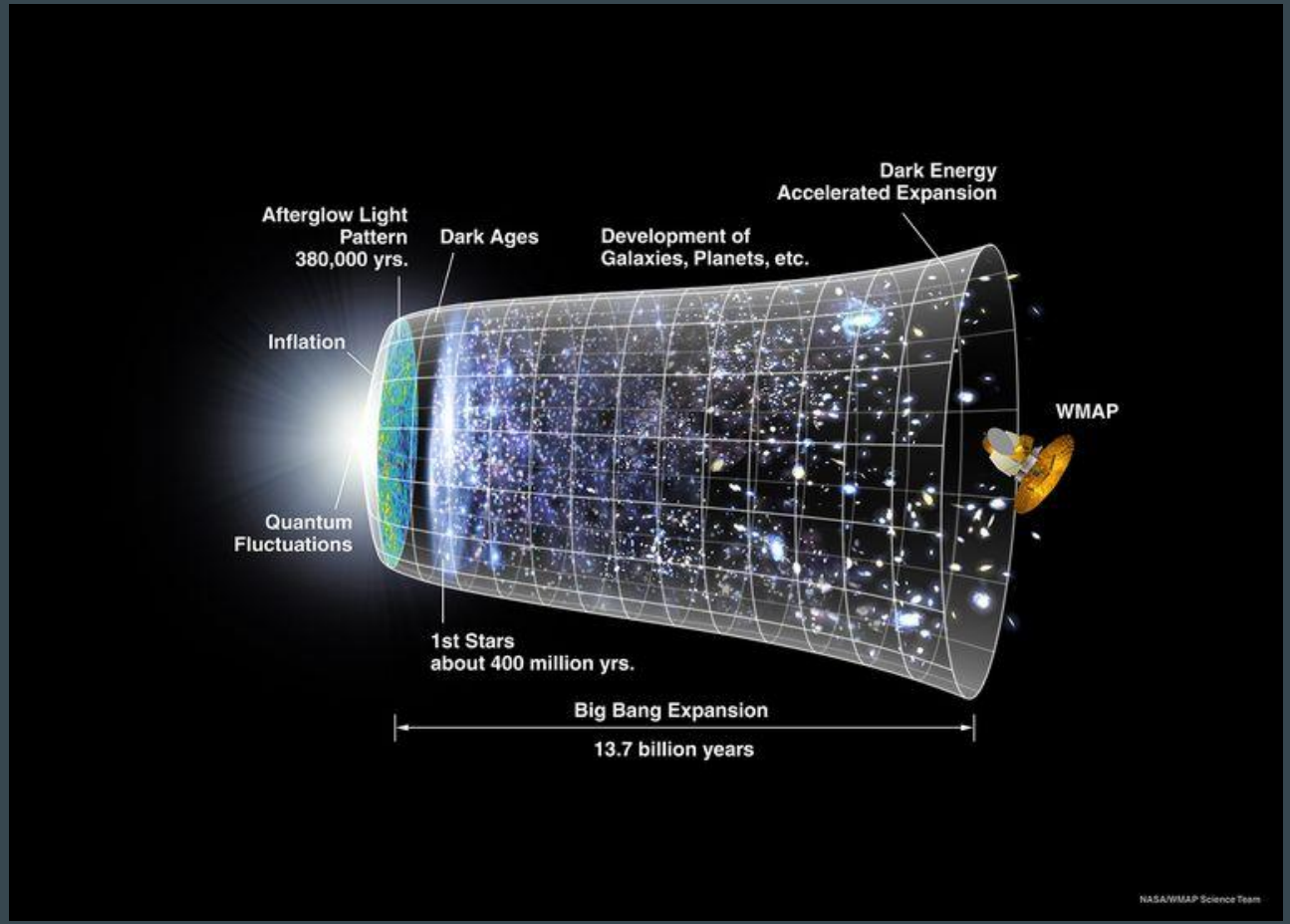
arXiv: 2007.05535 (w/ C. Dvorkin, accepted to PRD)

Cosmology in a nutshell

Parametrized by the **Lambda Cold Dark Matter model** (ΛCDM)



NASA/WMAP Science Team

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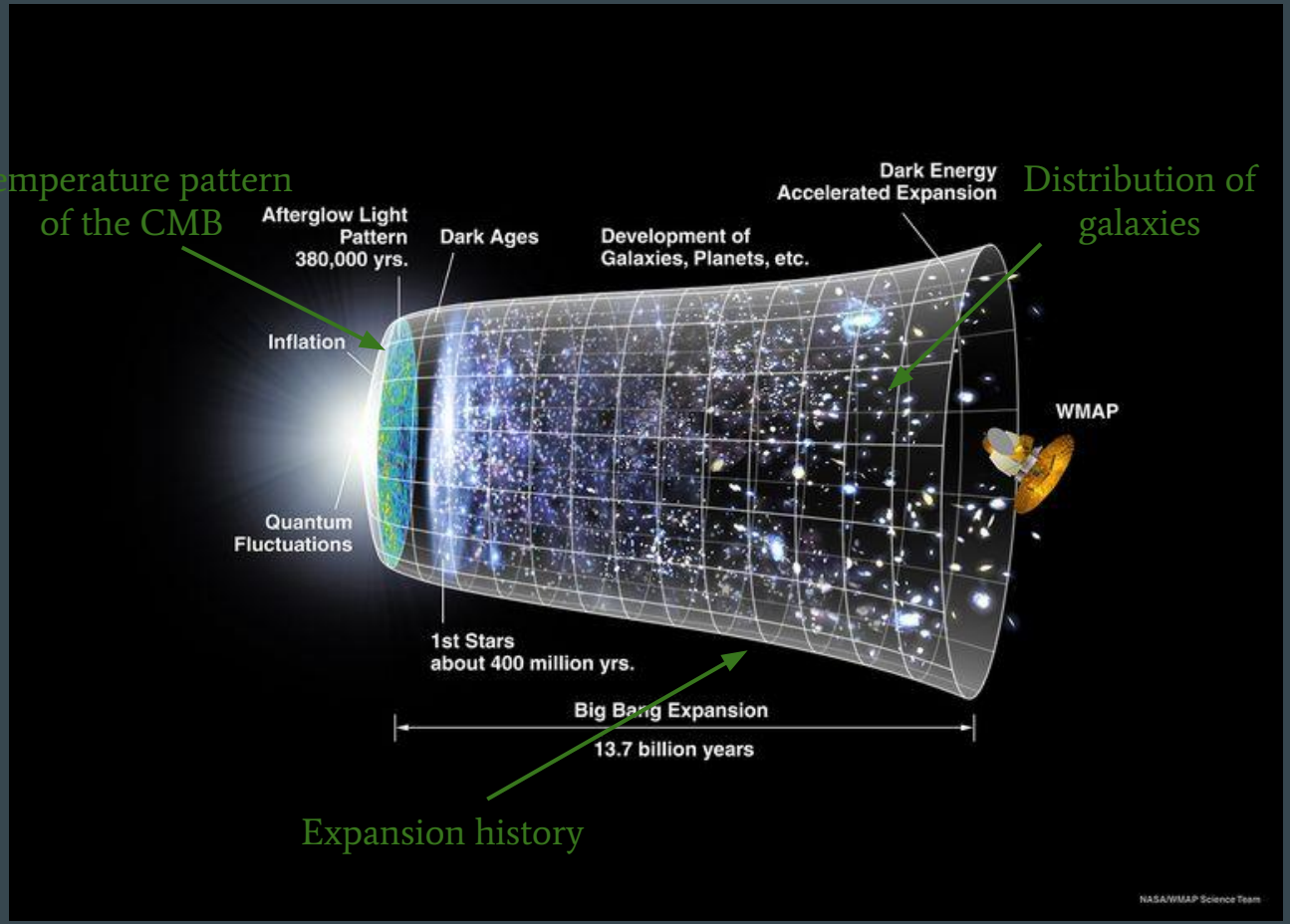


NASA/WMAP Science Team

Tensions in cosmology

With the avalanche of data over the past 10-20 years we are in the era of precision cosmology, where parameters are measured at the percent level.

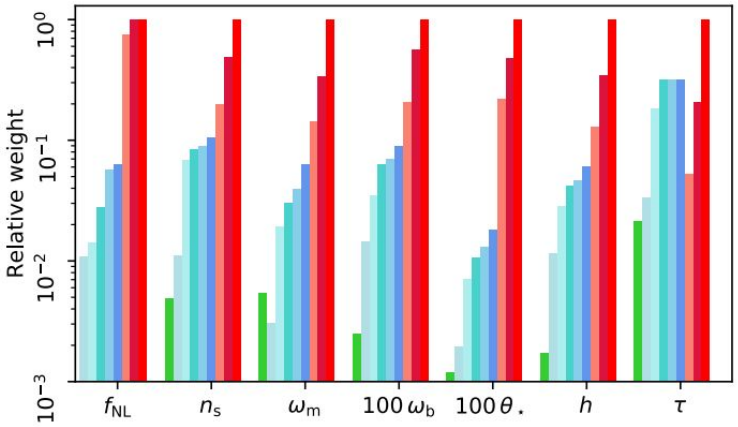


Fig. 13. Increase in the "statistical weight" (i.e., $1/\sigma^2$, where σ for each parameter comes from marginalising over the rest of the set) for a selection of ΛCDM parameters as a function of time. The bars represent the same divisions as in Figs. 11 and 12: pre-WMAP (green); WMAP1, WMAP3, WMAP5, WMAP7, and WMAP9 (blue shades); and Planck13, Planck15, and Planck18 (red shades).

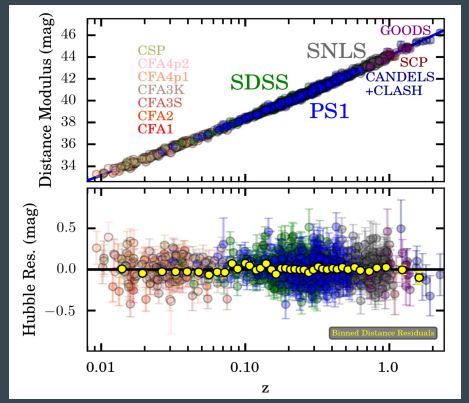
Planck (2020)

Tensions in cosmology

ΛCDM parameters are not **predicted** but rather **inferred** from observations*.

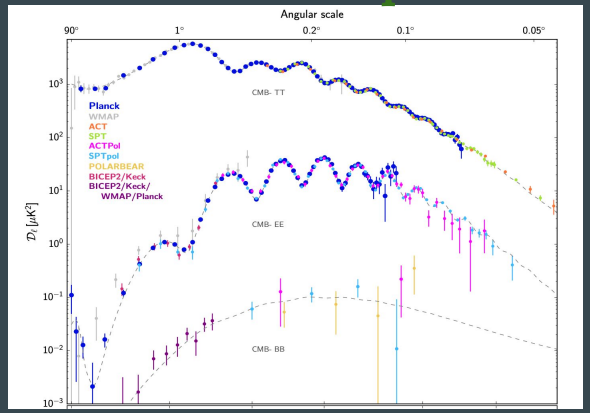
We can obtain **independent estimates** of the parameters from **different observables** in our single universe to check for consistency between our universe and the ΛCDM model.

Scolnic+ (2018)

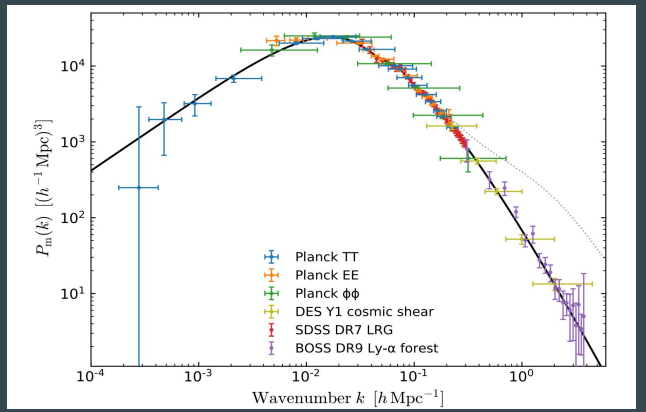


Expansion history

CMB anisotropies



Planck (2020)

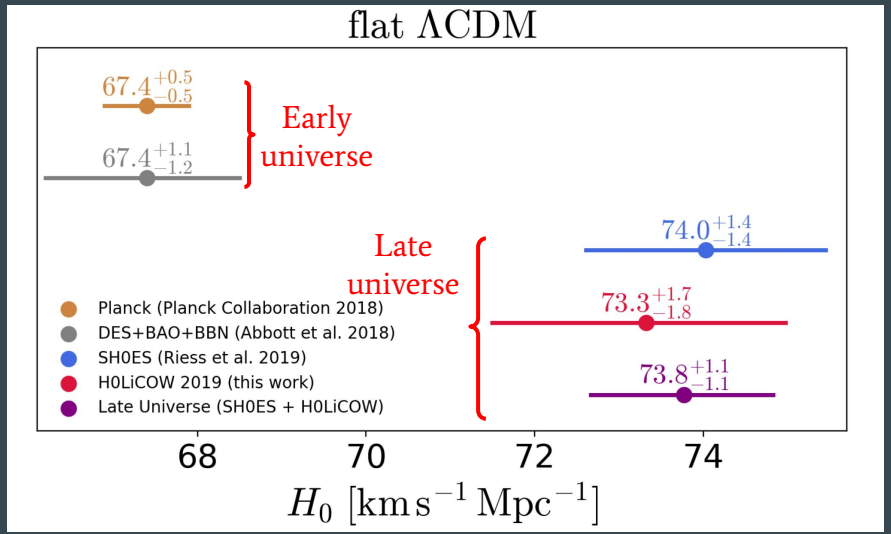


Planck (2020)

Clustering of matter

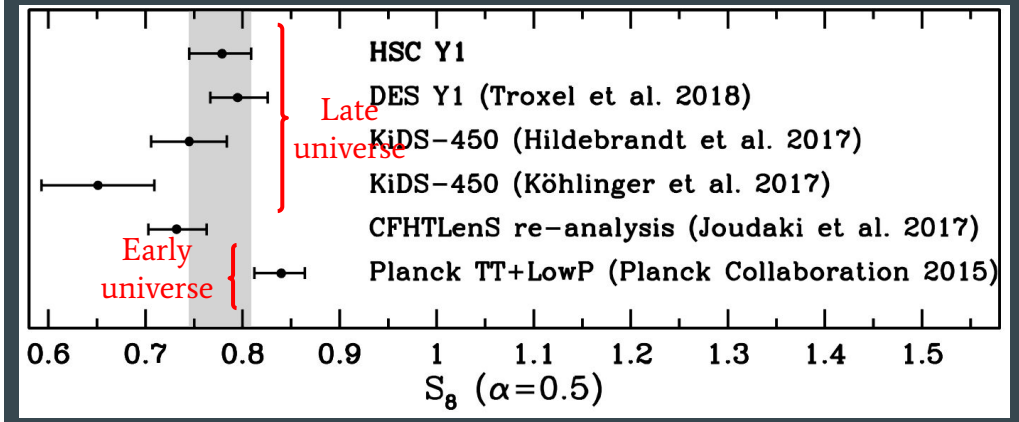
Tensions in cosmology

While individual datasets do not favor extensions to the base model, we see significant **tensions** between some of the ΛCDM (derived) parameters from different observables.



