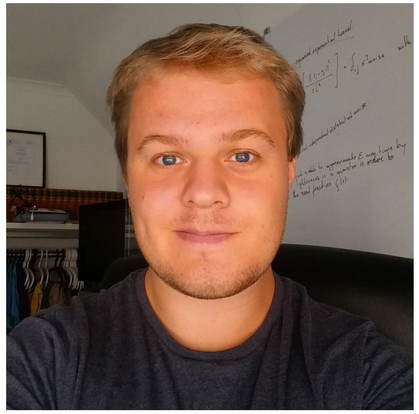
Mining for Dark Matter substructure: Learning from lenses without a likelihood

Johann Brehmer

New York University

DMWG seminar, RIKEN
February 17, 2020

Siddharth Mishra-Sharma



Joeri Hermans

Gilles Louppe

Kyle Cranmer

NYU

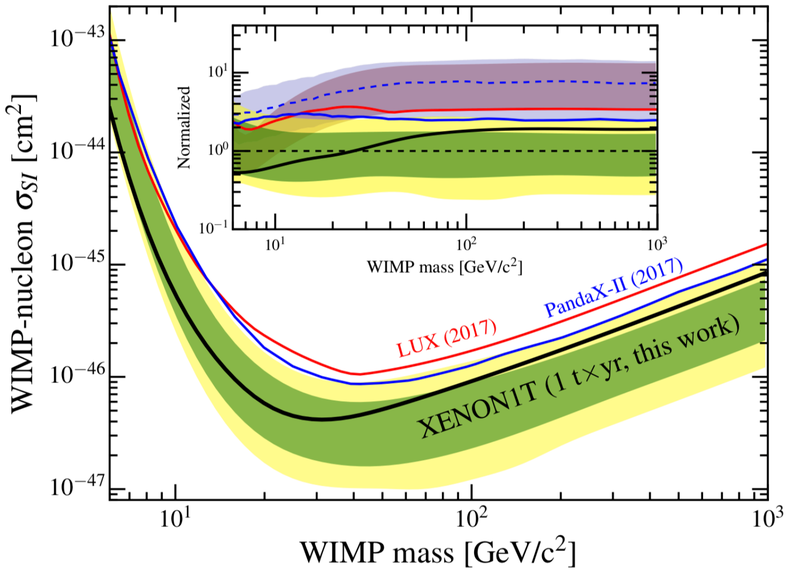
MSDSE
Moore - Sloan
Data Science Environments

diana hep

iris hep
Institute for Research and Innovation
in Software for High Energy Physics

The SCAILFIN Project
scailfin.github.io

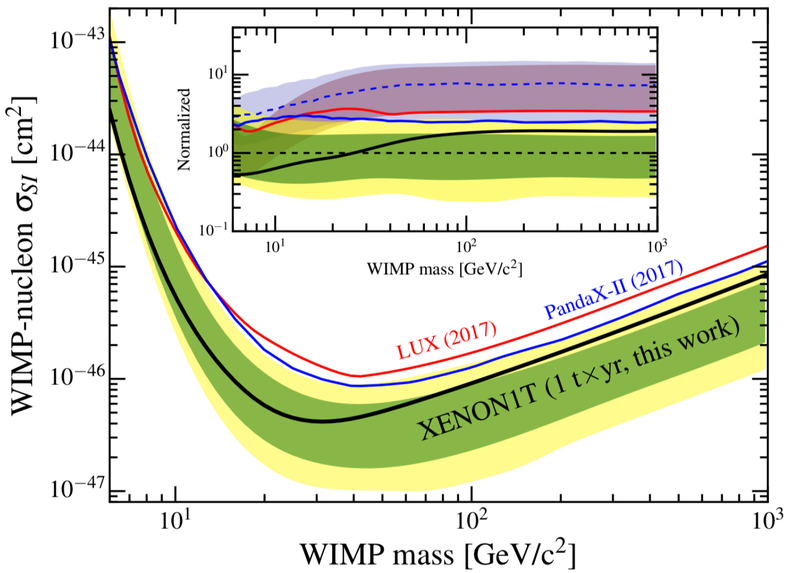
Dark matter



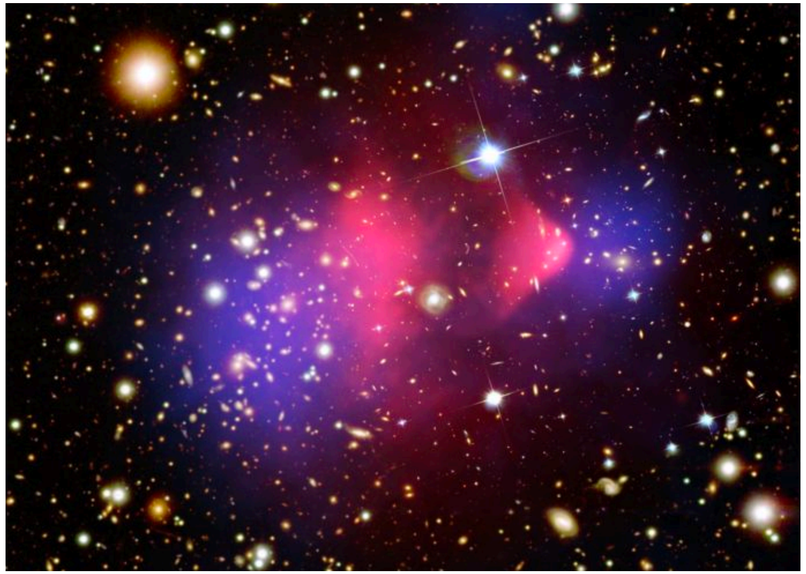
[XENON 1805.12562]

Non-gravitational interactions:
no evidence so far

Dark matter



[XENON 1805.12562]



[NASA]

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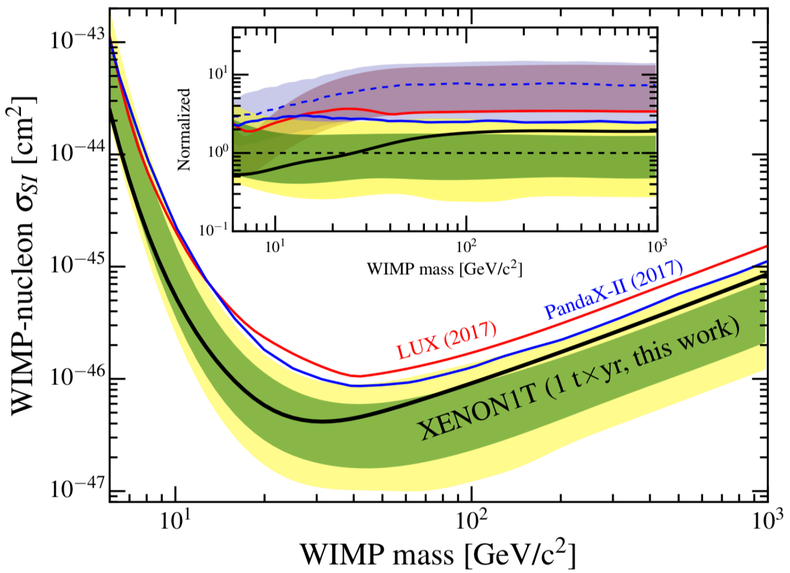
Gravitational interactions at large length scales: plenty of evidence, consistent with ΛCDM

Dark matter



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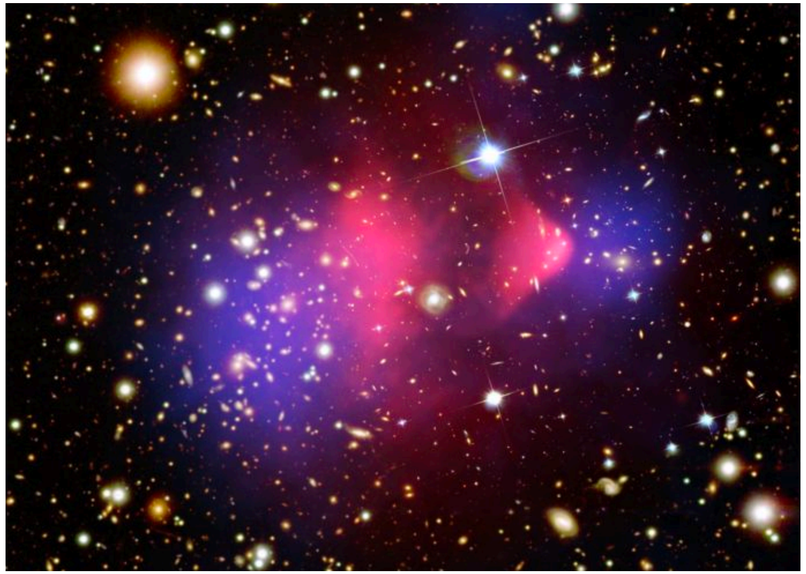

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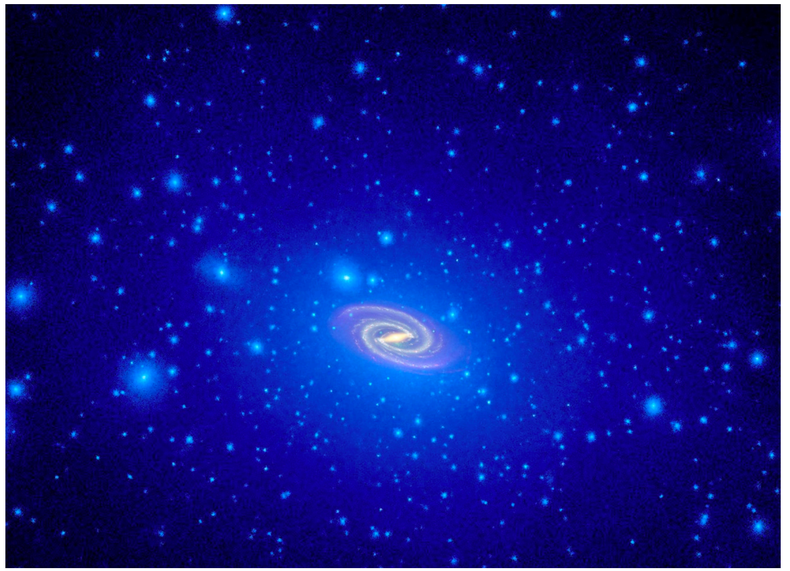


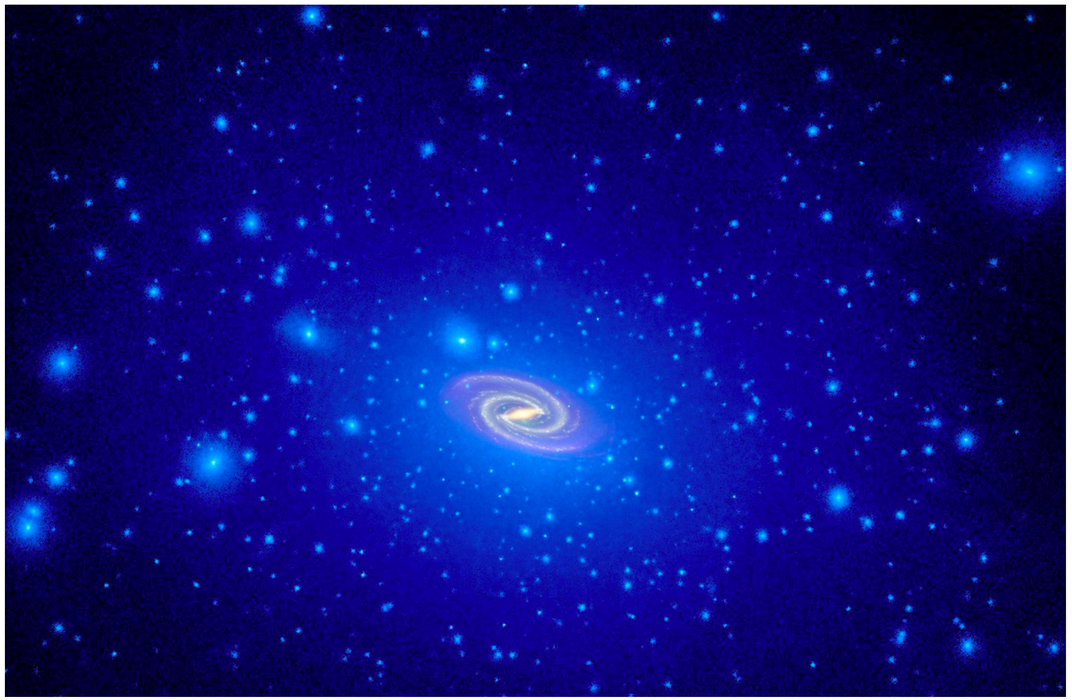
[T. Brown, J.Tumlinson]

Non-gravitational interactions: no evidence so far

Gravitational interactions at large length scales: plenty of evidence, consistent with ΛCDM

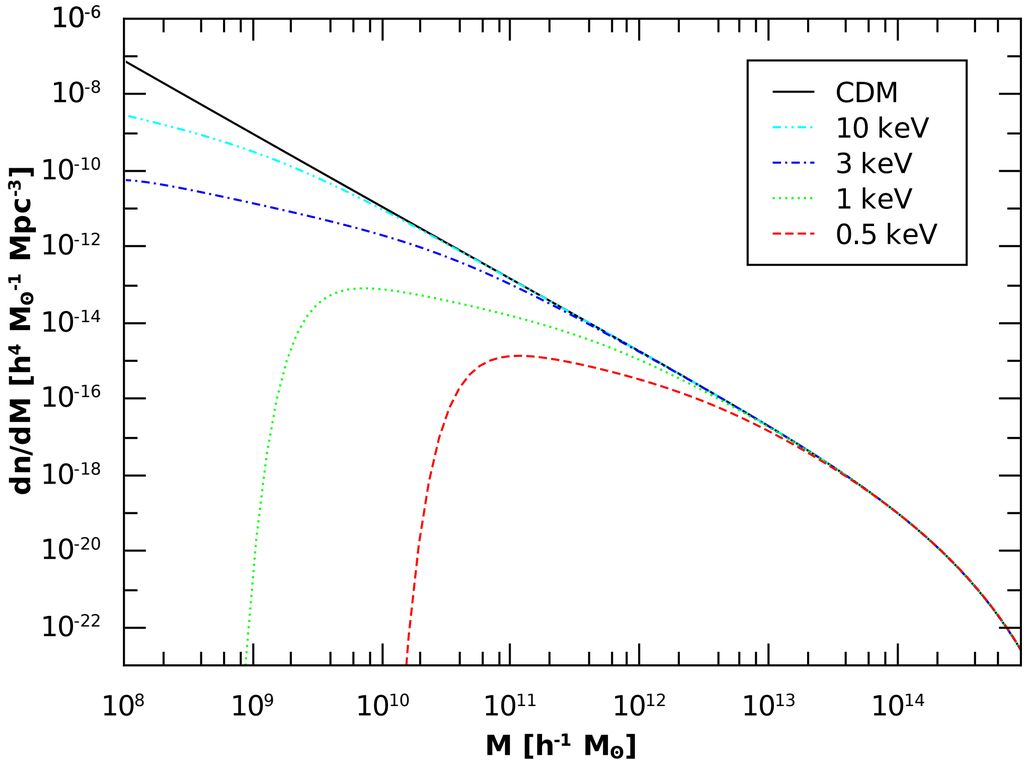
Gravitational interactions at small scales (DM substructure): beginning to be probed, many models predict deviations from ΛCDM

