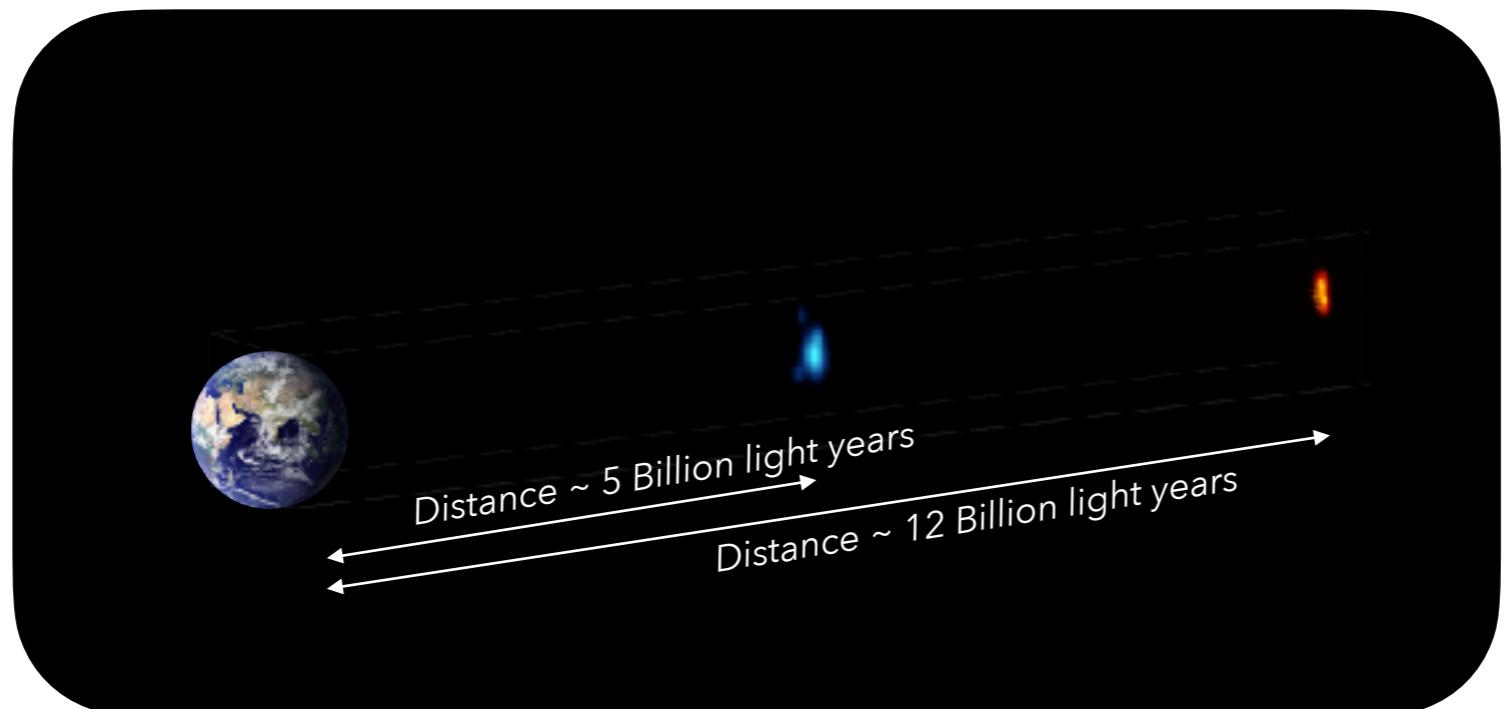


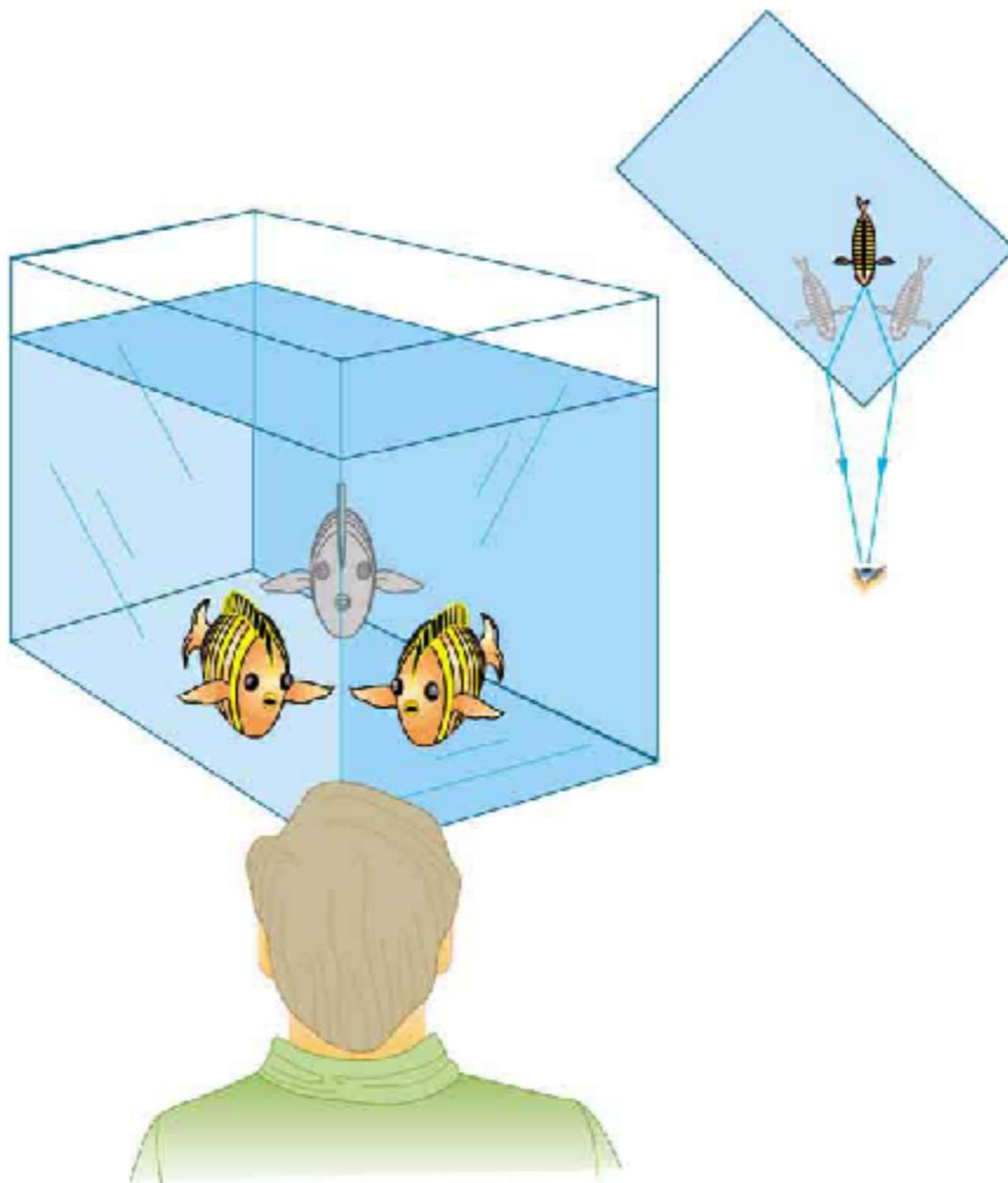
DATA-DRIVEN STRONG GRAVITATIONAL LENSING ANALYSIS IN THE ERA OF LARGE SKY SURVEYS

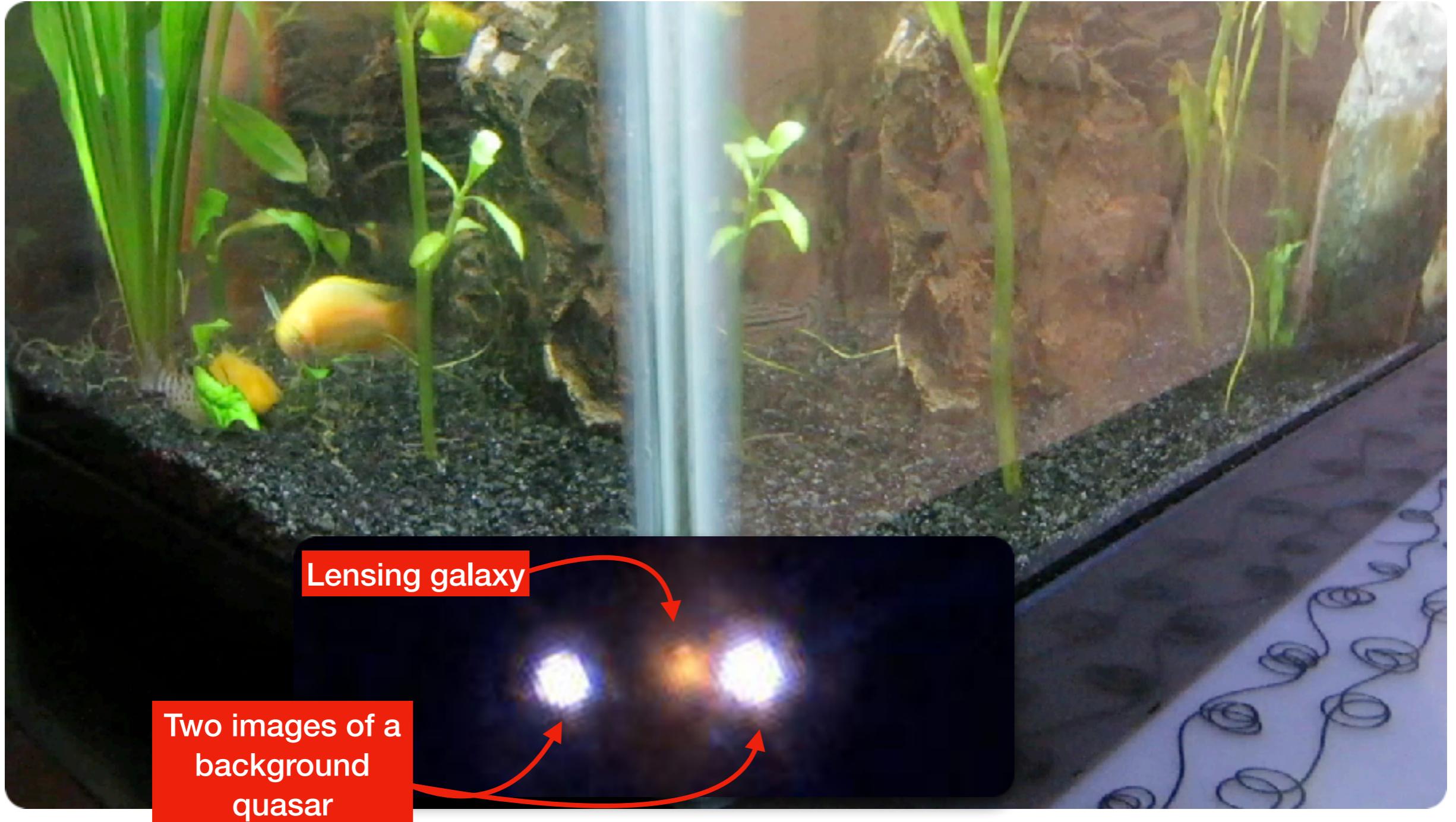
Laurence Perreault-Levasseur

STRONG GRAVITATIONAL LENSING

Formation of **multiple images** of a single distant object due to the **deflection of its light** by the **gravity** of intervening structures.







Lensing galaxy

Two images of a
background
quasar

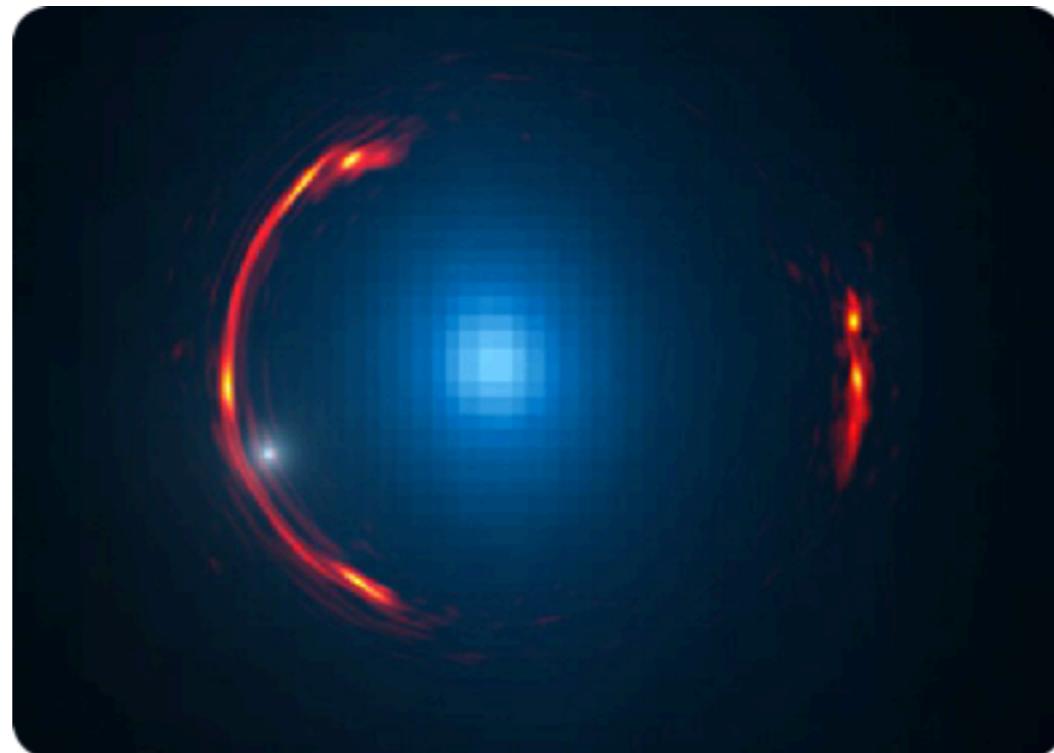




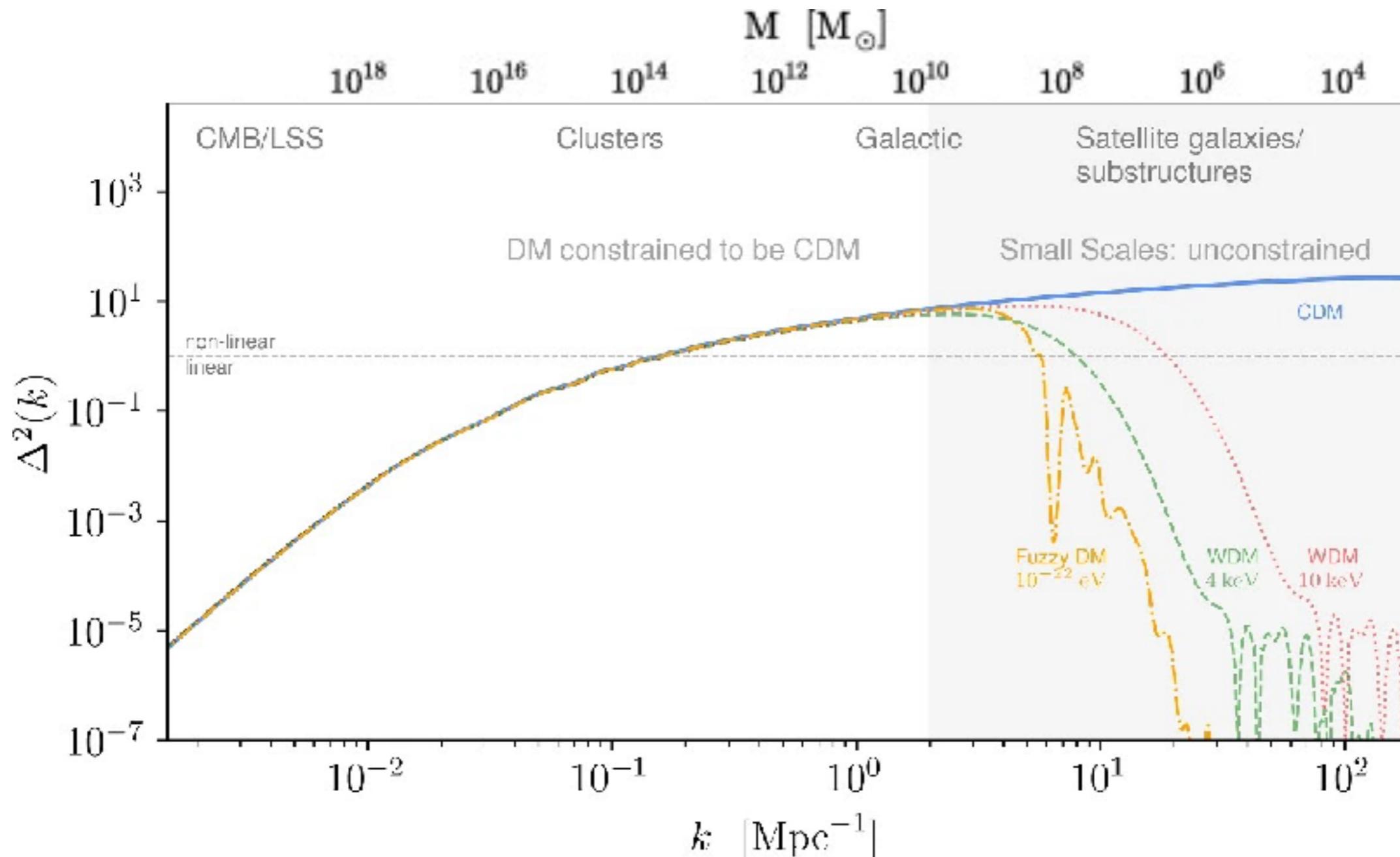
SCIENCE MOTIVATIONS FOR STRONG LENSING

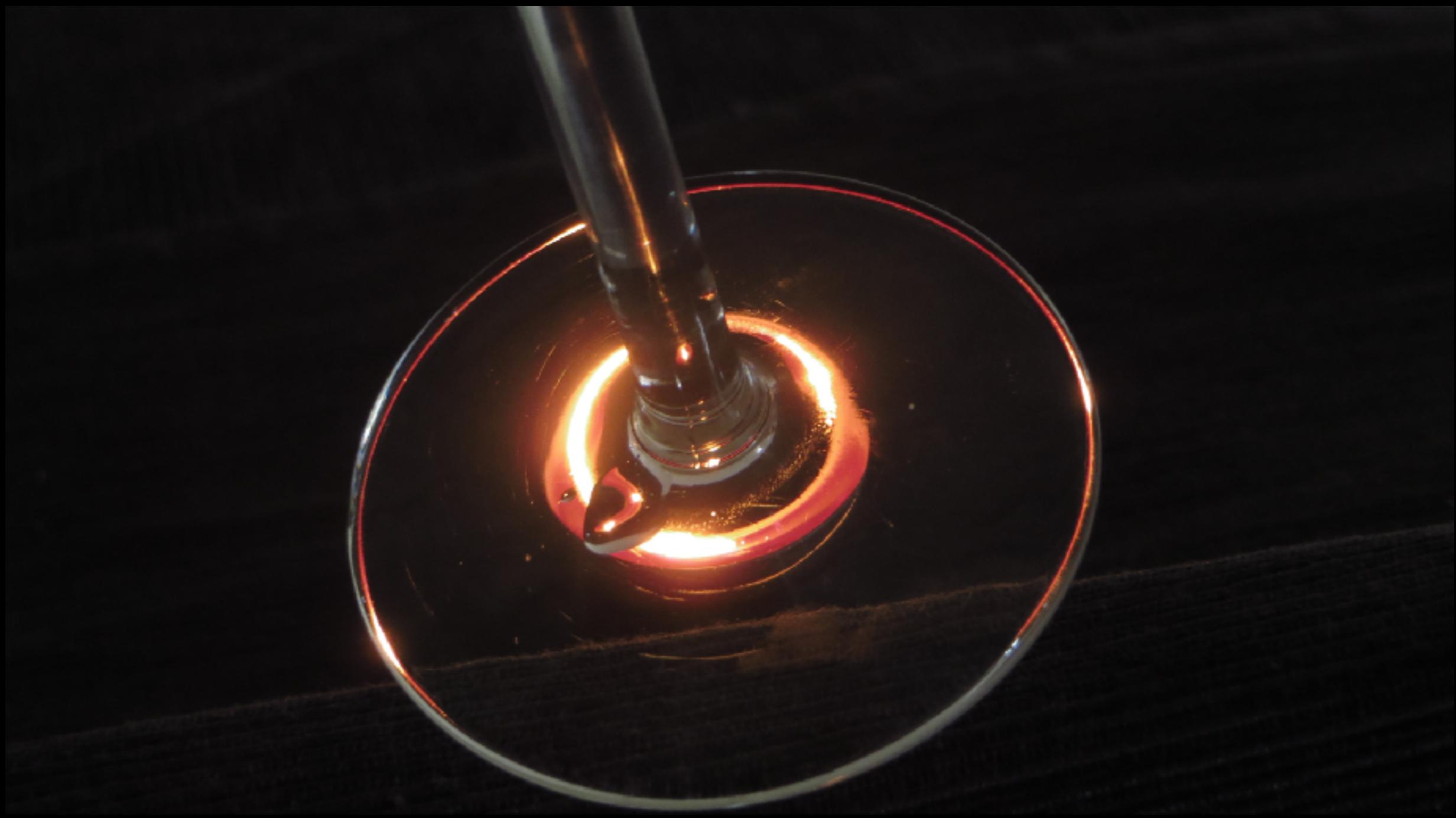
1 - Use lensing to probe the **distribution of matter** in the lensing structures.

- Distortions in images are caused by **gravity**.
- They can be used to map the **distribution of matter** in the lens.
- Particularly useful for studying **dark matter**.



MATTER POWER SPECTRUM

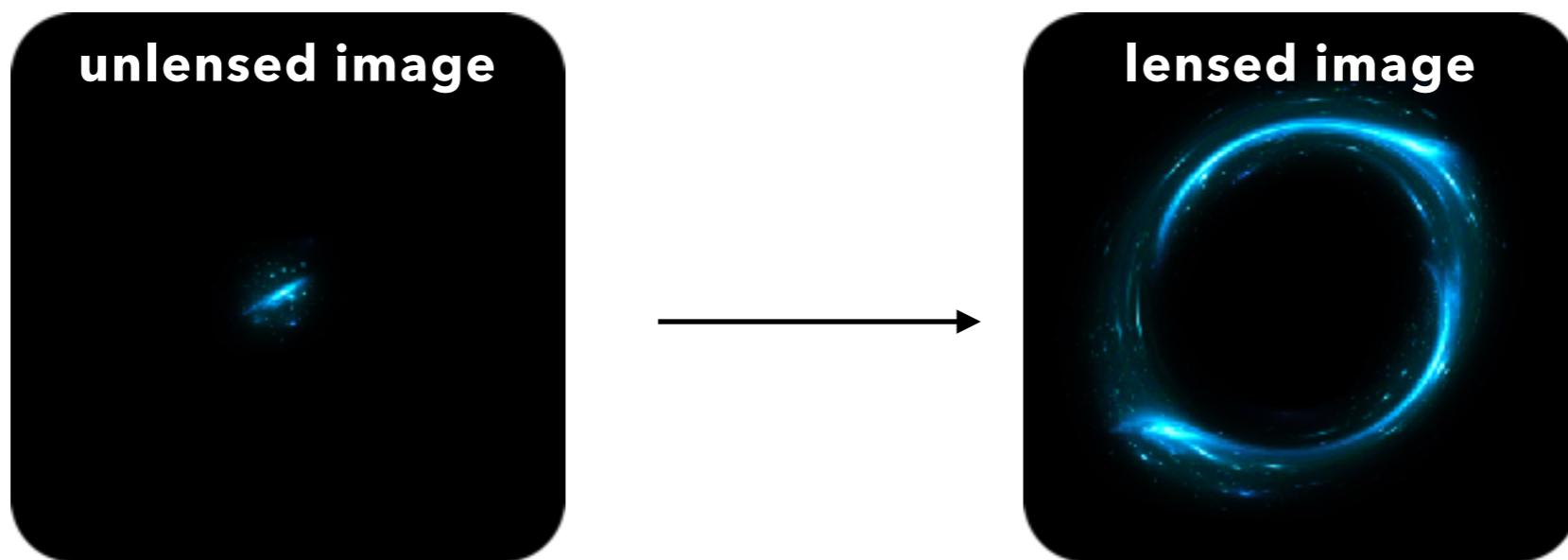




SCIENCE MOTIVATIONS FOR STRONG LENSING

2 - Use strong lensing as a **cosmic telescope**.

- Lensing **magnifies** the images of sources and makes them appear **brighter**.
- This allows us to study some of the most distant galaxies of the universe that would have been otherwise below our sensitivity or resolution limits.



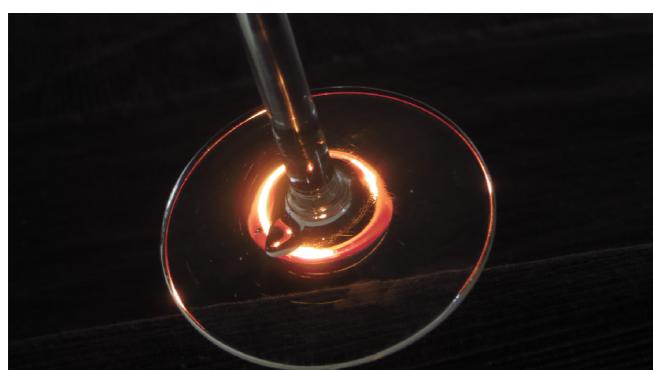
SCIENCE MOTIVATIONS FOR STRONG LENSING

3 - Measure **cosmological parameters** (H_0).

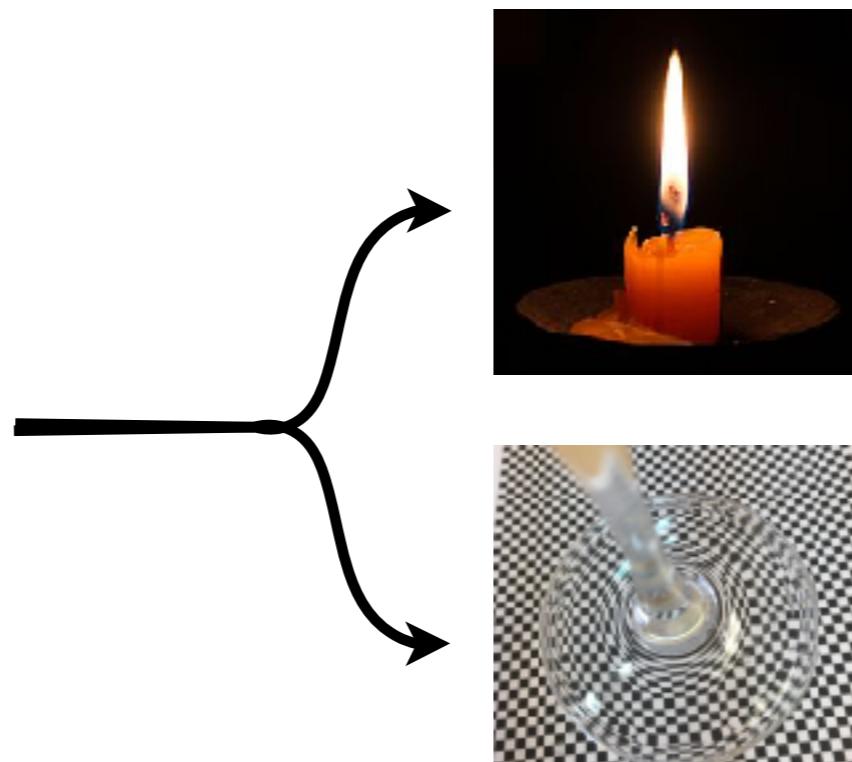
- Different images are produced because light follows **different paths**.
- These paths are of **different lengths**.
- If the source has time variability, this will cause **time delays** between different images.