Wong+ (2019)

Current expansion rate of the universe



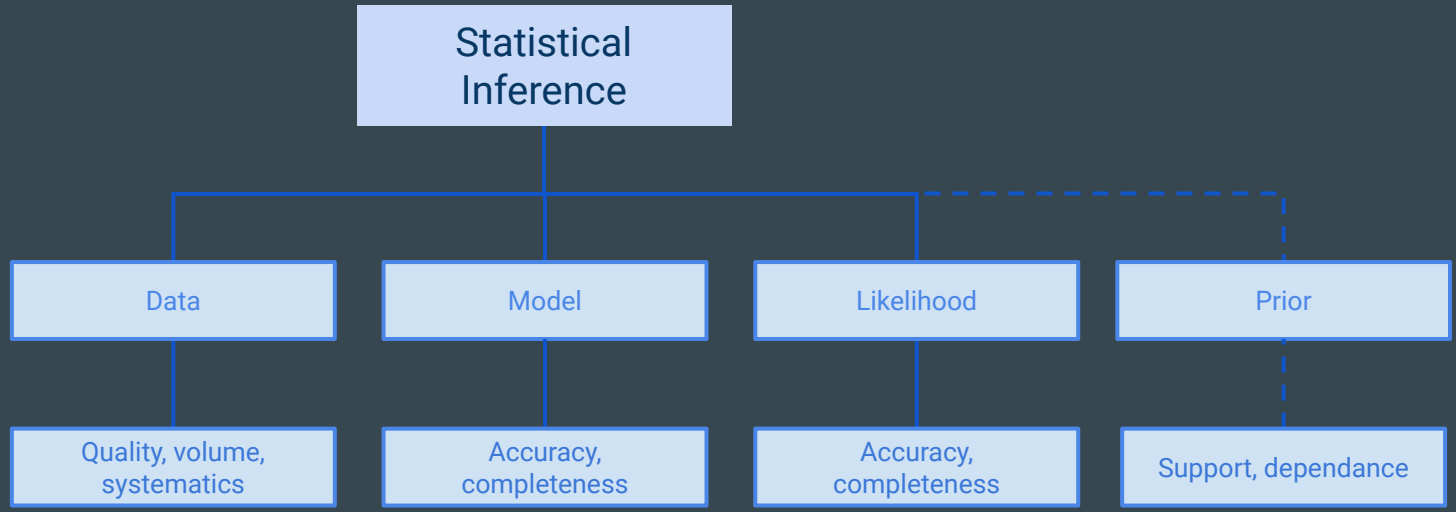
Growth of structure

Hikage+ (2019)

Tensions in cosmology

Are cosmological parameters as **accurate** as they are **precise**?

Without answering this question we can't know if tensions point to new physics.



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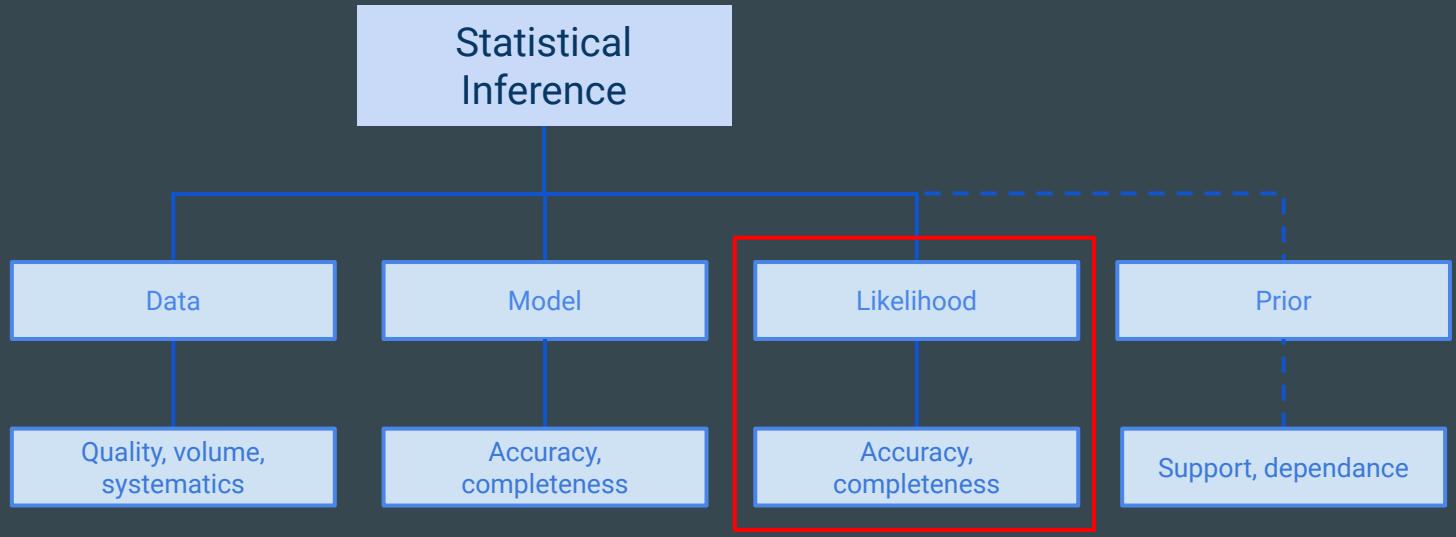

The Likelihood

The likelihood measures the extent to which a sample provides support for particular values in a statistical model.

Much of statistical inference is predicated on the likelihood:

- Maximum likelihood estimates
- likelihood ratio
- posteriors
- Bayes factor
- ...

Gaussian likelihoods

Gaussian likelihoods are very widespread: well understood, only need a covariance matrix, CLT...

$$p(\mathbf{x}|\boldsymbol{\mu}, \Sigma) = \frac{1}{\sqrt{2\pi|\Sigma|}} \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})\right]$$

CMB power spectra (*Planck* 2018)

maps. Specifically, the low-ℓ temperature (TT) likelihood is constructed by approximating the marginal distribution of the temperature angular power spectrum derived from Gibbs sampling-based component separation. The low-ℓ polarization (EE) likelihood is built by comparing a cross-frequency power spectrum of two foreground-corrected maps to a set of simulations. The temperature and polarization high-ℓ likelihoods (TT, TE, and EE) uses multiple cross-frequency spectra estimates, assuming smooth foreground and nuisance spectra templates and a Gaussian likelihood approximation.

Galaxy power spectrum (SDSS-III BOSS)

$D_V r_s^{\rm fid}/r_s = 1493 \pm 28, 1913 \pm 35$, and 2133 ± 36 Mpc. Assuming Gaussian likelihood, we provide a covariance matrix which contains the parameter constraints as well as their correlations (see appendix B).

Shear 2pt function (HSC)

$$-2\ln\mathcal{L}(\boldsymbol{p}) = \sum_{i,j}(d_i - m_i(\boldsymbol{p}))\,\mathrm{Cov}_{ij}^{-1}\,(d_j - m_j(\boldsymbol{p}))$$

Galaxy clustering + weak lensing (KiDS-1000)

6.2. Gaussian likelihood assumption

Along with the vast majority of large-scale structure cosmological analyses, we adopt a multivariate Gaussian likelihood. This is expected to be a generally excellent approximation if the summary statistics entering the likelihood have been averaged over many modes in the underlying fields. Exact likelihood expres-

Gaussian likelihoods

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However,

- CLT isn't always applicable (e.g. power spectra at small wavenumbers)
- For estimated covariance, marginalize over the true covariance (Gaussian → *t*-distribution)
- Systematic effects can introduce non-Gaussian correlations
- Physics giving rise to an observable: a nonlinear function of Gaussian RVs is not Gaussian distributed (CMB vs. galaxy distributions)

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Using a wrong likelihood introduces a source of **systematic uncertainty**:

can bias parameters inferred from some data → are tensions created/amplified by the use of wrong likelihoods?

Gaussian likelihoods

There isn't always a clear alternative/better likelihood:

Gaussianizing data →

ACT Thermal SZ one-point PDF (Hill+, 2015)

parameters to be broken. In this analysis, the data are not quite at the level needed to strongly break the cosmology–ICM degeneracy. The problem is made more challenging by the highly correlated, non-Gaussian nature of the PDF likelihood function (see Section V below), which we simplify by combining many of the bins in the tail of the tSZ PDF. With a more sophisticated approach to the likelihood function and wider, deeper maps, future measurements of the tSZ PDF should allow for a stronger breaking of the cosmology–ICM degeneracy.

Removing NG bins →

CFHTLenS shear correlation (Sellentin+, 2018)

As demonstrated in the previous section, the correlations between various data points of CFHTLenS give rise to non-Gaussianities at a 30% level according to our definition. Here, we present a preliminary study of how these non-Gaussianities might impact parameter constraints, by excluding the most contaminated data points from the likelihood. However, as essentially the entire CFHTLenS dataset is contaminated (see Fig. 3), such exclusions are clearly a suboptimal strategy. We nonetheless report our findings as intermediate results and postpone an update to a non-Gaussian likelihood to future work.

An alternative: data-driven likelihoods (DDLs)

Data-driven likelihoods are learned from data:

- We can think of (mock) data as independent draws from the underlying true likelihood function.
- We can estimate the data's PDF with sufficient samples from it.

The hope is that DDLs can accurately capture non-Gaussianities in the data.

An alternative: data-driven likelihoods (DDLs)

Gaussian Mixture Models (GMM)

$$\hat{p}_{\mathrm{GMM}}(\mathbf{x}) = \sum_{i=1}^{K} \phi_i \mathcal{N}(\mathbf{x}|\mu_i, \Sigma_i)$$

weights

unknown parameters

Use expectation maximization to find parameters, BIC to determine *K*.

Independent Component Analysis (ICA)

$$\mathbf{x} = \mathbf{A}\mathbf{s}$$

Rotate principal components to maximize statistical independence.

$$\hat{\mathbf{s}} \equiv \mathbf{x}_{\mathrm{ICA}} = \mathbf{W}\mathbf{x} = \{\mathbf{x}_{1,\mathrm{ICA}}, \ldots, \mathbf{x}_{N,\mathrm{ICA}}\}$$

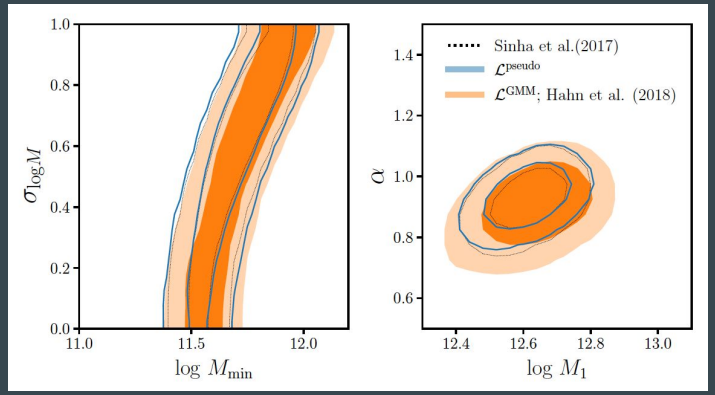
KDE

$$\hat{p}_{\mathrm{ICA}}(\mathbf{x}) = \prod_{n=1}^{N} \hat{p}_n(\mathbf{x})$$

An alternative: data-driven likelihoods (DDLs)

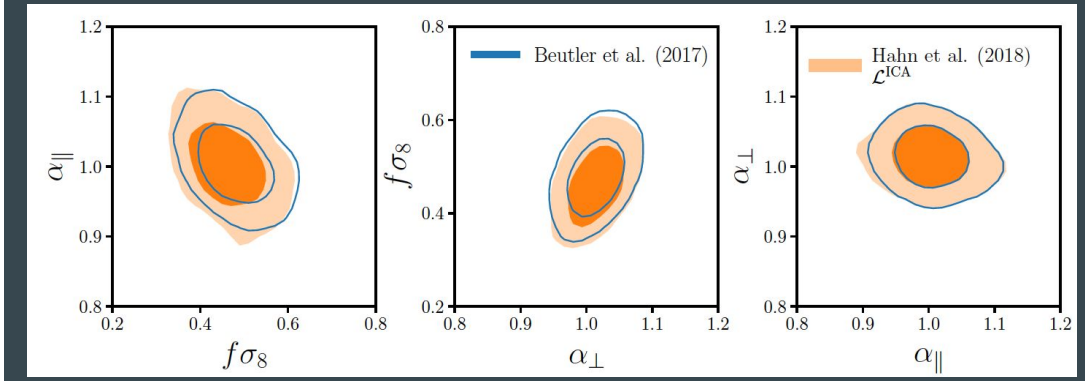
Hahn+ (2018): Large-scale structure with non-Gaussian likelihoods (<0.5σ shifts)

Group multiplicity function (with GMM)



20,000 mocks

Galaxy power spectrum (with ICA)



2,048 mocks

An alternative: data-driven likelihoods (DDLs)

Flow-based Likelihoods (FBLs, Diaz Rivero & Dvorkin 2020)