DM small-scale structure is a probe of its particle nature



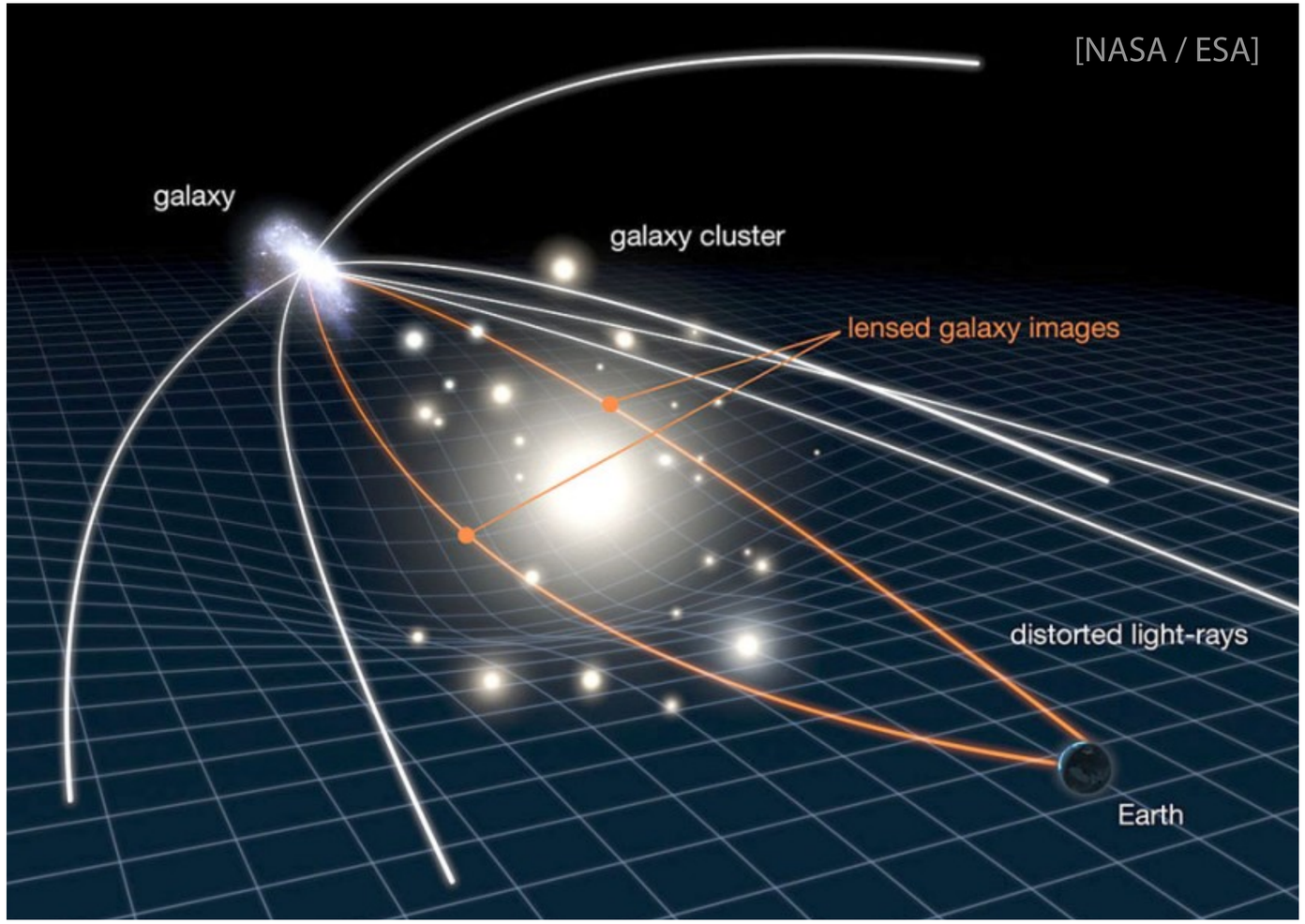
[T. Brown, J.Tumlinson]

Abundance of DM subhalos vs mass:



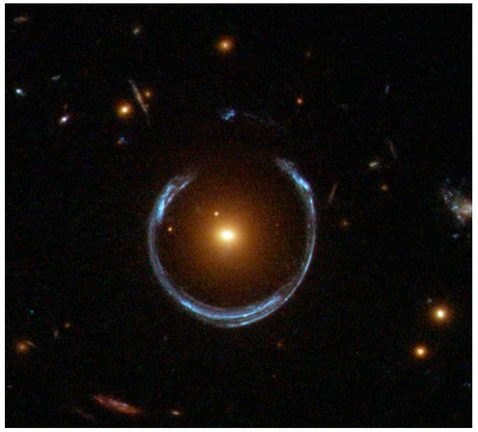
[R. Dunstan et al 1109.6291]

Strong gravitational lensing



Multiple images of quasars

Extended arcs from galaxies



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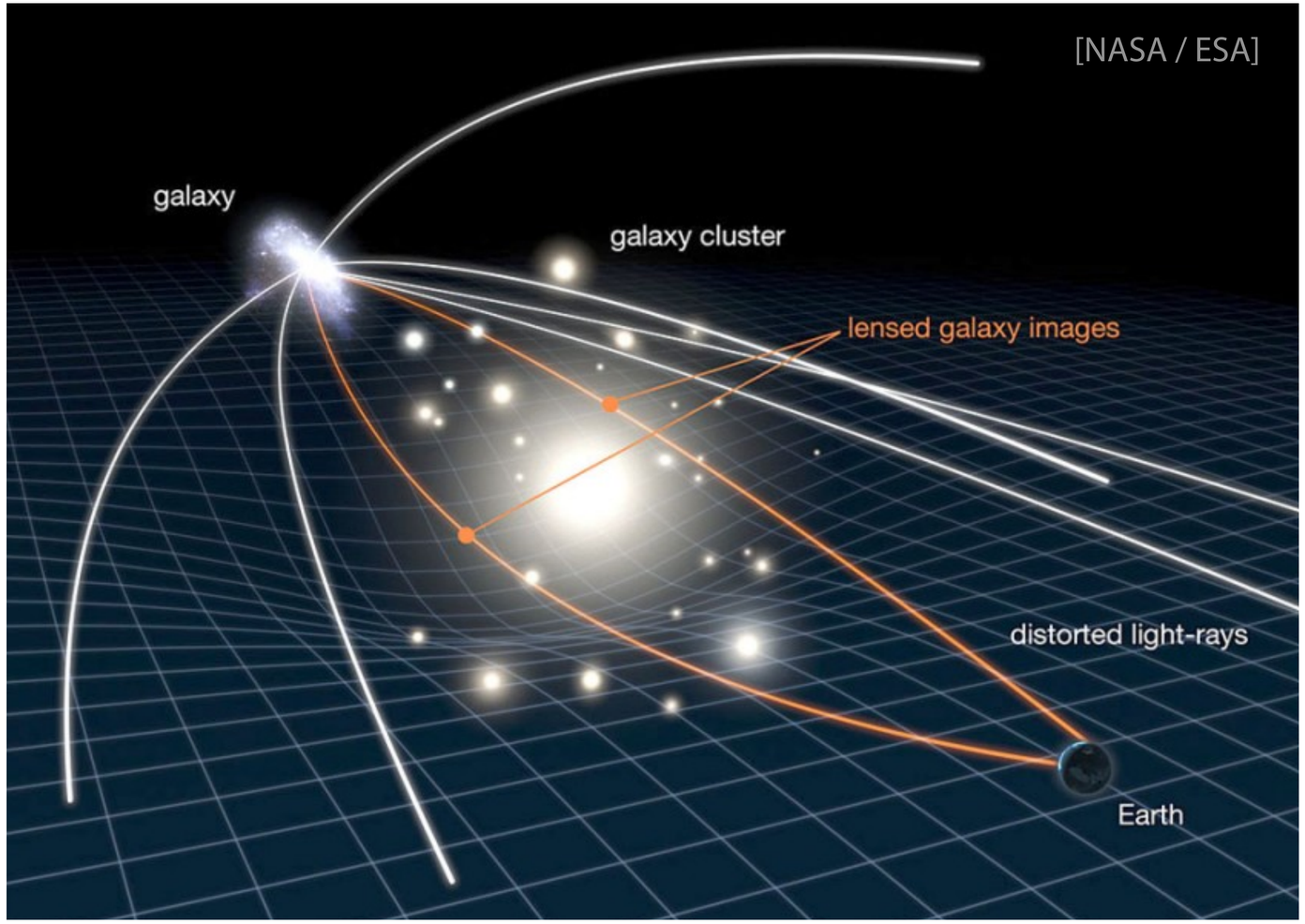

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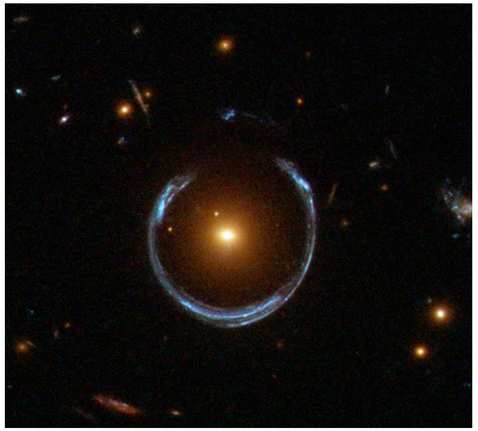
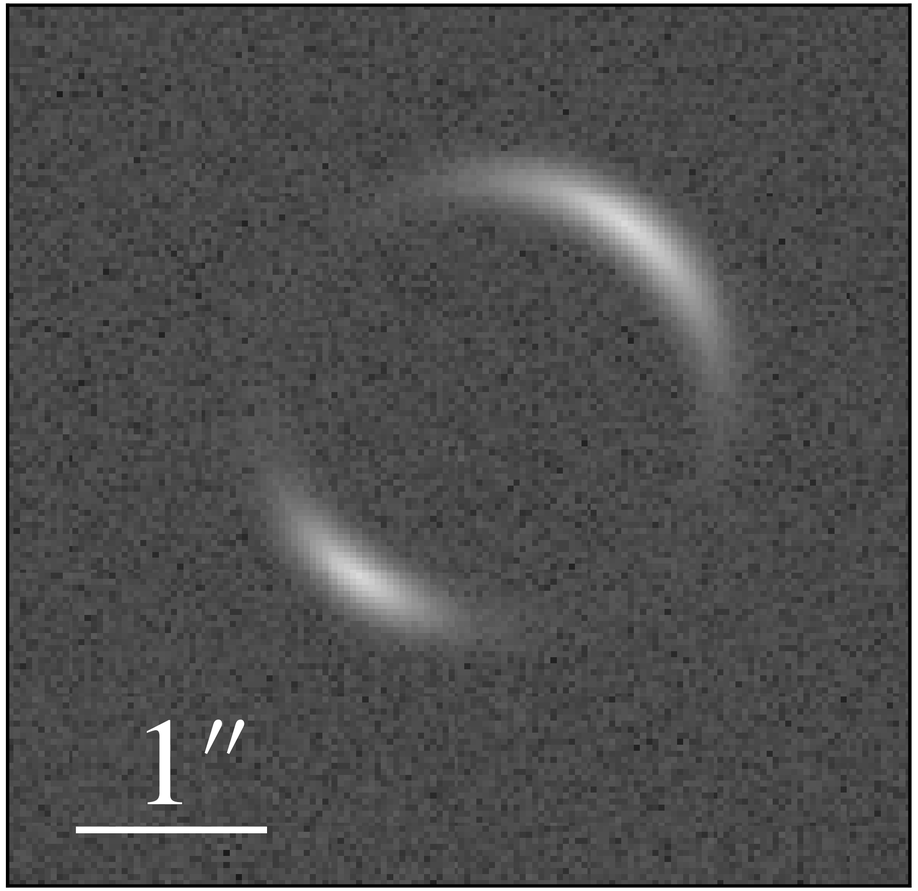
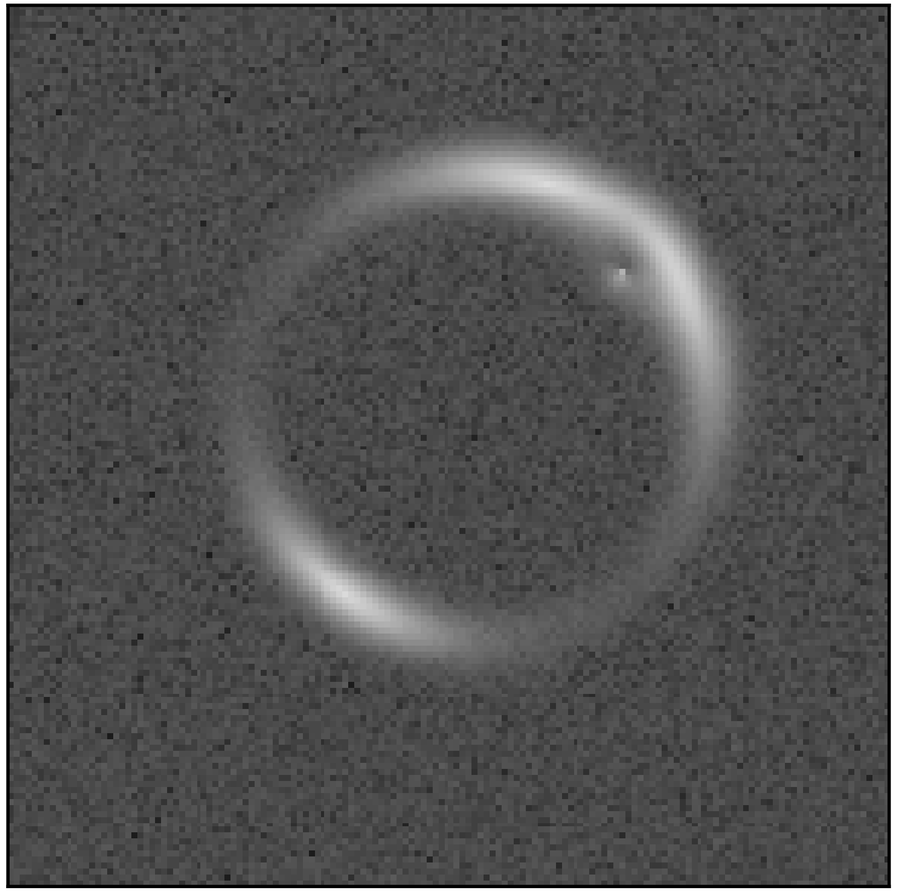