LENSING ANALYSIS

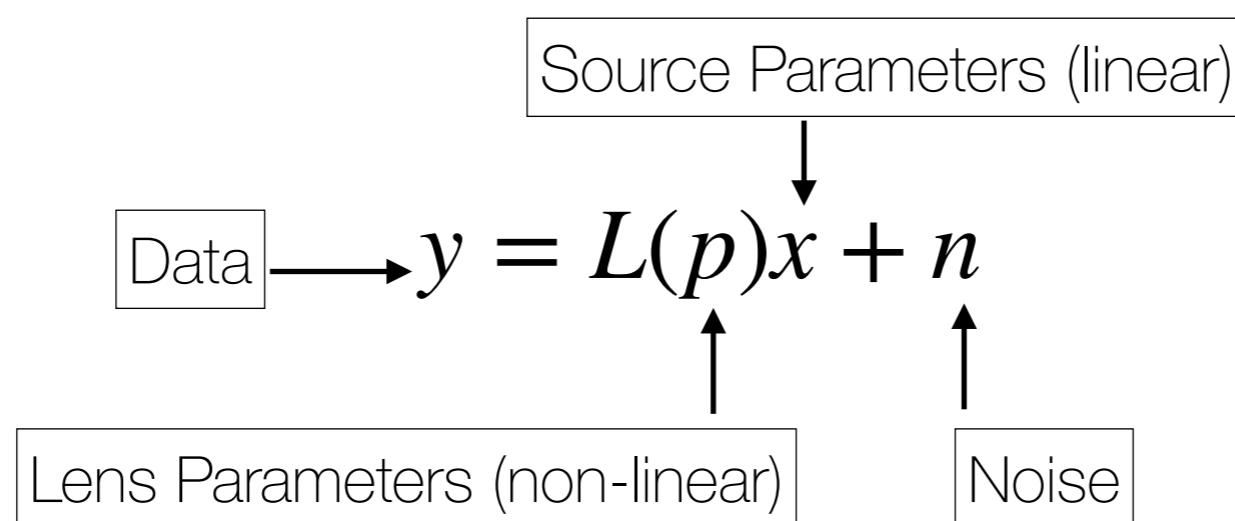


Data



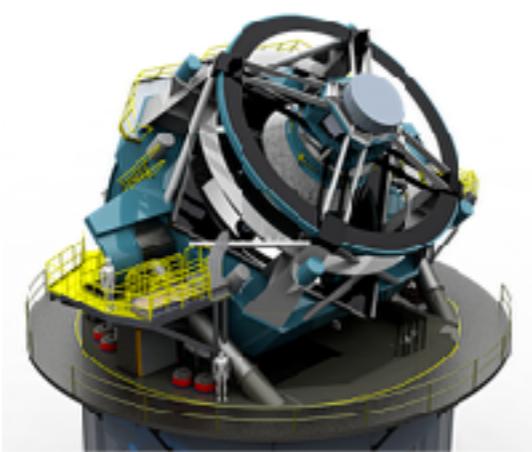
1: Morphology of the background source
(the true, undistorted image of the candle)

2: Matter distribution in the lens
(the shape of the wineglass)

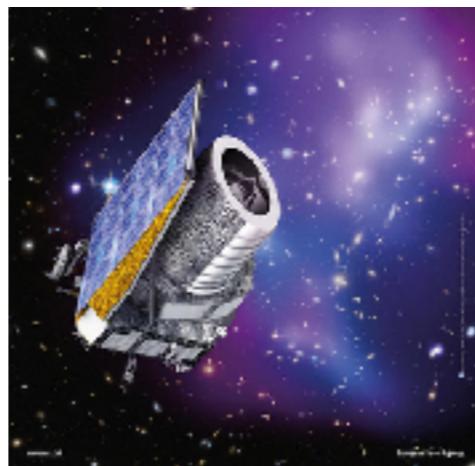


LOOKING INTO THE FUTURE

In the next few years, we're expecting to discover more than 170,000 new lenses.



LSST



Euclid
consortium



NANCY GRACE
Roman
SPACE TELESCOPE

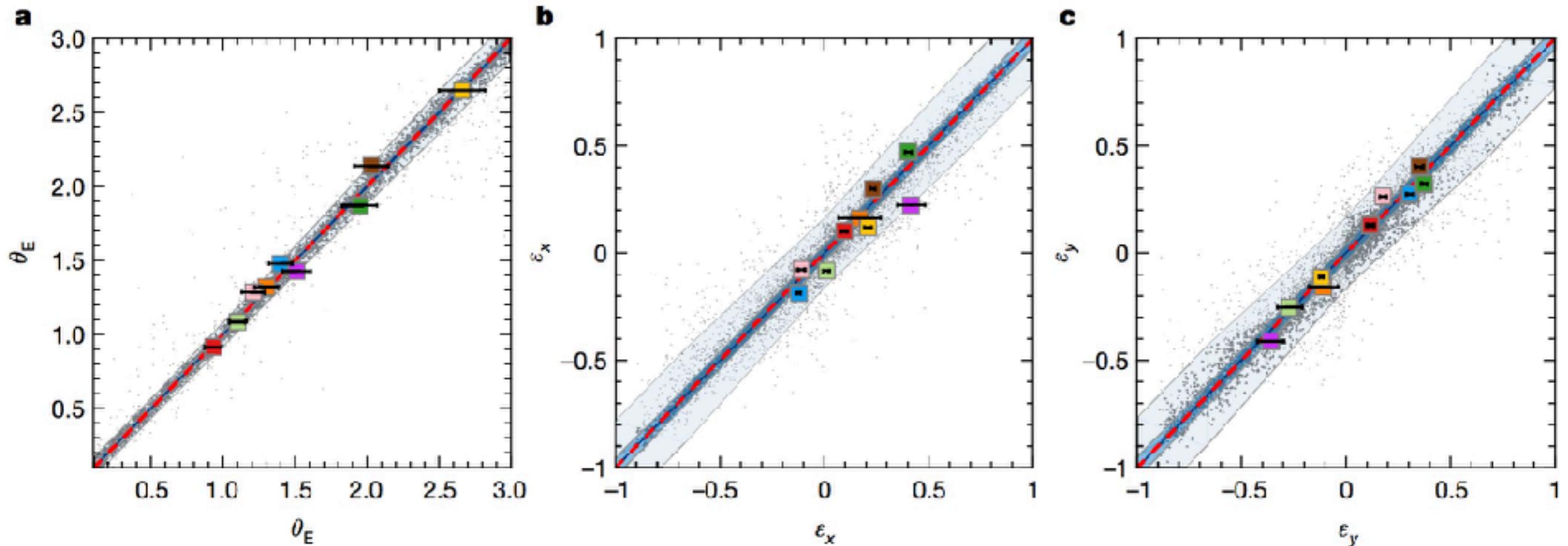
Methods for the future:

How are we going to analyze 170,000 lenses?

- Lens modeling is **very slow**.
- Simple lens model takes ~3 days

=> **1,400 years !**

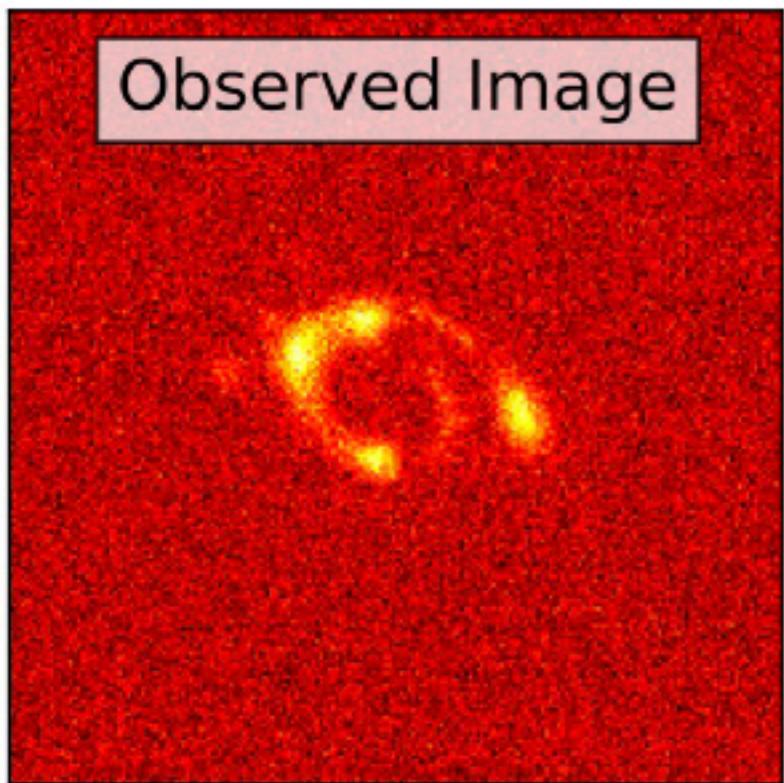
ESTIMATING THE MATTER DISTRIBUTION PARAMETERS WITH CNNS



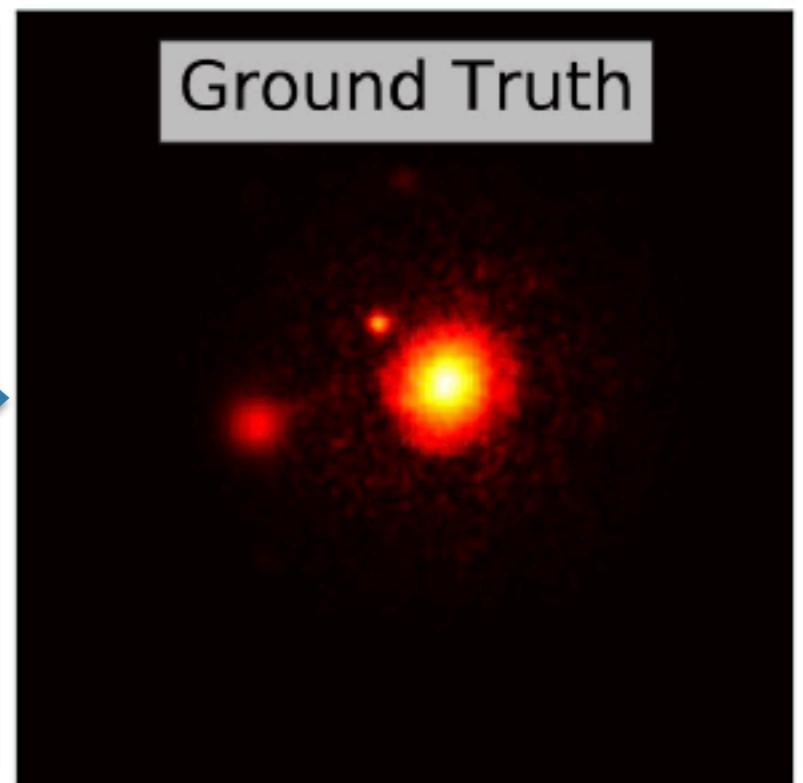
10 million times faster than traditional lens modeling.

0.01 seconds on a **single GPU**

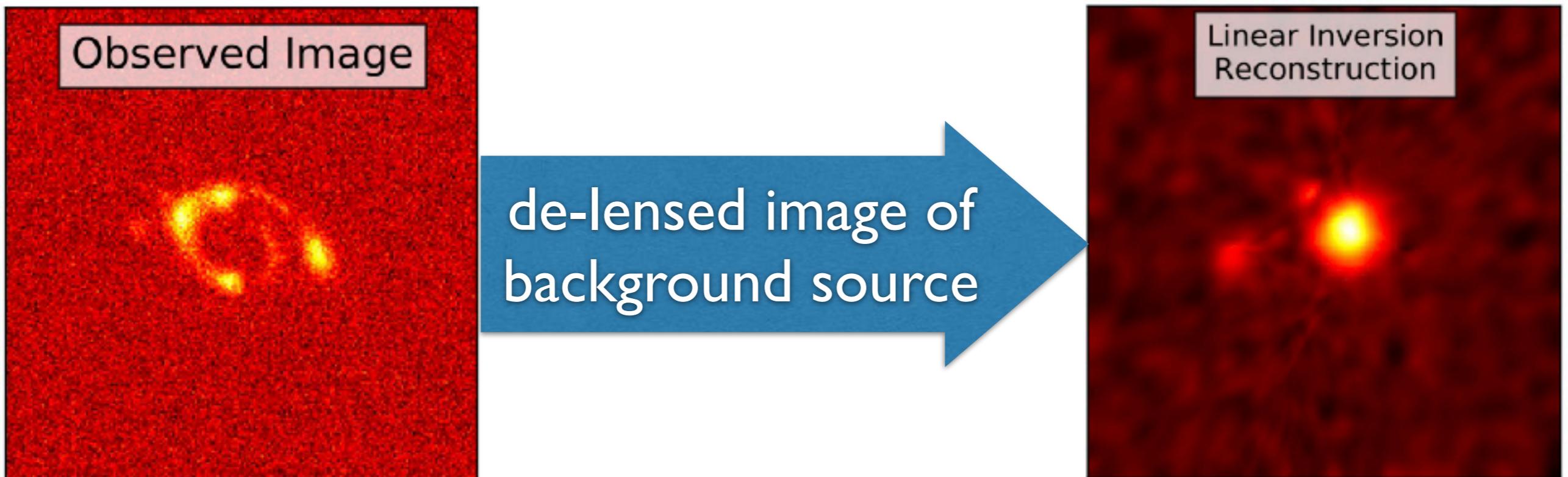
UNDISTORTED IMAGE OF THE BACKGROUND SOURCE



de-lensed image of
background source?

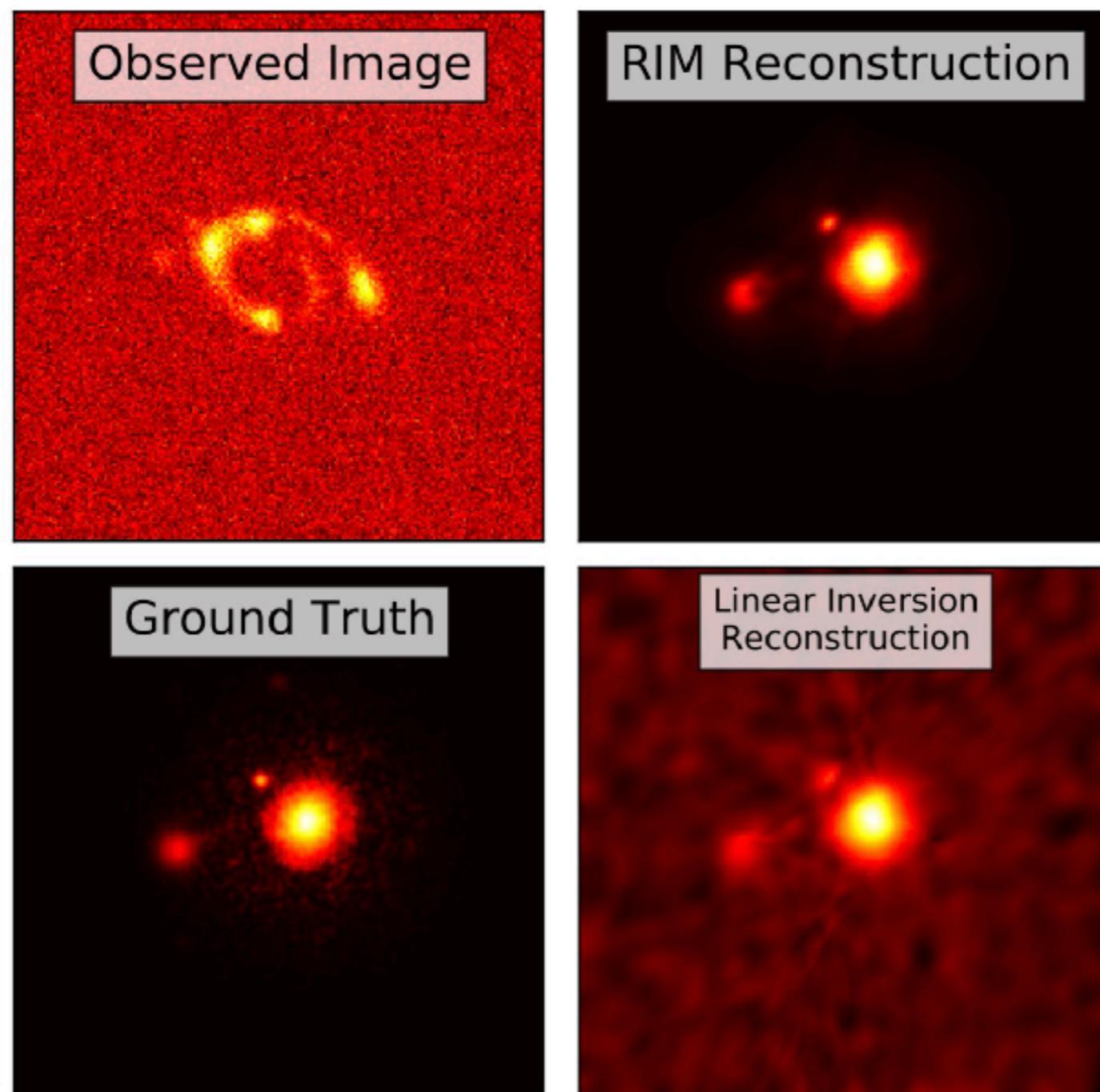


UNDISTORTED IMAGE OF THE BACKGROUND SOURCE

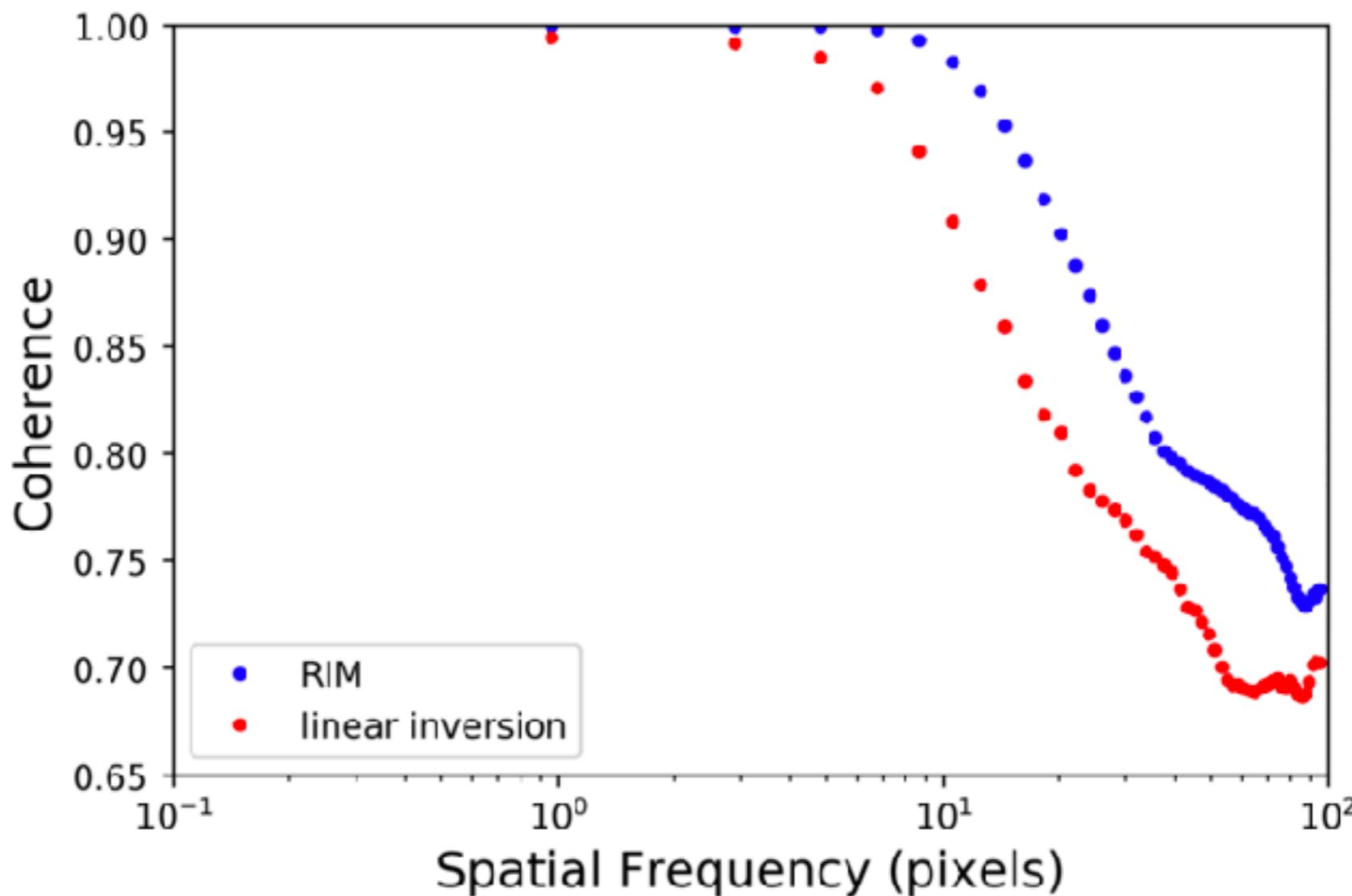


$$S = (L^T C_N^{-1} L + C_p^{-1})^{-1} L^T C_N^{-1} D$$

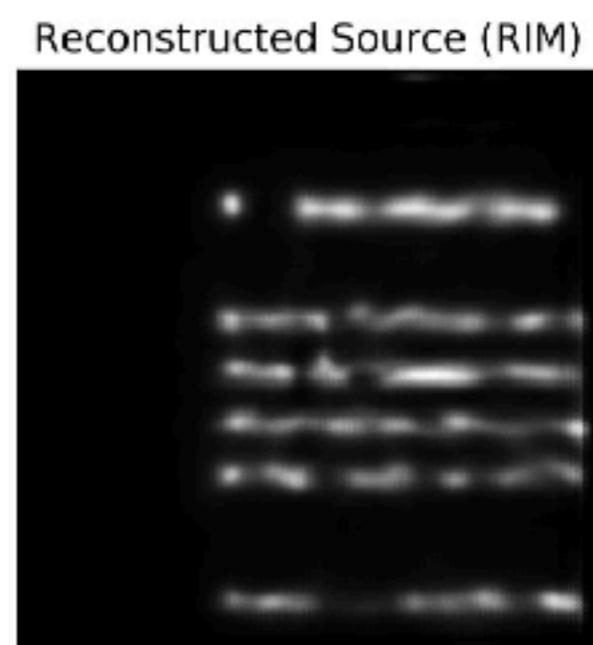
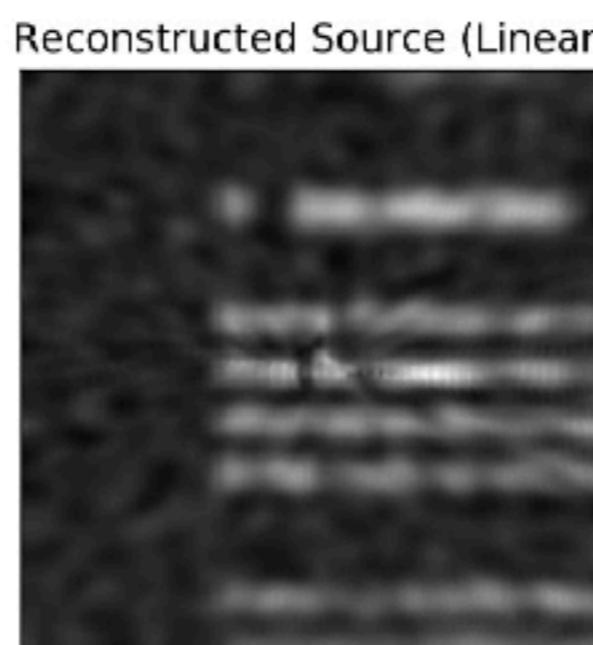
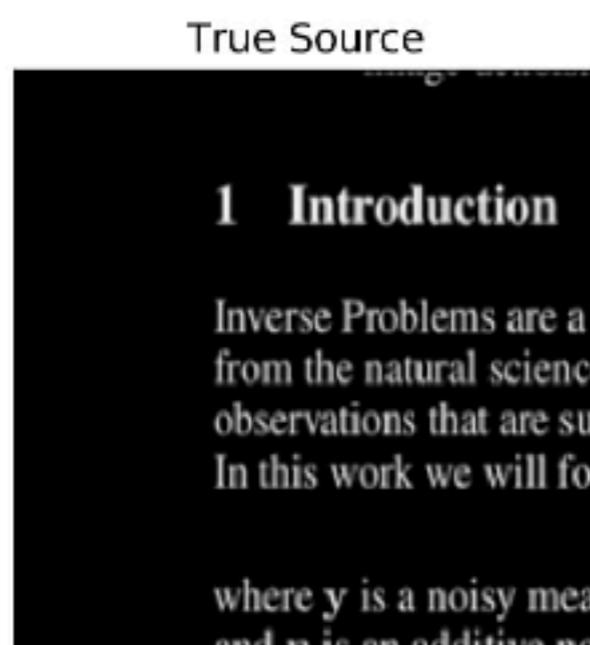
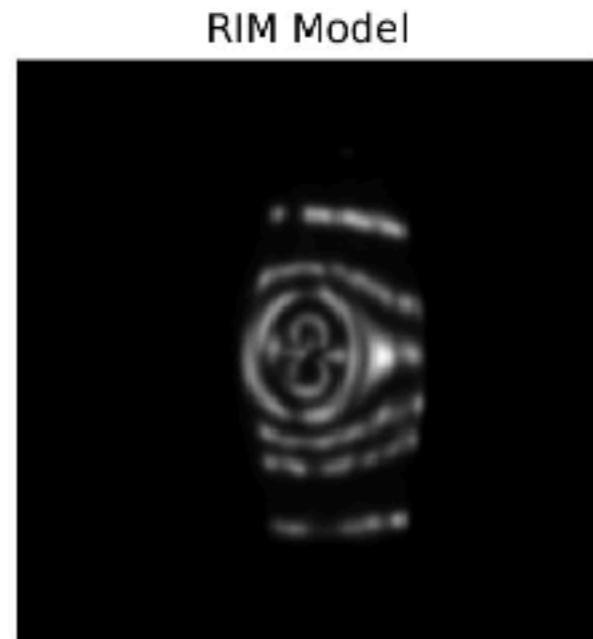
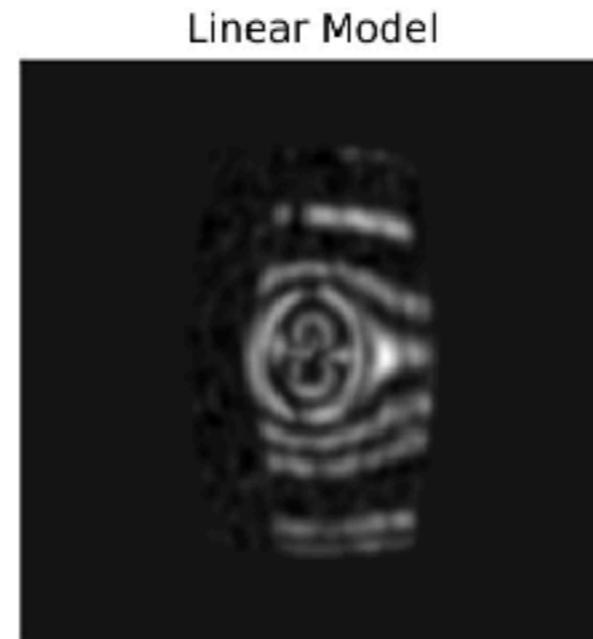
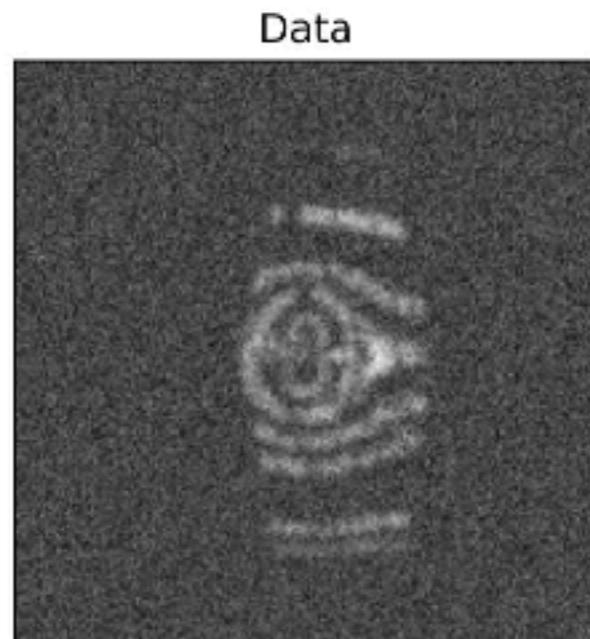
UNDISTORTED IMAGE OF THE BACKGROUND SOURCE WITH THE RECURRENT INFERENCE MACHINE (RIM)