→ I will introduce flow-based generative models

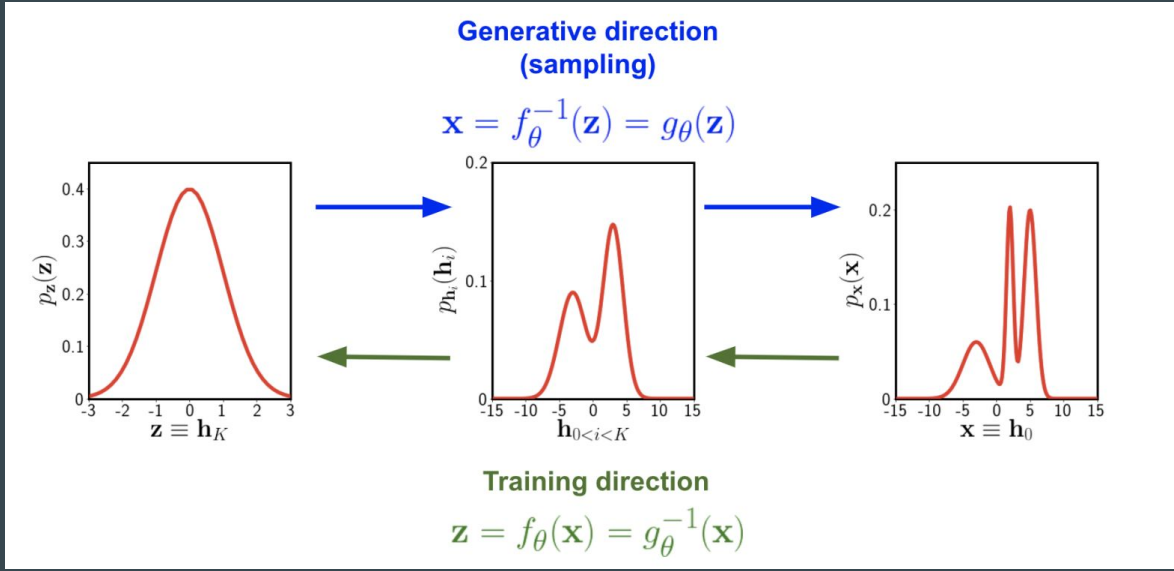
→ Their minimization objective is what we will call a flow-based likelihood

See also literature on **simulation-based inference** and **likelihood-free inference** (e.g. DELFI), which have used flows for density estimation as well!

Flow-based generative models

Generative models aim to learn the probability distribution that gave rise to data $\boldsymbol{x}$, such that new samples can be drawn.

In *flow-based models*, a simple distribution is repeatedly transformed to match $p(\boldsymbol{x})$.



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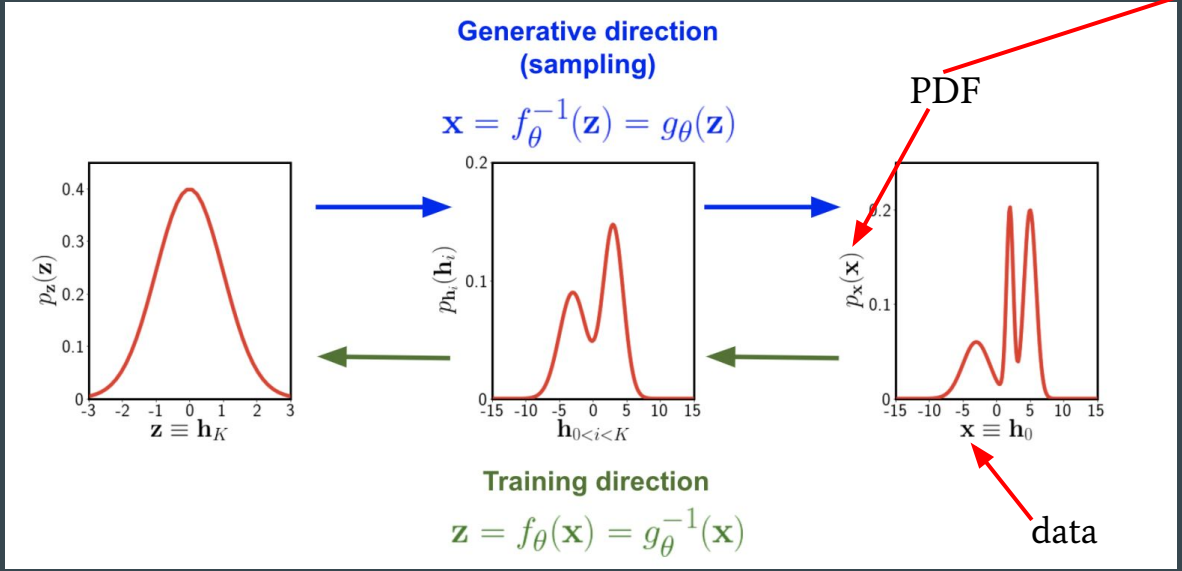

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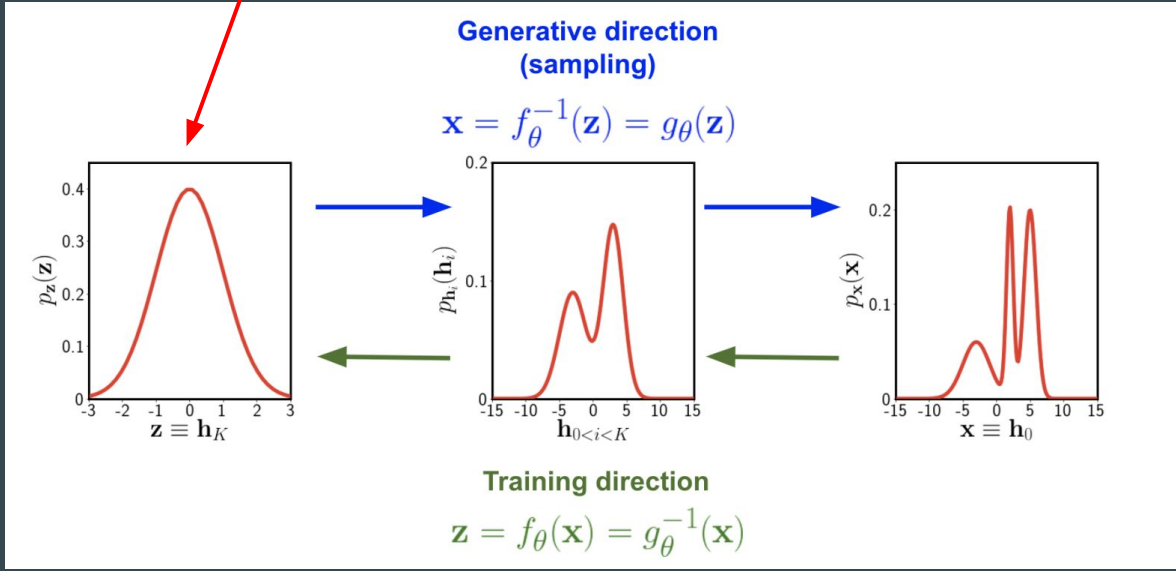

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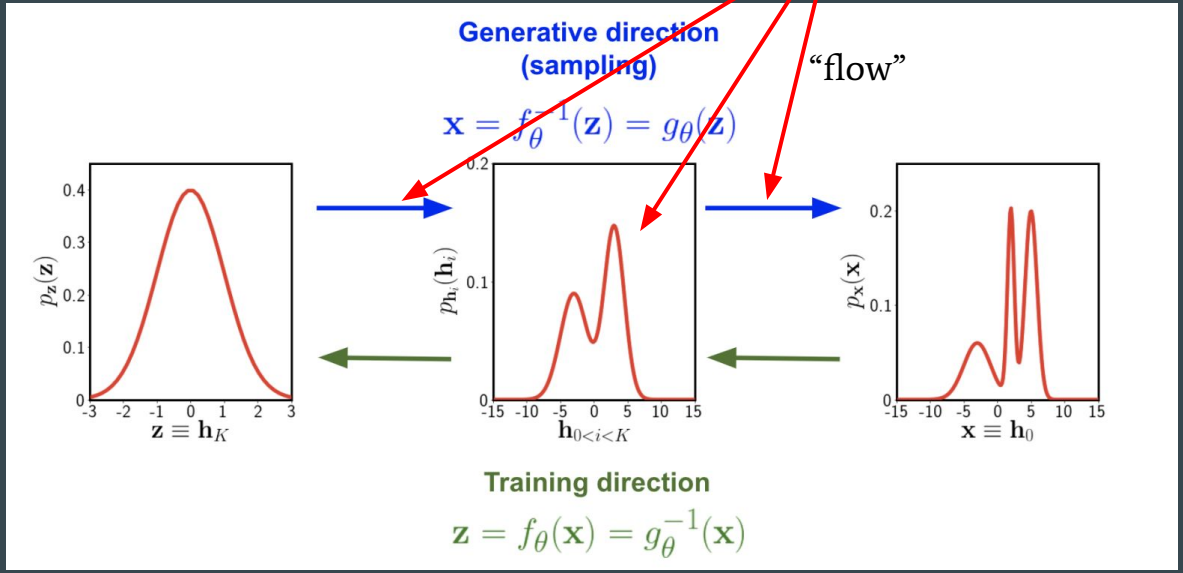

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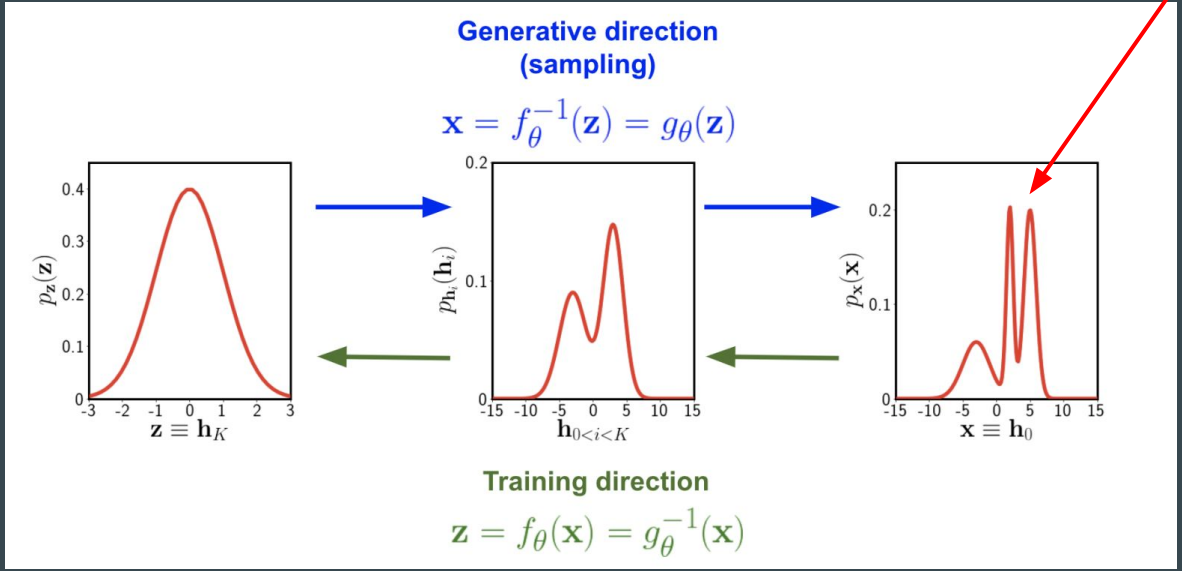

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In *flow-based models*, a simple distribution is repeatedly transformed to match p(***x***).

$$\mathbf{z} \sim p_{\mathbf{z}}(\mathbf{z})$$

$$\mathbf{x} \equiv \mathbf{h}_0 \underset{g_K}{\overset{f_1}{\longleftrightarrow}} \mathbf{h}_1 \underset{g_{K-1}}{\overset{f_2}{\longleftrightarrow}} \ldots \underset{g_2}{\overset{f_{K-1}}{\longleftrightarrow}} \mathbf{h}_{K-1} \underset{g_1}{\overset{f_K}{\longleftrightarrow}} \mathbf{h}_K \equiv \mathbf{z}$$

$$f = f_1 \circ f_2 \circ \ldots f_K$$

$$g = g_1 \circ g_2 \circ \ldots g_K$$

$$\mathbf{x} = g_\theta(\mathbf{z}) = f_\theta^{-1}(\mathbf{z})$$

$$\mathbf{z} = g_\theta^{-1}(\mathbf{x}) = f_\theta(\mathbf{x})$$

Flow-based generative models

Generative models aim to learn the probability distribution that gave rise to data $\boldsymbol{x}$, such that new samples can be drawn.

In *flow-based models*, a simple distribution is repeatedly transformed to match $p(\boldsymbol{x})$.

$$\log p_{\mathbf{x}}(\mathbf{x}) = \log p_{\mathbf{z}}(\mathbf{z}) + \log \left| \det \left(\frac{d\mathbf{z}}{d\mathbf{x}} \right) \right|$$

$$= \log p_{\mathbf{z}}(\mathbf{z}) + \sum_{i=1}^{K} \log \left| \det \left(\frac{d\mathbf{h}_i}{d\mathbf{h}_{i-1}} \right) \right|$$

Flow-based generative models

The goal is to train a model to learn these transformations.

- Transformations can involve (invertible) neural networks to make them very expressive.
- The loss is the negative log-likelihood over the training set.

$$\mathcal{L} = -\frac{1}{|\mathcal{D}|} \sum_{\mathbf{x} \in \mathcal{D}} \log p_\theta(\mathbf{x})$$

If training is successful, the learned likelihood == the true data likelihood == a DDL.

Flow-based generative models

BUT, transformations must

- be easily invertible,
- have an easy-to-compute Jacobian determinant (scales as N^3),

which limits their expressivity.

Different tricks in the literature:

- Restrict the form of the transformation to exploit identities
- Make Jacobian triangular by making transformations auto-regressive or splitting up dimensions and applying affine transformations

Ideally also want quick density estimation **and** sampling.