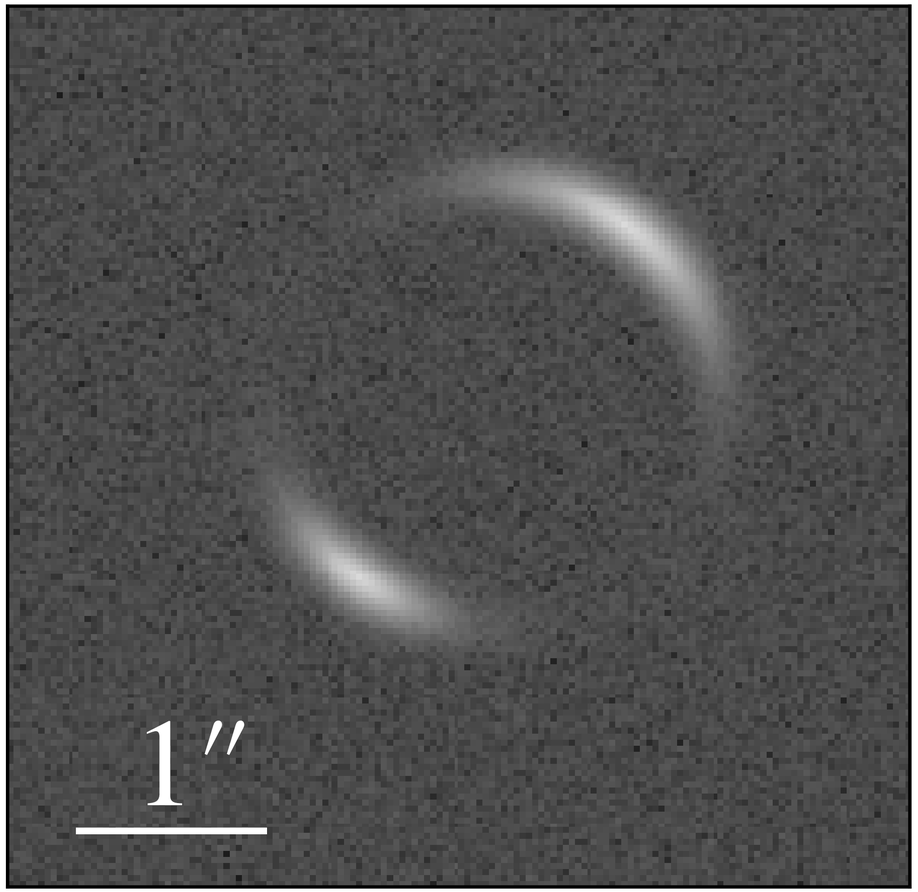
Subhalos affect strong lensing



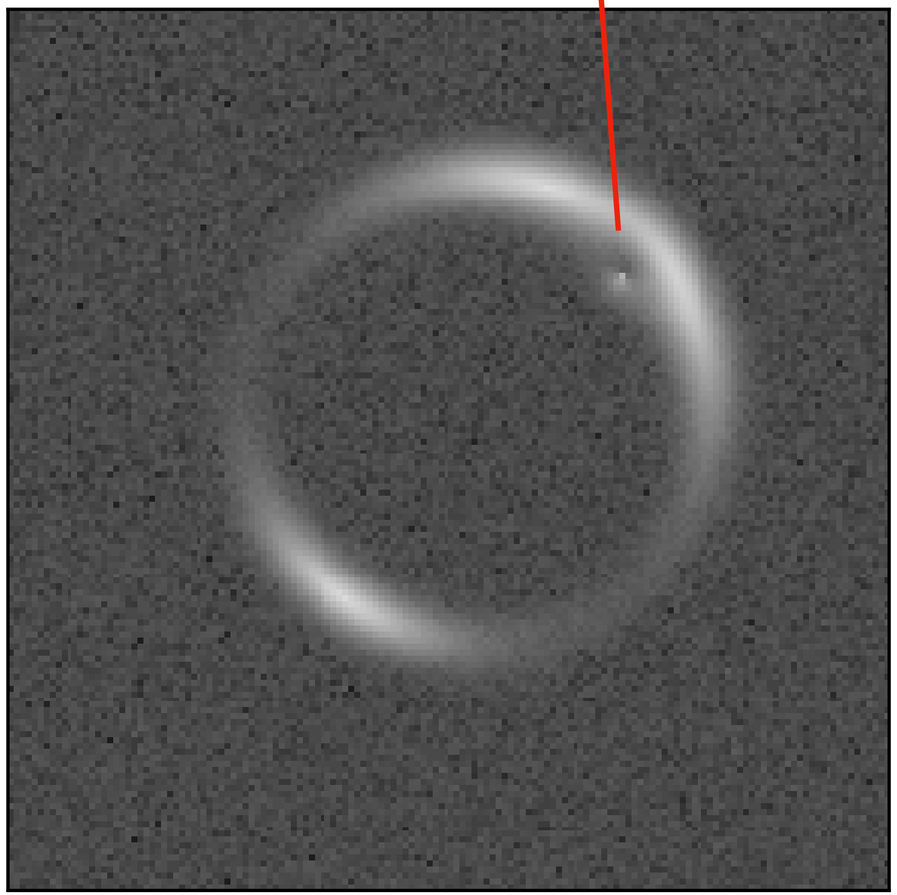


Subhalos affect strong lensing

Smooth halo only

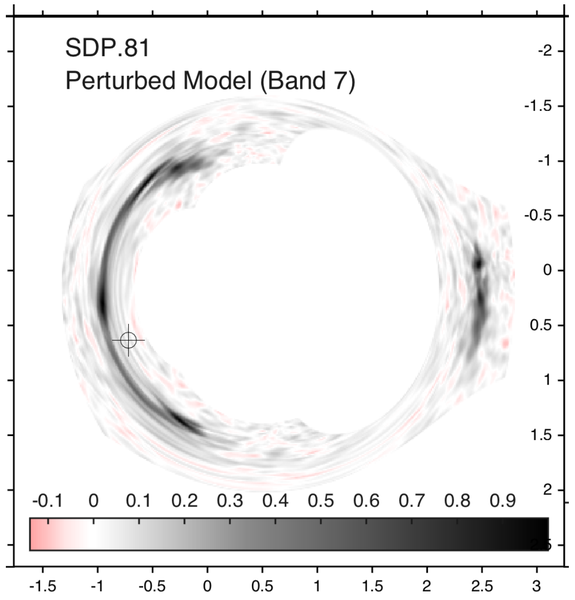


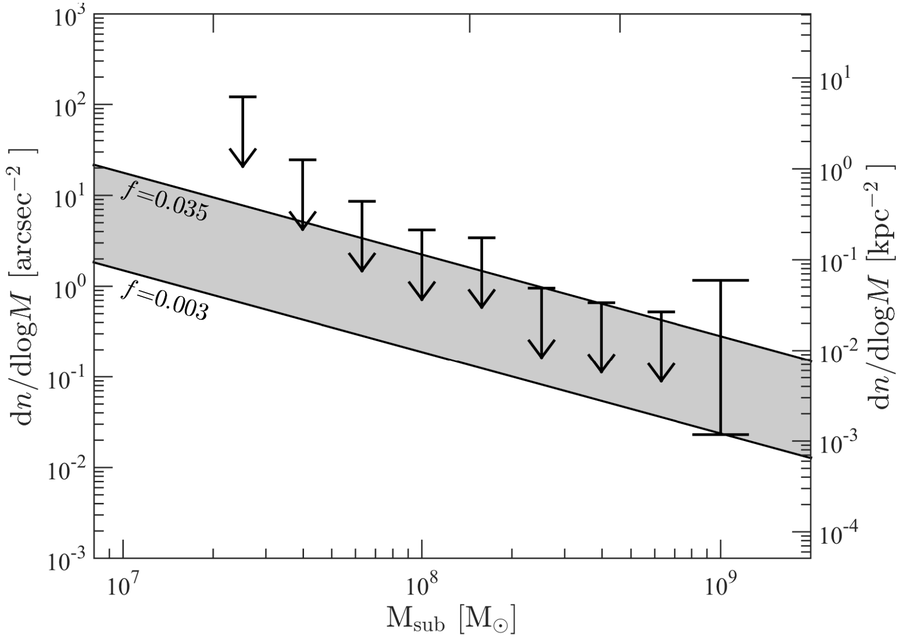
Smooth halo + subhalo



Inference clump by clump

- Individual heavy subhalos leave a relatively clear signal and can be identified [Hezaveh et al 1601.01388]





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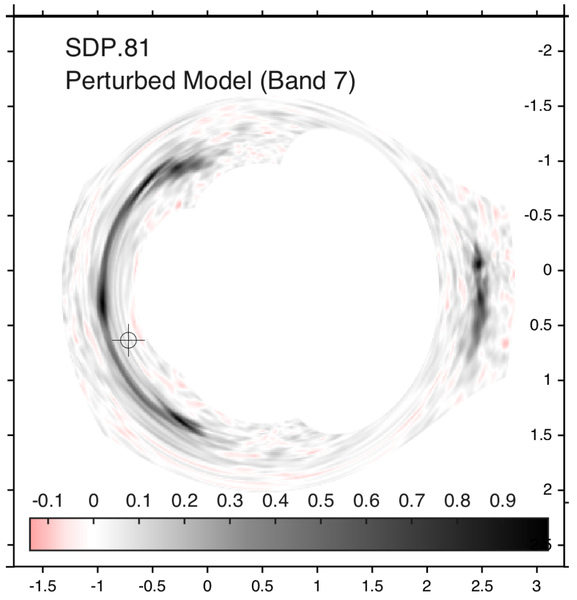
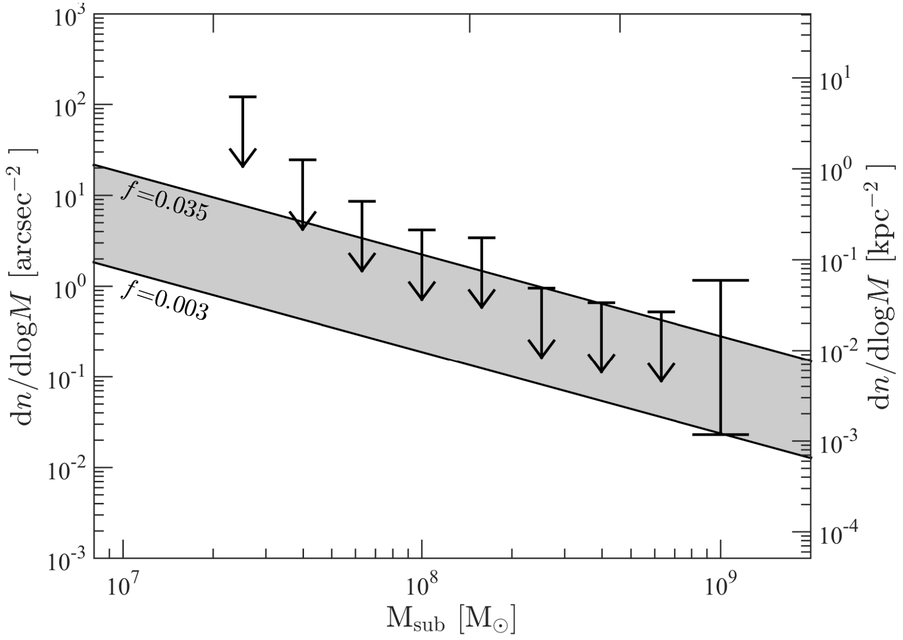
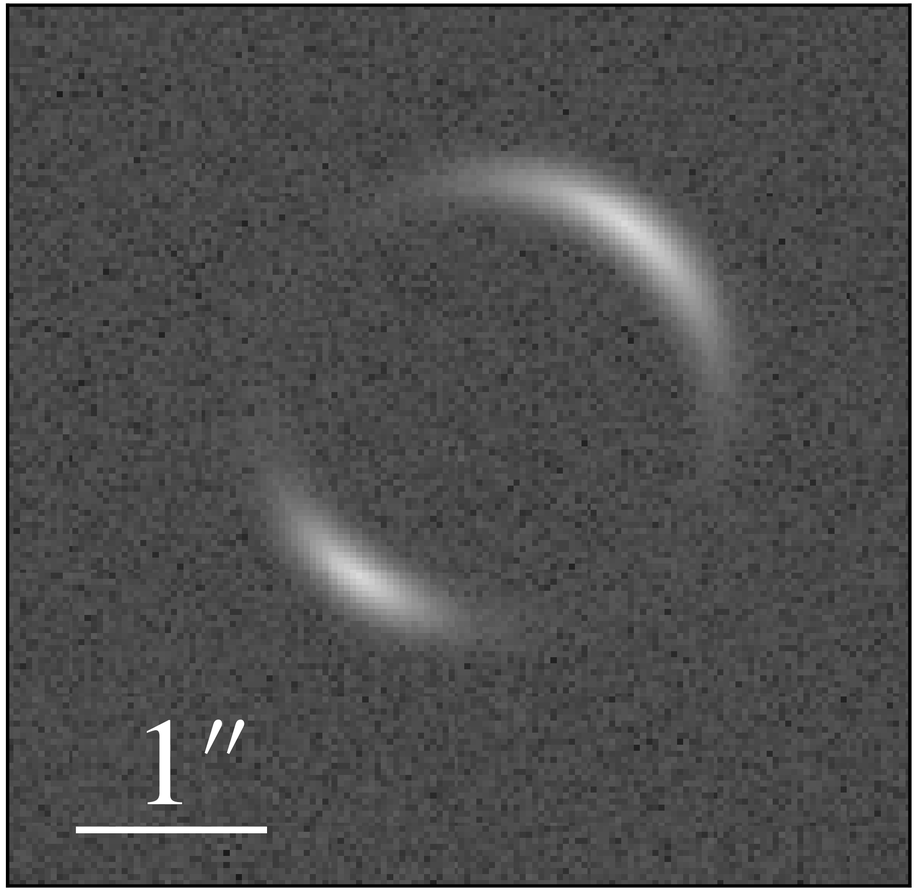
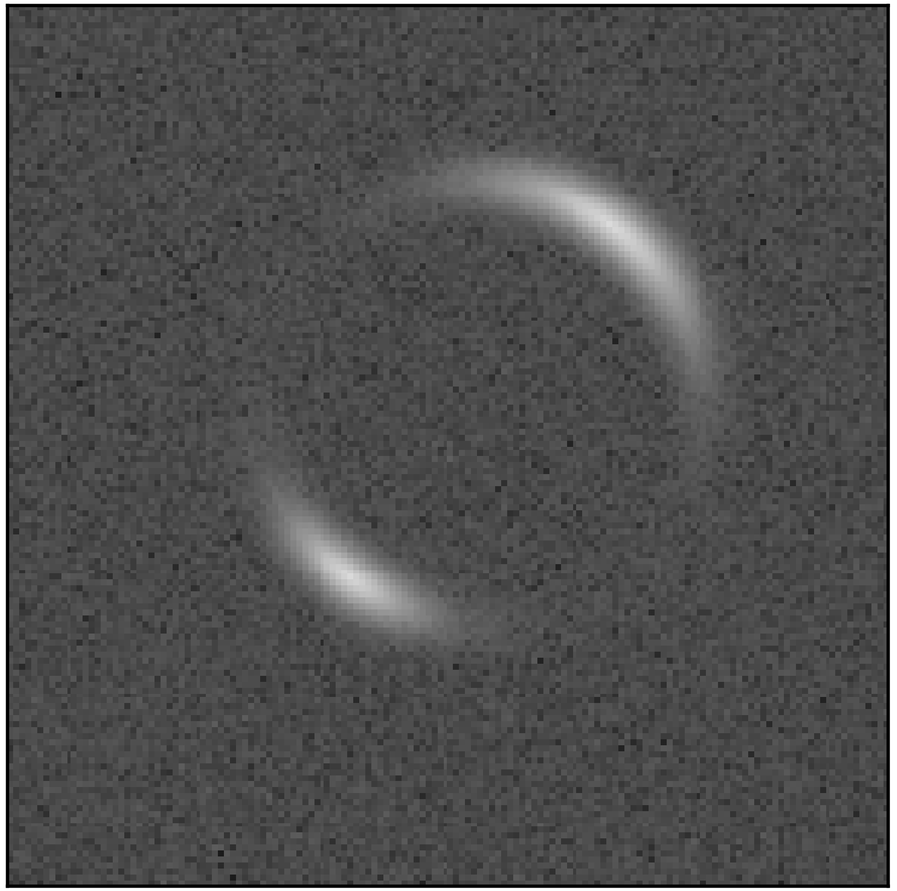