BACKGROUND SOURCE RECONSTRUCTION: COMPARISON TO MAXIMUM LIKELIHOOD METHODS

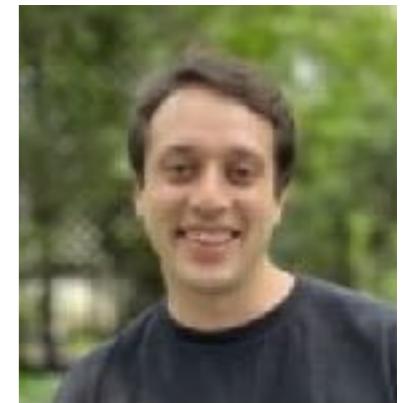


EXAMPLES OUTSIDE THE TRAINING DATA

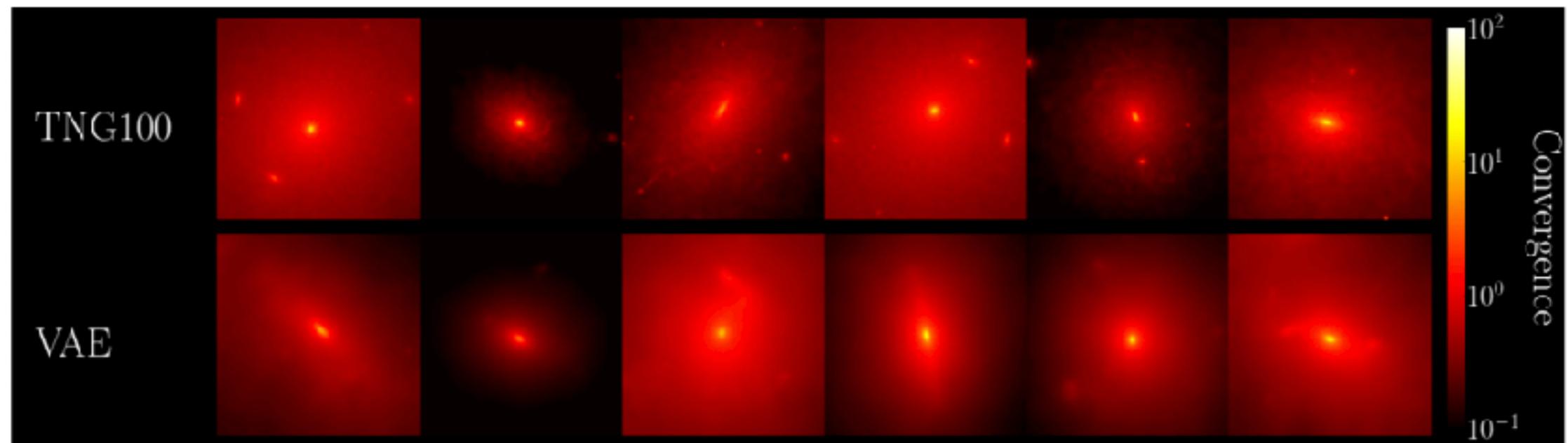




SIMULATED GALAXIES GENERATED WITH A VARIATIONAL AUTOENCODER

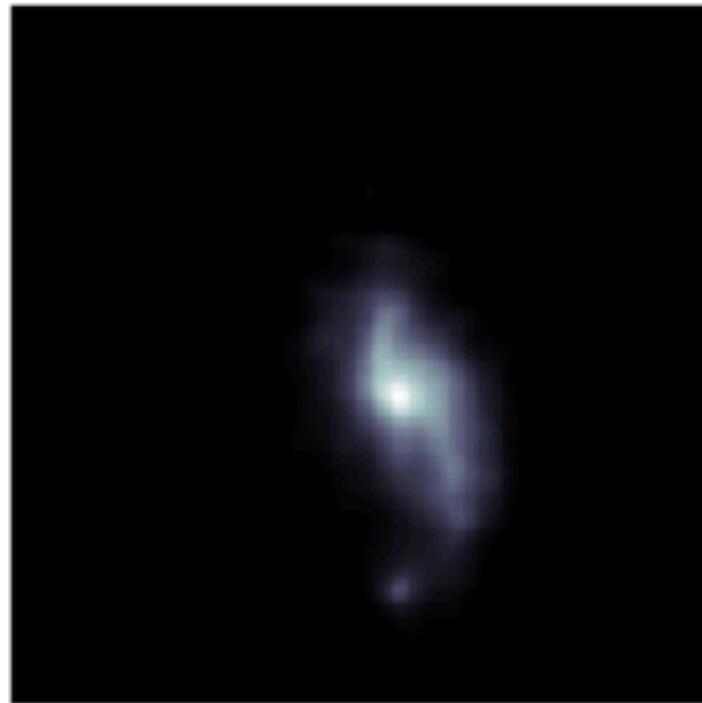


Alexandre Adam

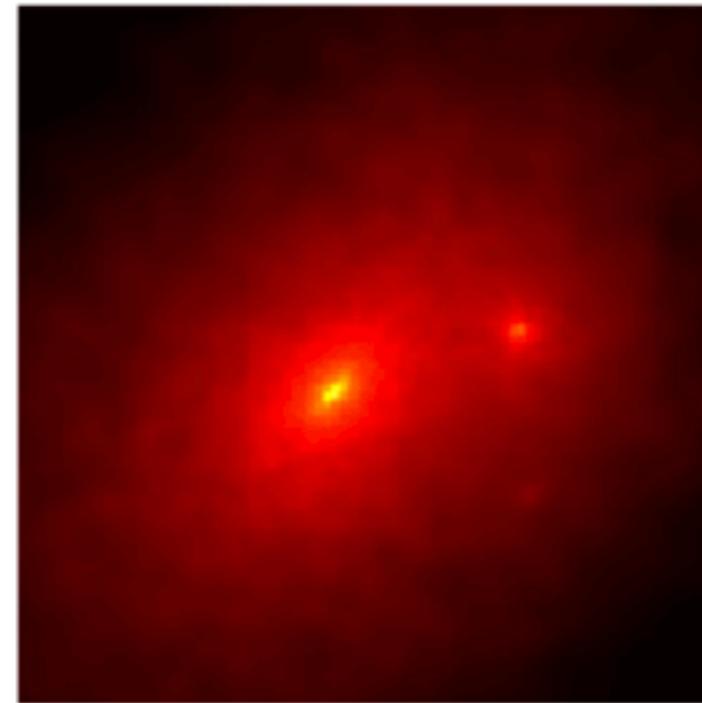


TRAINING ON HYDRODYNAMICAL SIMULATIONS

Ground Truth



Background

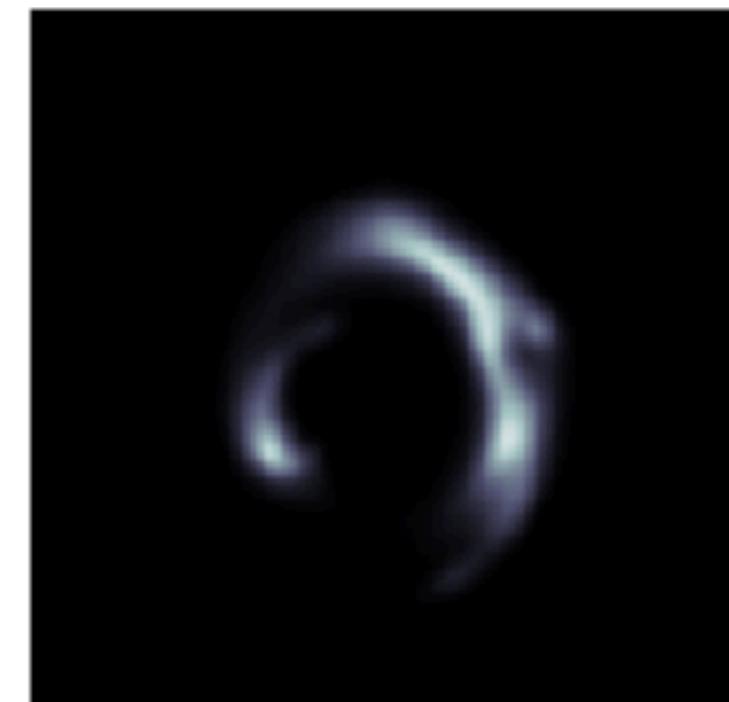
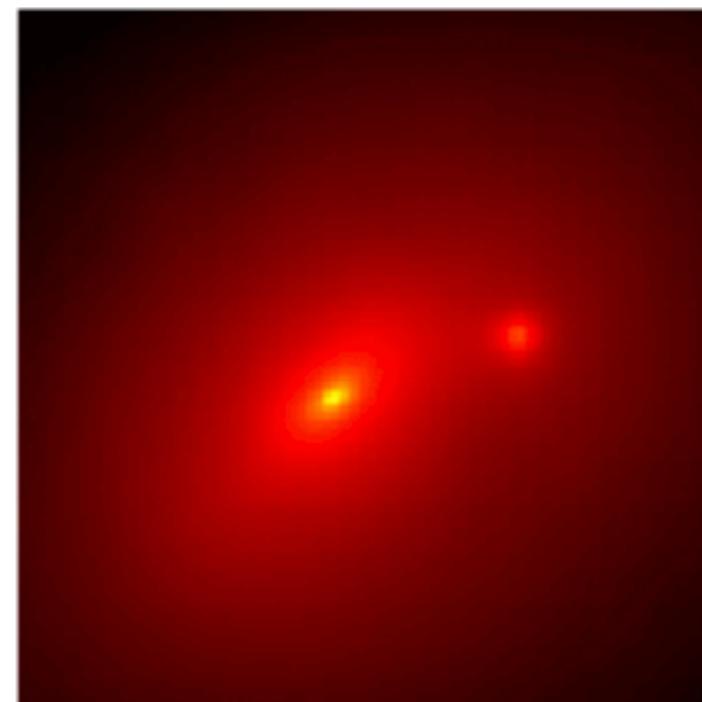
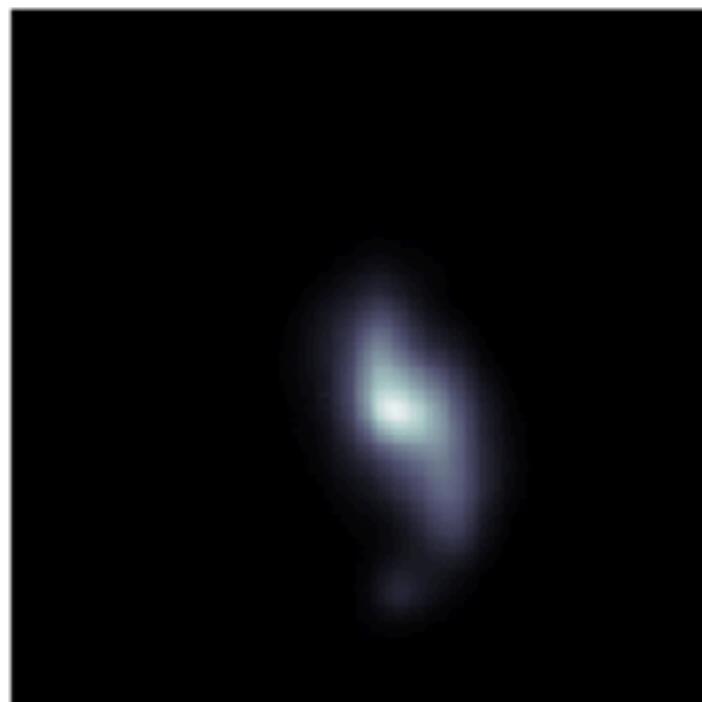


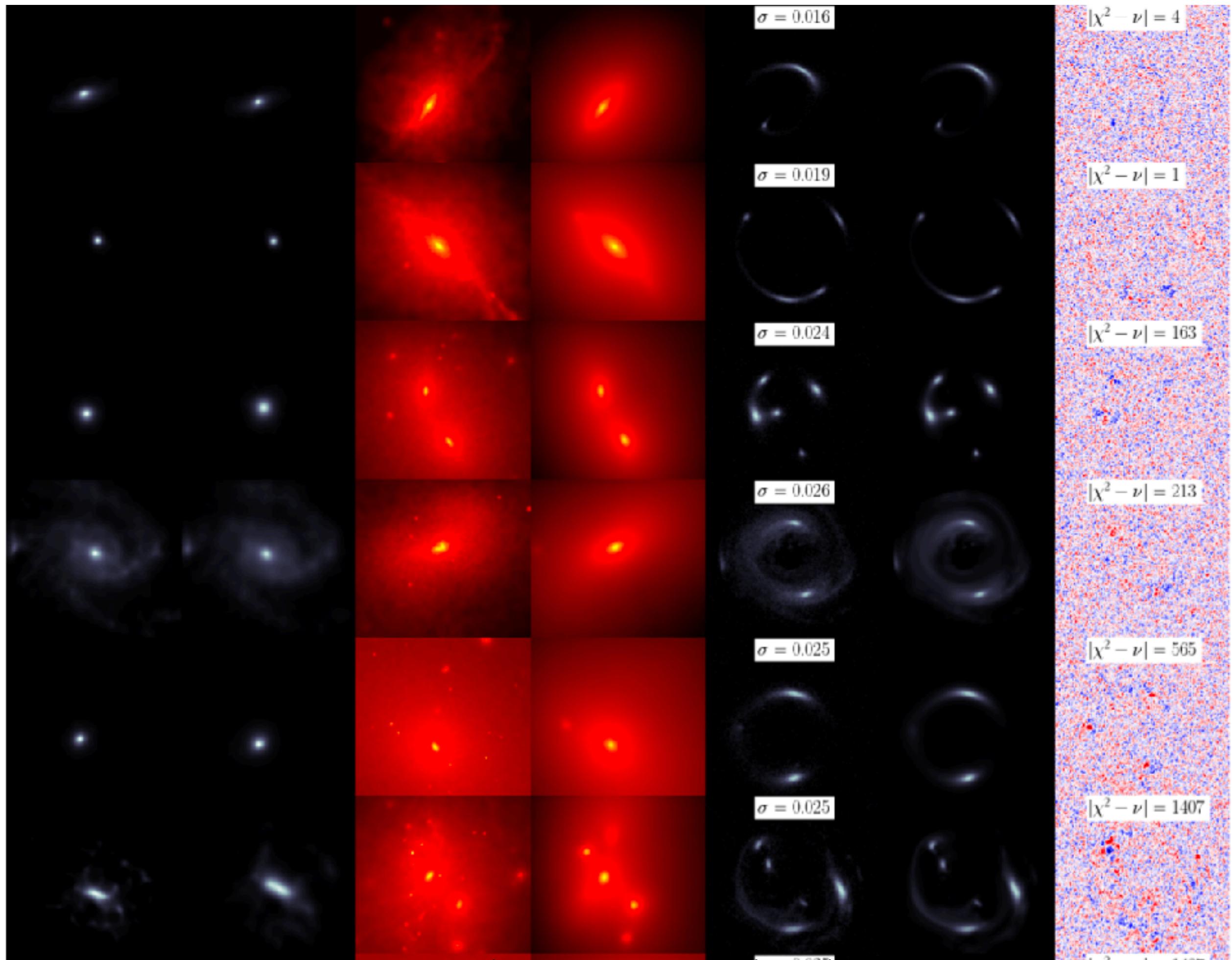
Foreground



Lensed Image

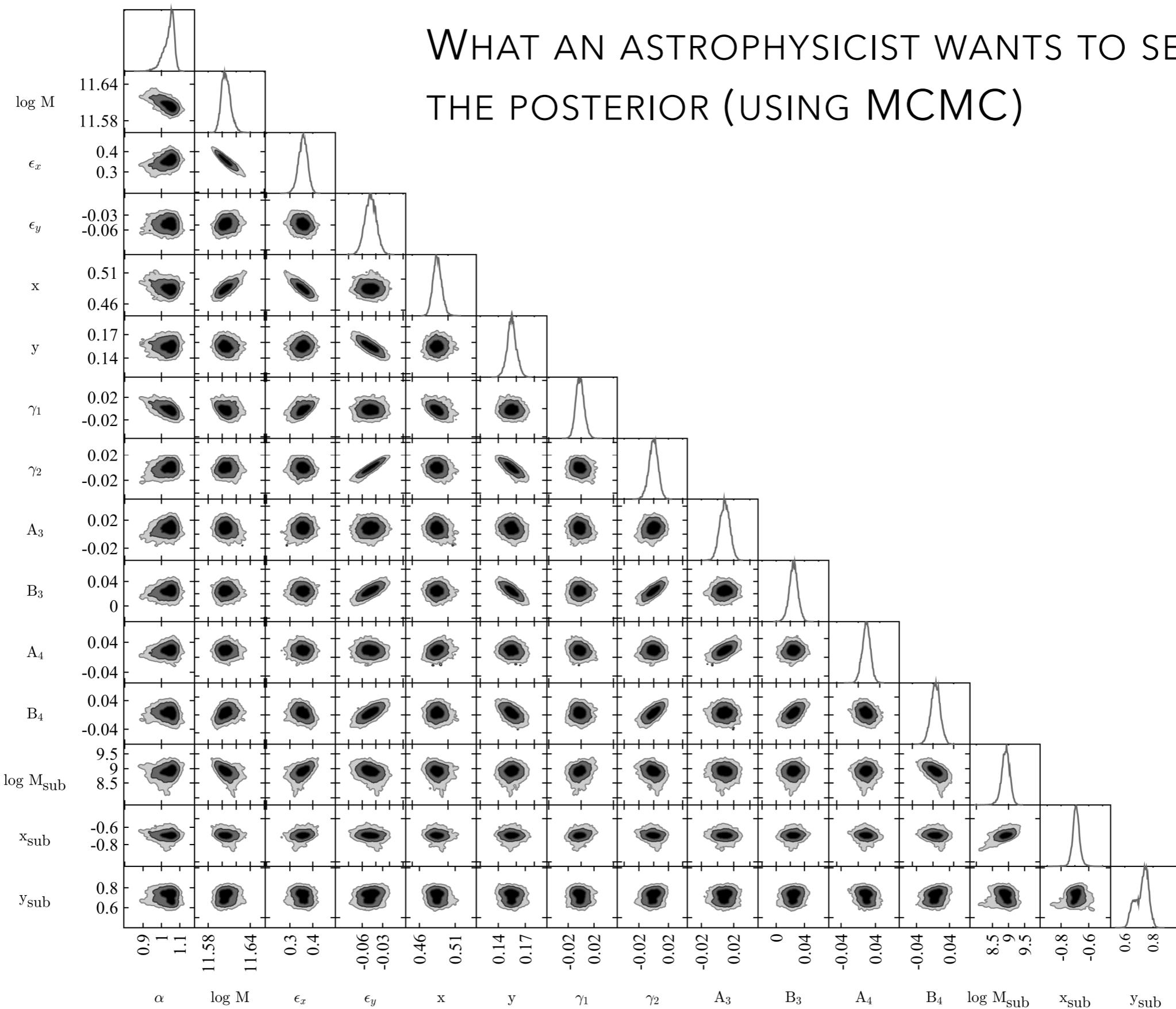
Prediction



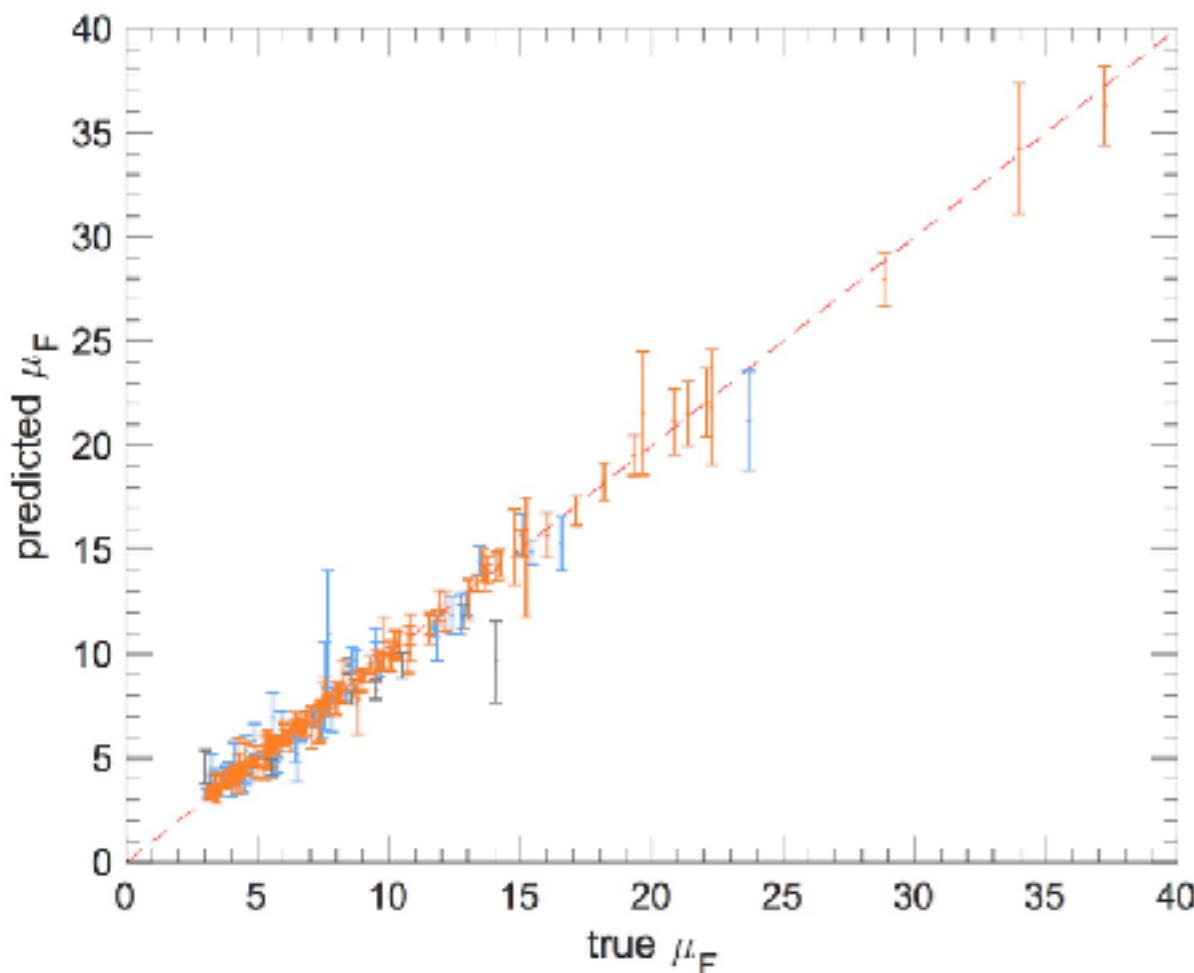


Adam, Perreault-Levasseur, Hezaveh, Welling, ApJ, 2023, arXiv:2301.04168

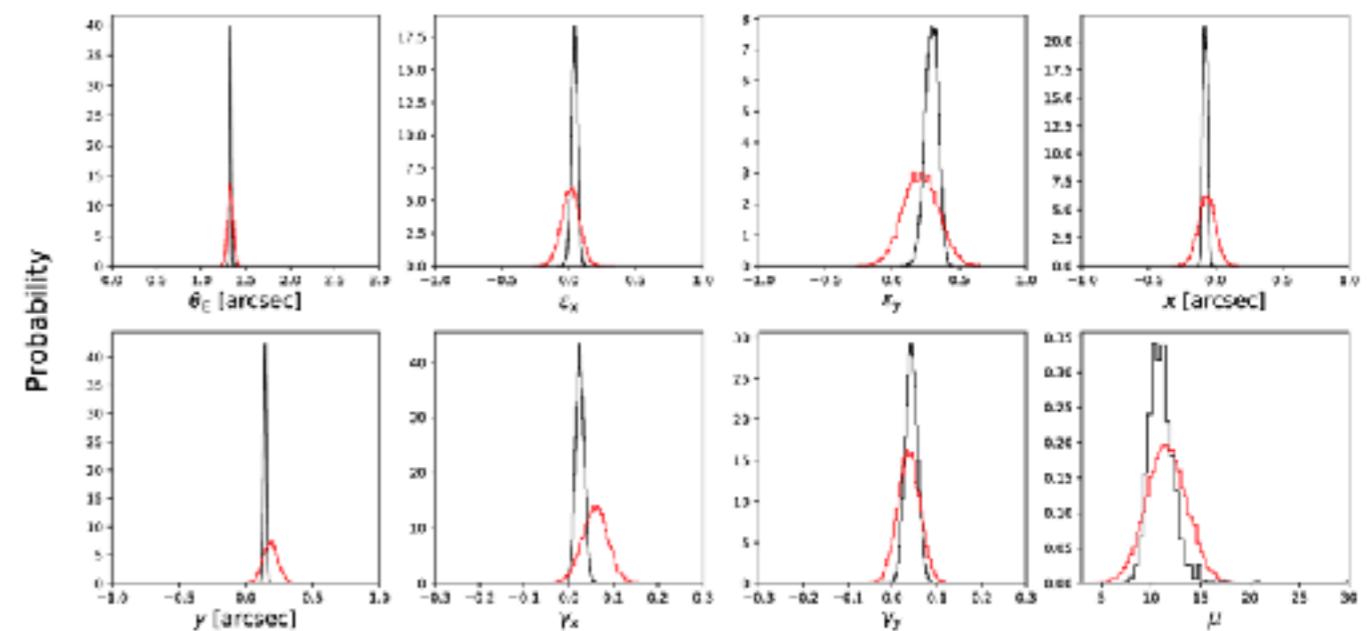
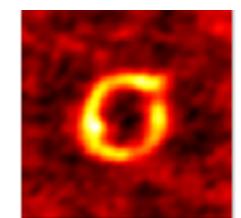
WHAT AN ASTROPHYSICIST WANTS TO SEE: THE POSTERIOR (USING MCMC)



UNCERTAINTY ESTIMATION WITH APPROXIMATE BAYESIAN NEURAL NETWORKS



Max-likelihood lens modeling (black)
Neural Networks (red)



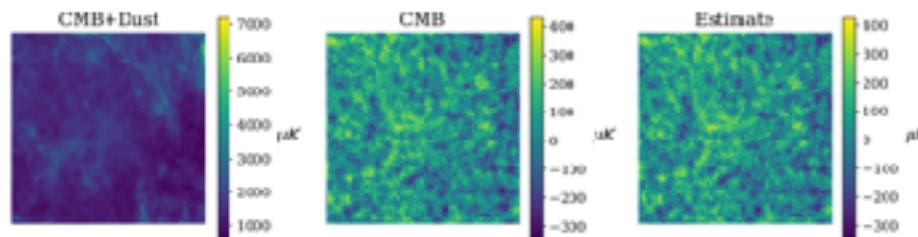
Variational Inference to Approximate Bayesian Neural Networks

Pros:

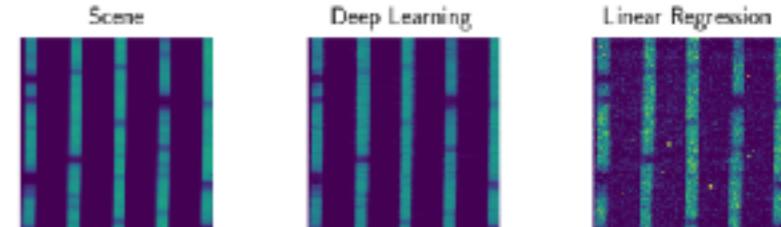
- ▶ Amortized.
- ▶ Requires few hundred forward passes at evaluation time (to collect samples). Still very fast.
- ▶ Marginalizes implicitly over parameters we do not wish to explicitly model.
- ▶ With good coverage probabilities, one can use importance sampling of the output distribution to get an unbiased posterior. (Provided one can actually write this posterior)

Caveats:

- ▶ The variational distributions (Bernouilli) are extremely simplistic, therefore even if we attempt to use them to approximate the true weight distributions, that approximation could be bad and yield inaccurate uncertainties.