Flow-based generative models

Glow (Kingma & Dhariwal 2018)

Fast likelihood-free cosmology with neural density estimators and active learning

Justin Alsing,[1,2,3]★ Tom Charnock[4], Stephen Feeney[2] and Benjamin Wandelt[2,5]
[1]*Oskar Klein Centre for Cosmoparticle Physics, Stockholm University, Stockholm SE-106 91, Sweden*
[2]*Center for Computational Astrophysics, Flatiron Institute, 162 5th Ave, New York City, NY 10010, USA*
[3]*Imperial Centre for Inference and Cosmology, Department of Physics, Imperial College London, Blackett Laboratory, Prince Consort Road, London SW7 2AZ, UK*
[4]*Sorbonne Université, CNRS, UMR 7095, Institut dâĂŹAstrophysique de Paris, 98 bis bd Arago, 75014 Paris, France*
[5]*Sorbonne Université, Institut Lagrange de Paris (ILP), 98bis boulevard Arago, F-75014 Paris, France*

arXiv:1903.00007

Constraining the Reionization History using Bayesian Normalizing Flows

Héctor J. Hortúa, Luigi Malagò, Riccardo Volpi

Machine Learning and Optimization Group,
Romanian Institute of Science and Technology (RIST),
Cluj-Napoca, Romania

arXiv:2005.07694

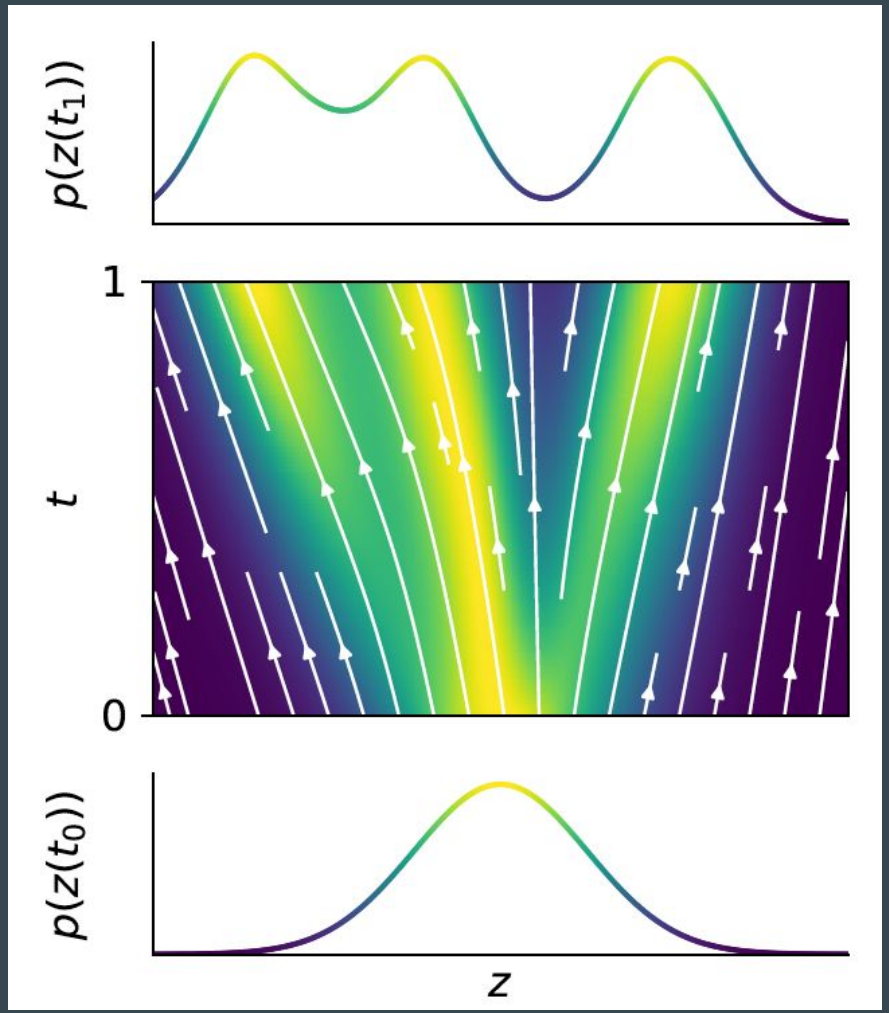
FFJORD (Grathwohl+ 2018)

Transformation from prior to data is seen as evolution in time.

$$\frac{\partial \mathbf{z}(t)}{\partial t} = f(\mathbf{z}(t), t; \theta)$$

$$\frac{\partial \log p(\mathbf{z}(t))}{\partial t} = -\mathrm{Tr}\left(\frac{\partial f}{\partial \mathbf{z}(t)}\right)$$

$$\log p(\mathbf{z}(t_1)) = \log p(\mathbf{z}(t_0)) - \int_{t_0}^{t_1} \mathrm{Tr}\left(\frac{\partial f}{\partial \mathbf{z}(t)}\right) dt.$$



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neural network

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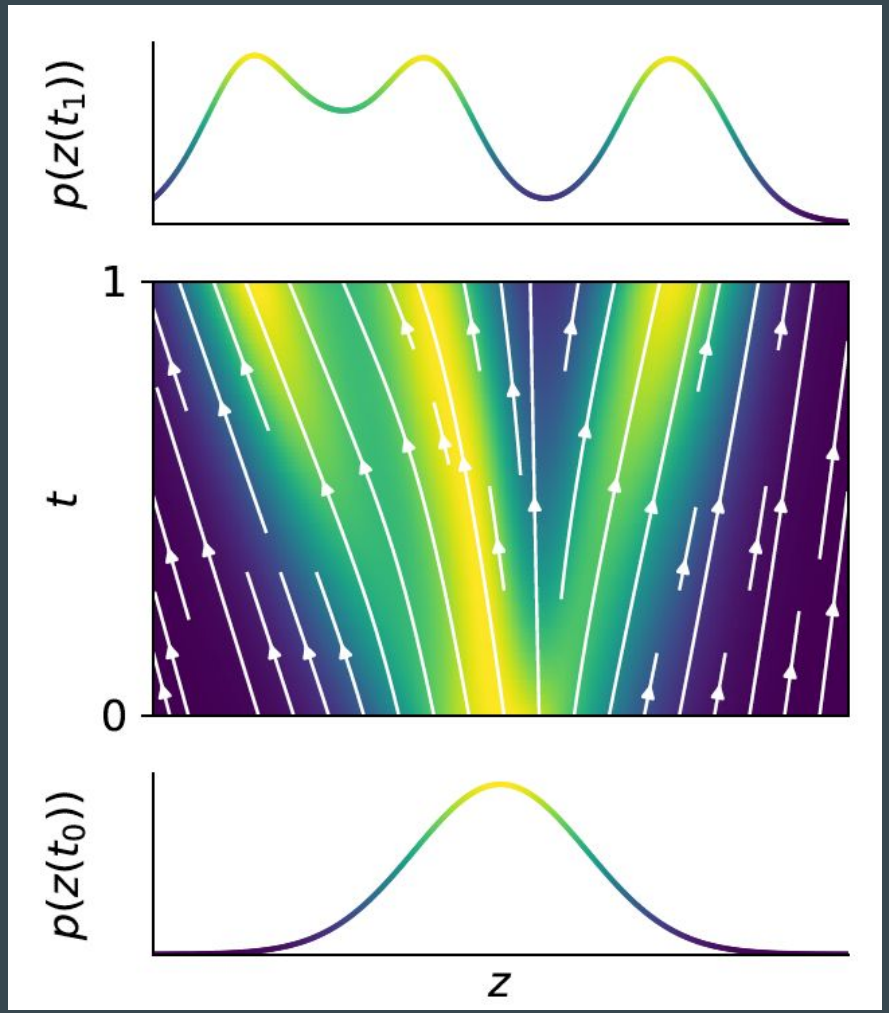
data

prior (IC)



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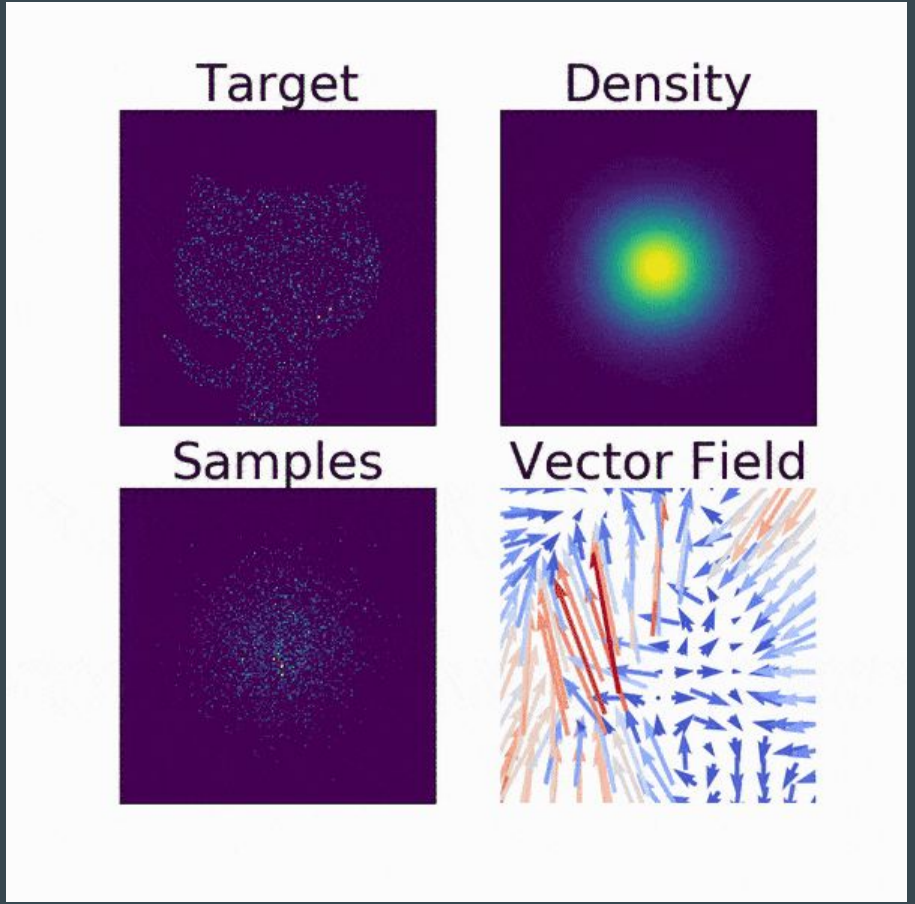
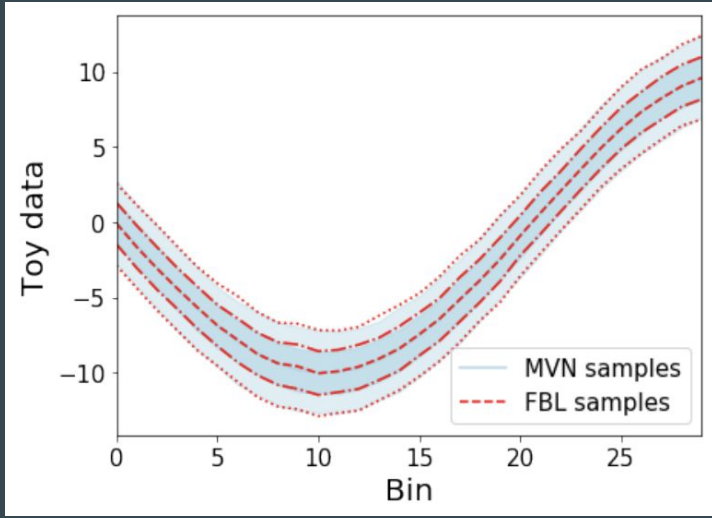
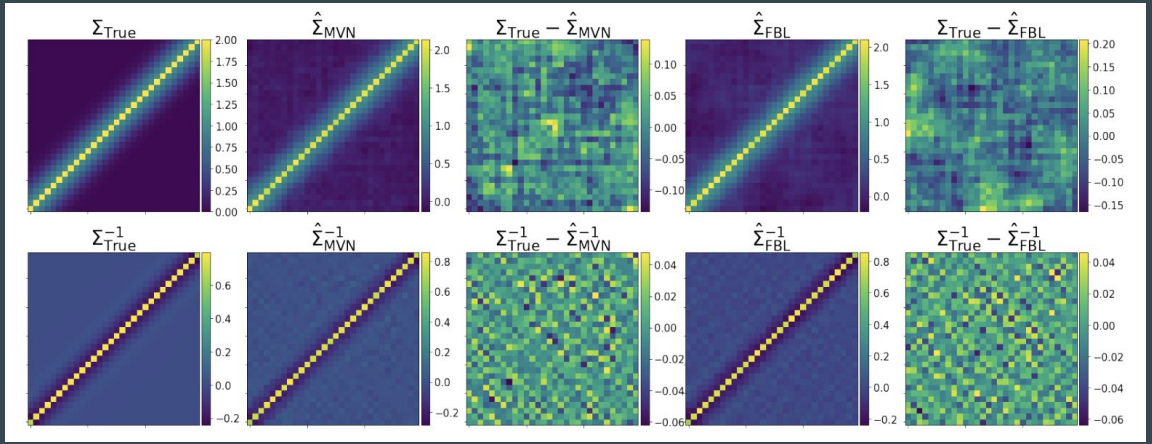
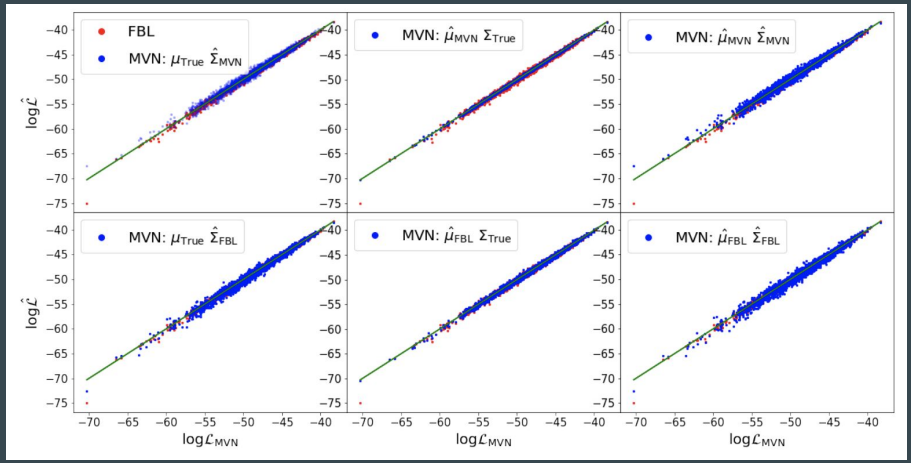