- Transdimensional inference allows simultaneously inferring multiple individual subhalos and population-level parameters [B. Brewer et al 1508.00662; T. Daylan et al 1706.06111]
- Works for subhalos $\sim 10^9 \mathrm{M}_\odot$, scales poorly to many lighter subhalos (or many observed lenses)

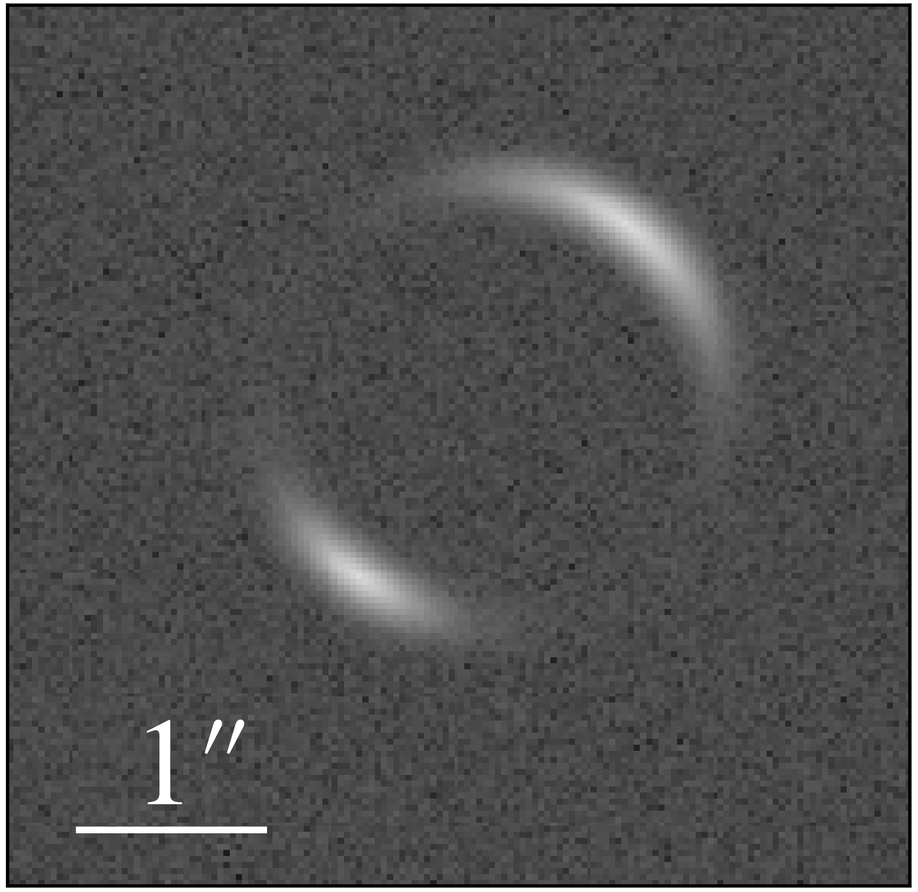
Many light subhalos collectively affect strong lensing



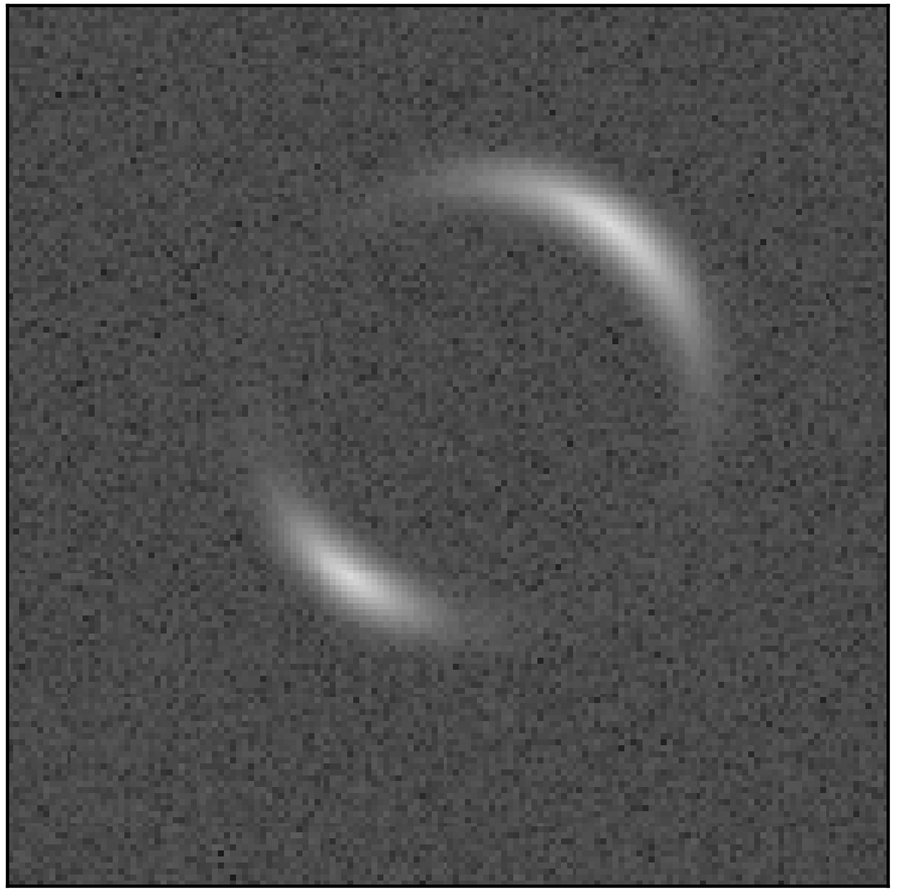


Many light subhalos collectively affect strong lensing

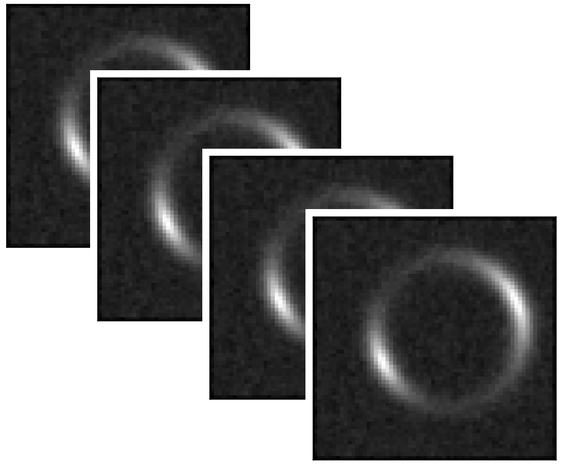
Smooth halo only

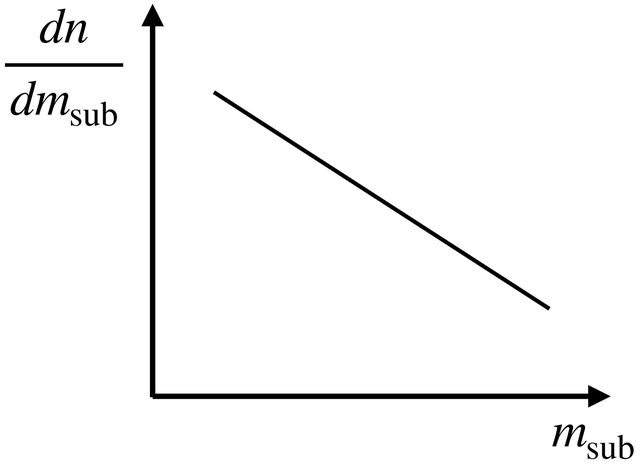


Smooth halo + subhalos



Goal: Scalable inference for small subhalos

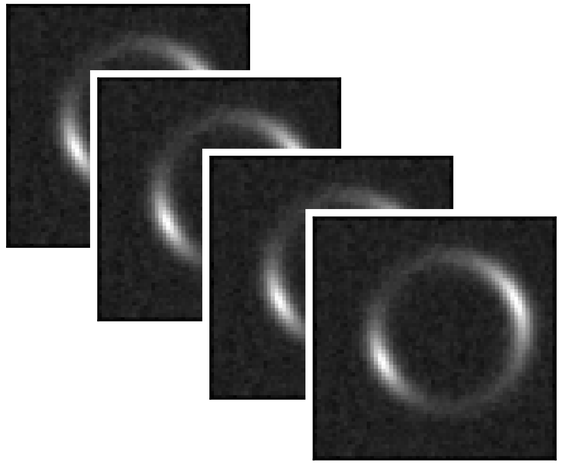


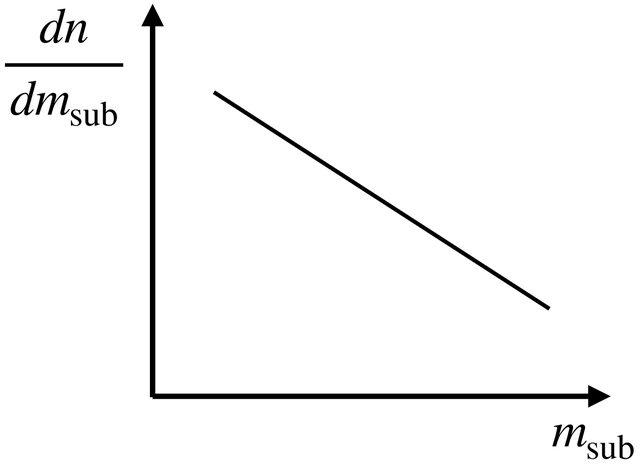


Future surveys (LSST, Euclid) are expected to deliver large samples of galaxy-galaxy strong lenses [Collett et al 1507.02657]

Goal: infer subhalo mass distribution through collective effects of many light subhalos

Goal: Scalable inference for small subhalos





Future surveys (LSST, Euclid) are expected to deliver large samples of galaxy-galaxy strong lenses [Collett et al 1507.02657]

Goal: infer subhalo mass distribution through collective effects of many light subhalos

⇒ Need inference technique that

- scales to many lenses
- can deal with a large number of subhalos
- captures subtle effects in high-dimensional image data

A key challenge is that
we cannot calculate the likelihood function.

Modeling strong lensing

Model parameters

Subhalo mass function parameters

θ

Modeling strong lensing

Model parameters

Subhalo mass function parameters

θ

Latent variables

Source / host halo properties

z_{source} z_{lens}

Subhalo number, masses, positions

n_{sub} $\{z_{\mathrm{sub}\,i}\}$

$$p(z_{\mathrm{source}}) \quad p(z_{\mathrm{lens}}) \quad p(n_{\mathrm{sub}}|\theta) \prod_{i}^{n_{\mathrm{sub}}} p(z_{\mathrm{sub}\,i}|\theta)$$

Modeling strong lensing

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Subhalo number, masses, positions

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Observables

Observed lens image

x

$p(z_{\rm source})$ $p(z_{\rm lens})$ $p(n_{\rm sub}|\theta) \prod_i^{n_{\rm sub}} p(z_{{\rm sub}\,i}|\theta)$ $p(x|z_{\rm source}, z_{\rm lens}, \{z_{{\rm sub}\,i}\})$

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Observables

Observed lens image

x

We can easily write a simulator that samples from

$$p(x, z|\theta) = p(z_{\mathrm{source}}) \quad p(z_{\mathrm{lens}}) \quad p(n_{\mathrm{sub}}|\theta) \prod_i^{n_{\mathrm{sub}}} p(z_{\mathrm{sub}\,i}|\theta) \qquad p(x|z_{\mathrm{source}}, z_{\mathrm{lens}}, \{z_{\mathrm{sub}\,i}\})$$

Prediction (simulation)

Modeling strong lensing

Model parameters

Subhalo mass function parameters

θ

Latent variables

Source / host halo properties

$z_{\rm source}$ $z_{\rm lens}$

Subhalo number, masses, positions

$n_{\rm sub}$ $\{z_{{\rm sub}\,i}\}$

Observables

Observed lens image

x

The key quantity for inference is the marginal likelihood

$$p(x|\theta) = \int \mathrm{d}z_{\rm source} \int \mathrm{d}z_{\rm lens} \sum_{n_{\rm sub}} \int \mathrm{d}^{n_{\rm sub}} z_{\rm sub} \quad p(z_{\rm source}) \quad p(z_{\rm lens}) \quad p(n_{\rm sub}|\theta) \prod_i^{n_{\rm sub}} p(z_{{\rm sub}\,i}|\theta) \quad p(x|z_{\rm source}, z_{\rm lens}, \{z_{{\rm sub}\,i}\})$$

Inference

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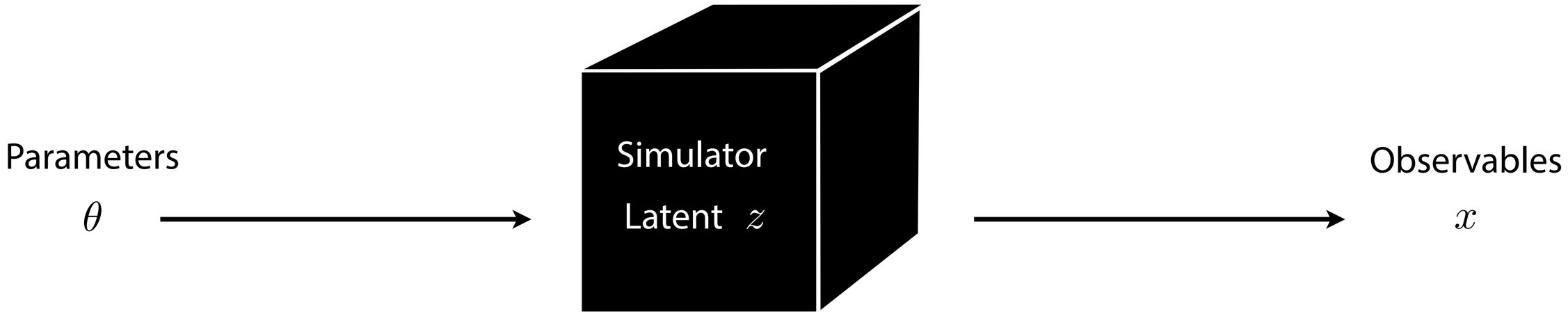
Unfortunately, it is intractable:
we cannot compute the integral over this huge latent space. This is a major challenge for inference.

Similarly, MCMC based on $p(x, z|\theta)$ is extremely inefficient.
(More subtle: We cannot sample from $p(z|x, \theta)$ efficiently.)