CMB Cleaning



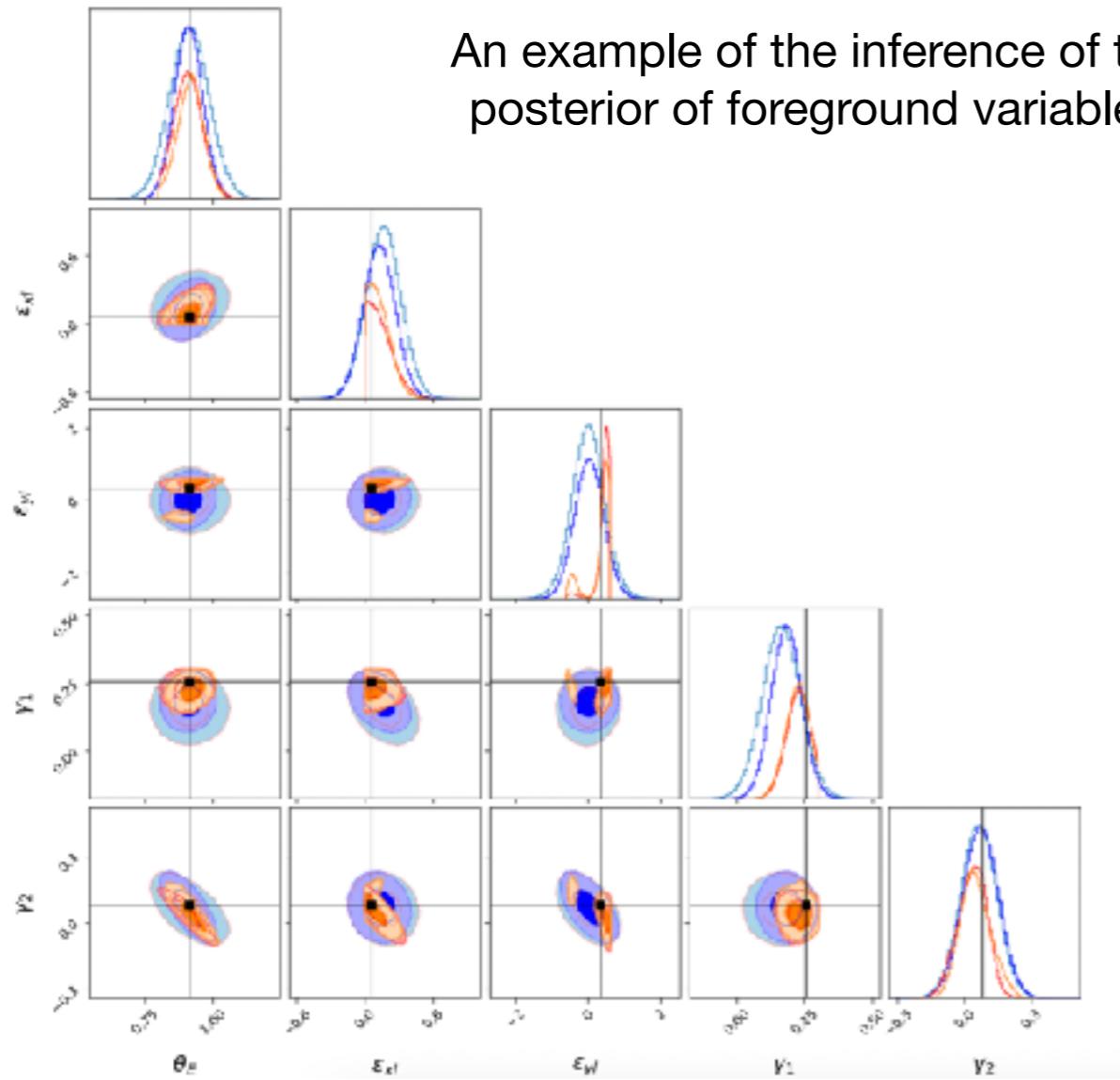
IR Spectrometer De-noising

Same problem remains regardless of the variational distribution used: there is no way of quantifying how well we approximate the true weight distributions

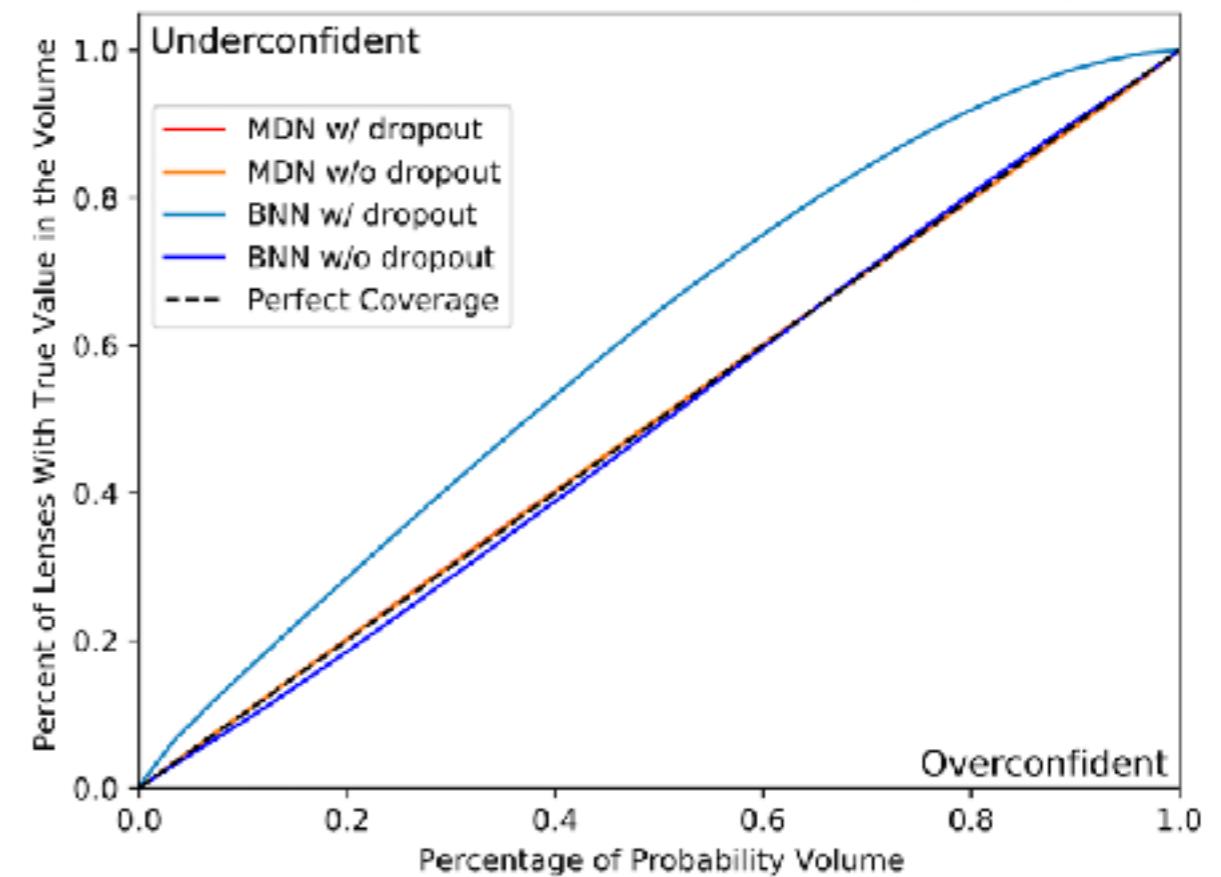
UNCERTAINTY ESTIMATION WITH SIMULATION-BASED INFERENCE METHODS



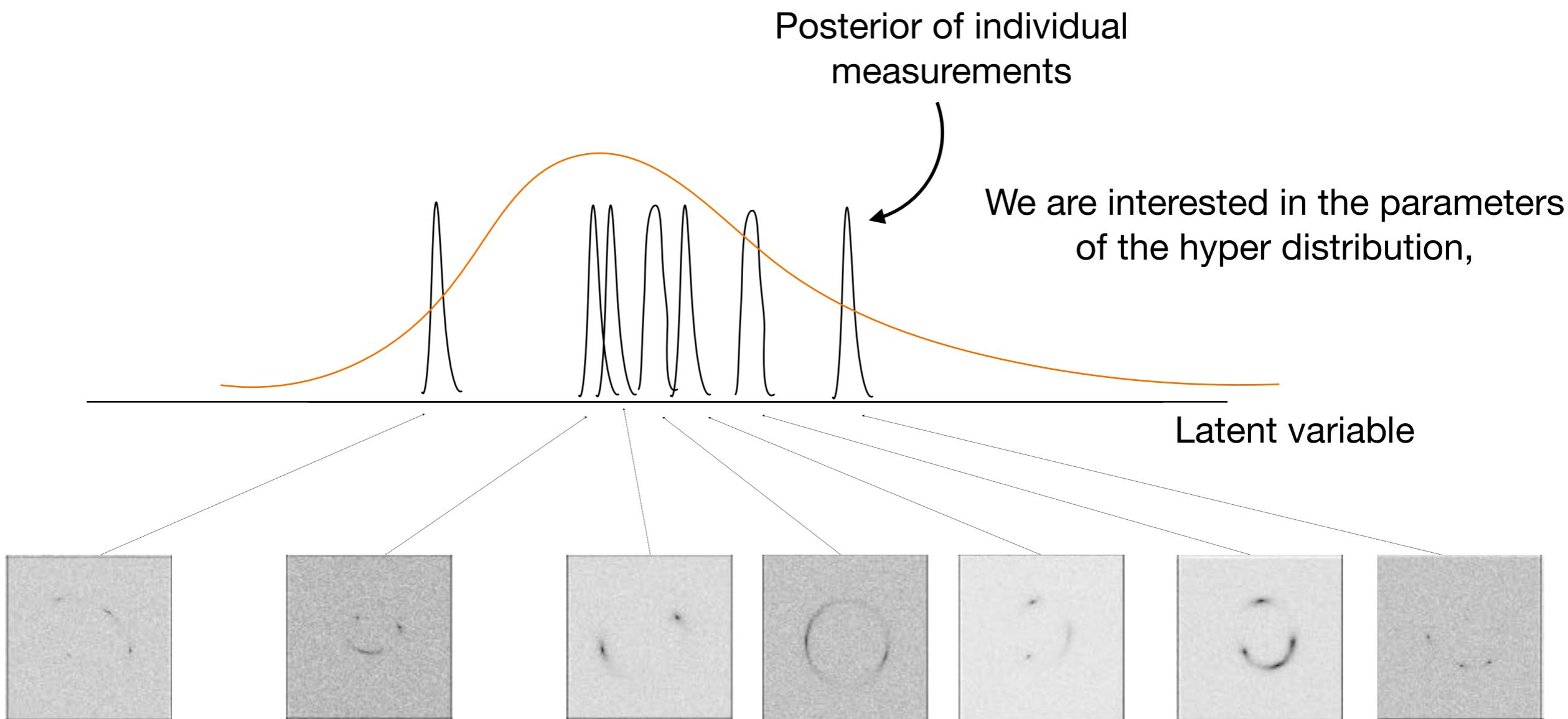
An example of the inference of the posterior of foreground variables



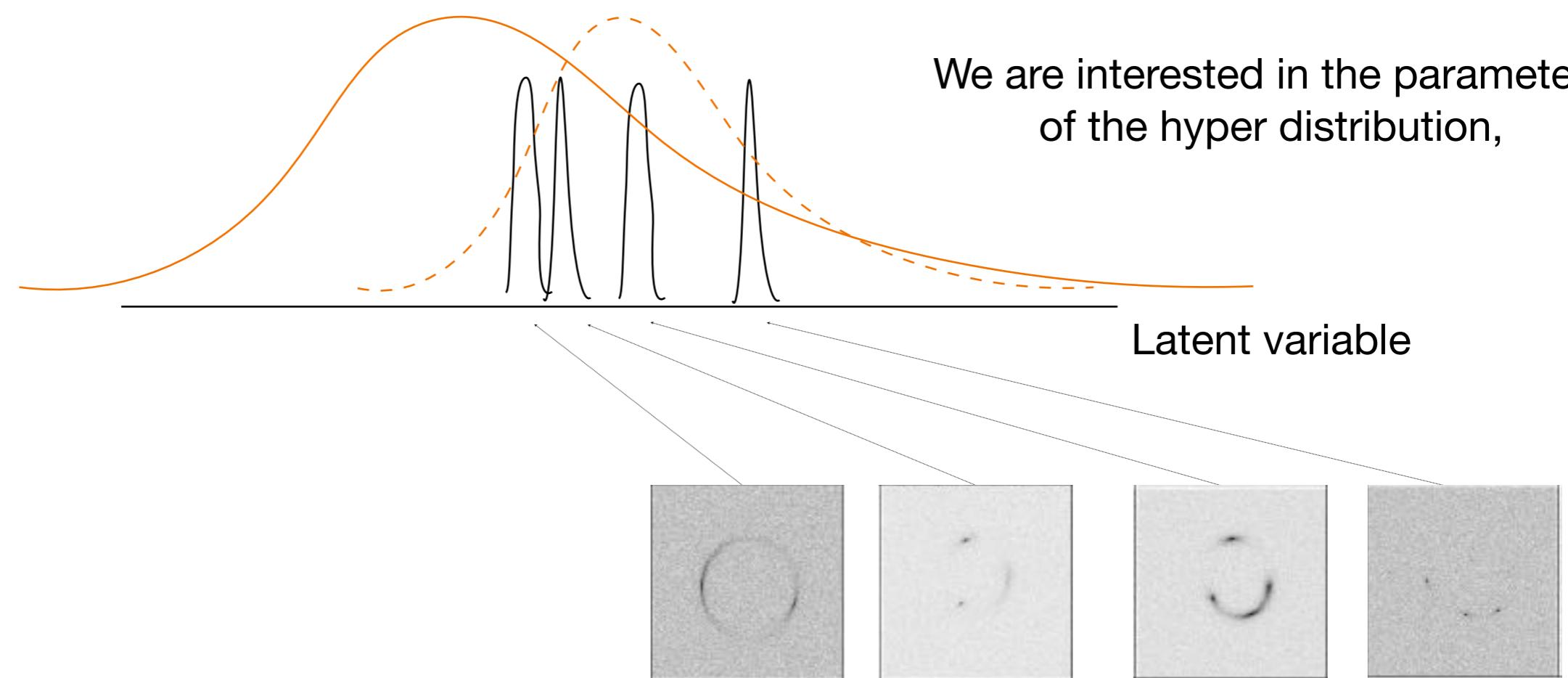
Coverage probabilities



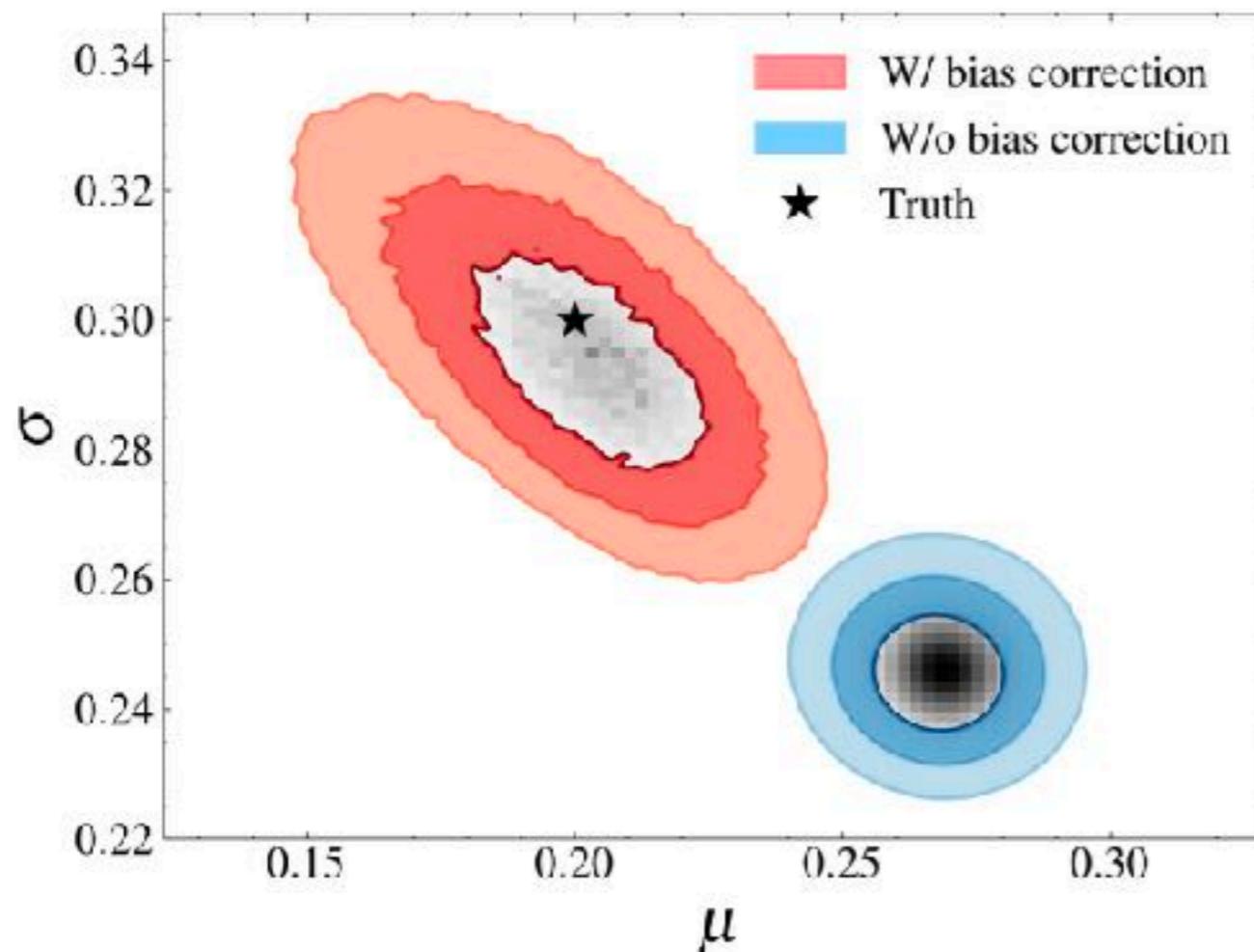
Hierarchical Bayesian inference



Hierarchical Bayesian inference



Hierarchical Bayesian inference



Ronan
Legin



Connor
Stone

UNCERTAINTY ESTIMATION WITH SIMULATION-BASED INFERENCE METHODS

Pros:

- ▶ Use the **power of ML to find a compress statics**, and even if it is biased, we can get unbiased error estimate, the only drawback would be sub-optimal precision. (Provided the simulation pipeline is accurate!)
- ▶ A well-defined statistical framework that can: be relatively **fast**, deal with **complex distributions**, model **joint posteriors**.
- ▶ Use a neural density estimator to get the joint distribution $p(\text{data}, \text{parameter})$, no need for the epsilon parameter in ABC.
- ▶ Can **change the prior** from data point to data point without retraining the ML compressor.
- ▶ Once we have the posterior, can **generate samples** that are consistent with data (this is really important for ‘interrogating the black box’)

Caveats:

- ▶ Hard to marginalize implicitly over parameters, we need to **explicitly** model them.
- ▶ We don’t model the uncertainty of the density estimator itself. (But it’s a fairly simple ML model, and except for very pathological problems it’s reasonable to expect that we are in interpolation mode).
- ▶ Limited to **low-dimensional posteriors** (10s maximum).
- ▶ Requires an **accurate simulation pipeline**.

NEURAL RATIO ESTIMATORS

$$P(x, \theta)$$

Class #1
 $\{(x_1, \theta_1), (x_2, \theta_2), \dots, (x_N, \theta_N)\}$

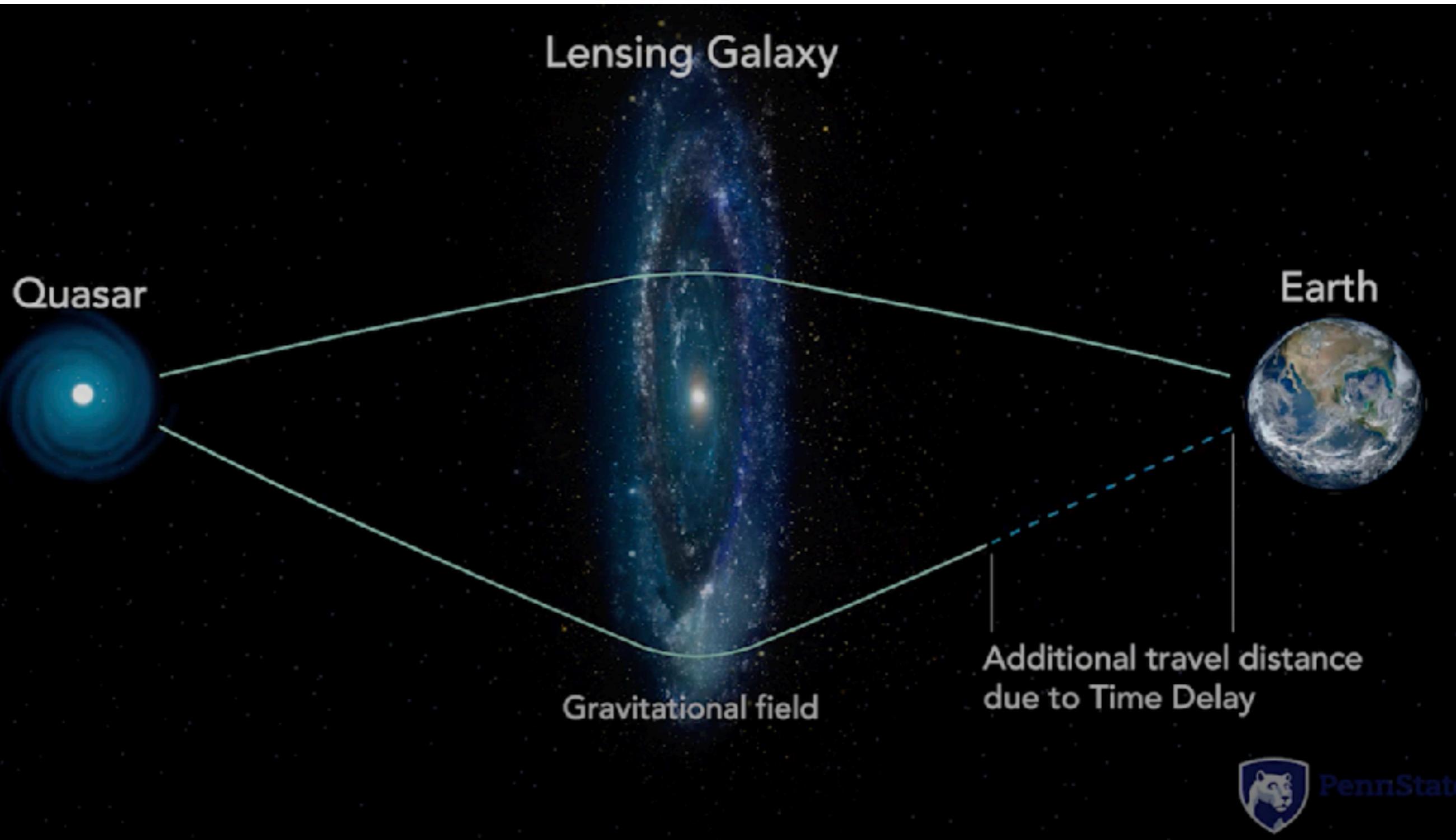
$$P(x)P(\theta)$$

Class #2
 $\{(x_1, \theta_1), (x_2, \theta_2), \dots, (x_M, \theta_M)\}$

Classify

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

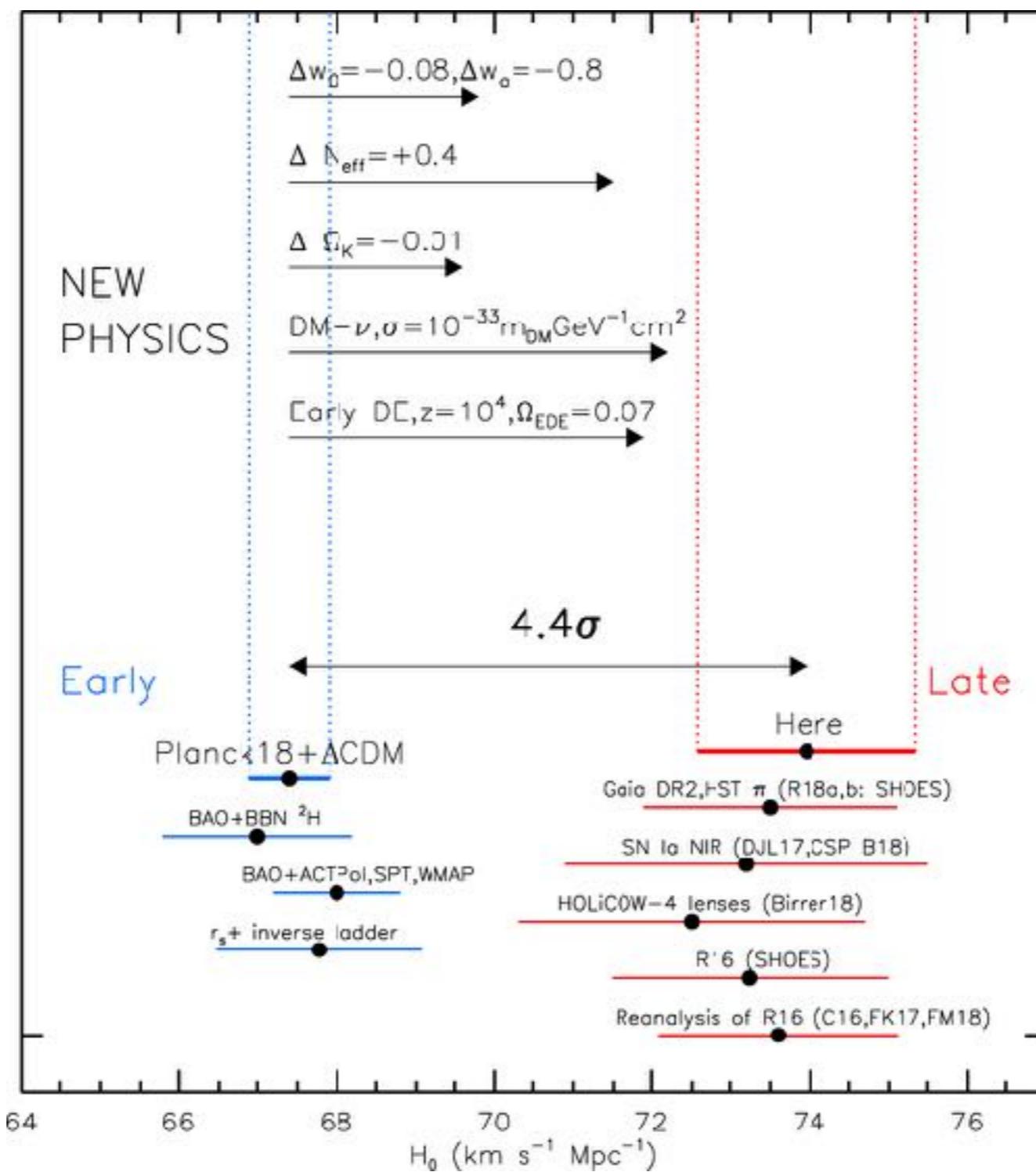
H₀ INFERENCE WITH TIME DELAY COSMOGRAPHY



Penn State

THE HUBBLE CONSTANT

DISCREPANCY BETWEEN MEASUREMENTS



H₀ INFERENCE WITH NEURAL RATIO ESTIMATORS

$$P(\theta, x)$$
$$p(\text{H}_0, \text{[Figure: Signal traces and heatmap]})$$

$$P(\theta)P(x)$$
$$p(\text{H}_0)p(\text{[Figure: Signal traces and heatmap]})$$

Class #1

$$\{(x_1, \theta_1), (x_2, \theta_2), \dots, (x_N, \theta_N)\}$$

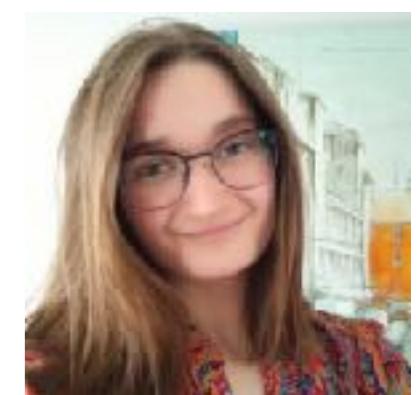
Class #2

$$\{(x_1, \theta_1), (x_2, \theta_2), \dots, (x_M, \theta_M)\}$$

Classify

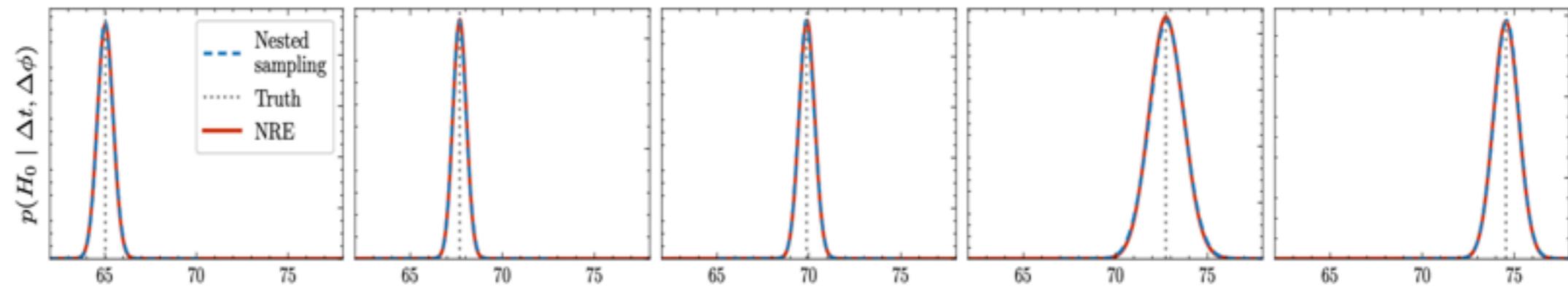
$$r(x, \theta) = \frac{p(x, \theta)}{p(x)p(\theta)} = \frac{p(\theta | x)}{p(\theta)}$$