Samples vs likelihood quality

Non-singular covariance



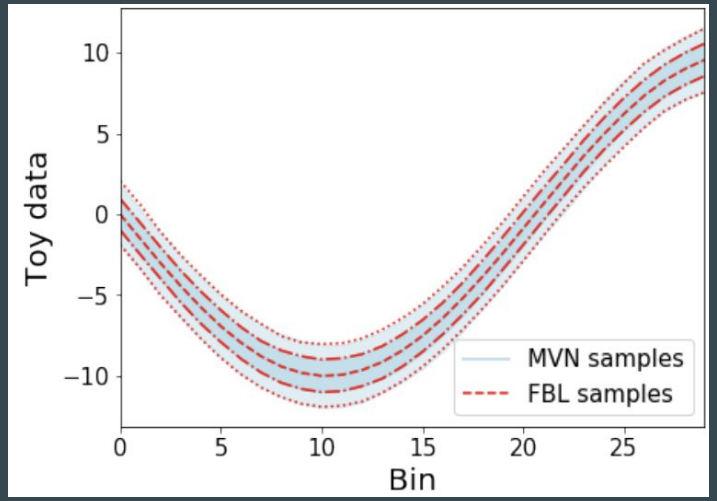


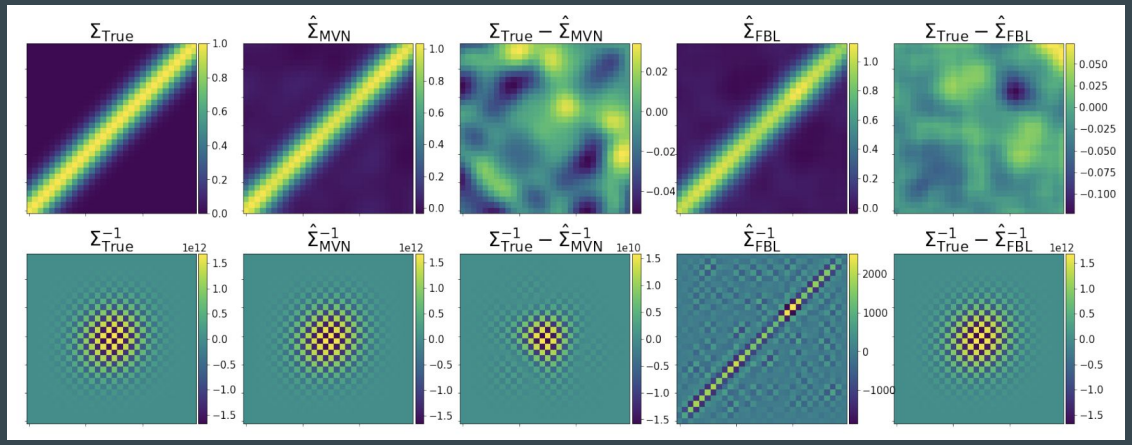


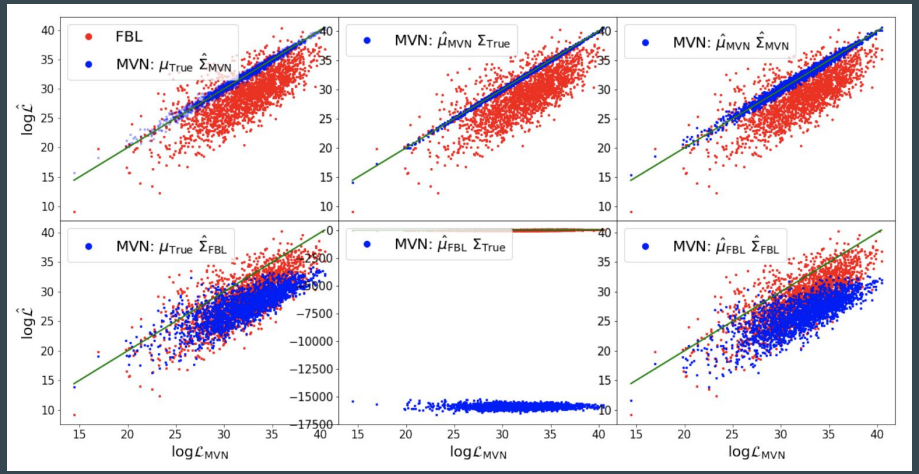
Diaz Rivero & Dvorkin (2020)

Samples vs likelihood quality

Singular covariance







Diaz Rivero & Dvorkin (2020)

Quantifying non-Gaussianity in a dataset

We propose identifying non-Gaussianities (NG) in three ways:

1. ***t*-statistic of skewness and excess kurtosis for every bin in the data**

$$t = \frac{\hat{\beta} - \beta_{\text{null}}}{\text{SE}(\hat{\beta})}$$

0 for a Gaussian

Diaz Rivero & Dvorkin (2020)

Quantifying non-Gaussianity in a dataset

We propose identifying non-Gaussianities (NG) in three ways:

2. **Transcovariance matrix (Sellentin+ 2018)**, which considers the Gaussianity of all pairs of data points

$$s_i^{u,v} = x_i^u + x_i^v$$

$$\frac{1}{b}\sum_{a=1}^{b}[\mathcal{K}(s_a^{u,v}) - \mathcal{N}(0,2)]^2 \equiv S_{u,v}^{+}$$

$$\epsilon_u^{+} = \sum_{v \neq u} S_{u,v}^{+}$$

Should be equal for whitened Gaussian data

Total non-Gaussian contamination for each bin

Diaz Rivero & Dvorkin (2020)

Quantifying non-Gaussianity in a dataset

We propose identifying non-Gaussianities (NG) in three ways:

3. **KL divergence of (the data w.r.t. a MVN)** vs (MVN with itself) (Hahn+ 2018)

$$D_{n,m}(p||q) = \int p(\mathbf{x}) \log \frac{p(\mathbf{x})}{q(\mathbf{x})} d\mathbf{x}$$

$$\hat{D}_{n,m}(p||q) = \frac{d}{n} \sum_{i=1}^{n} \log \frac{\nu_k(i)}{\rho_k(i)} + \log \frac{m}{n-1}$$

Unbiased kNN estimator (Wang+ 2009)

Diaz Rivero & Dvorkin (2020)

Quantifying non-Gaussianity in a dataset

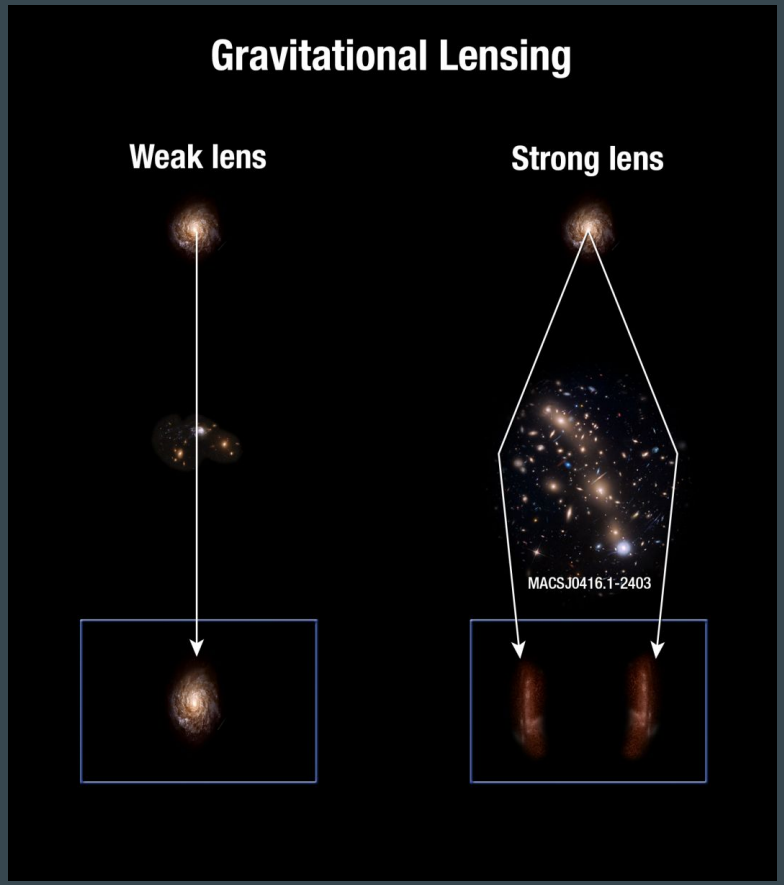
Going forward we will:

1. Apply these three tests to a mock dataset to look at the different ways in which NG can manifest themselves.

2. Generate samples from the three DDLs to assess whether each likelihood has successfully captured the NGs.

Diaz Rivero & Dvorkin (2020)

Weak gravitational lensing



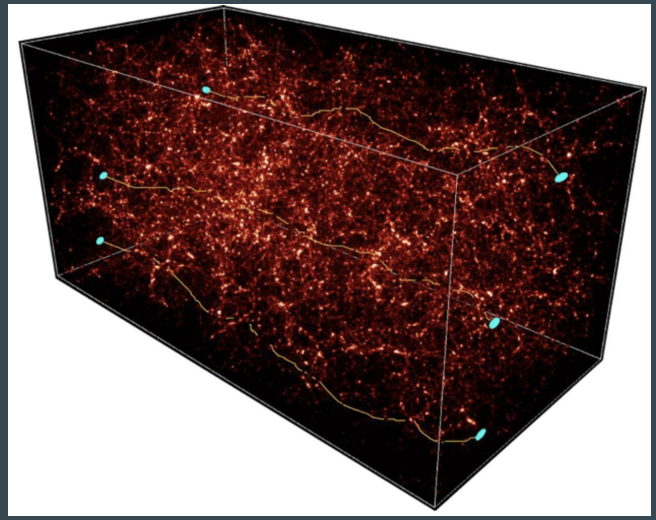
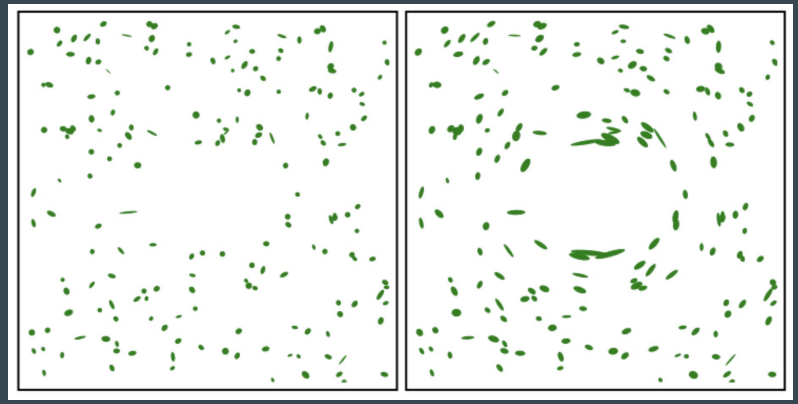


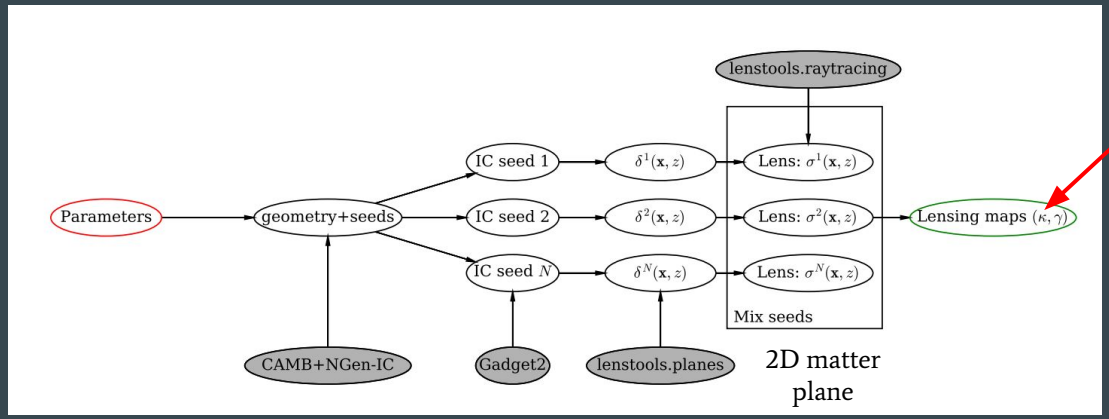
Figure credit: HETDEX

Statistical correlations in the shapes of millions of galaxies



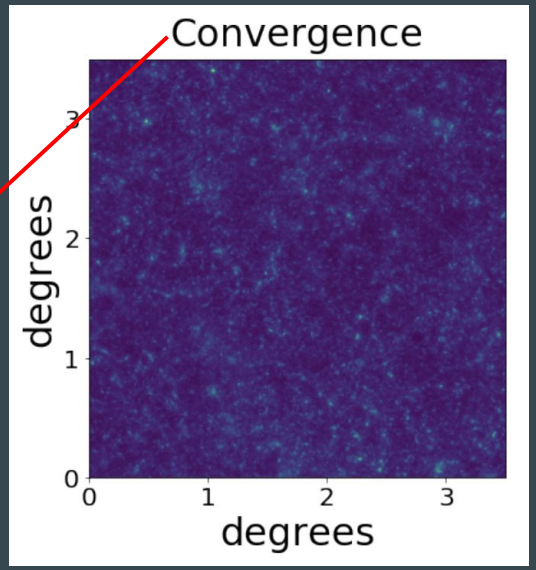
Simulated weak lensing data

Simulated 75,000 mock convergence maps using LensTools (Petri 2016)



Petri (2016)