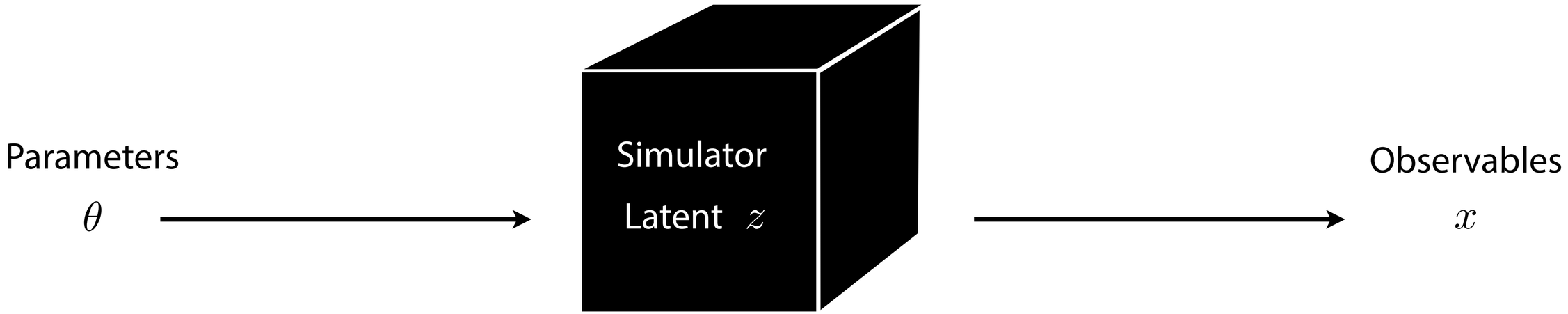
Inference

Simulation-based (“likelihood-free”) inference



Prediction:
- Well-understood mechanistic model
- Simulator can generate samples $x \sim p(x|\theta)$

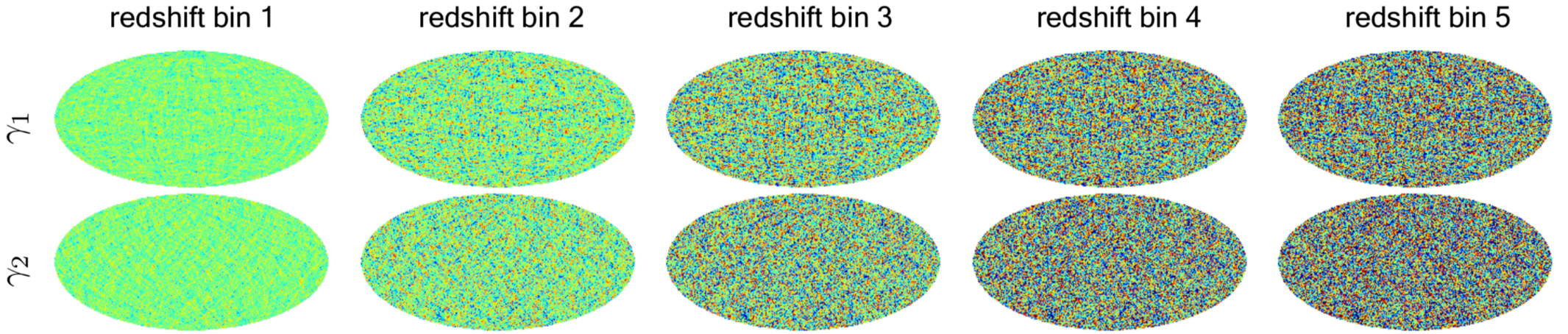
Simulation-based ("likelihood-free") inference



Prediction:
- Well-understood mechanistic model
- Simulator can generate samples $x \sim p(x|\theta)$

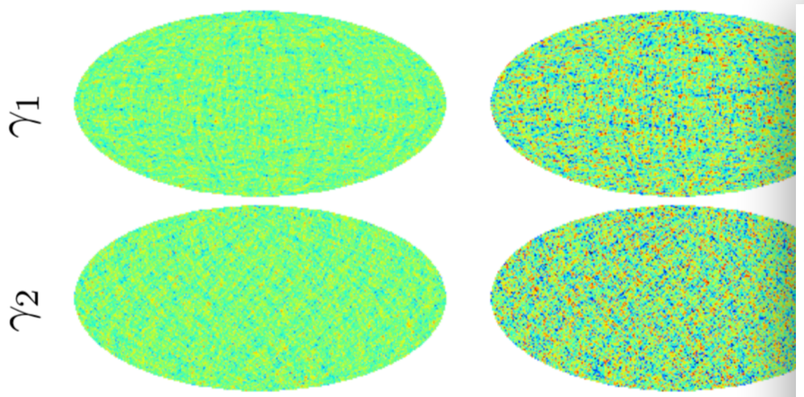
Inference:
- Likelihood $p(x|\theta) = \int \mathrm{d}z\, p(x, z|\theta)$ is intractable
- Inference is challenging

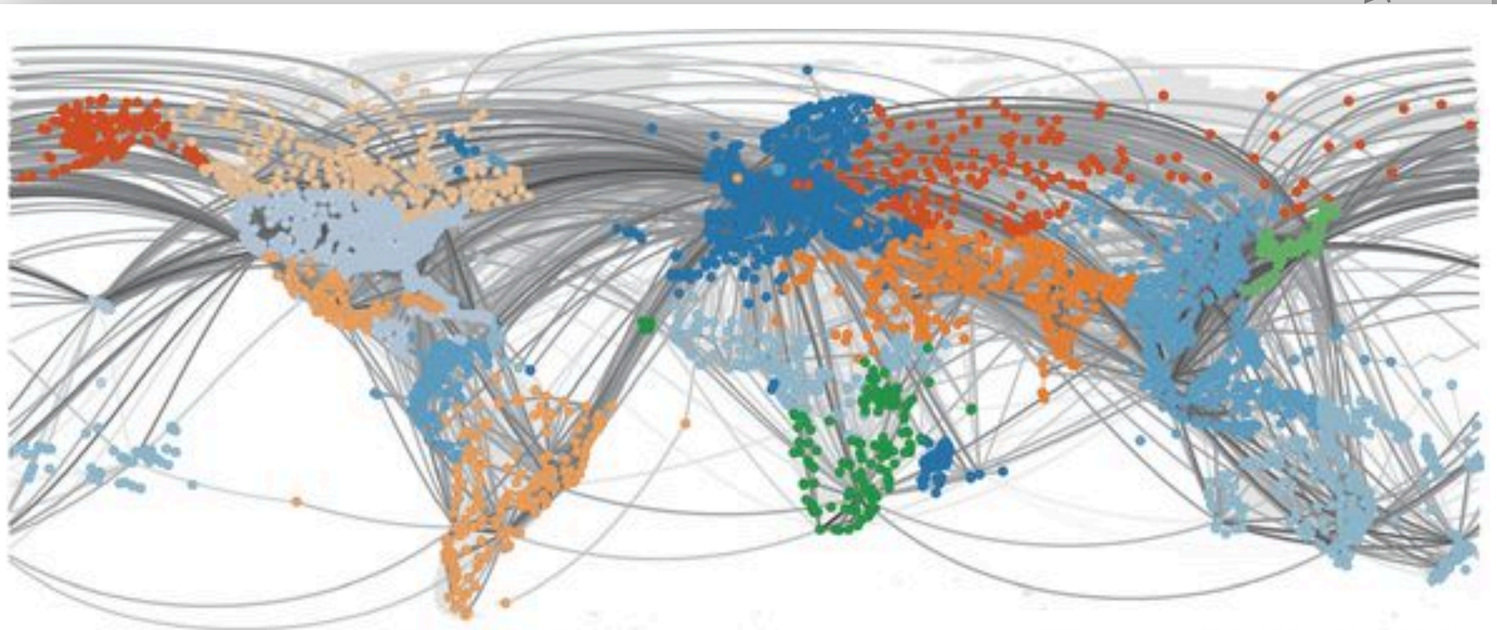
Simulation-based inference appears all over science



[J. Alsing, T. Charnock, S. Feeney, B. Wandeelt 1903.00007]

Simulation-based inference appears all over science

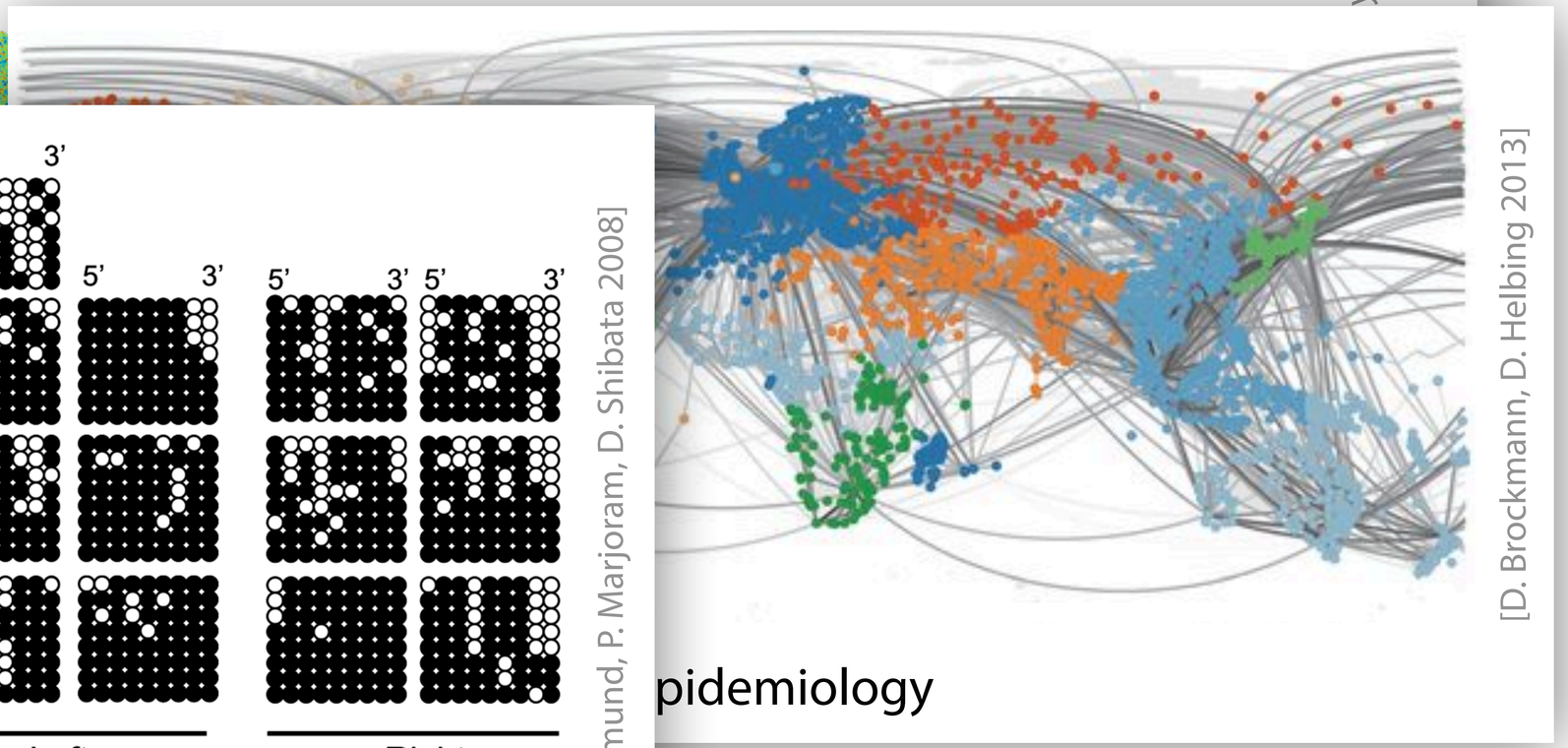




Epidemiology

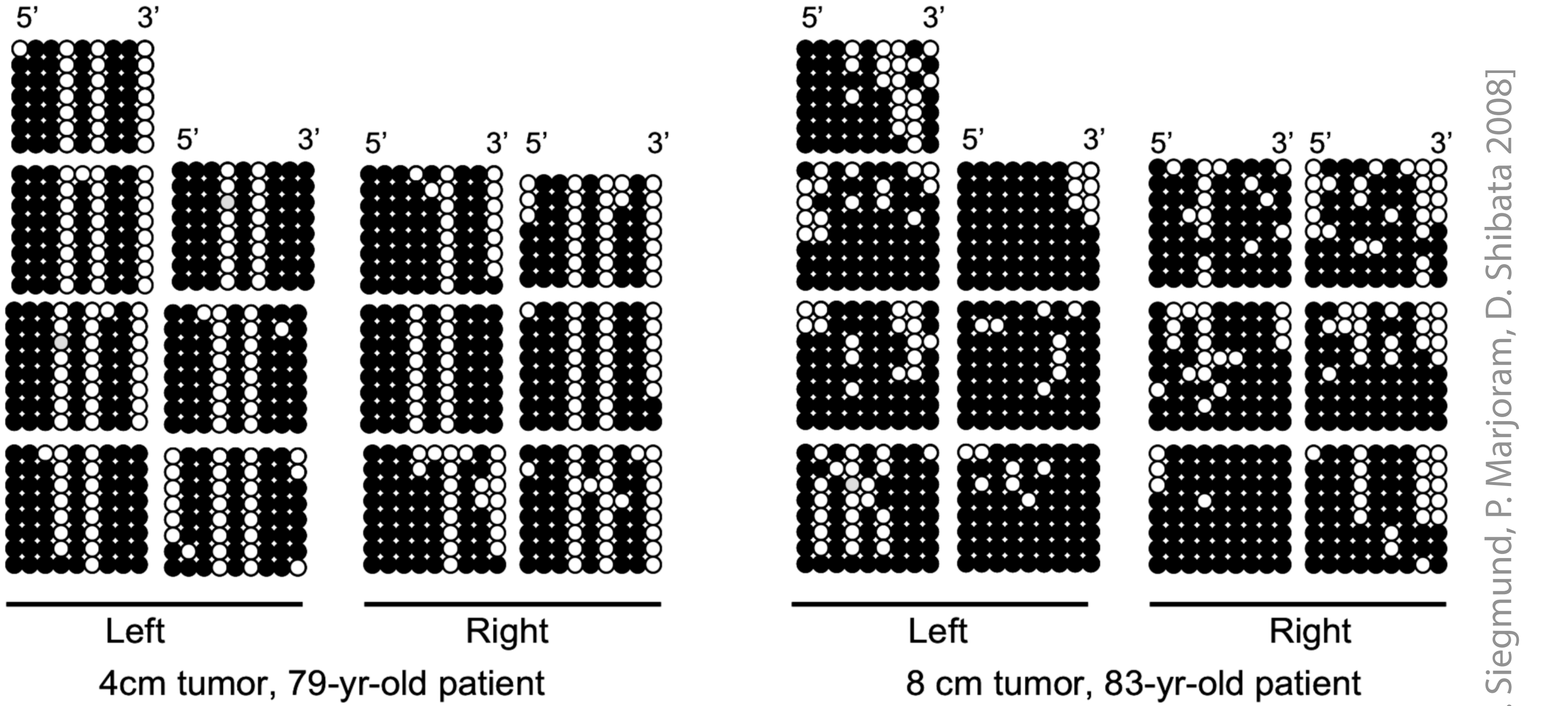
[D. Brockmann, D. Helbing 2013]

Simulation-based inference appears all over science



[D. Brockmann, D. Helbing 2013]

pidemiology

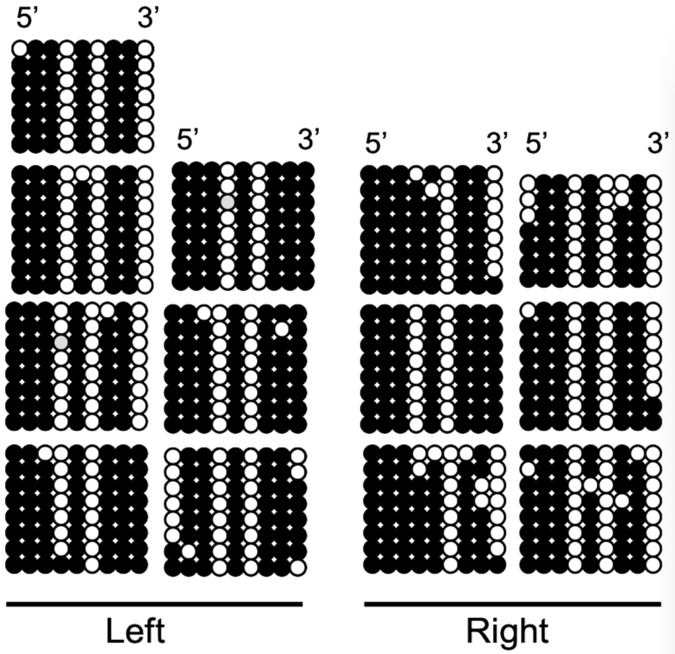


[K. Siegmund, P. Marjoram, D. Shibata 2008]