H₀ INFERENCE WITH NEURAL RATIO ESTIMATORS

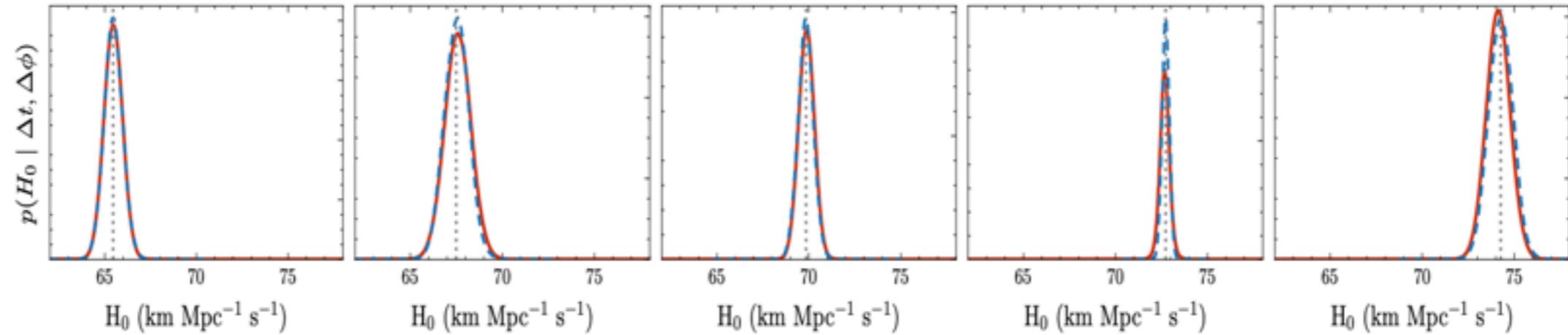


Ève Campeau-Poirier

Doubles



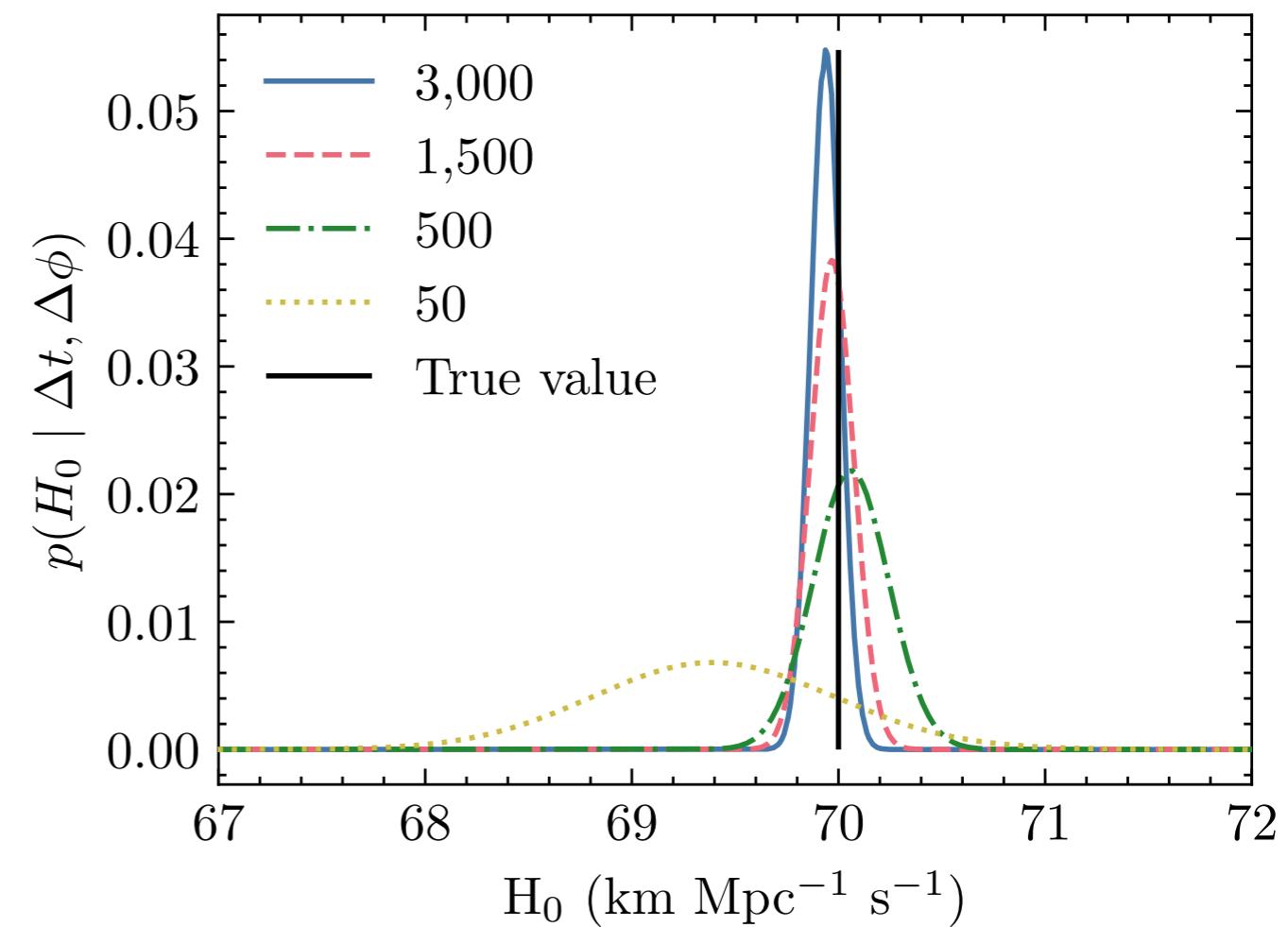
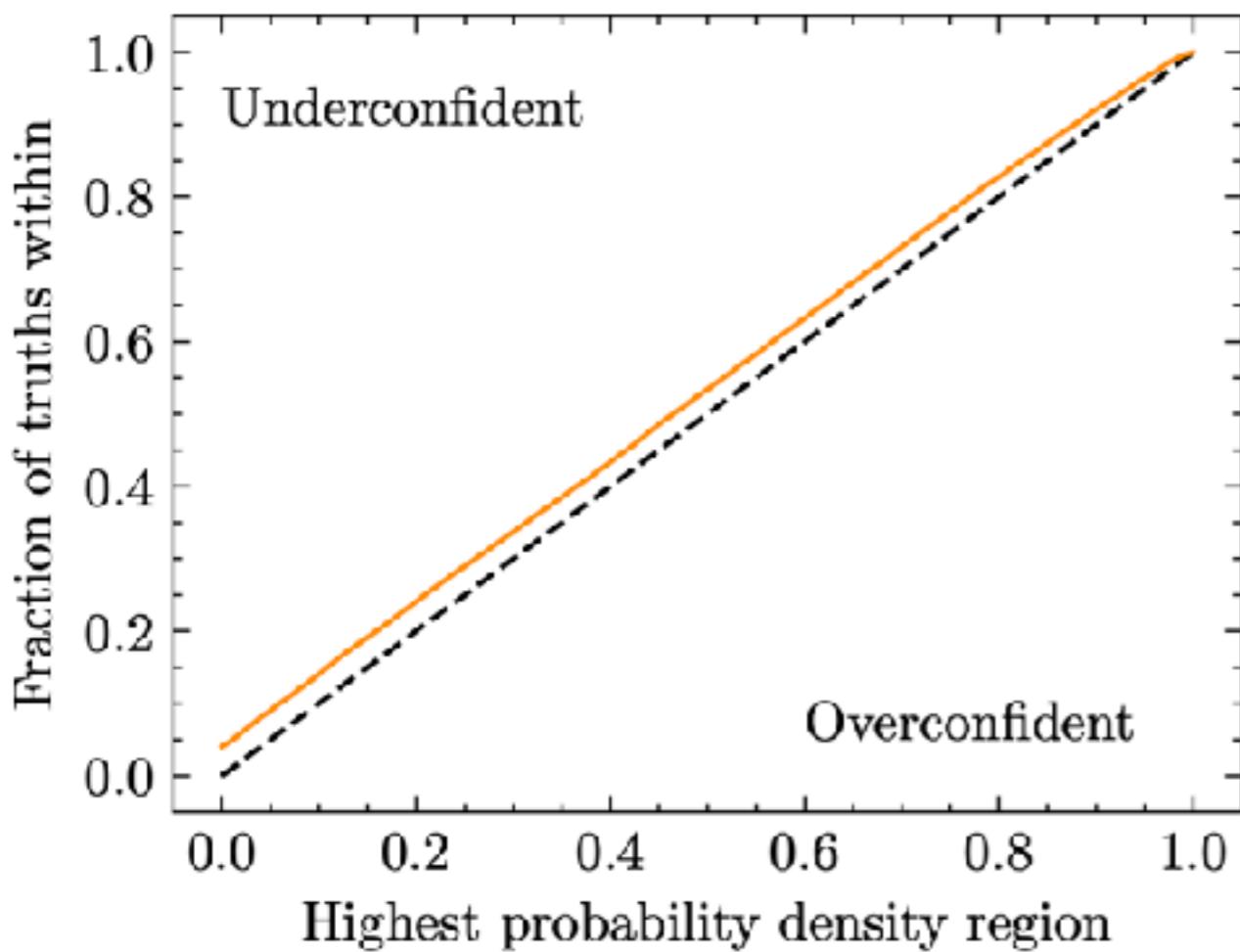
Quads



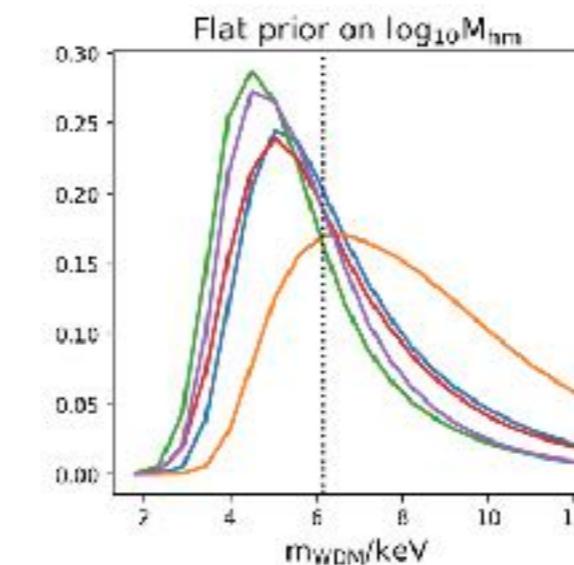
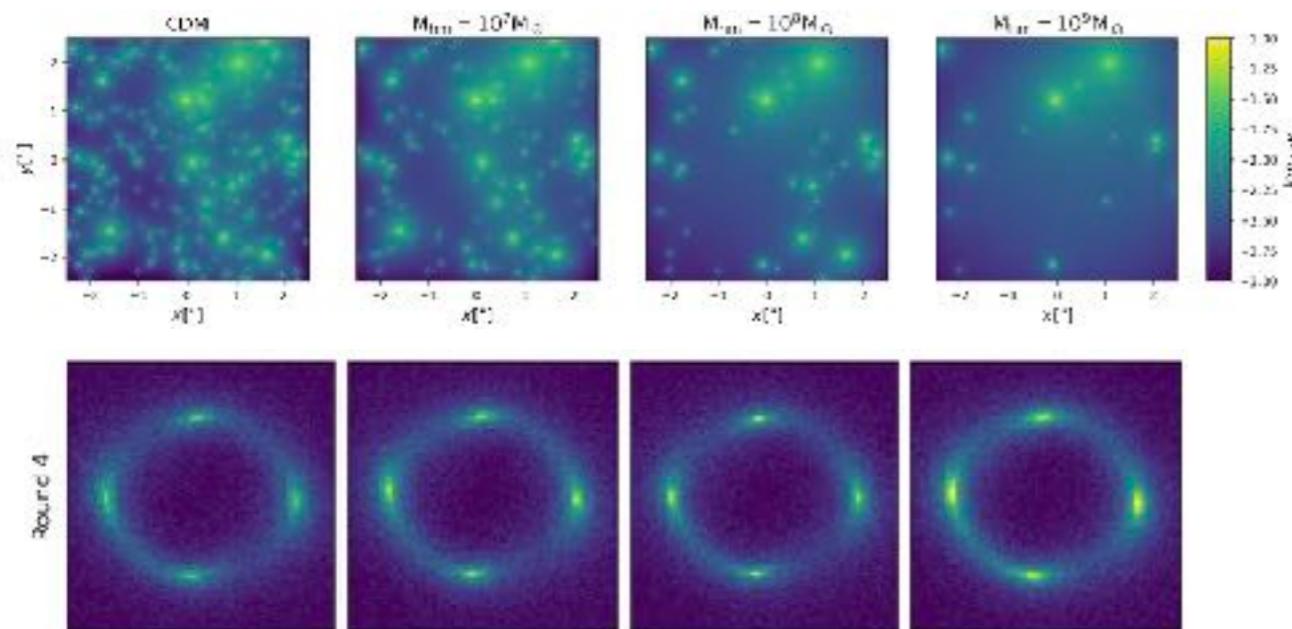
H₀ INFERENCE WITH NEURAL RATIO ESTIMATORS



Ève Campeau-Poirier



Estimating the dark matter particle temperature with Neural Ratio Estimators



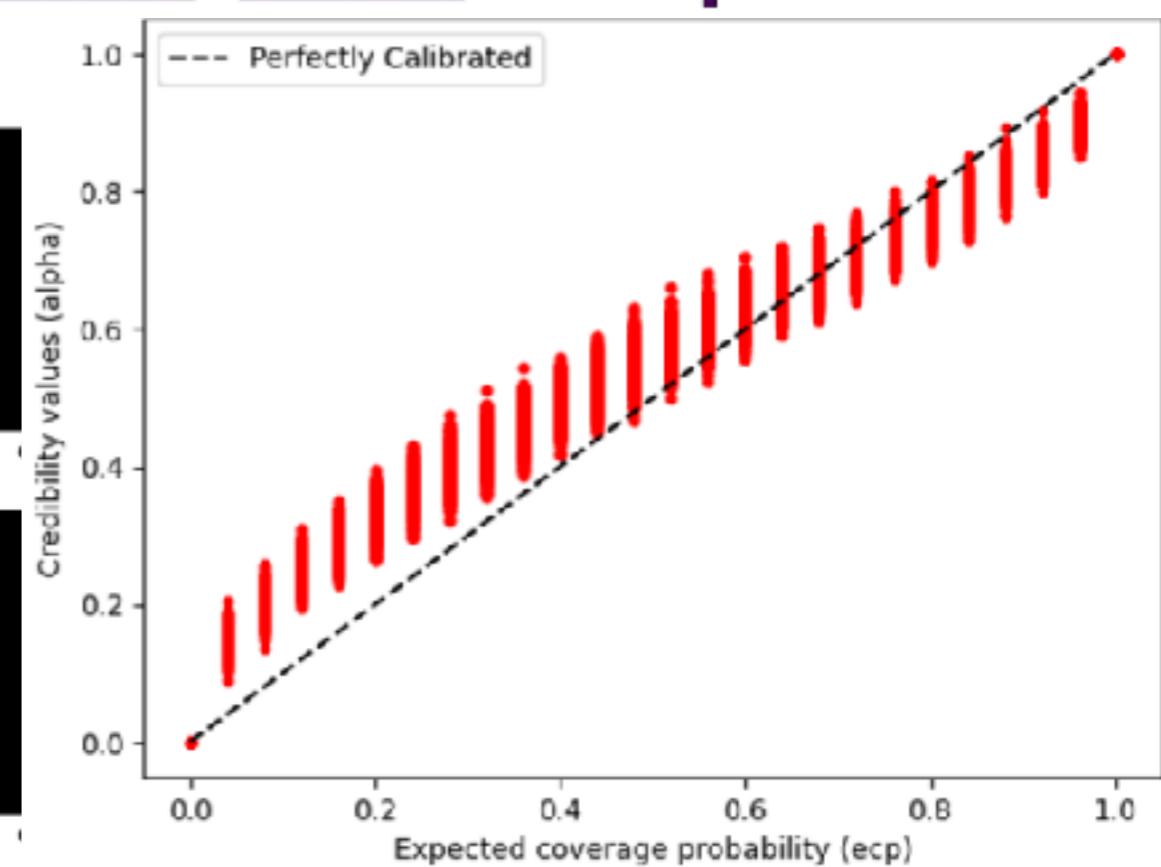
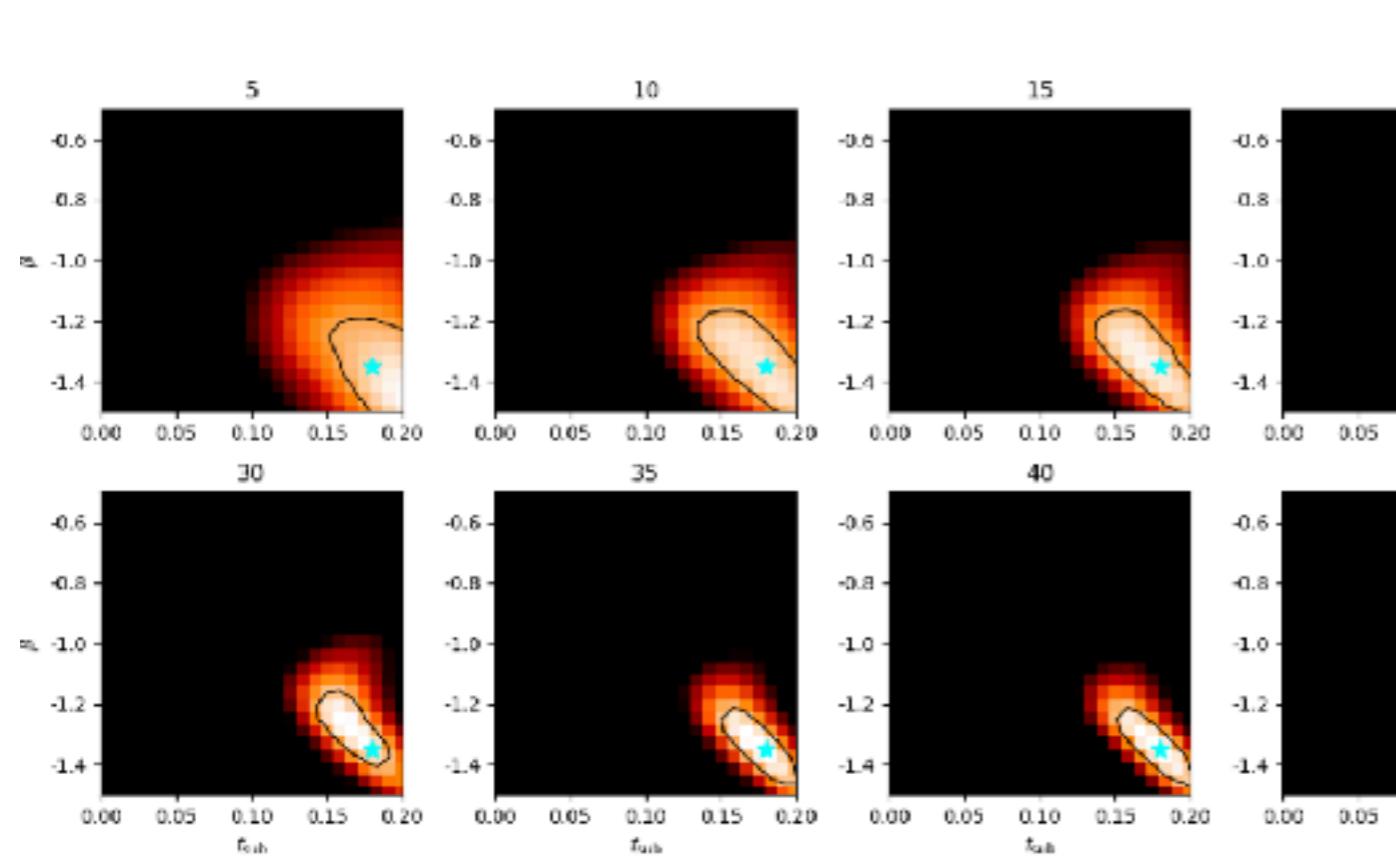
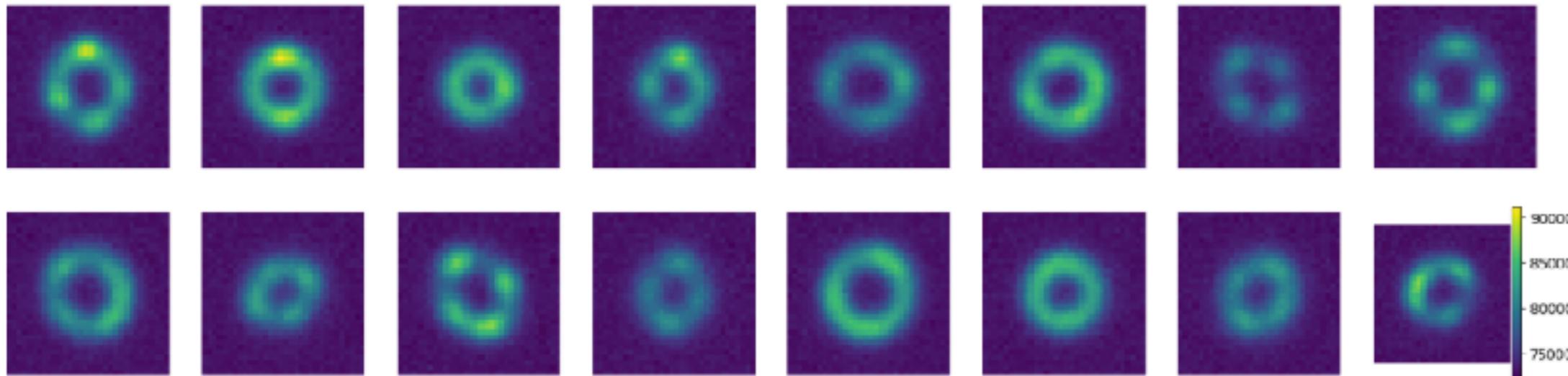
Adam
Coogan

Anau Montel, Coogan et al. 2022, arXiv:2205.09126
Coogan et al., NeurIPS 2020 ML4PS Workshop

ESTIMATING THE SENSITIVITY OF LSST TO THE BREAK AND SLOPE OF THE DARK MATTER MASS FUNCTION



Andreas
Filipp



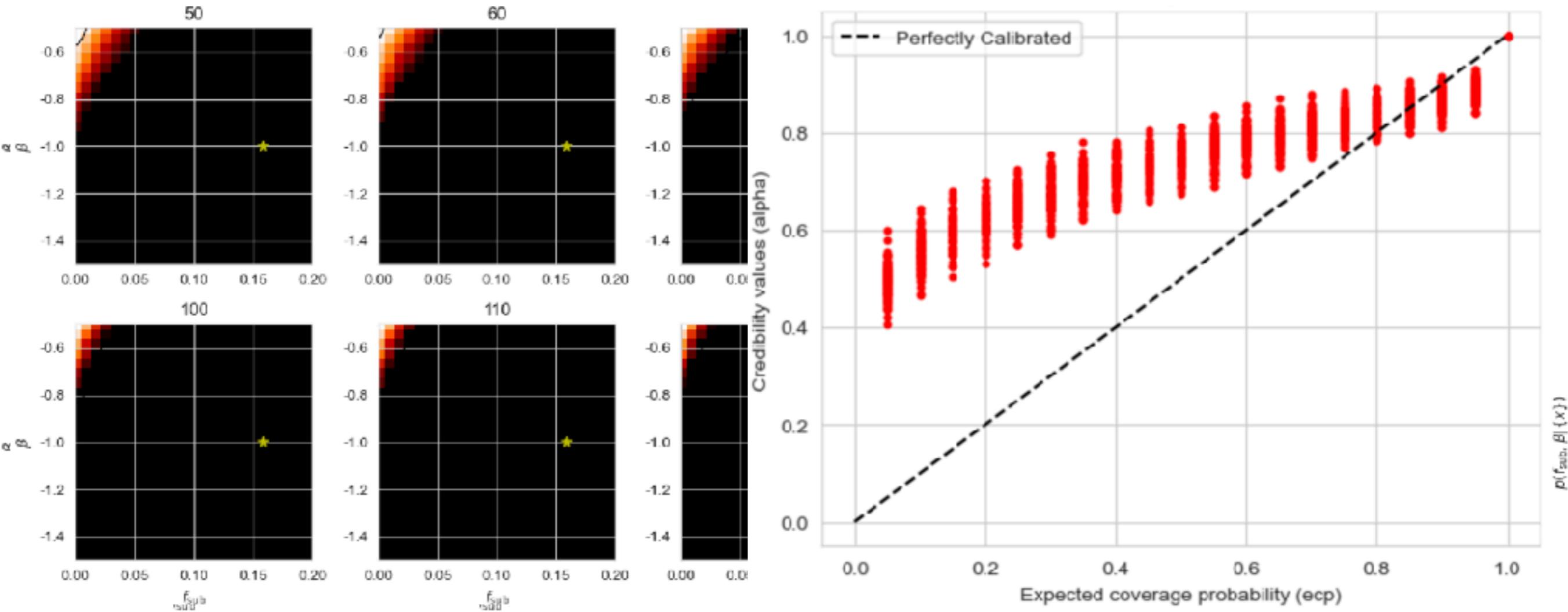
TESTING FOR ROBUSTNESS TO MODEL MISSPECIFICATION

Training on SIS (spherically symmetric lenses)...



And testing on galaxies with slight ellipticities, $q=0.98$

Andreas
Filipp



RATIO ESTIMATION METHODS

Pros:

- ▶ Can marginalize implicitly over large number of nuisance parameters

Caveats:

- ▶ Because we have marginalized, we've lost the capability to generate samples consistent with the observations.
- ▶ From experiments, it seems easy to find examples where the NN is very brittle and sensitive to model misspecification.
- ▶ So far: no real way of quantifying the uncertainty of the ratio estimator itself. All the guarantees are in terms of convergence to a specific ratio in the limit of perfect training. Is this always realistic?

TACKLING AN UNSOLVED PROBLEM: HIGH DIMENSIONAL INFERENCE

How do we infer the posteriors of high-dimensional parameters (e.g., an image or spectra)?

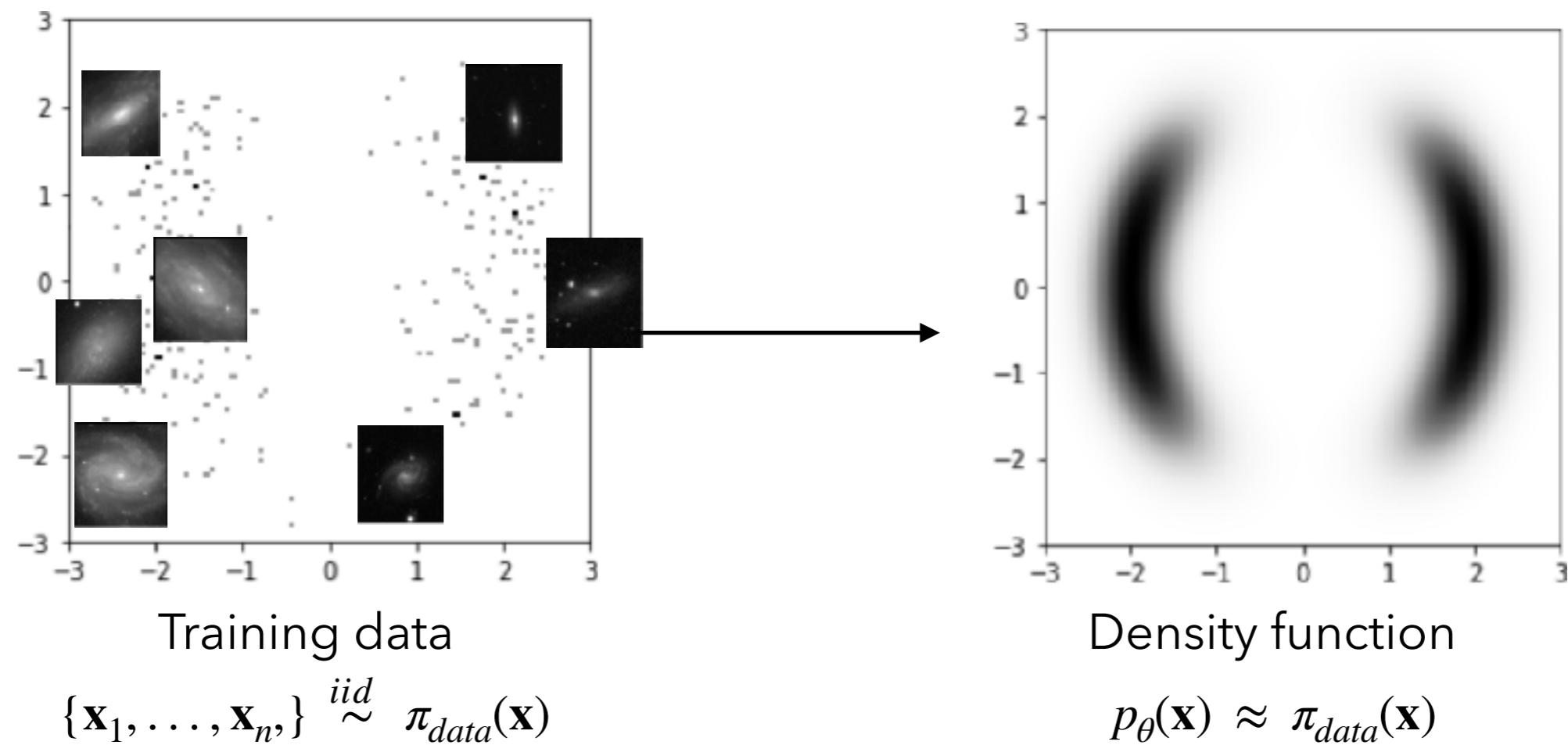
Obstacles:

- 1) How do we encode complex priors
- 2) How we sample such high-dimensional posteriors (even if we could compute them)

LEARNING THE PRIOR EXPLICITLY

Can we learn our high-dimensional prior explicitly from data?
i.e. can we learn a generative model that will produce samples from that distribution?