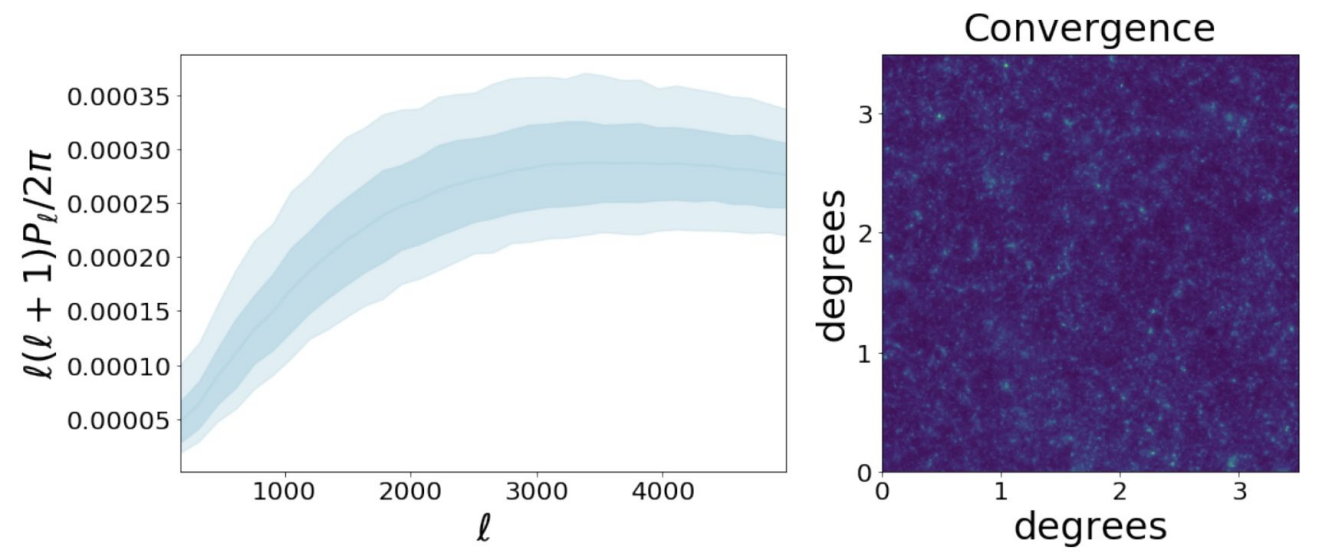
3D matter distribution (*N*-body sim)



Simulated weak lensing data

Simulated 75,000 mock convergence maps using LensTools (Petri 2016) and calculated the weak lensing convergence power spectrum:

$$P_\ell = \frac{1}{2\ell+1}\sum_{m=-\ell}^{\ell} |a_{\ell,m}|^2$$



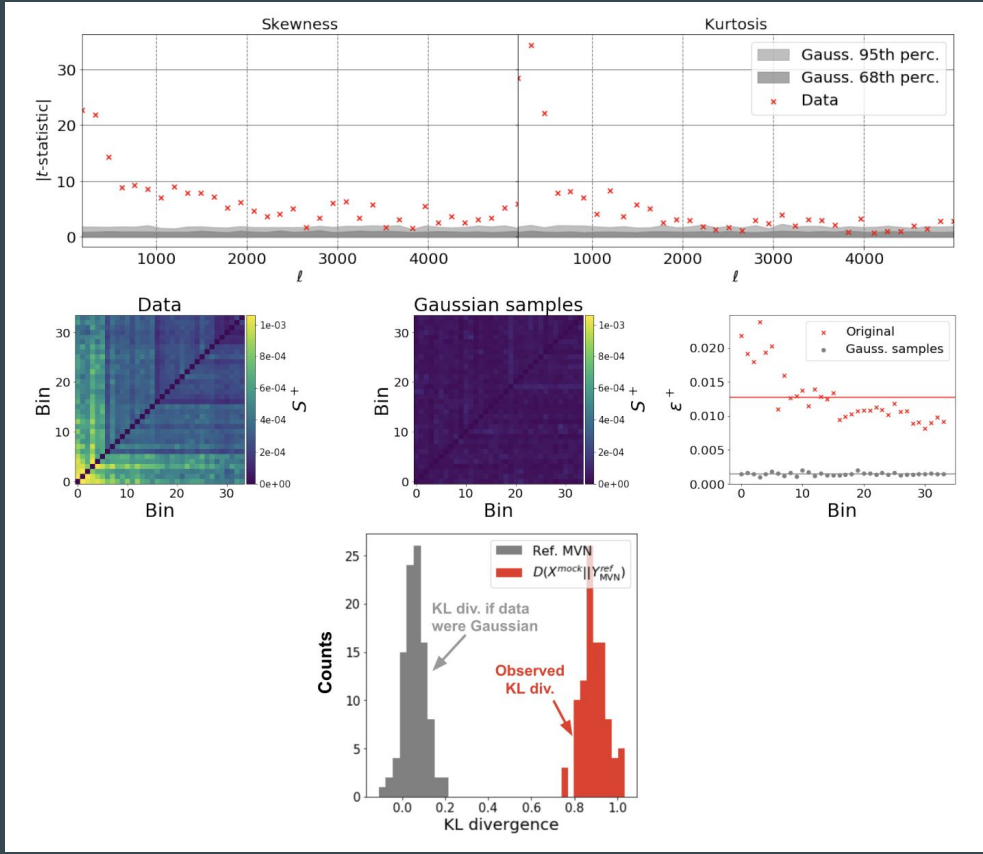
Rivero & Dvorkin (2020)

NG in the weak lensing convergence power spectrum

Test 1: t-stat of skewness and kurtosis

Test 2: transcovariance matrix

Test 3: KL divergence



Diaz Rivero & Dvorkin (2020)

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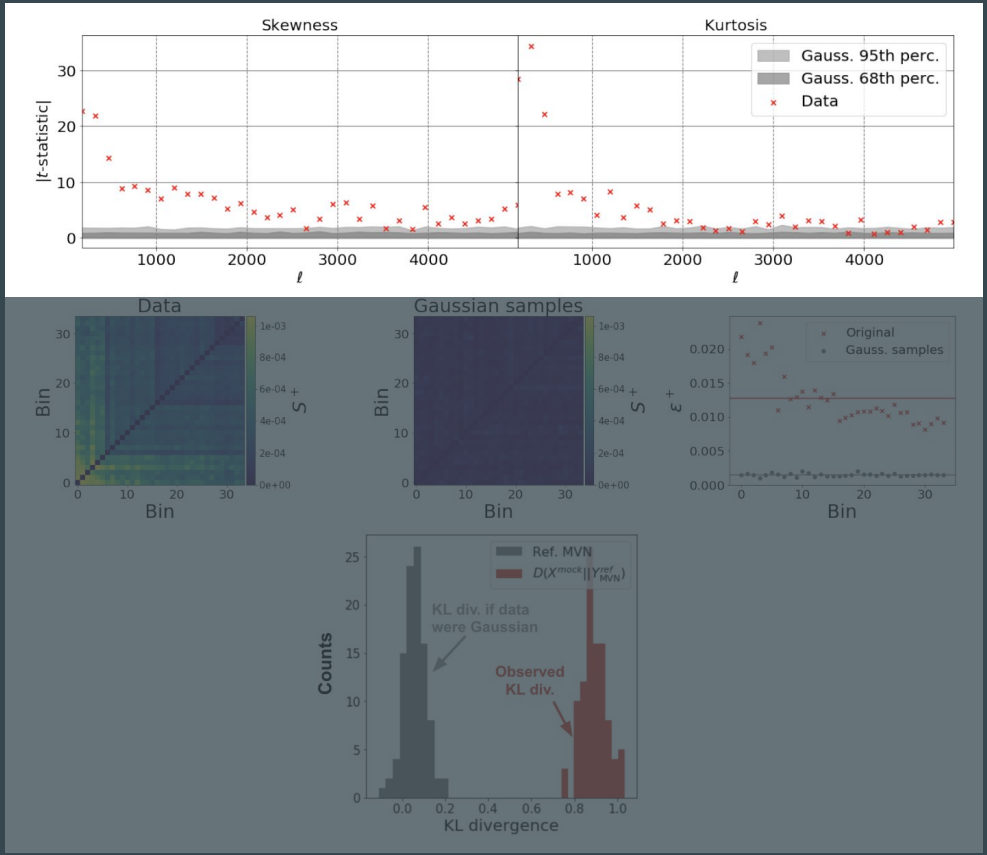

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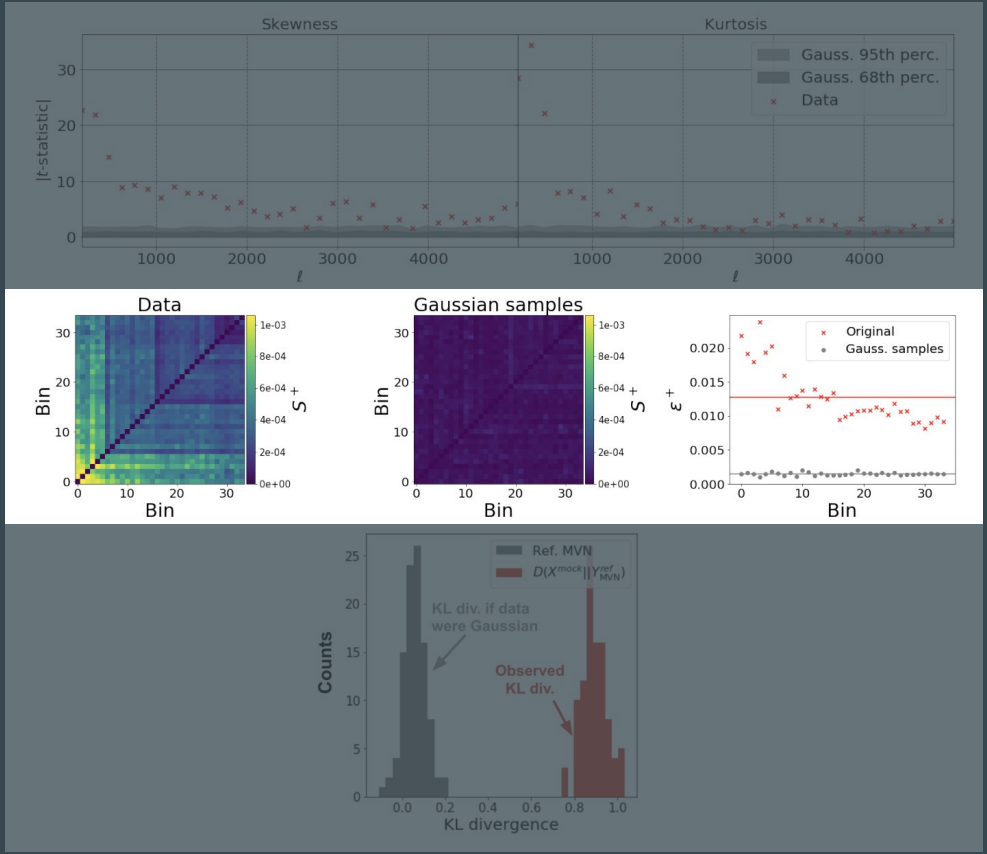

Diaz Rivero & Dvorkin (2020)

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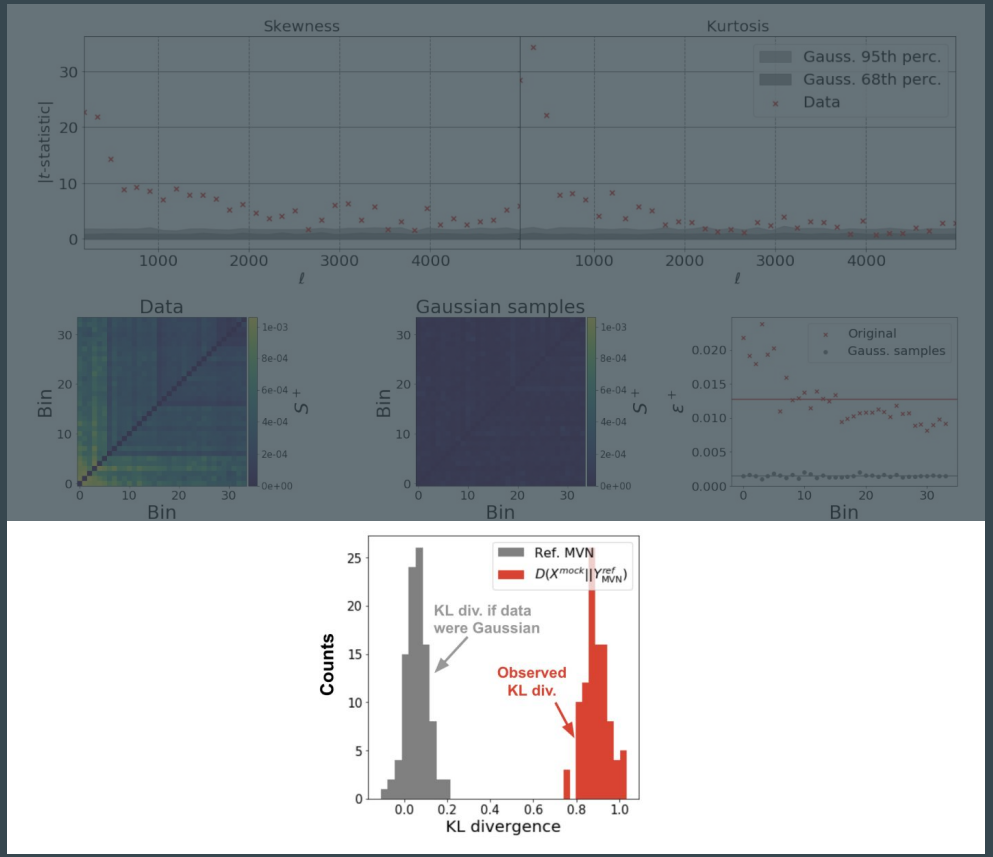
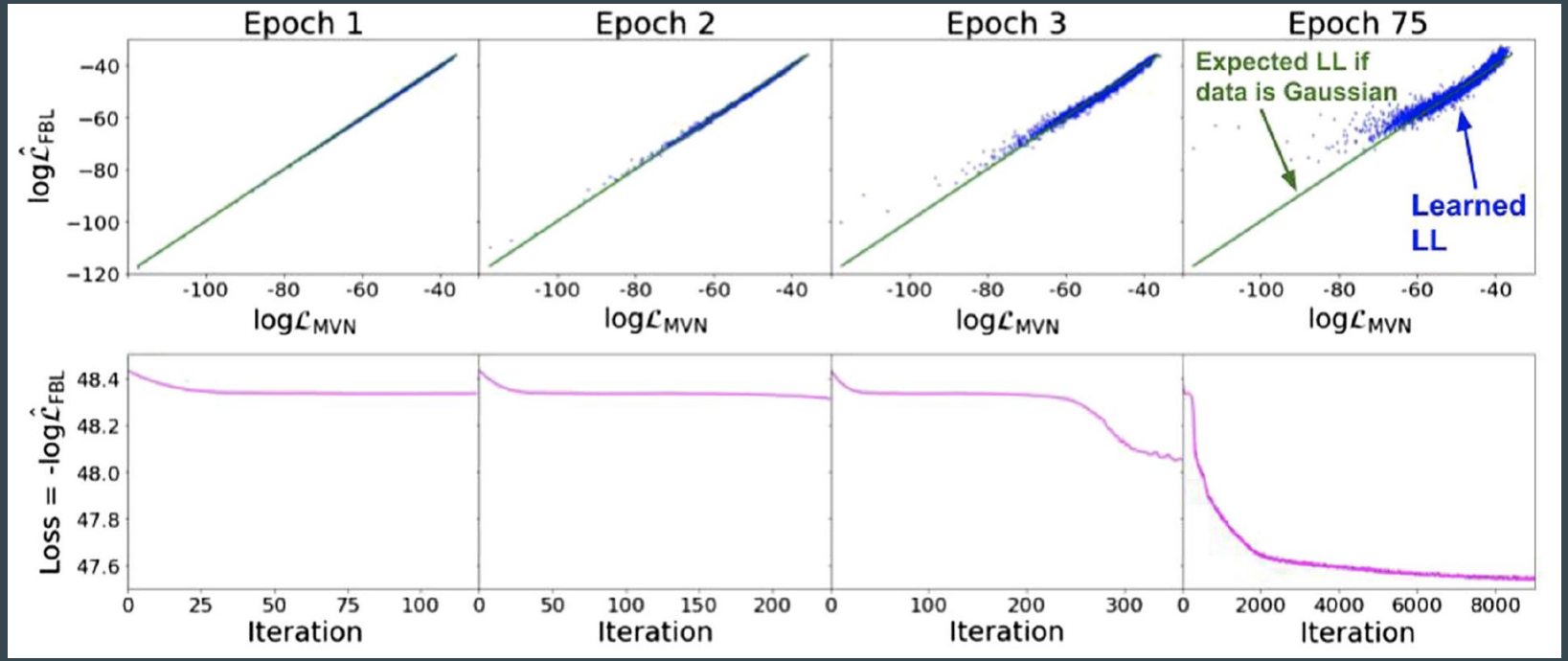