Genetics

Simulation-based inference appears all over science

[D. Brockmann, D. Helbing 2013]



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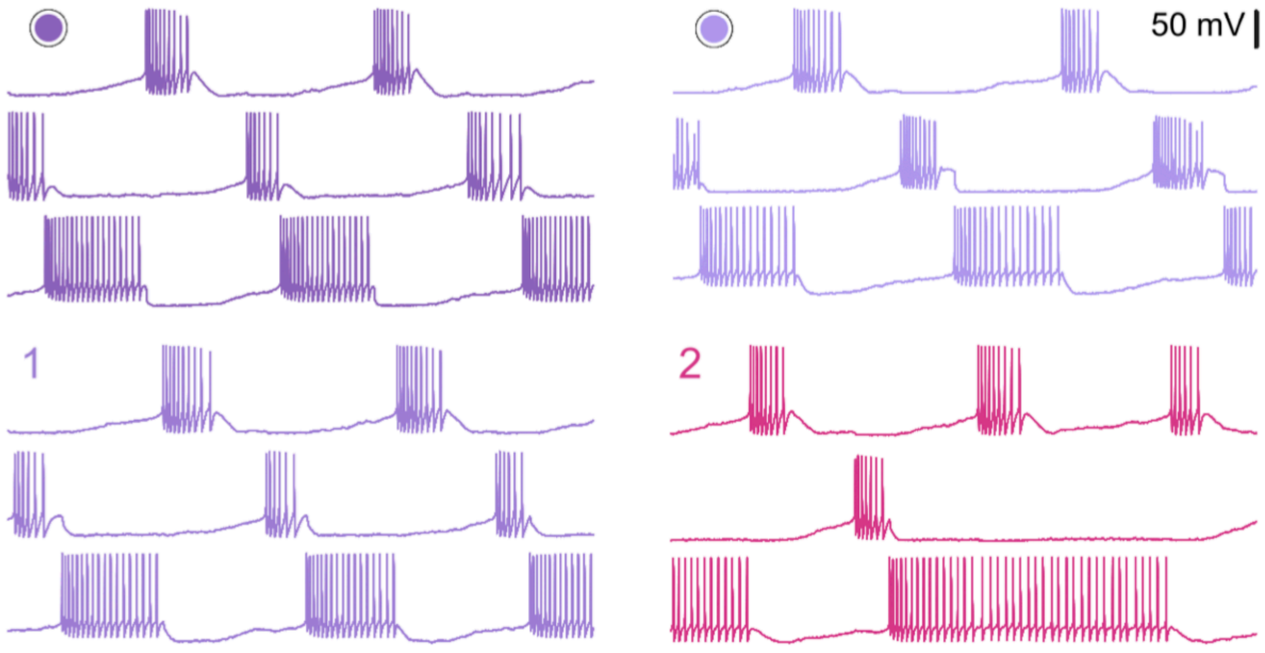
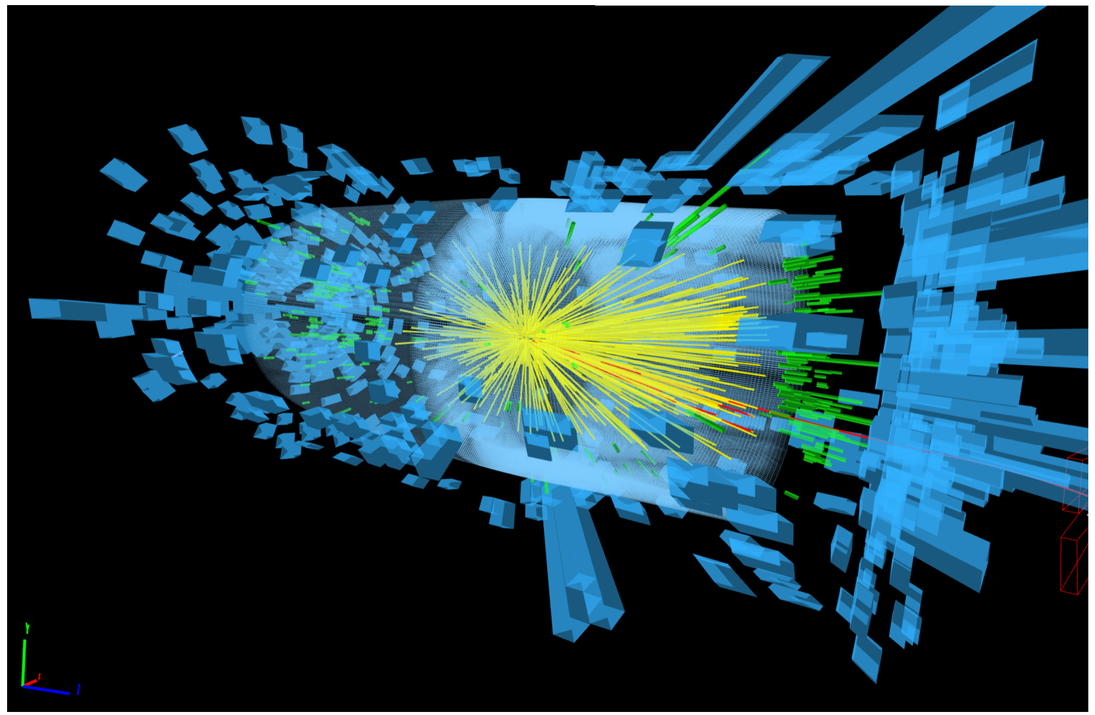


Neuroscience

[Pedro J. Goncalves et al. biorxiv:10.1101/838383]

Simulation-based inference appears all over science



[CMS]

Particle physics

redshift bin 4

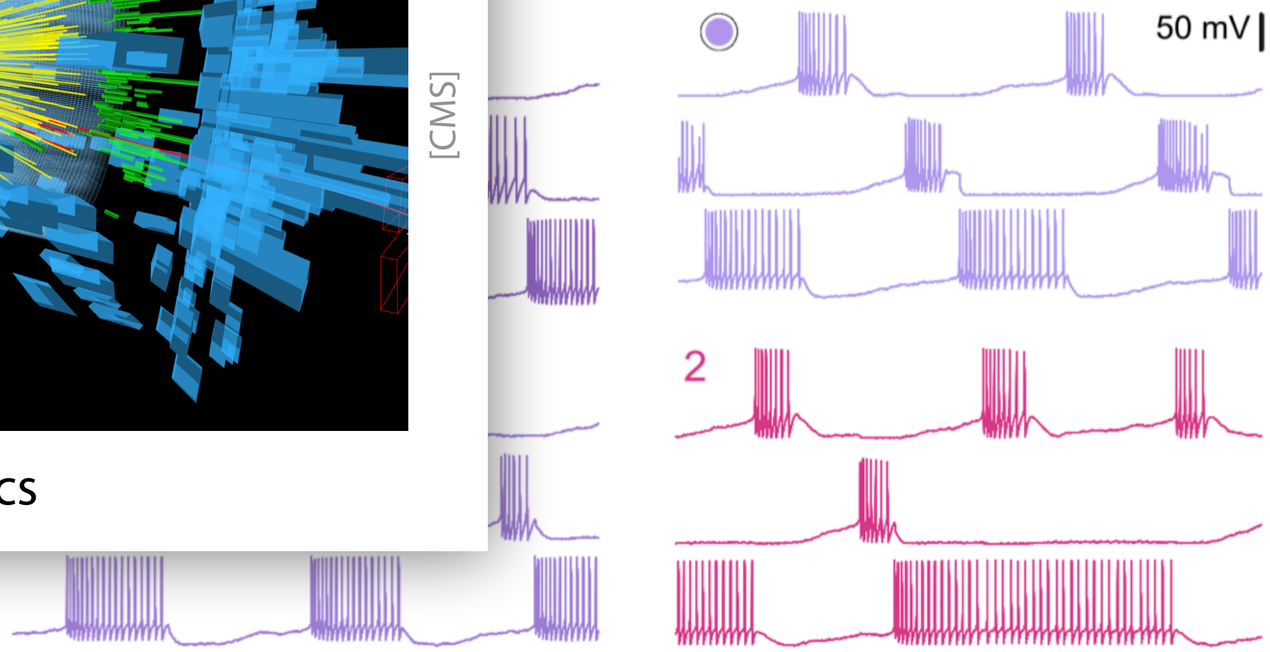
redshift bin 5

[D. Brockmann, D. Helbing 2013]

5’

4cm tumor, 79-yr-old patient

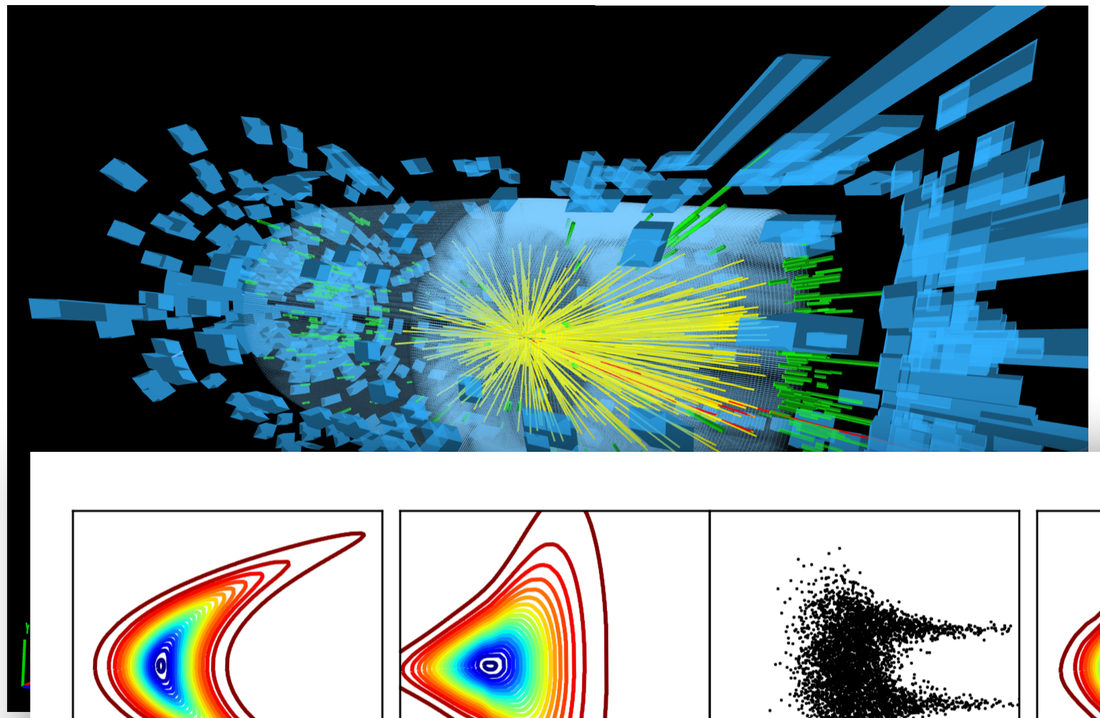
Ger



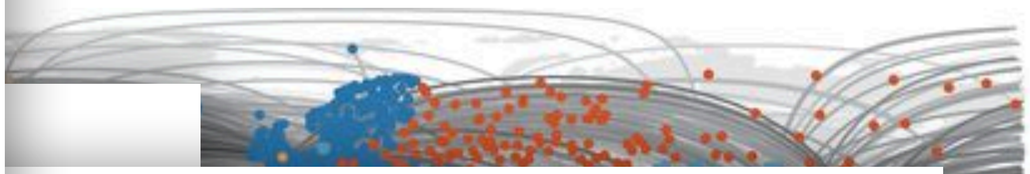
[Pedro J. Goncalves et al. biorxiv:10.1101/838383]

Neuroscience

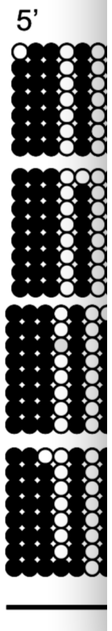
Simulation-based inference appears all over science

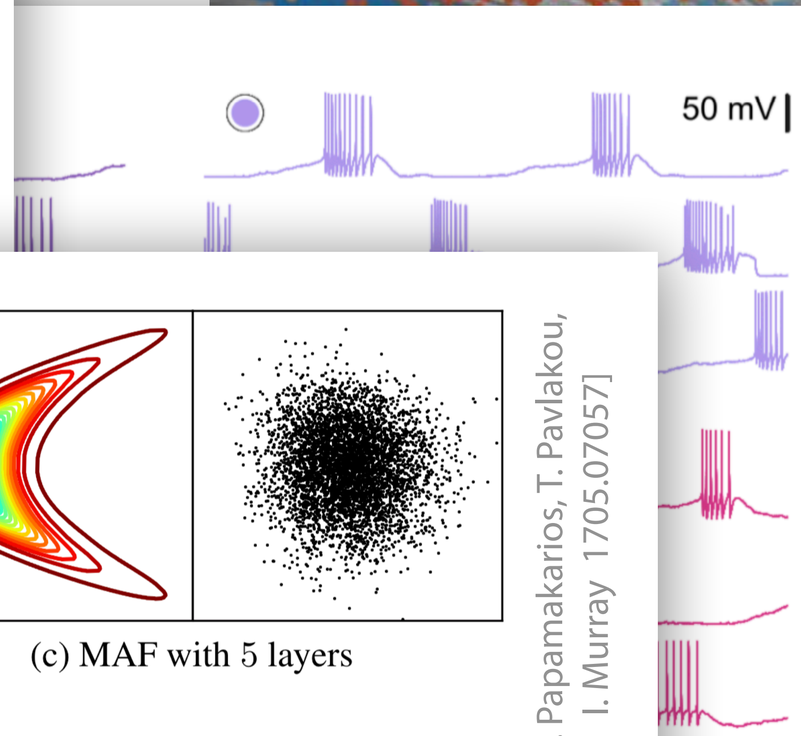


[CMS]



[D. Brockmann, D. Helbing 2013]





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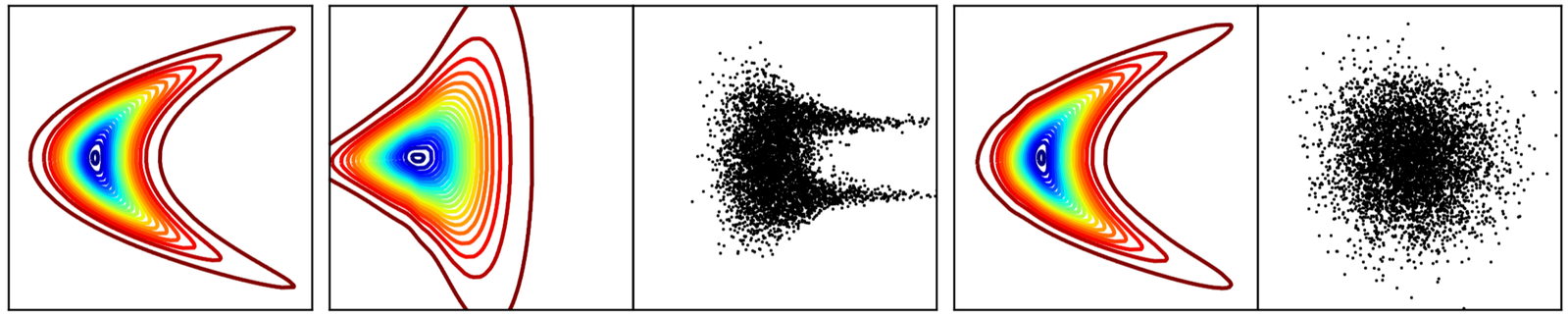