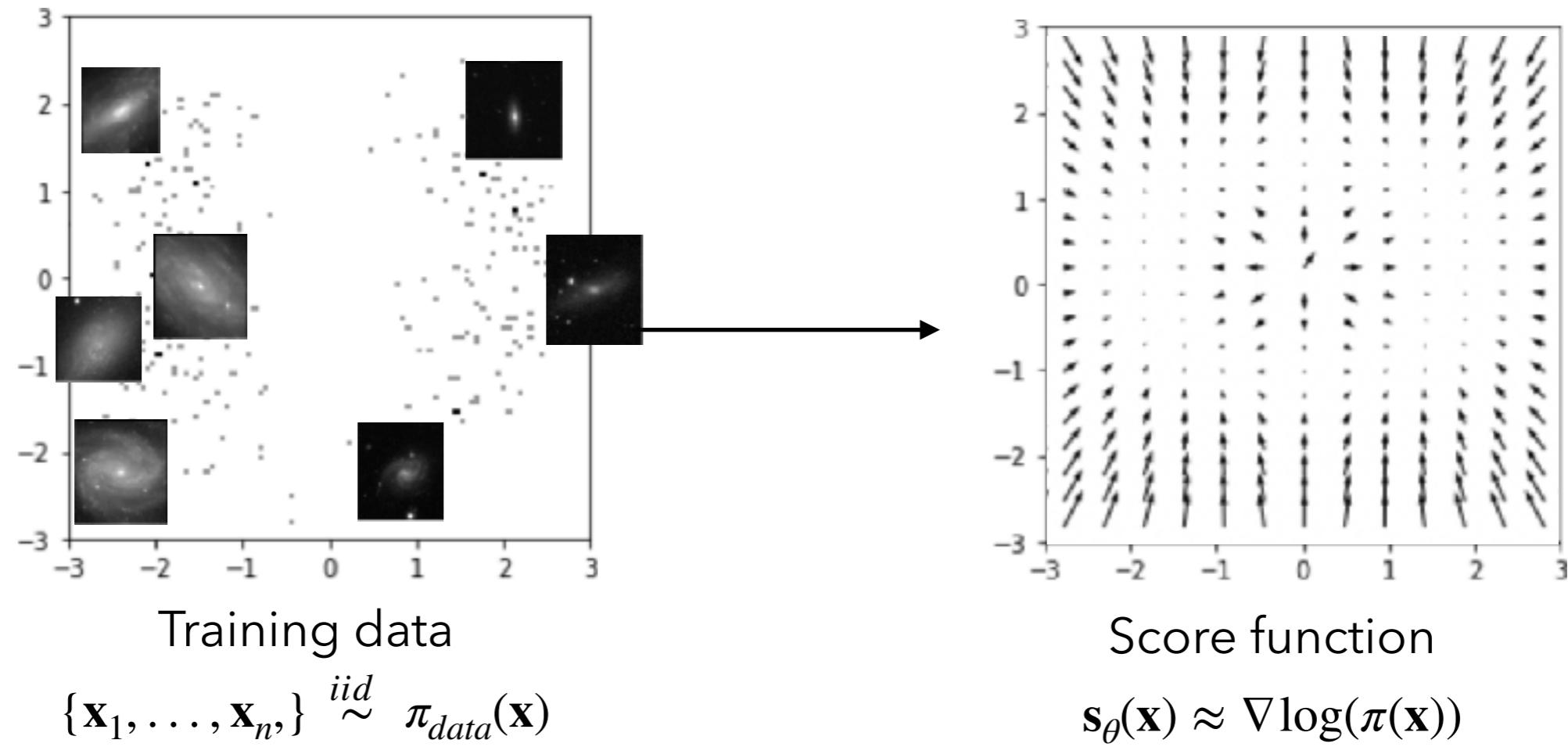
How can we do this from samples (e.g. data)? Modeling the density?



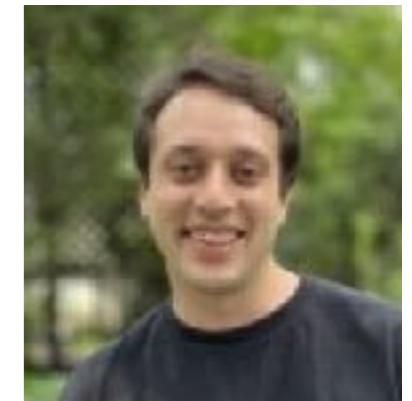
SCORE MODELING

Turns out that if I want to sample a distribution, the only thing I need to learn is its **score**, which does not include the normalization constant and only uses local information

$$\mathbf{s}(\mathbf{x}) = \nabla_{\mathbf{x}} \log(\pi(\mathbf{x}))$$



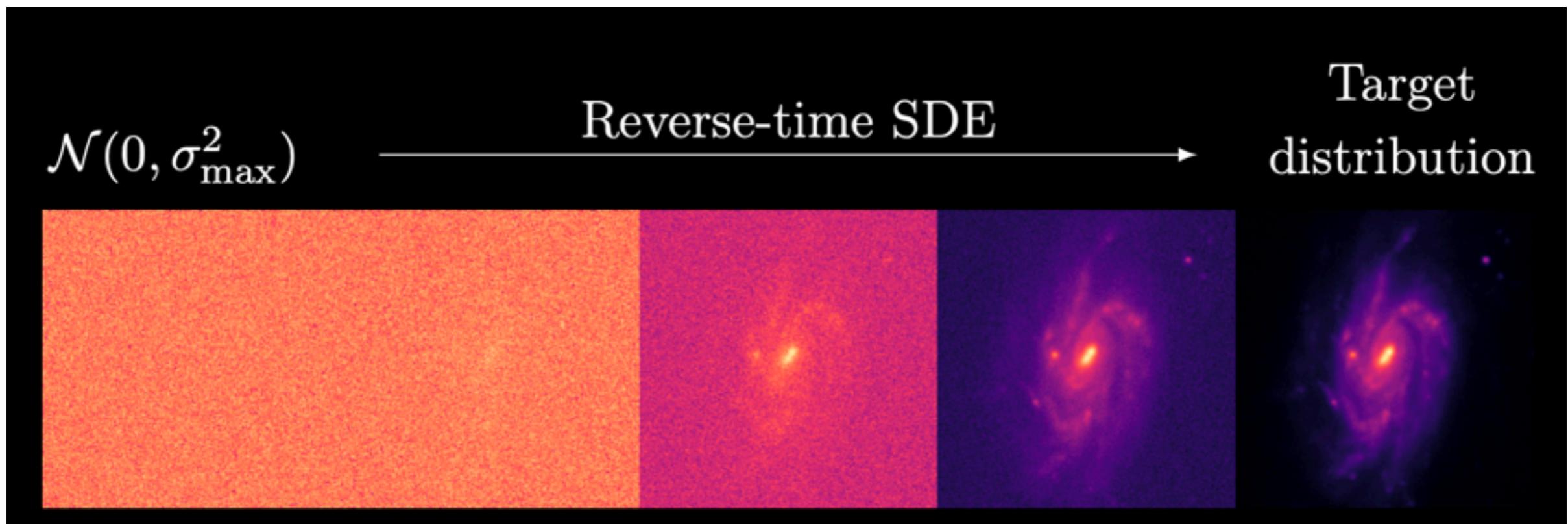
SCORE-BASED MODELING

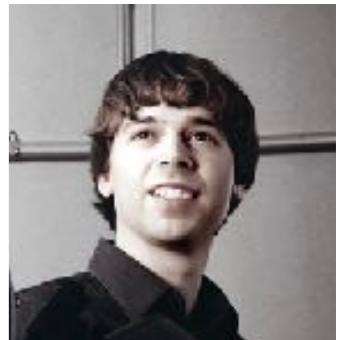
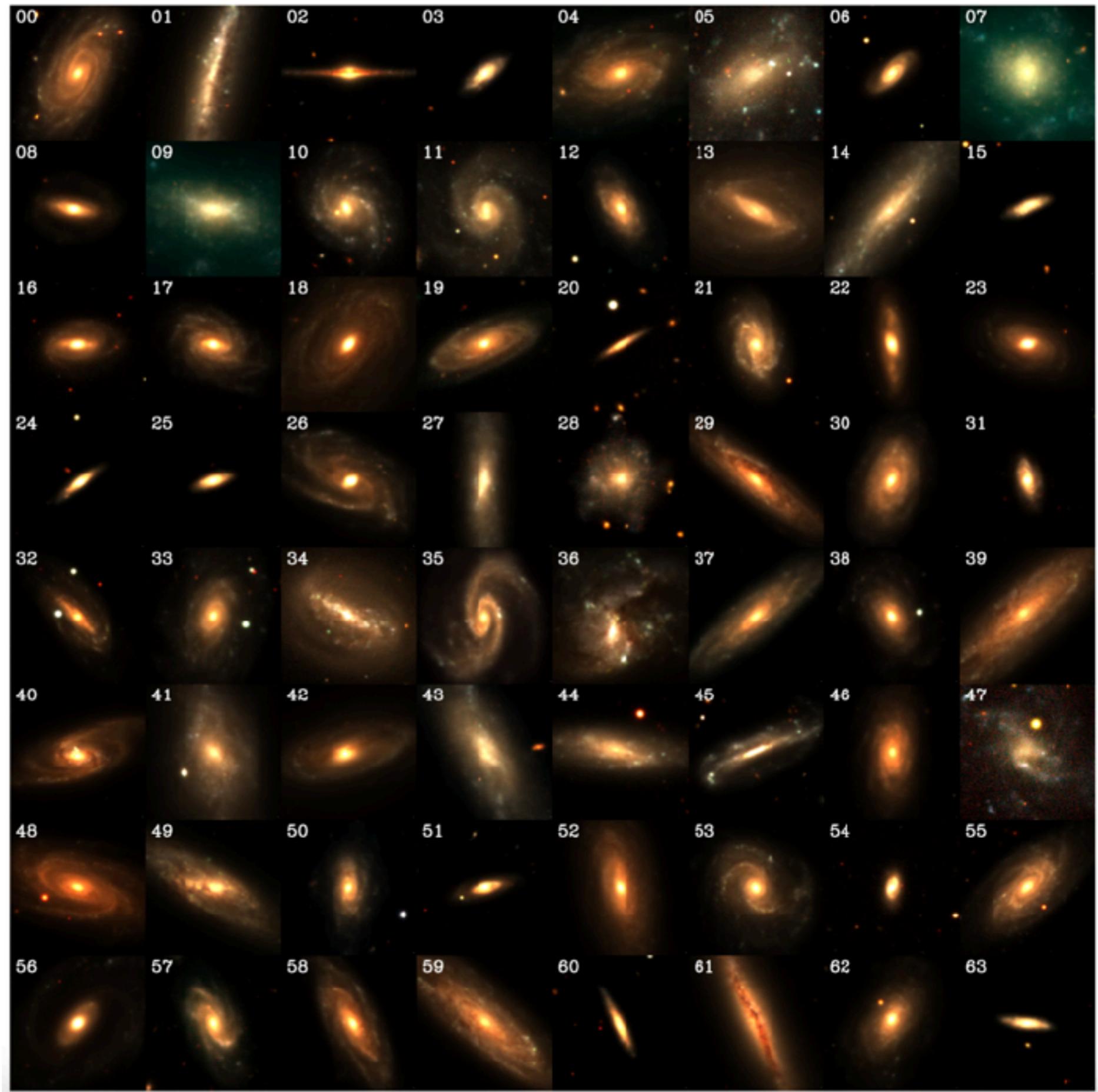


Alexandre Adam

We model the score of the prior

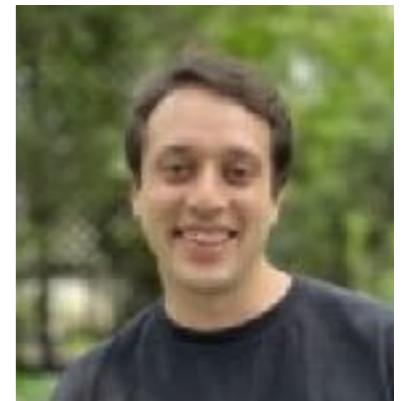
$$s_\theta(x) \equiv \nabla_x \log p_\theta(x)$$





Connor
Stone

SCORE-BASED MODELING



Now if we want to sample from the posterior, its score is all we need:

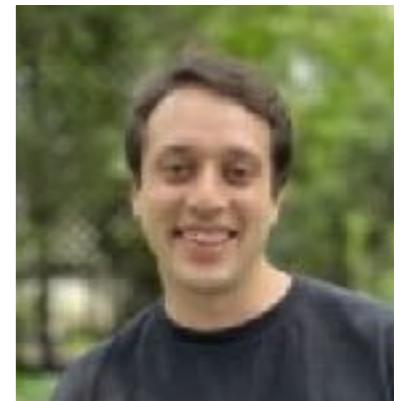
Alexandre Adam

$$\nabla_x \log p(x | y)$$

To a good approximation, we can calculate the likelihood score analytically if we assume it's Gaussian and we know the lensing matrix.

This is the prior score we learnt from the training data

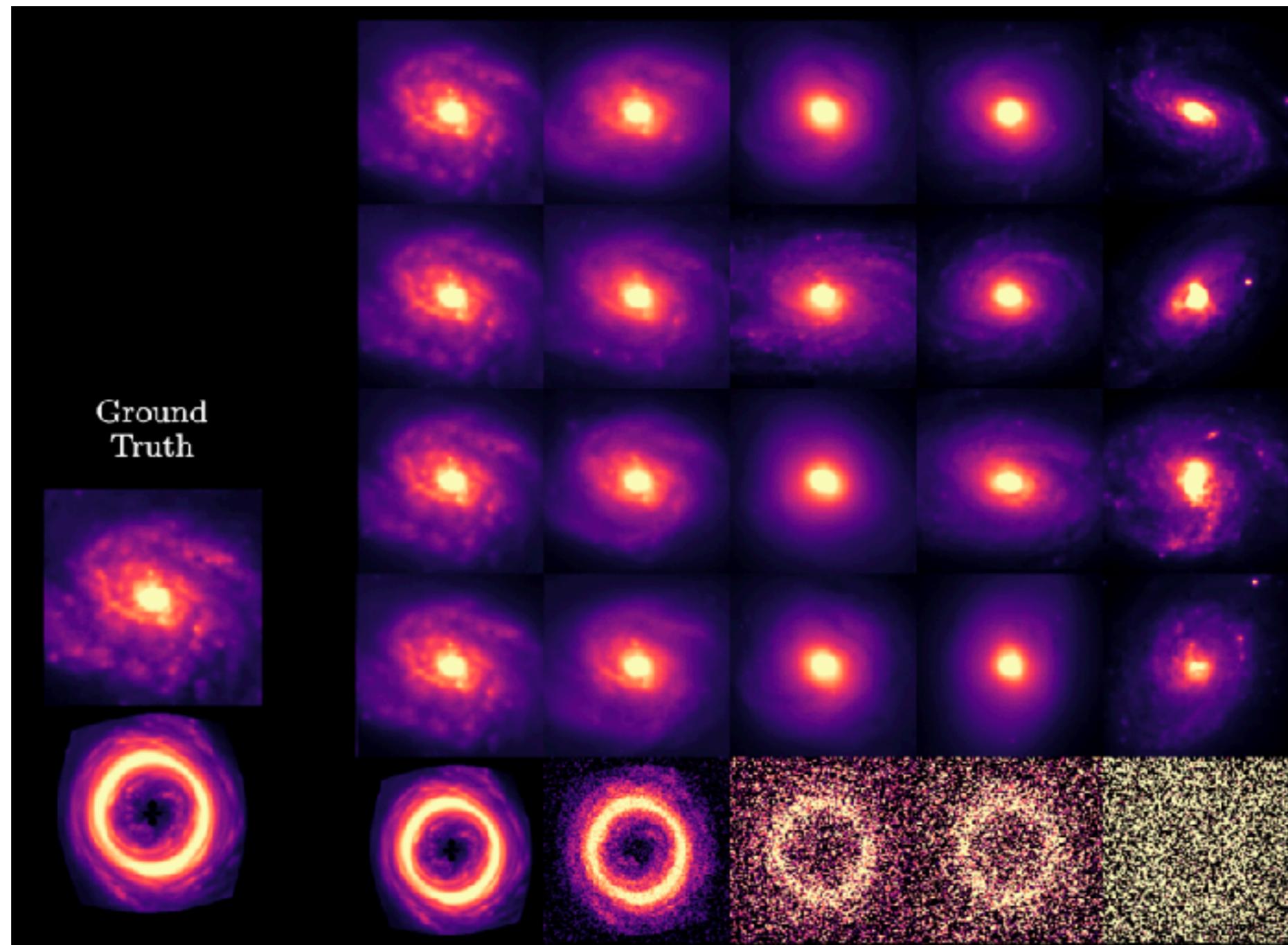
SCORE-BASED MODELING



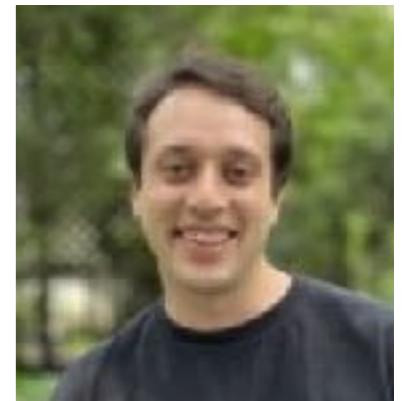
Now if we want to sample from the posterior, its score is all we need:

Alexandre Adam

$$\nabla_x \log p(x | y) = \nabla_x \log p(y | x) + \nabla_x \log p_\theta(x)$$



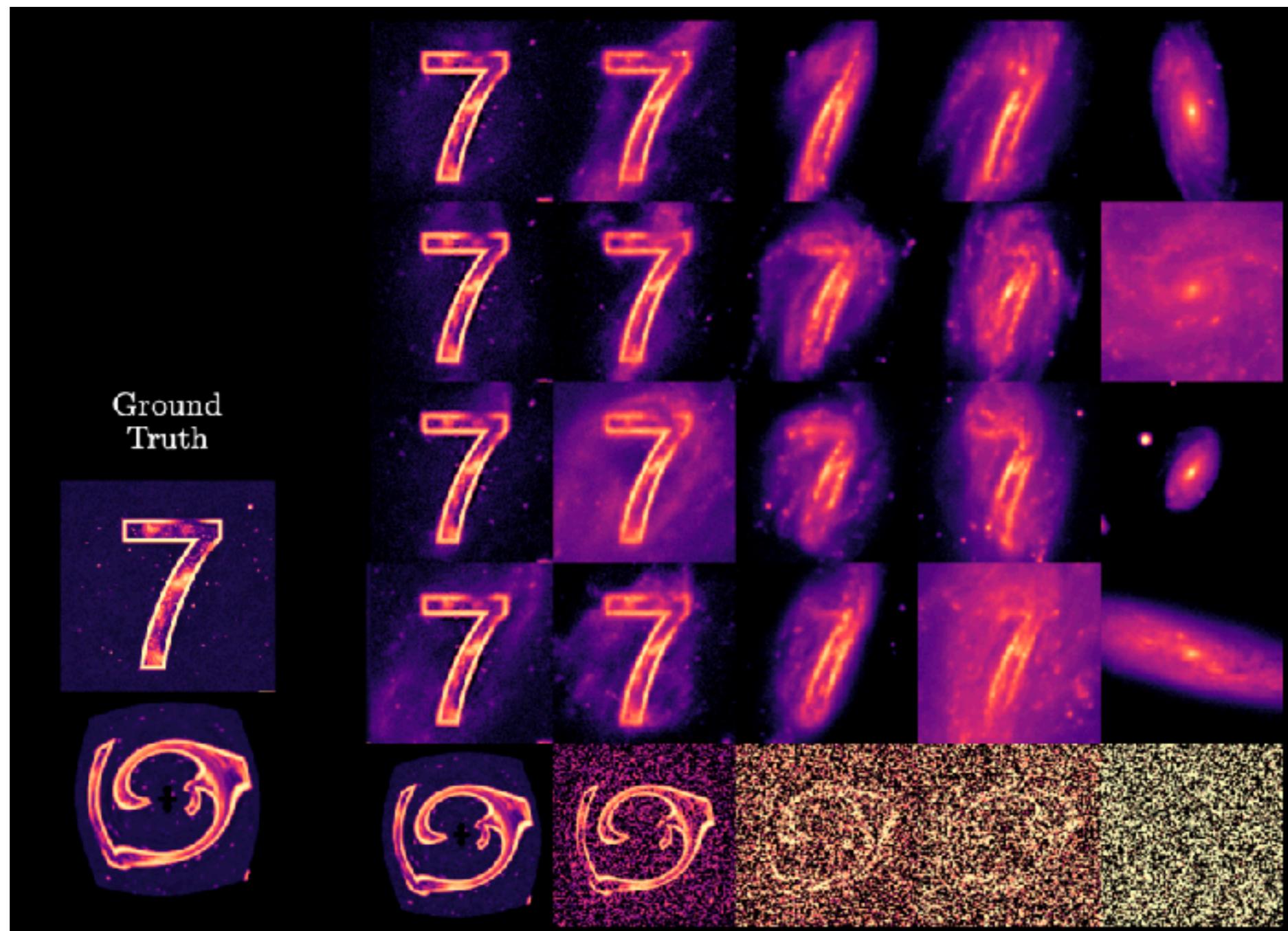
OUT OF DISTRIBUTION TESTS



Now if we want to sample from the posterior, its score is all we need:

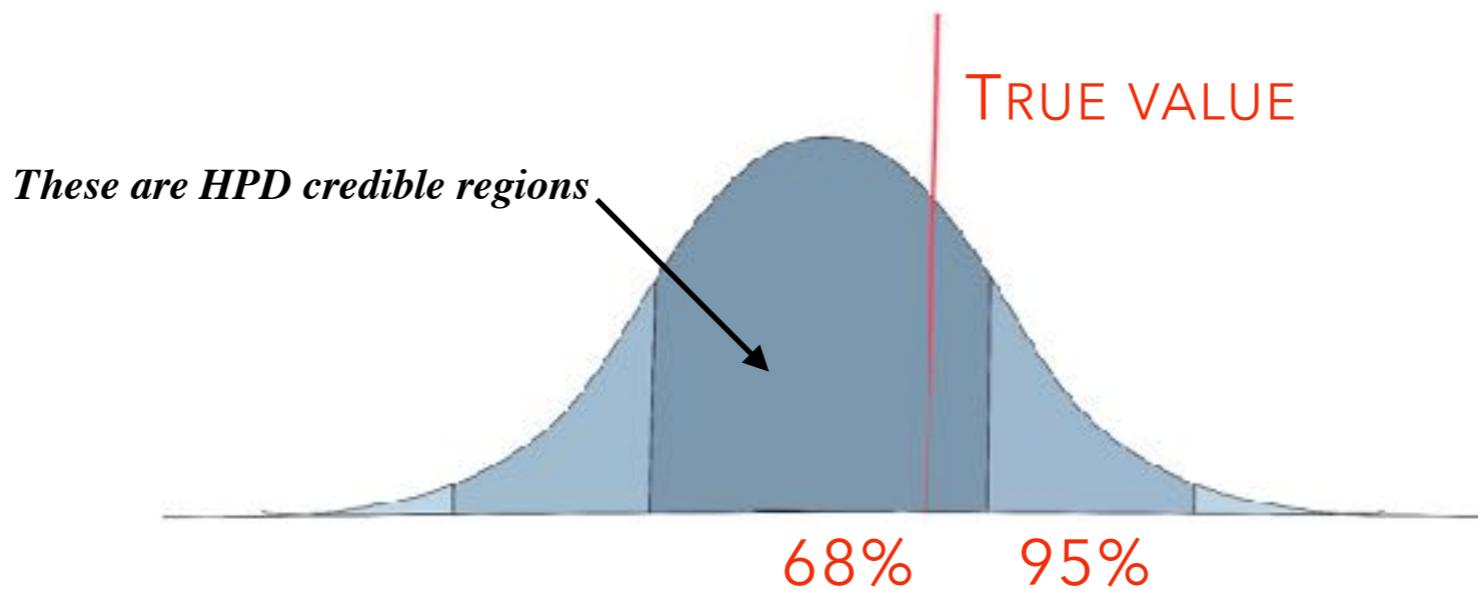
Alexandre Adam

$$\nabla_x \log p(x|y) = \nabla_x \log p(y|x) + \nabla_x \log p_\theta(x)$$



ARE THESE UNCERTAINTIES ACCURATE?

The expected coverage probability of a credible region is the proportion of the time that the region contains the true value of interest.



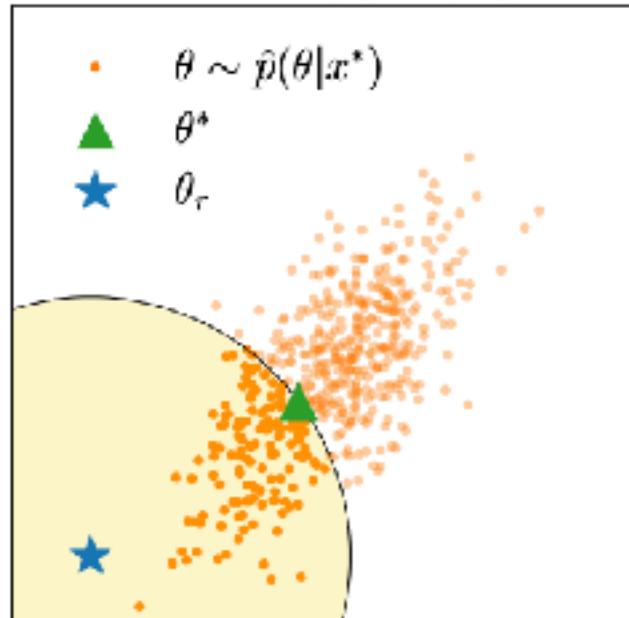
For an accurate posterior estimator, the expected coverage probability is equal to the probability mass of the credible region.