Diaz Rivero & Dvorkin (2020)

FBL for the convergence power spectrum

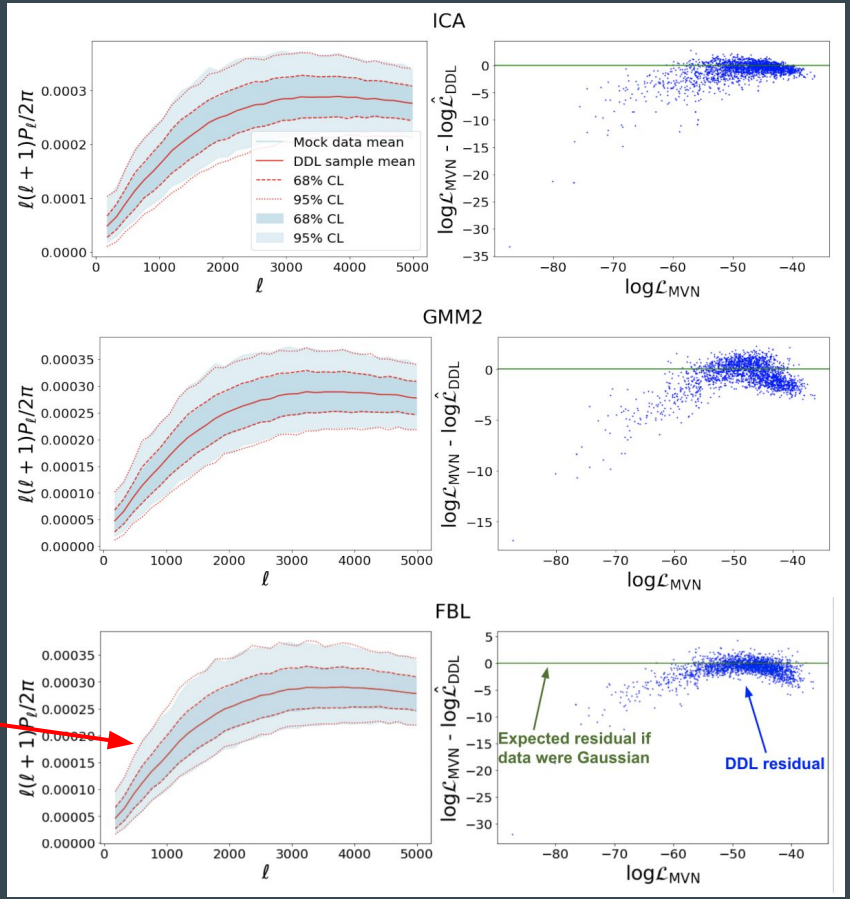
Training the model: whitened data, Adam opt., ELU activation function, 80/10/10 split



Diaz Rivero & Dvorkin (2020)

FBL for the convergence power spectrum

Samples drawn from the DDL



Diaz Rivero & Dvorkin (2020)

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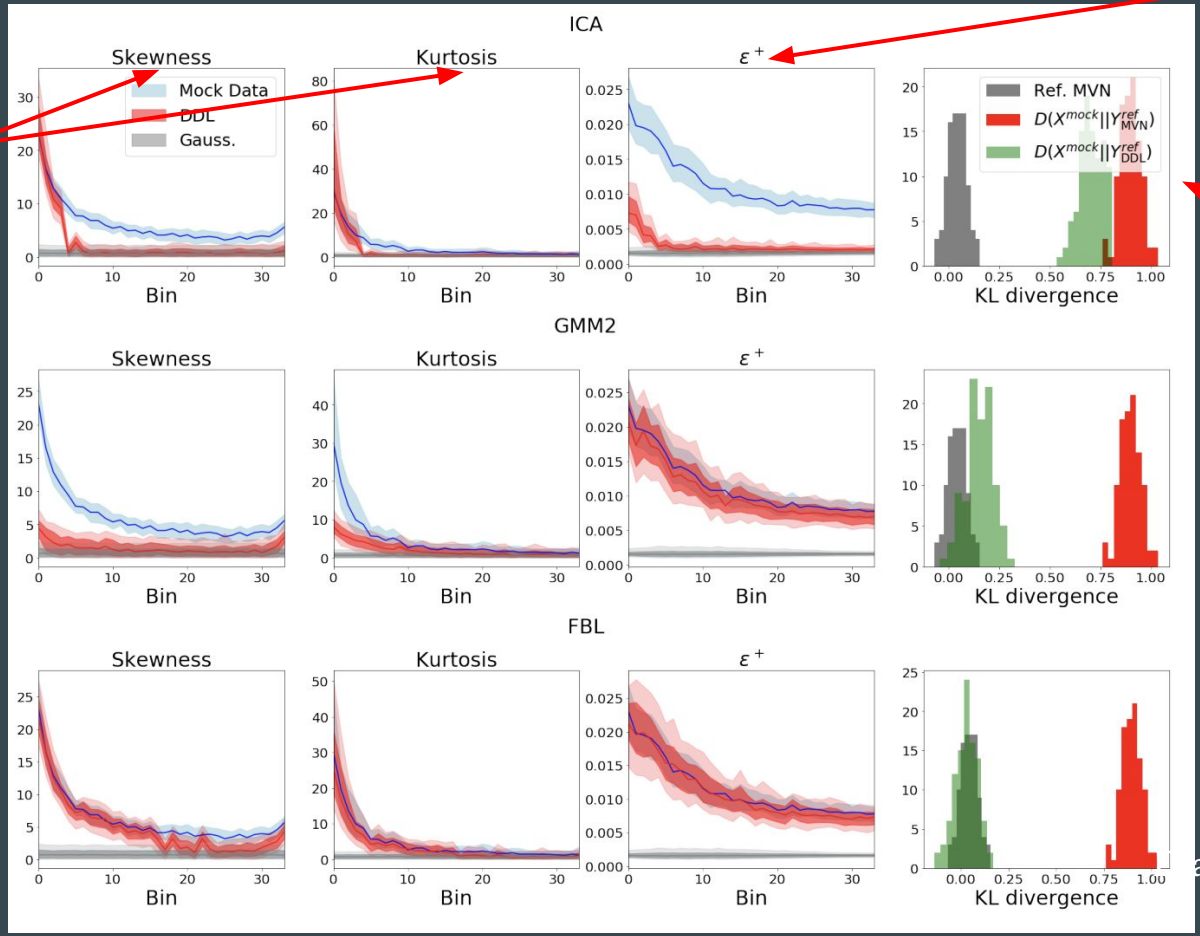

az Rivero & Dvorkin (2020)

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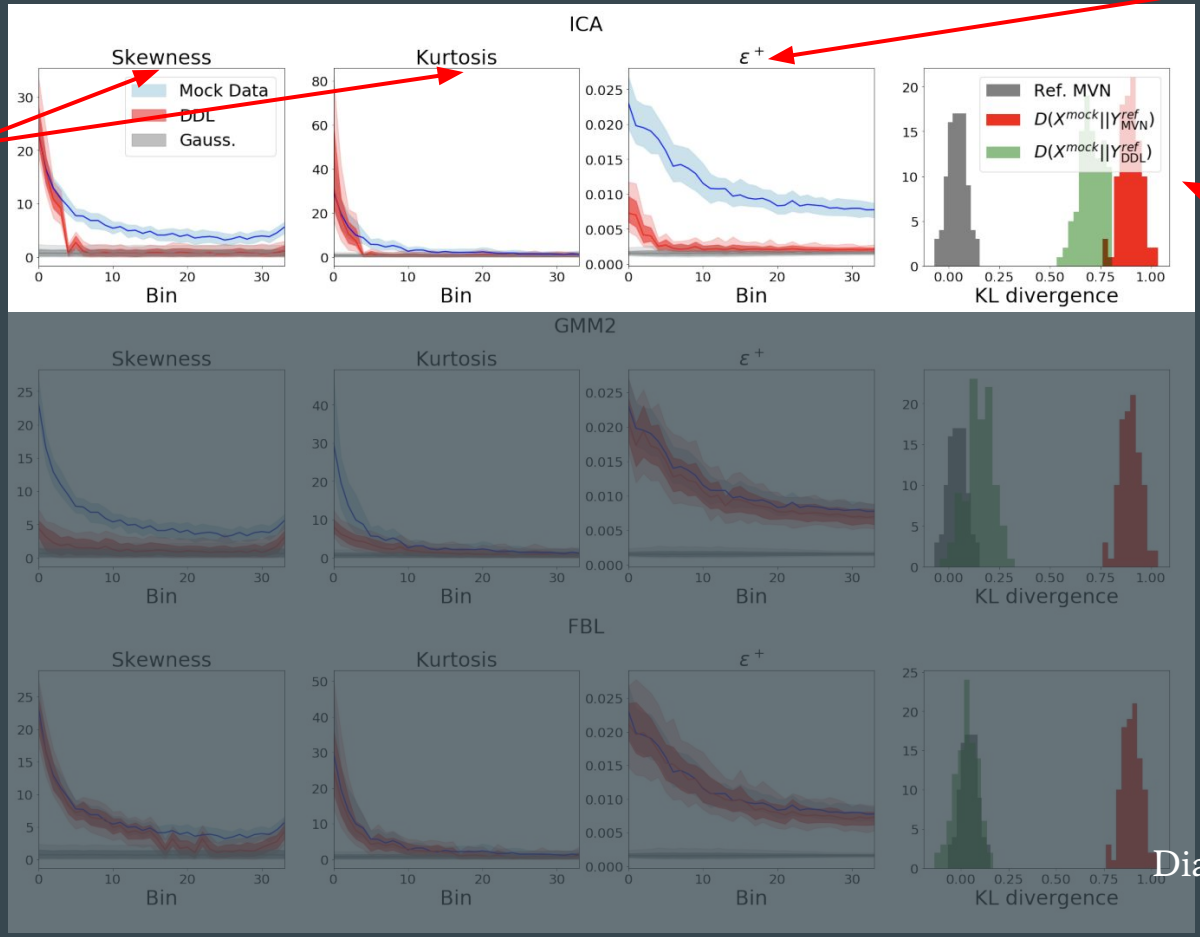
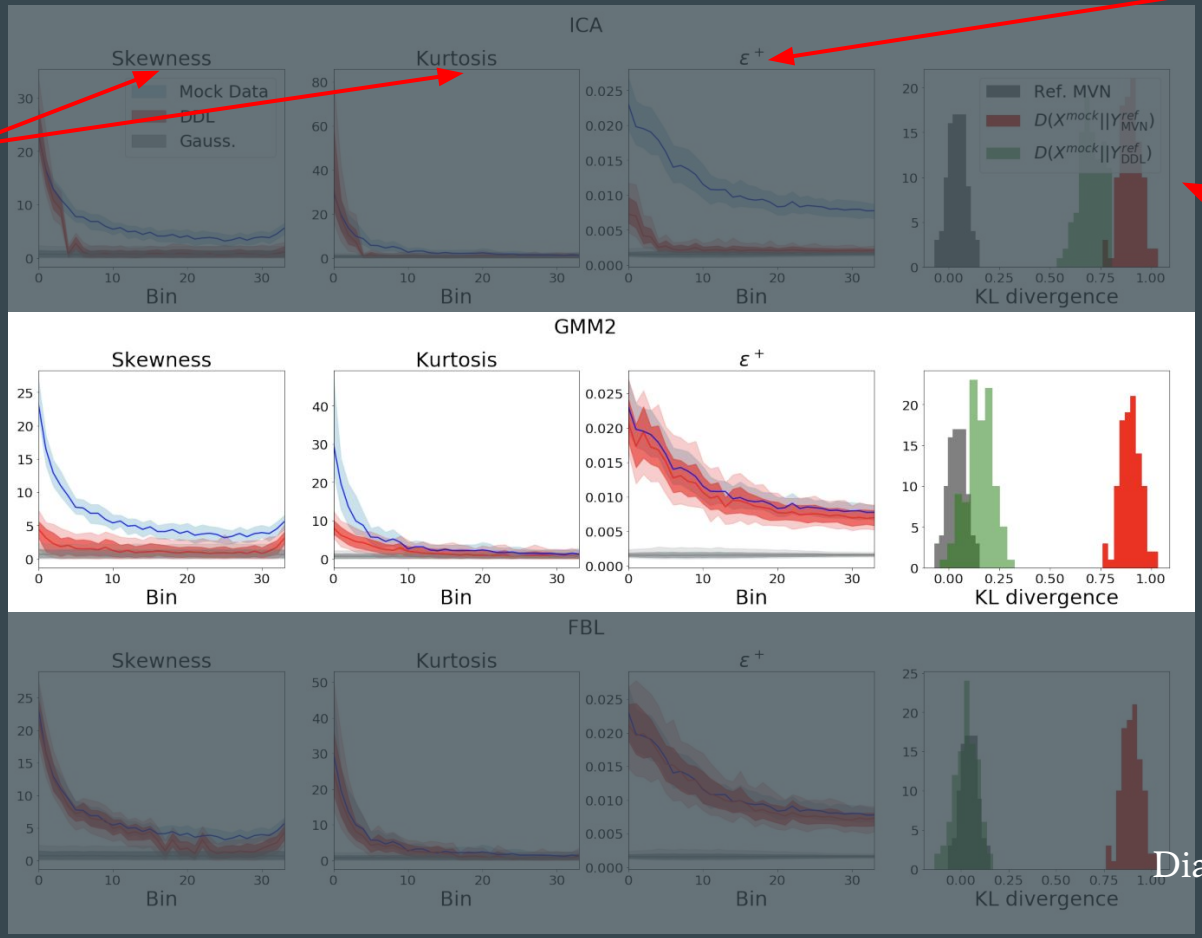