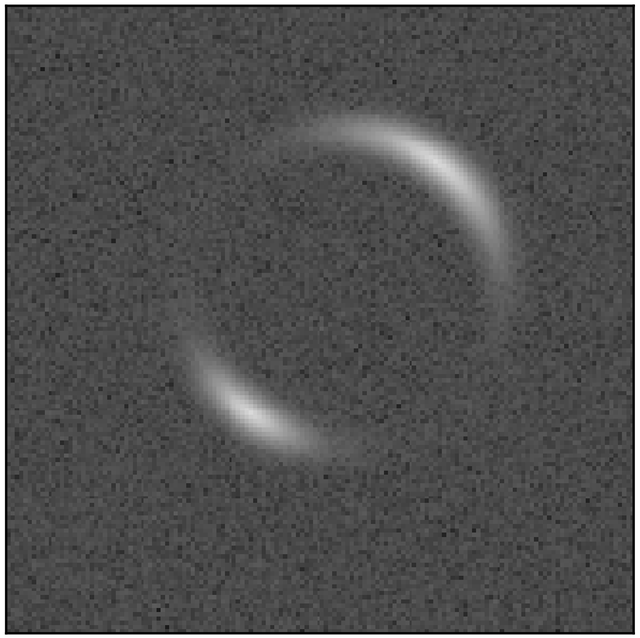
(a) Target density (b) MADE with Gaussian conditionals (c) MAF with 5 layers

[G. Papamakarios, T. Pavlakou, I. Murray 1705.07057]

Computer Science / Machine Learning / Statistics

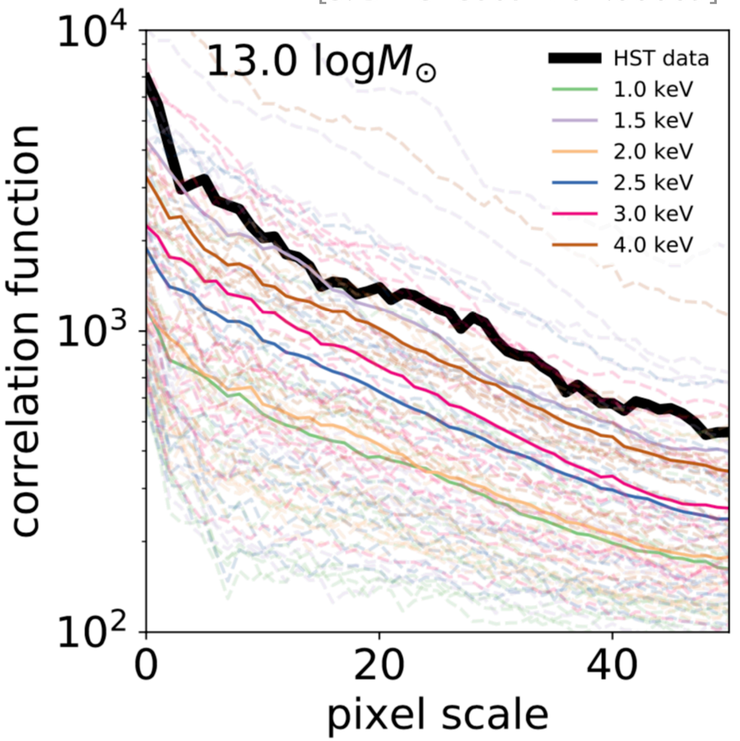
Traditionally, inference is made possible with summary statistics.

Solve it with summary statistics



High-dimensional observable data x
(pixel values)

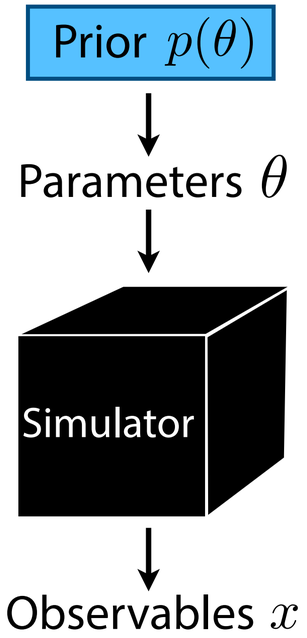
[S. Birrer et al 1702.00009]



Low-dimensional summary statistics x'
(e.g. correlation functions)

Approximate Bayesian Computation (ABC)

[D. Rubin 1984]



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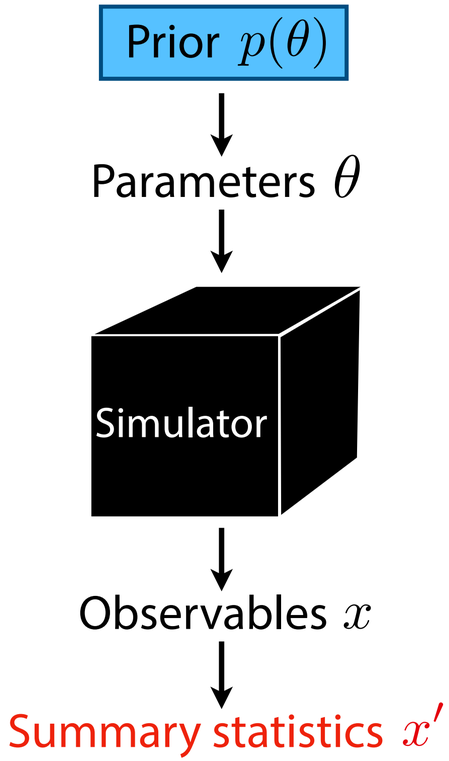

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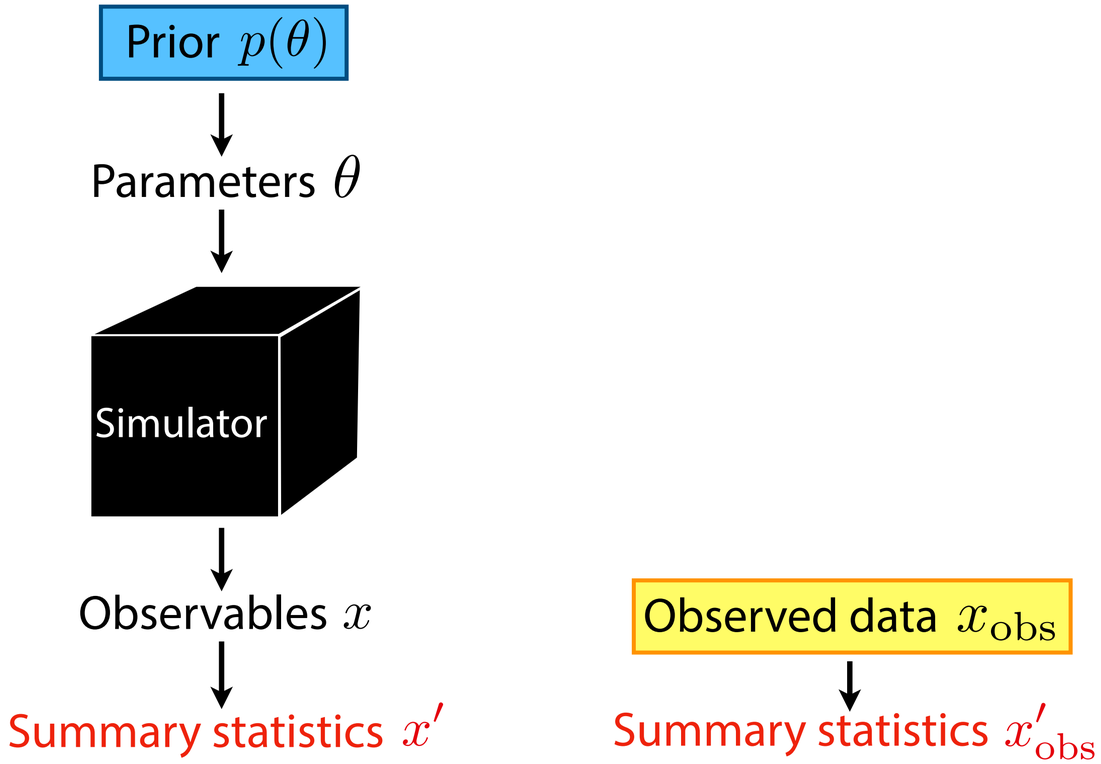

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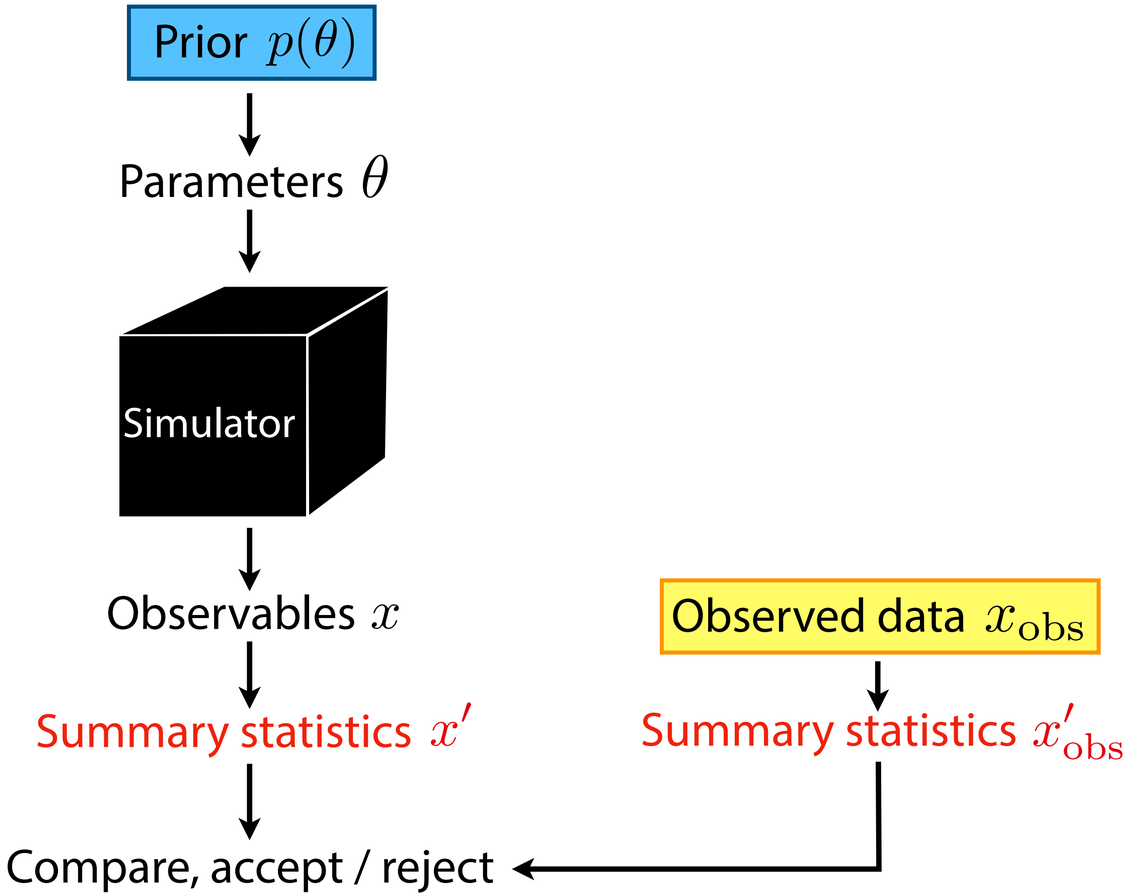

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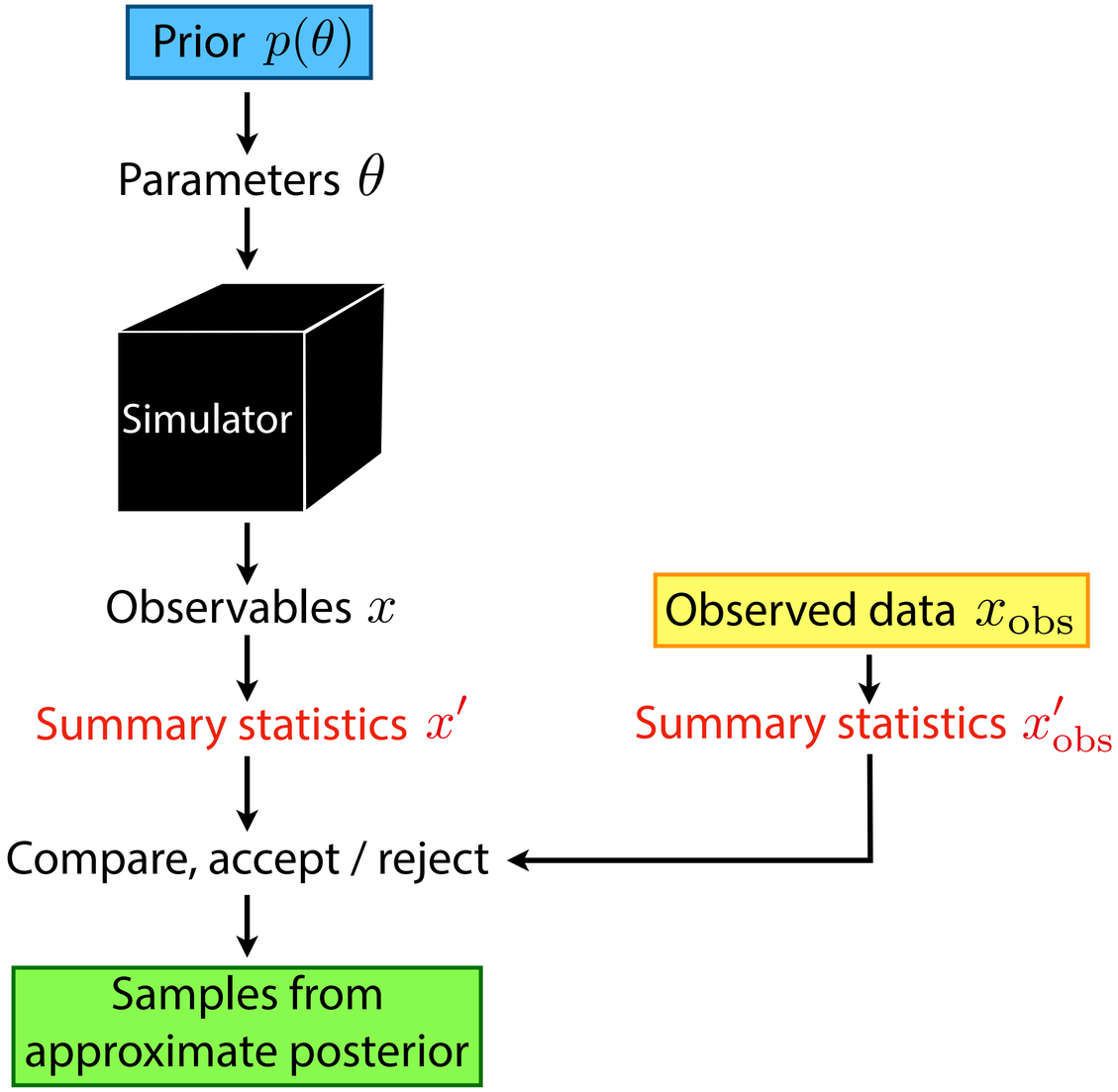