COVERAGE TEST FOR ACCURACY

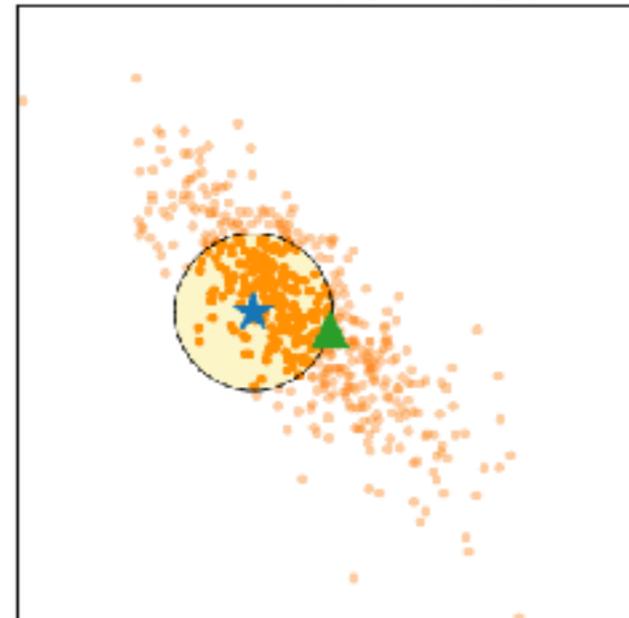


Pablo Lemos

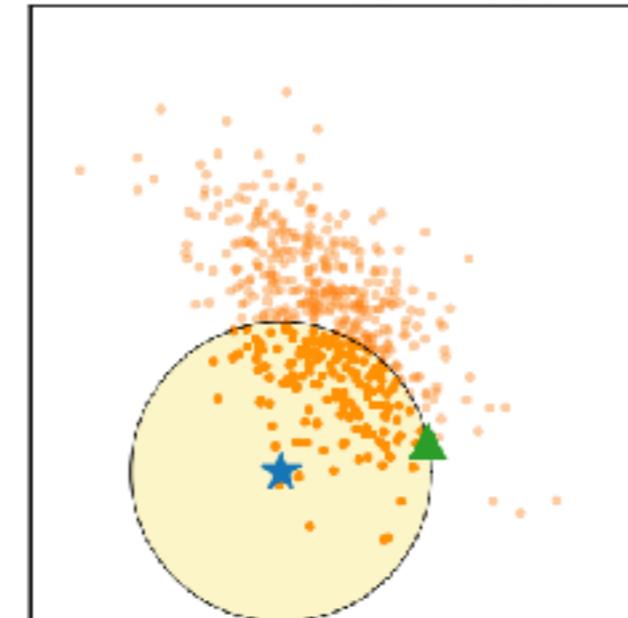
Simulation 1 ($x_1^* \sim p(\cdot | \theta_1^*)$)



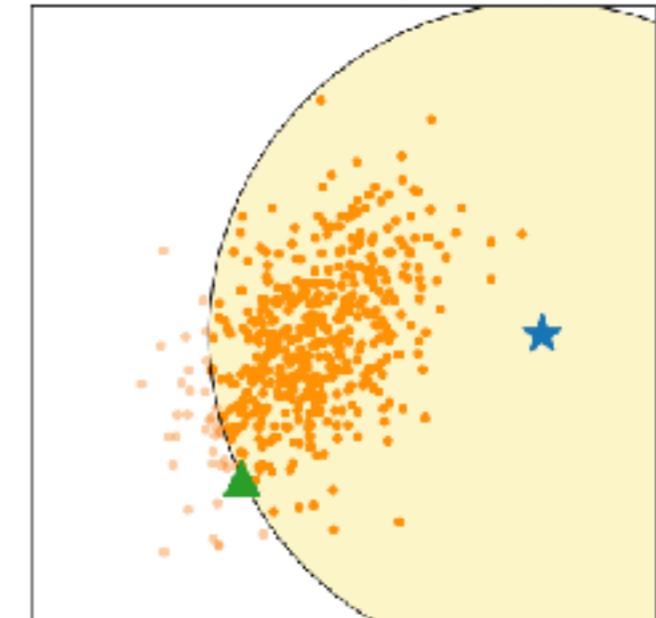
Simulation 2 ($x_2^* \sim p(\cdot | \theta_2^*)$)



Simulation 3 ($x_3^* \sim p(\cdot | \theta_3^*)$)



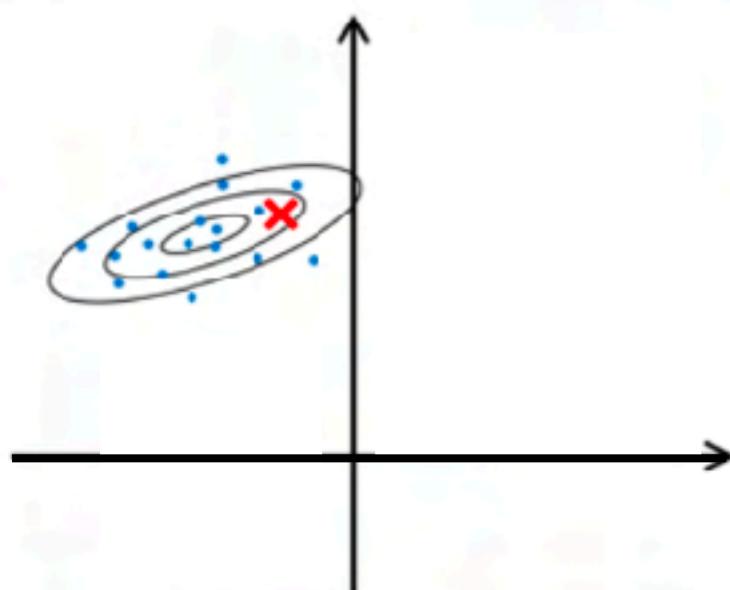
... Simulation N ($x_N^* \sim p(\cdot | \theta_N^*)$)



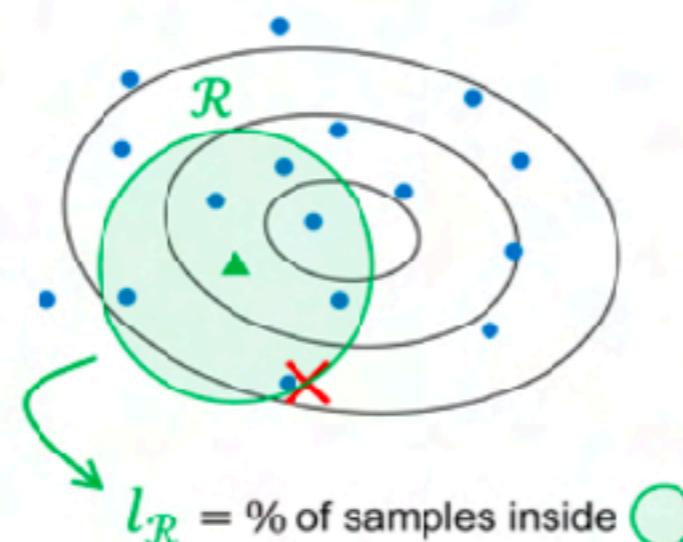
pip install tarp

COVERAGE TEST FOR ACCURACY WITH RANDOM POINTS (TARP)

Step 1
Generate Simulations



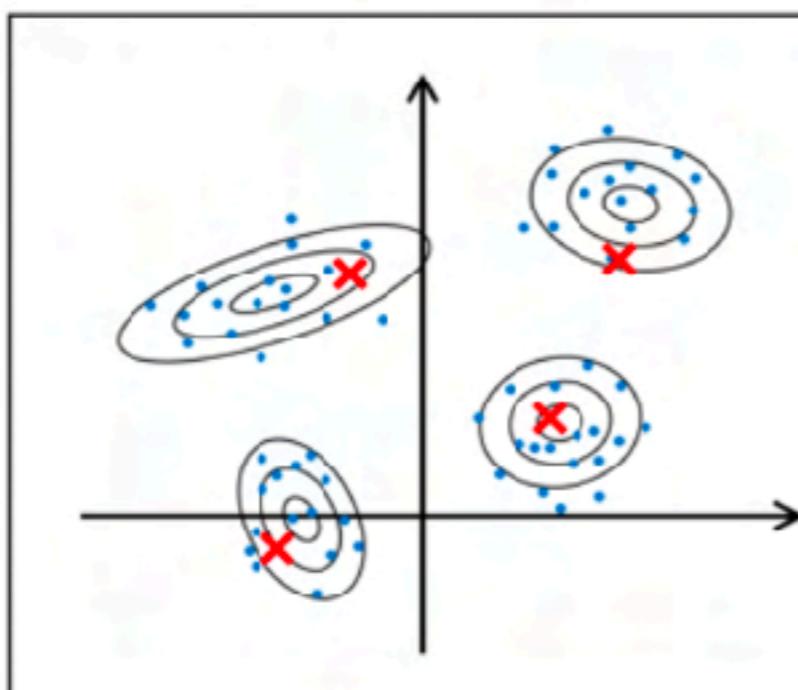
Step 2
Estimate Credibility Level



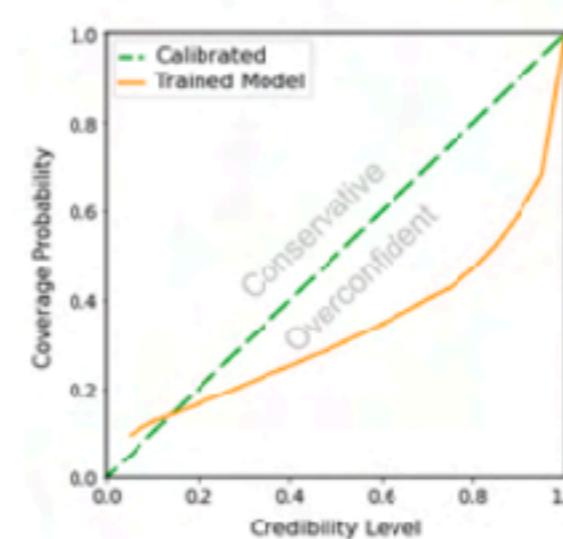
Step 3
Estimate Coverage Probability

$$C_R = \% \text{ of regions with smaller or equal credibility level than } l_R$$
$$= \frac{|\{\mathcal{R}_i : l_{\mathcal{R}_i} \leq l_R\}|}{|\{\mathcal{R}_i\}|}$$

Step 4
Repeat over multiple truth in test set



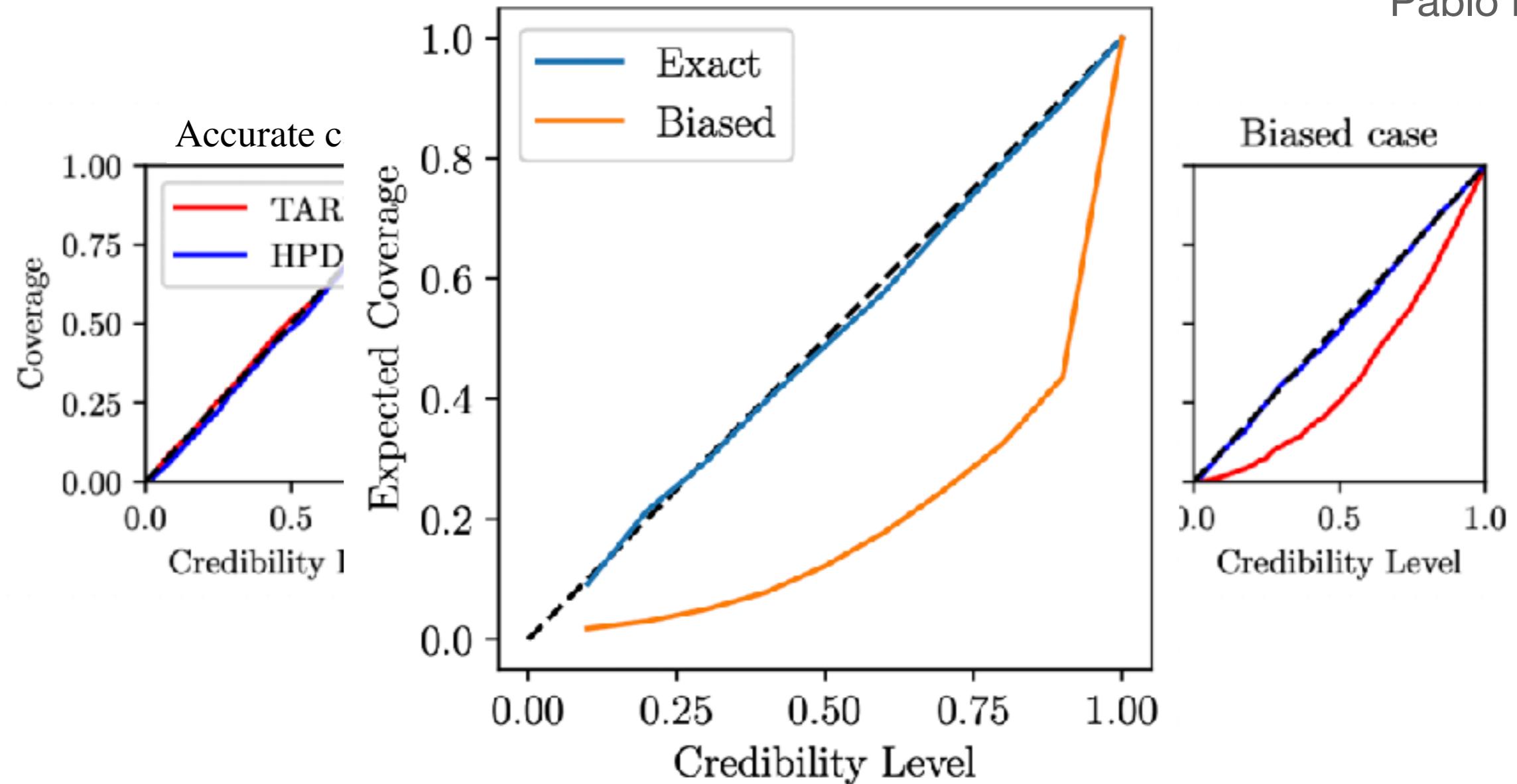
Step 5
Calculate and plot expected coverage probability curve



COVERAGE TEST FOR ACCURACY



Pablo Lemos

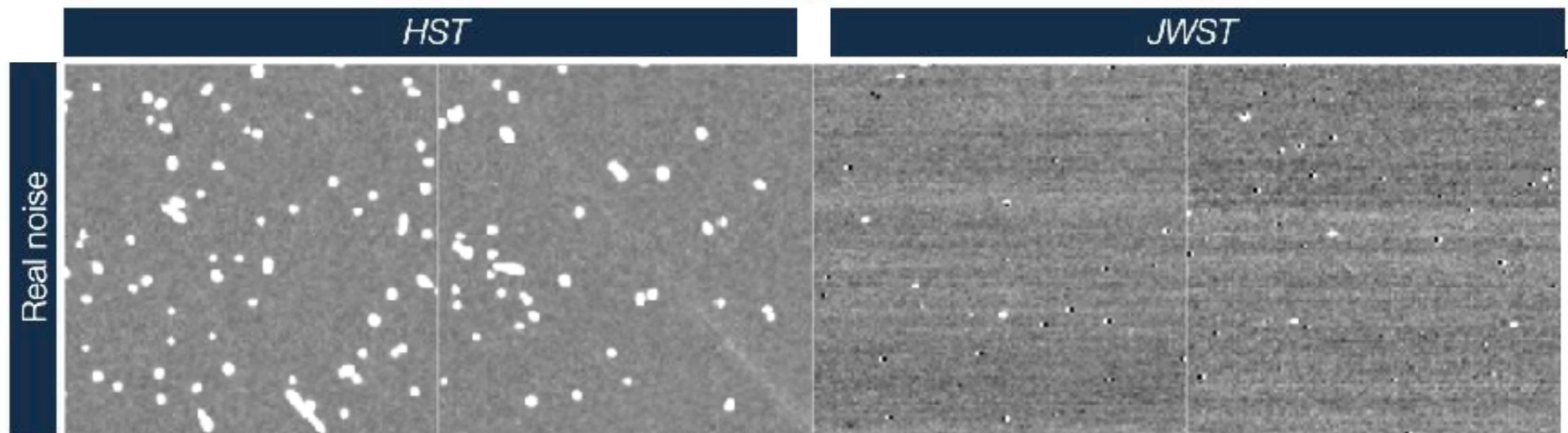


DEALING WITH REALISTIC NOISE: BEYOND GAUSSIANITY



Alexandre Adam

Ronan Legin

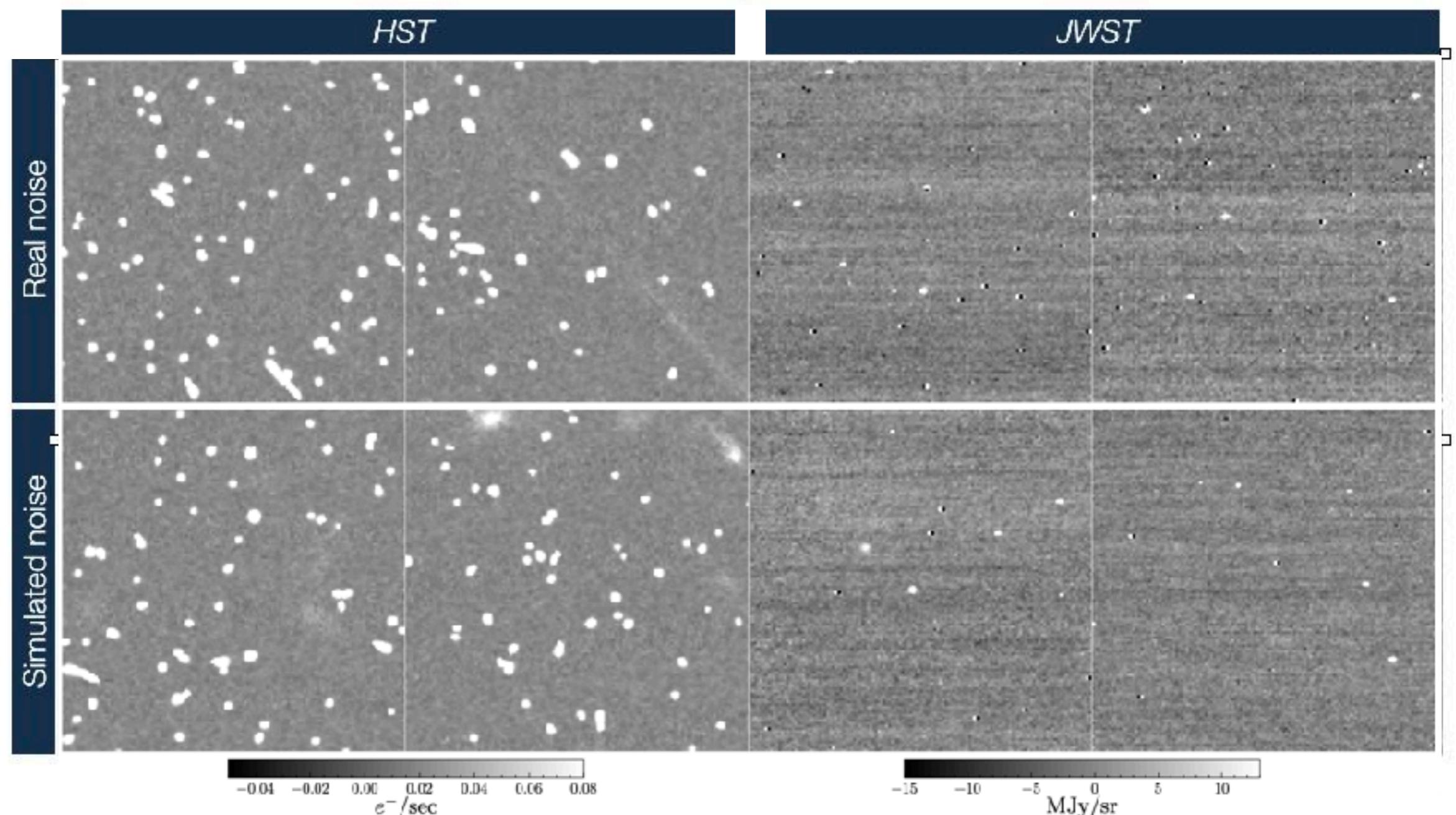


DEALING WITH REALISTIC NOISE: BEYOND GAUSSIANITY

SLIC: SCORE-BASED LIKELIHOOD CHARACTERIZATION

Since we have learnt a generative model of the additive noise, it can now be used in a simulation pipeline to get new, independent realizations of noise:

$$P(\mathbf{x}_O | \eta) = Q(\mathbf{x}_O - \mathbf{M}(\eta))$$



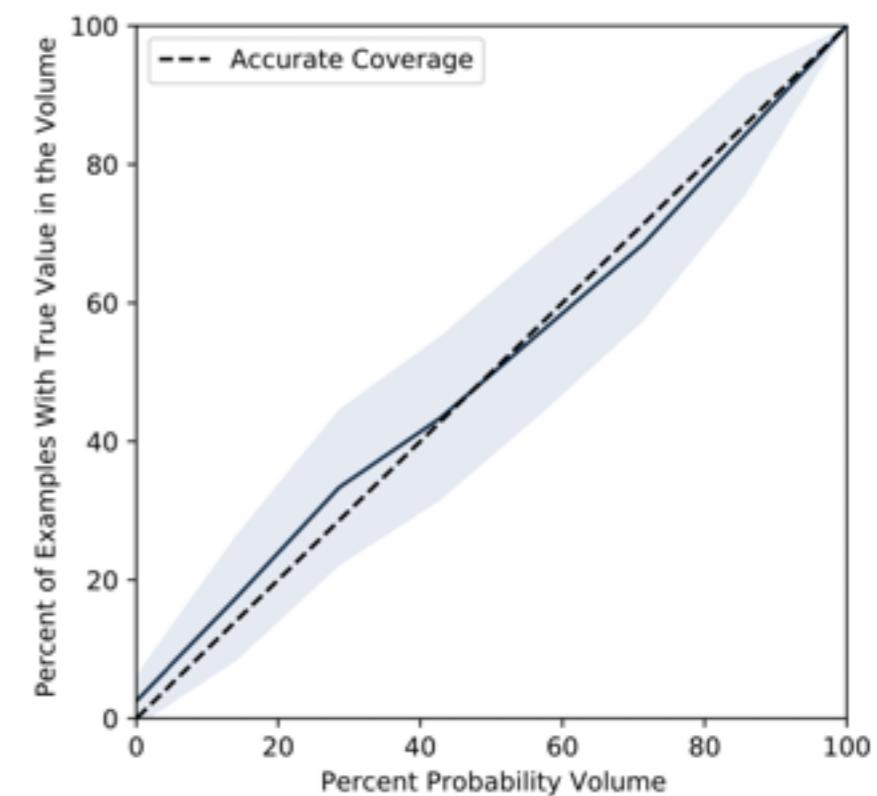
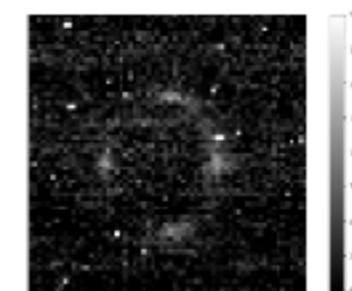
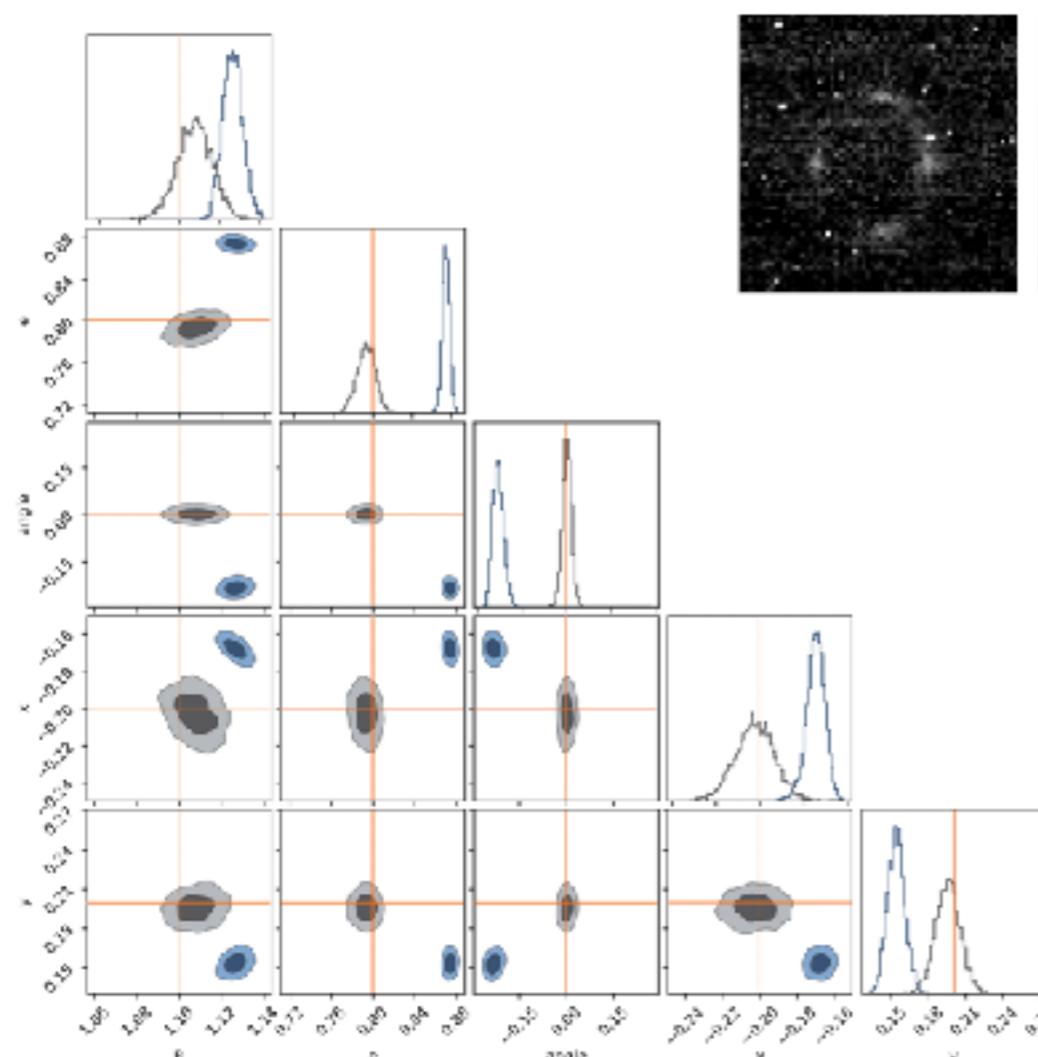
DEALING WITH REALISTIC NOISE: BEYOND GAUSSIANITY

SLIC: SCORE-BASED LIKELIHOOD CHARACTERIZATION

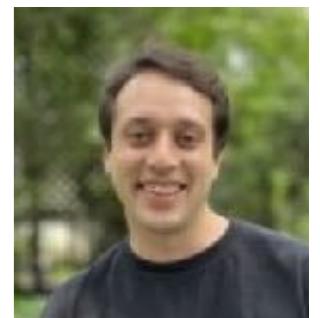
$$\mathbf{s}(\mathbf{x}_0) = \partial \log Q(\mathbf{x}_0) / \partial \mathbf{x}$$

$$P(\mathbf{x}_O | \eta) = Q(\mathbf{x}_O - \mathbf{M}(\eta))$$

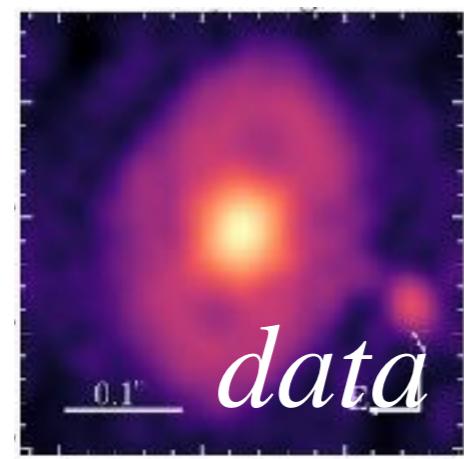
$$\eta_{i+1} = \eta_i + \tau \nabla_{\mathbf{x}} \log Q(\mathbf{x}_o - \mathbf{M}(\eta)) \nabla_{\eta} M(\eta_i) + \sqrt{2\tau}\xi$$



PSF-DECONVOLUTION

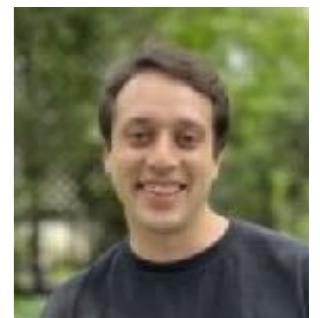


Alexandre Adam



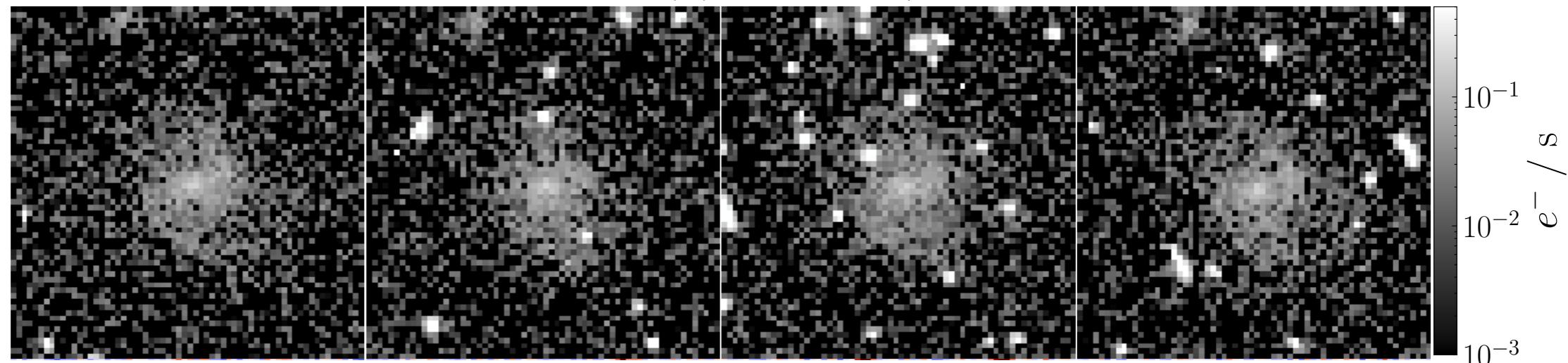
$$= PSF \left(\begin{matrix} \text{data} \\ x \end{matrix} \right) + n$$

PSF-DECONVOLUTION (FOR HST)