Diaz Rivero & Dvorkin (2020)

FBL for the convergence power spectrum

Test 2: transcovariance matrix

Test 1: t-stat of skewness and kurtosis



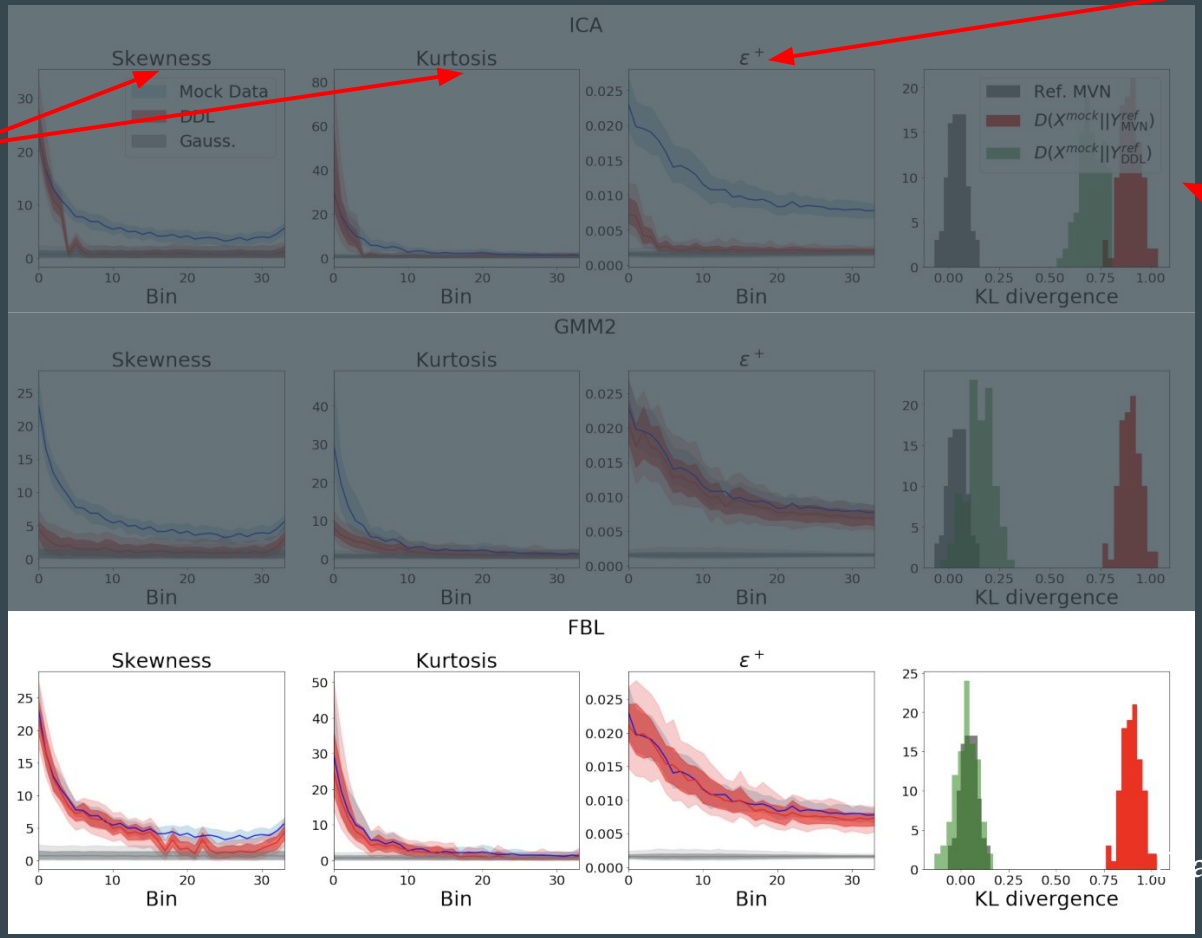
Test 3: KL divergence

Diaz Rivero & Dvorkin (2020)

FBL for the convergence power spectrum

Test 2: transcovariance matrix

Test 1: t-stat of skewness and kurtosis



Test 3: KL divergence

az Rivero & Dvorkin (2020)

Implications

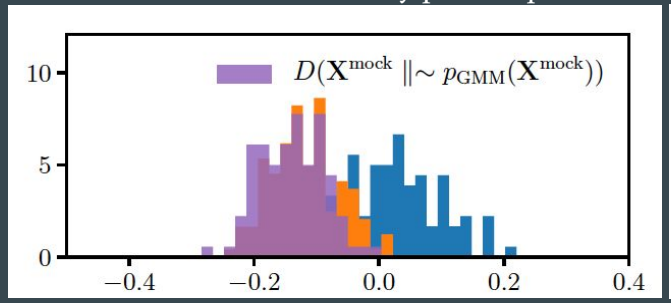
For our mock weak lensing data, GMM and ICA fail at capturing different NG, while the FBL does much better.

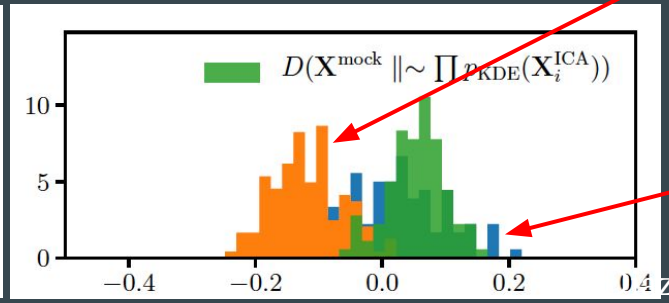
Data volume is not the only thing that determines the success/failure of a DDL: some **understanding of the NG** present in the data is crucial to select the right model.

- E.g. ICA inadequate for NGs across bins

FBL flexibility can preclude them from a trial-and-error procedure that other DDLs can require.

Galaxy power spectrum w/ 2,048 mocks (Hahn+ 2018)





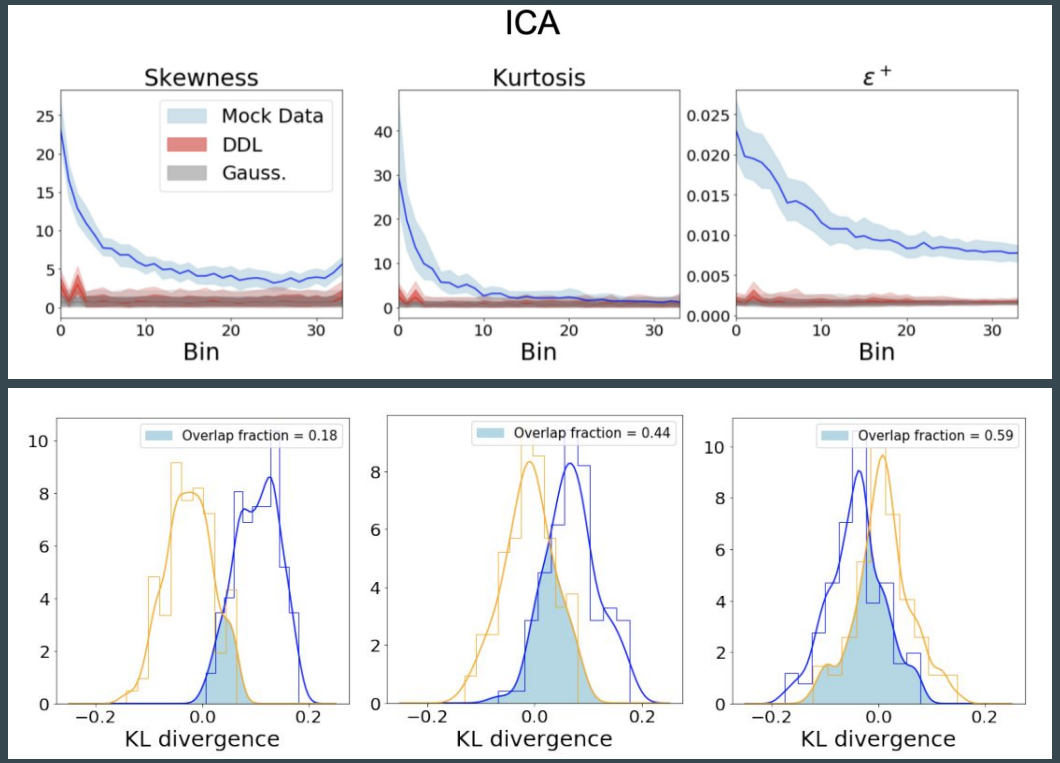
orange = data

Blue = gaussian

z Rivero & Dvorkin (2020)

Implications

But **data volume** obviously matters too! With 2,048 mocks...



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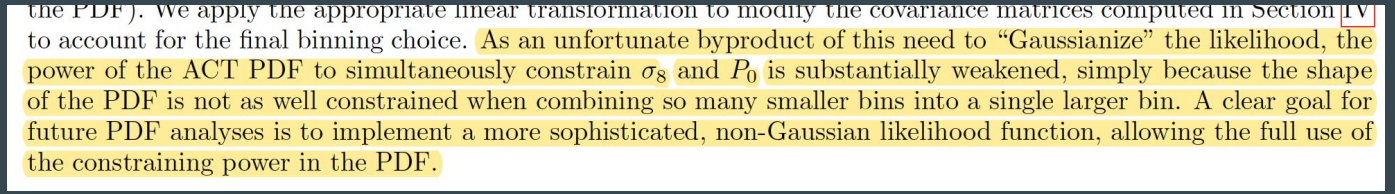
Implications

WL in particular is interesting because:

- Seems to have some **significant non-Gaussianities**, even on scales where cosmic variance doesn't dominate (see also Sellentin+ 2016, 2018 1 & 2).
- Some WL works (inadvertently) **Gaussianize the data** (e.g. combining bins) before inferring parameters, potentially destroying useful information, and conclude NG doesn't shift parameters (Lin+ 2019, Taylor+ 2019, Alsing+ 2019).


the PDF). We apply the appropriate linear transformation to modify the covariance matrices computed in Section IV to account for the final binning choice. As an unfortunate byproduct of this need to "Gaussianize" the likelihood, the power of the ACT PDF to simultaneously constrain σ_8 and P_0 is substantially weakened, simply because the shape of the PDF is not as well constrained when combining so many smaller bins into a single larger bin. A clear goal for future PDF analyses is to implement a more sophisticated, non-Gaussian likelihood function, allowing the full use of the constraining power in the PDF.

ACT Thermal SZ one-point PDF (Hill+, 2015)

- **Shortcomings of ICA** in addressing pairwise non-Gaussian correlations in WL data: works have used ICA dimensionality reduction before inferring parameters from weak lensing data and concluded NG don't impact parameter constraints considerably (Gupta+, 2018).

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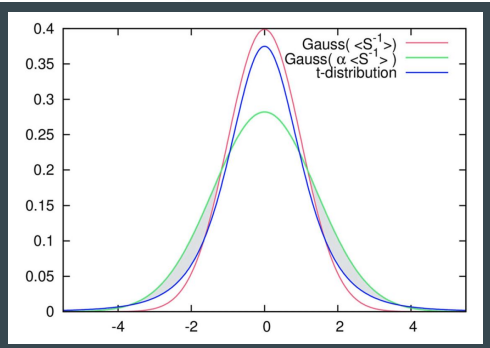
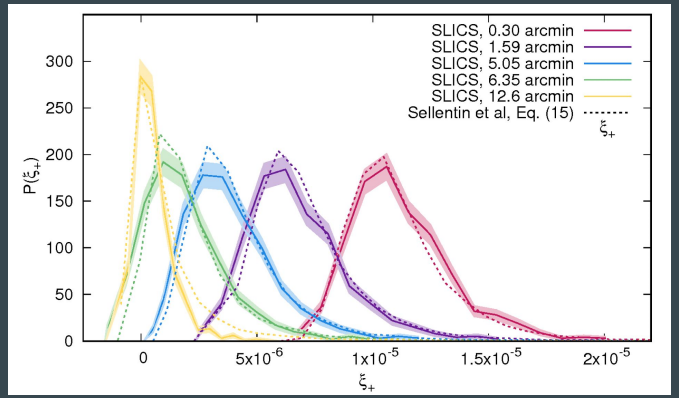
Questions?

Non-Gaussianity in weak lensing data

Estimating covariances
(Sellentin+ 2016)

$$p(\boldsymbol{x}|\boldsymbol{\mu}, \hat{\Sigma}, N) = \int d\Sigma \mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu}, \Sigma)\, p(\Sigma|\hat{\Sigma}, N)$$





Shear correlation function non-Gaussianity (Sellentin+ 2018, 1 & 2)