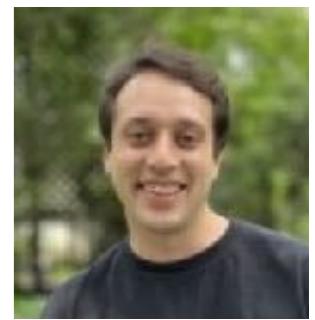


Alexandre Adam

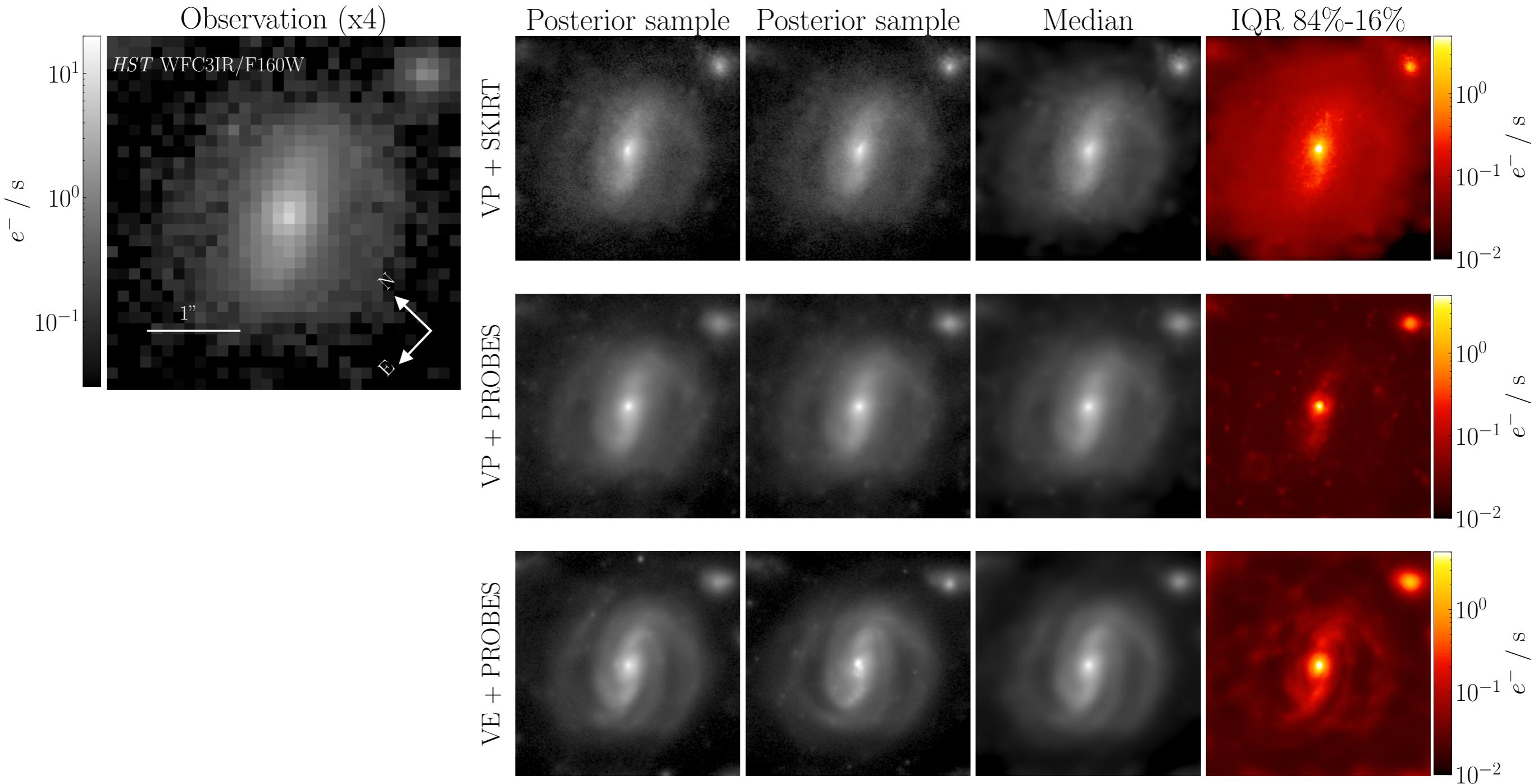
Observations (\mathbf{y}), *HST* ACS/F814W



PSF-DECONVOLUTION (FOR HST)

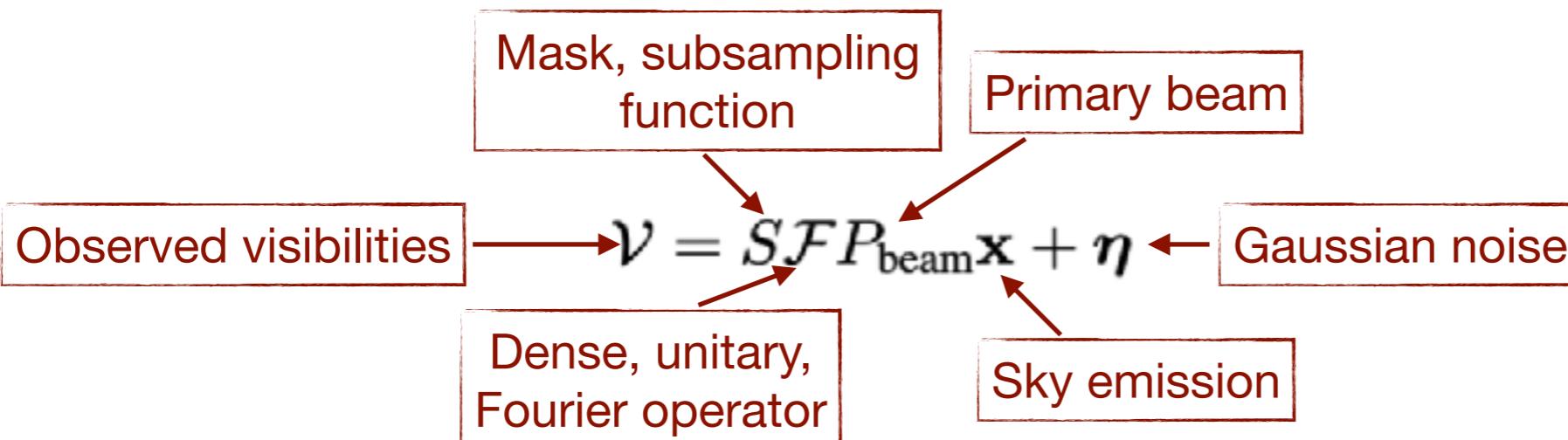


Alexandre Adam

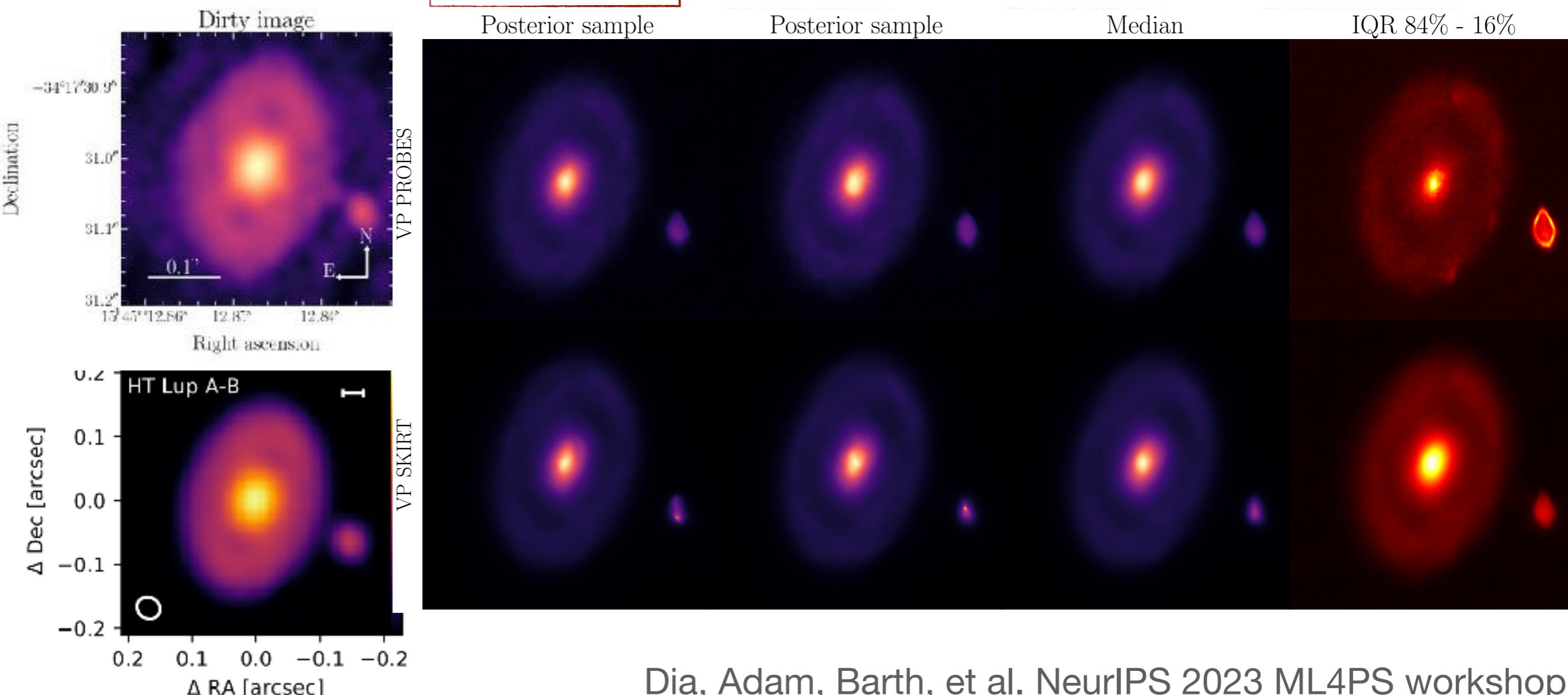


PSF-DECONVOLUTION FOR INTERFEROMETRIC DATA

With Score-Based Diffusion Models



Noé Dia



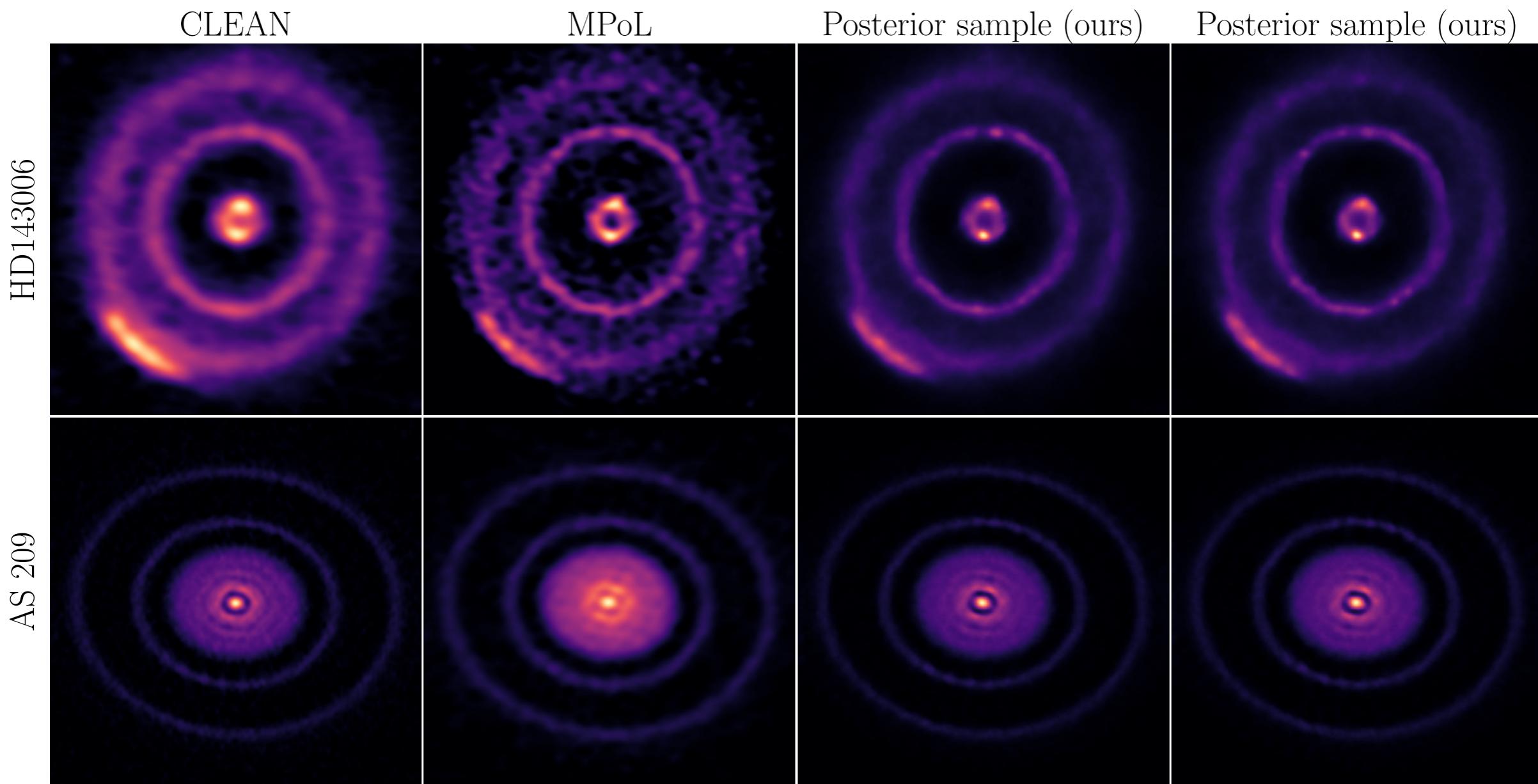
PSF-DECONVOLUTION FOR INTERFEROMETRIC DATA

With Score-Based Diffusion Models

$$\mathcal{V} = S\mathcal{F}P_{\text{beam}}\mathbf{x} + \boldsymbol{\eta}$$



Noé Dia

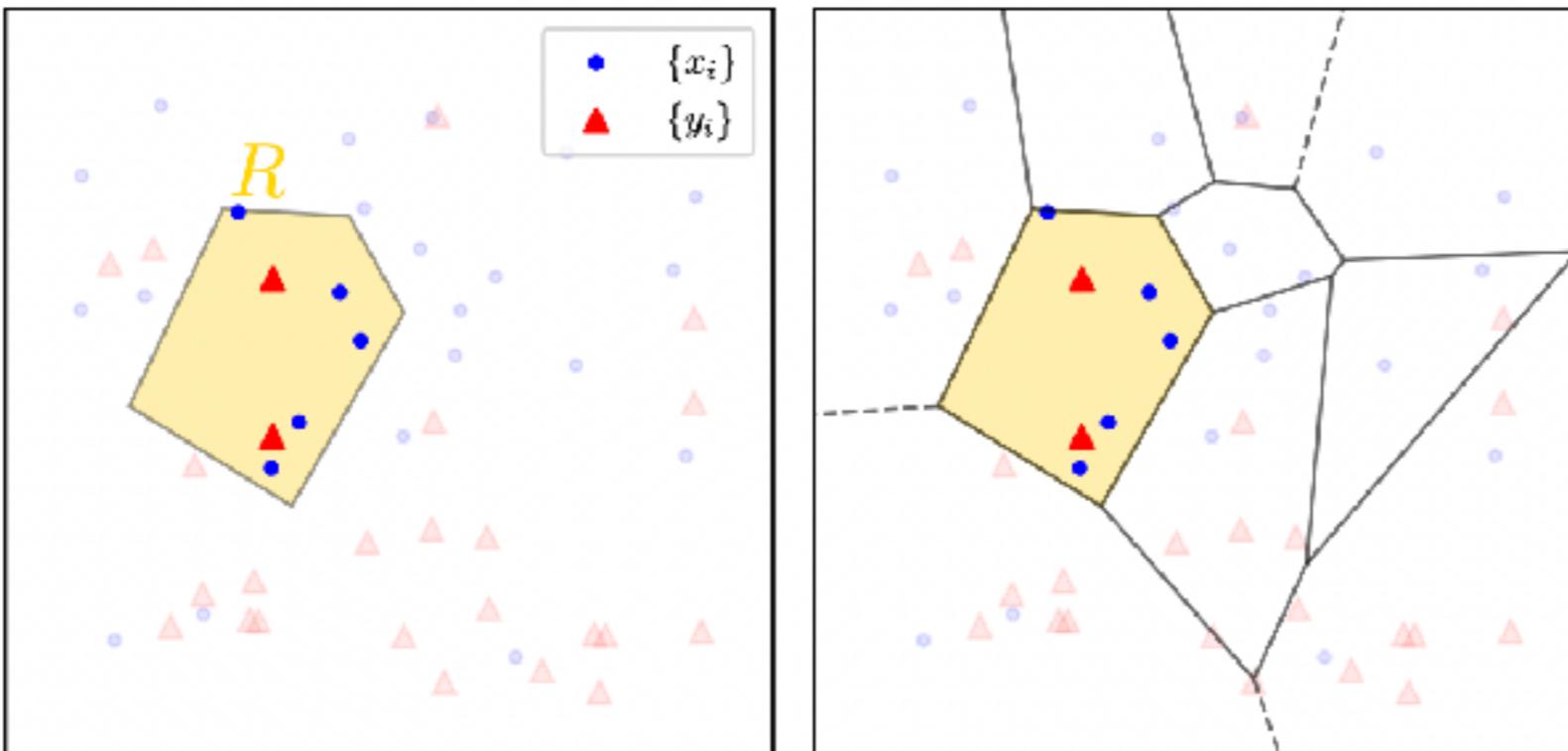


PQMASS: PROBABILISTIC ASSESSMENT OF GENERATIVE MODELS USING PROBABILITY MASS ESTIMATION



Sammy Sharief

Pablo Lemos



$$k(\mathbf{x}, R) \sim \mathcal{B}(n, \mathbb{P}_p(R))$$

$$\{k(\mathbf{x}, R_i)\}_{i=1 \dots n_R} \sim \mathcal{M}\left(n, \{\mathbb{P}_p(R_i)\}_{i=1 \dots n_R}\right)$$

$$\hat{N}_{x,i} \equiv n\hat{p}_{R_i}, \quad \hat{N}_{y,i} \equiv m\hat{p}_{R_i},$$

$$\hat{p}_{R_i} \equiv \frac{k(\mathbf{x}, R_i) + k(\mathbf{y}, R_i)}{n+m}.$$

$$\chi^2_{\text{PQM}} \equiv \sum_{i=1}^{n_R} \left[\frac{(k(\mathbf{x}, R_i) - \hat{N}_{x,i})^2}{\hat{N}_{x,i}} + \frac{(k(\mathbf{y}, R_i) - \hat{N}_{y,i})^2}{\hat{N}_{y,i}} \right]$$

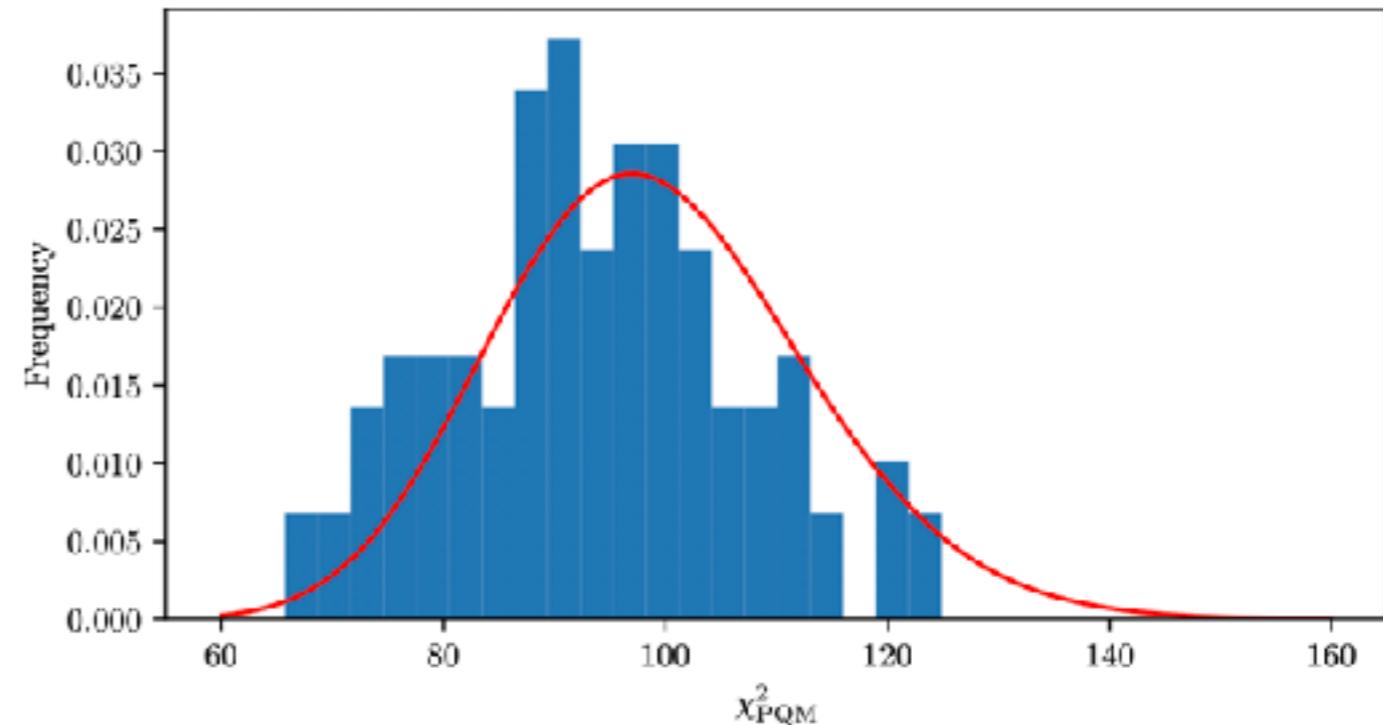
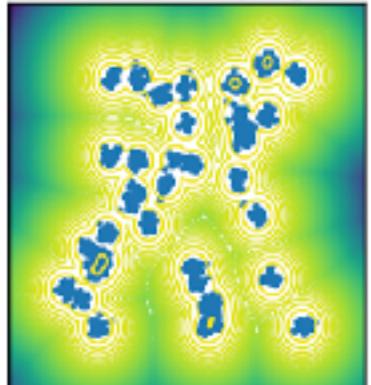
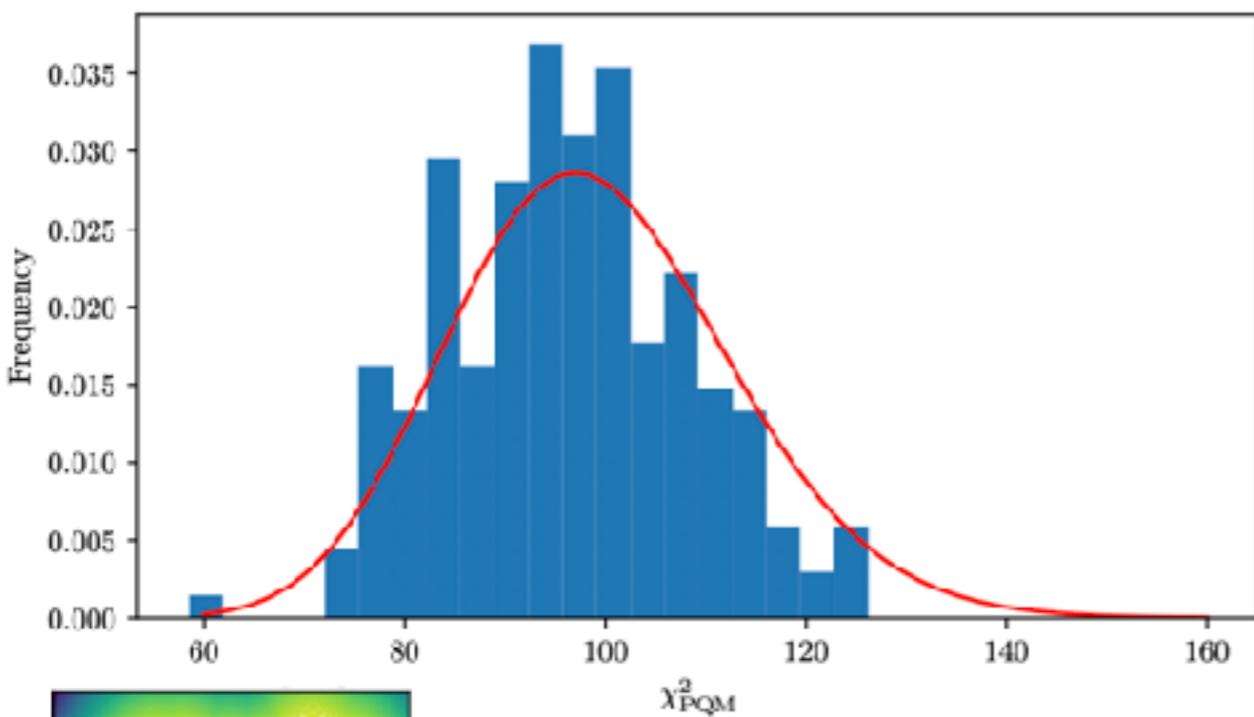
PQMASS: PROBABILISTIC ASSESSMENT OF GENERATIVE MODELS USING PROBABILITY MASS ESTIMATION



Sammy Sharief

Pablo Lemos

Given any sampling distribution, or generative model, if two sets of samples are generated from the same distribution, then the statistic χ^2_{PQM} follows a chi-square distribution with $n_R - 1$ degrees of freedom.

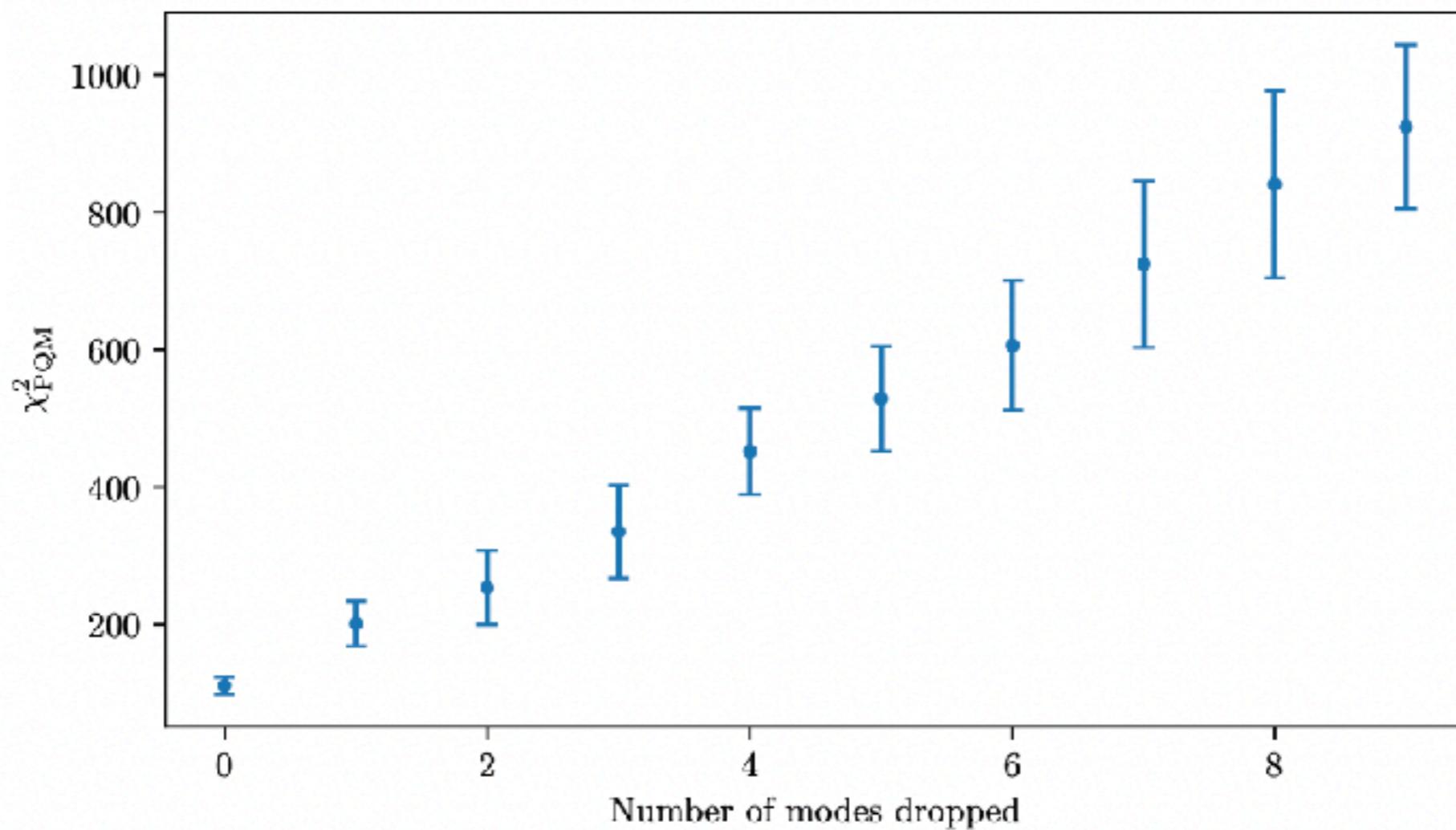
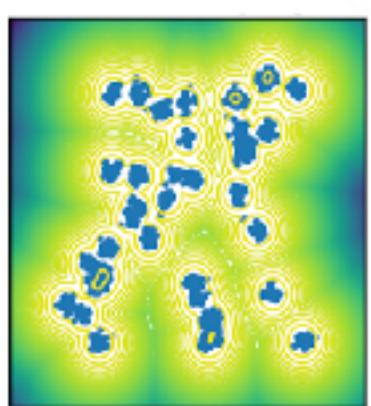


PQMASS: PROBABILISTIC ASSESSMENT OF GENERATIVE MODELS USING PROBABILITY MASS ESTIMATION



Sammy
Sharief

Pablo Lemos



PQMASS: PROBABILISTIC ASSESSMENT OF GENERATIVE MODELS USING PROBABILITY MASS ESTIMATION



Sammy
Sharief

Pablo Lemos