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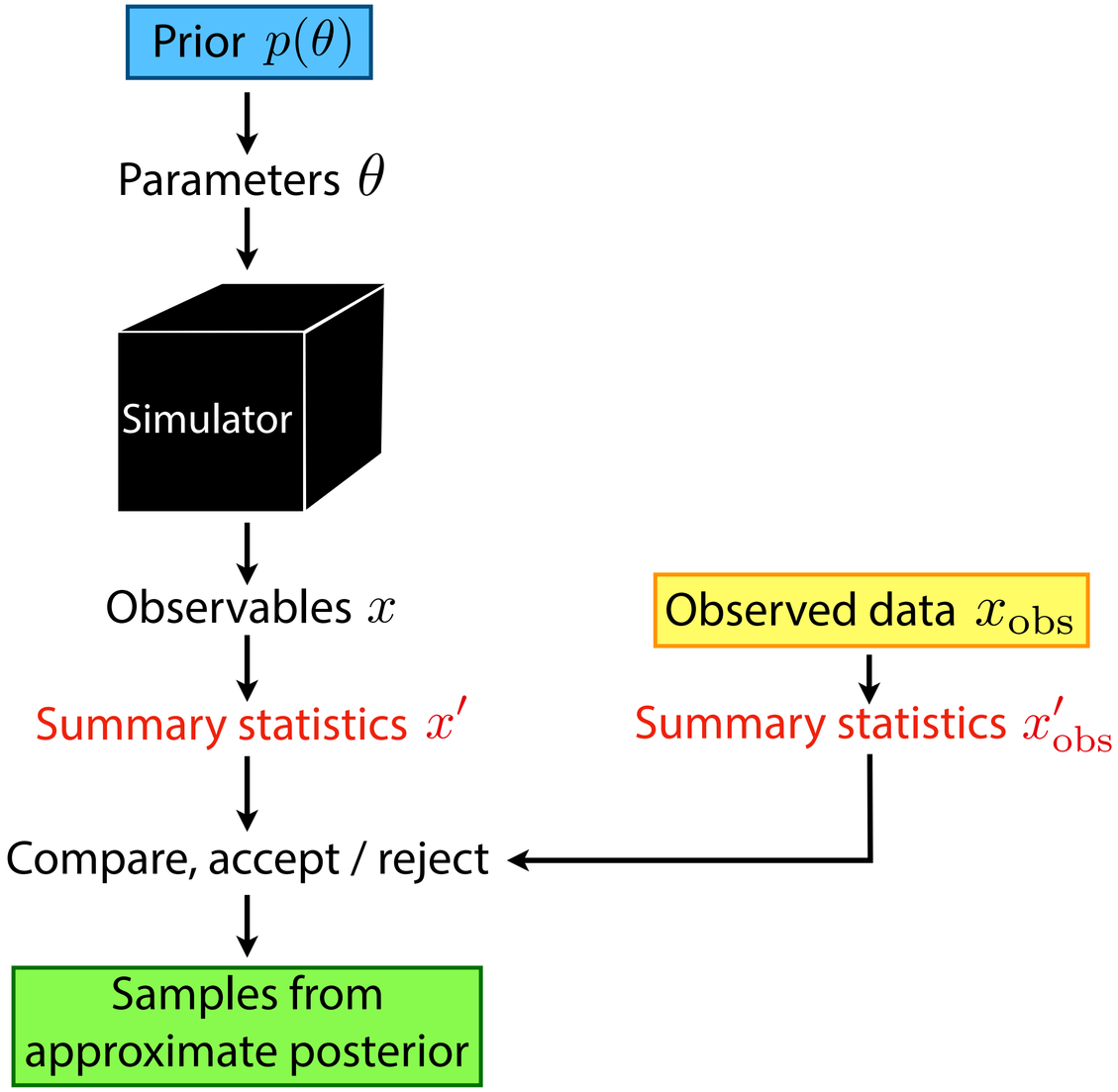
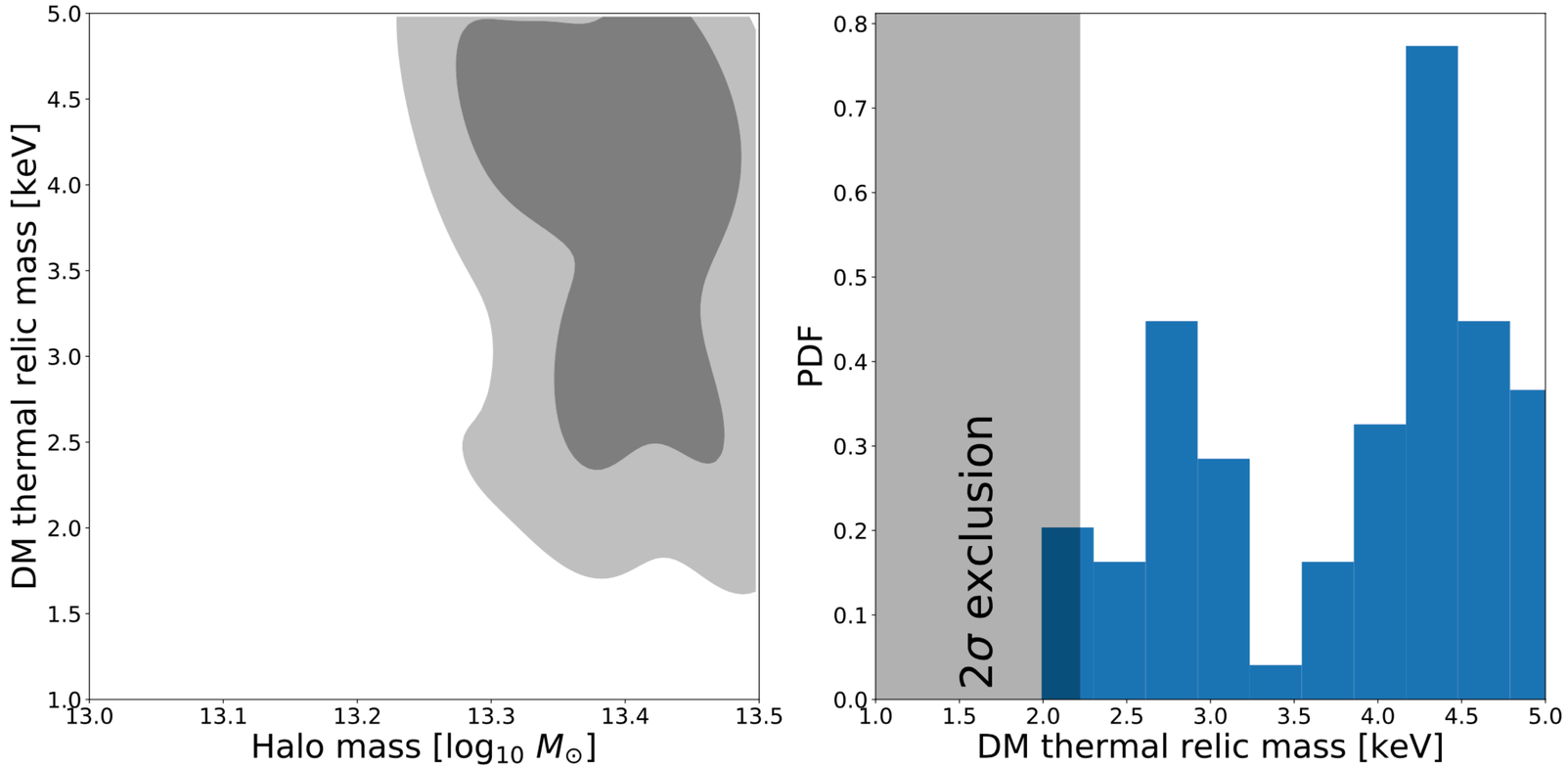


- Reduction to summary statistics makes inference possible, but throws away information
- Rejection algorithm can be very sample inefficient

Substructure ABC

[S. Birrer et al 1702.00009]



- Successful proof of principle application on HST data (RXJ1131-1231)
- Summary statistics based on correlation functions: results may be overly conservative
- Poor sample efficiency of ABC rejection: “posterior not converged”

Now, we can also use machine learning
to enable inference.

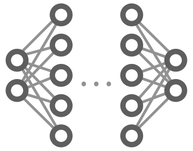
[K. Cranmer, JB, G. Louppe 1911.01429]

The likelihood ratio trick

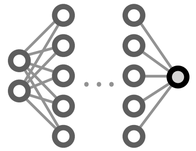
- Generative Adversarial Networks (GANs):

[I. Goodfellow et al. 1406.2661]

Generator
(intractable likelihood $p_{\text{gen}}(x)$)



Examples
(intractable likelihood $p_{\text{true}}(x)$)



Discriminator

The likelihood ratio trick

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[I. Goodfellow et al. 1406.2661]

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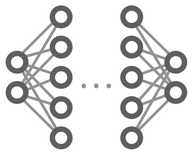

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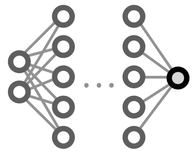


Discriminator

Discriminator learns decision function

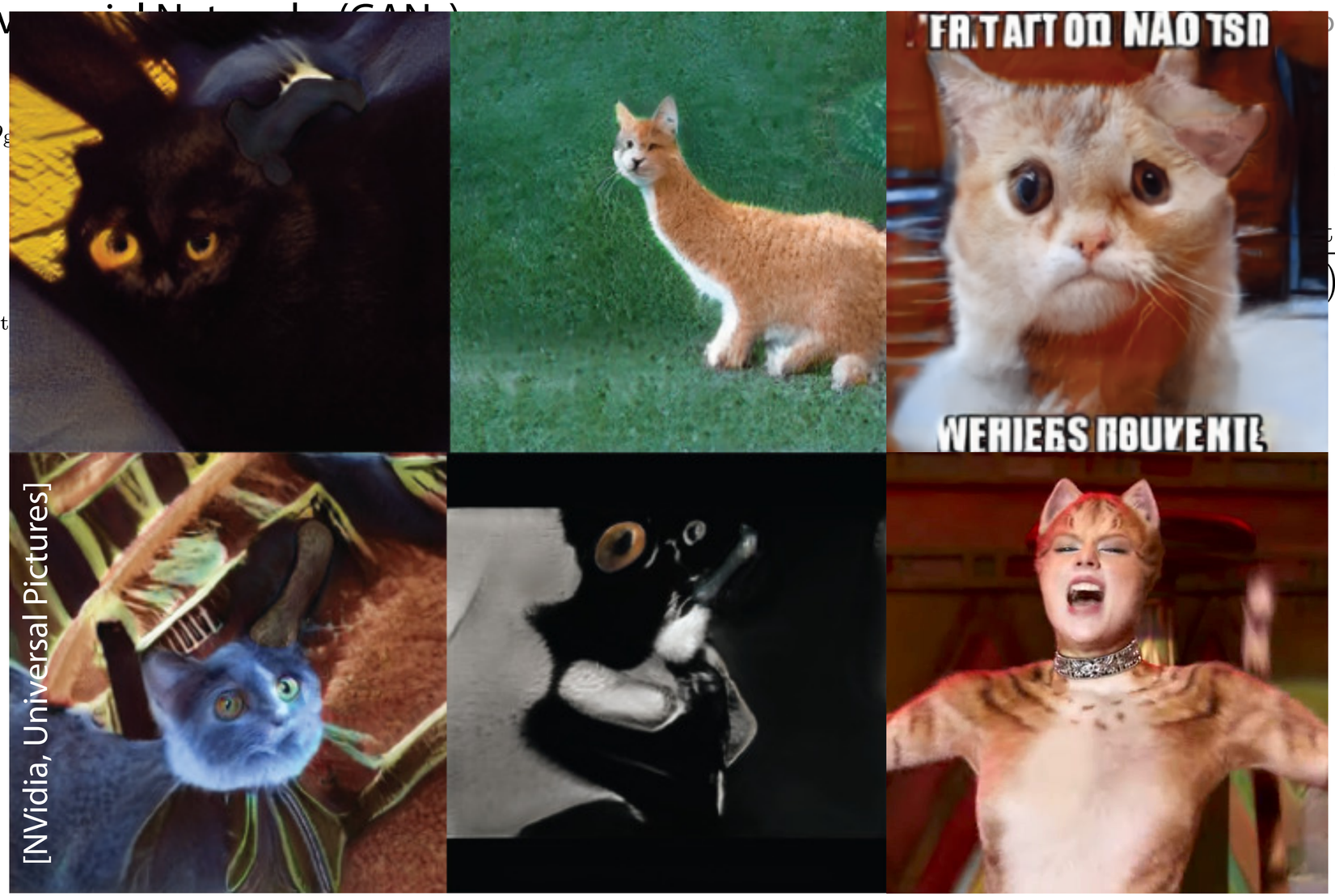
$$s(x) \rightarrow \frac{p_{\text{true}}(x)}{p_{\text{gen}}(x) + p_{\text{true}}(x)}$$

The likelihood ratio trick

- Generative Adv[illegible]Networks (GANs) [Goodfellow et al. 1406.2661]

Generator
(intractable likelihood p_g

Examples
(intractable likelihood p_t

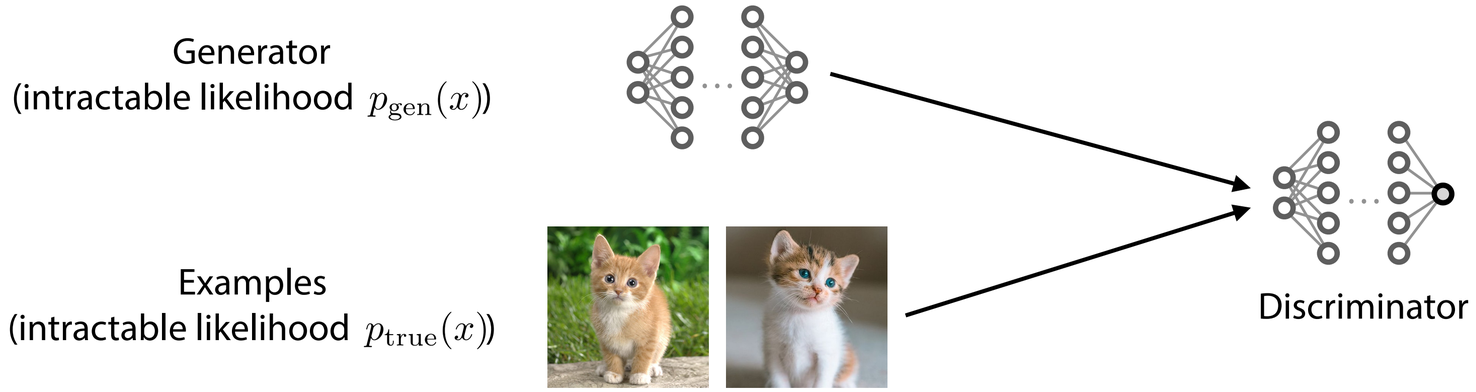


decision function

$$\frac{\text{true}(x)}{) + p_{\text{true}}(x)}$$

The likelihood ratio trick

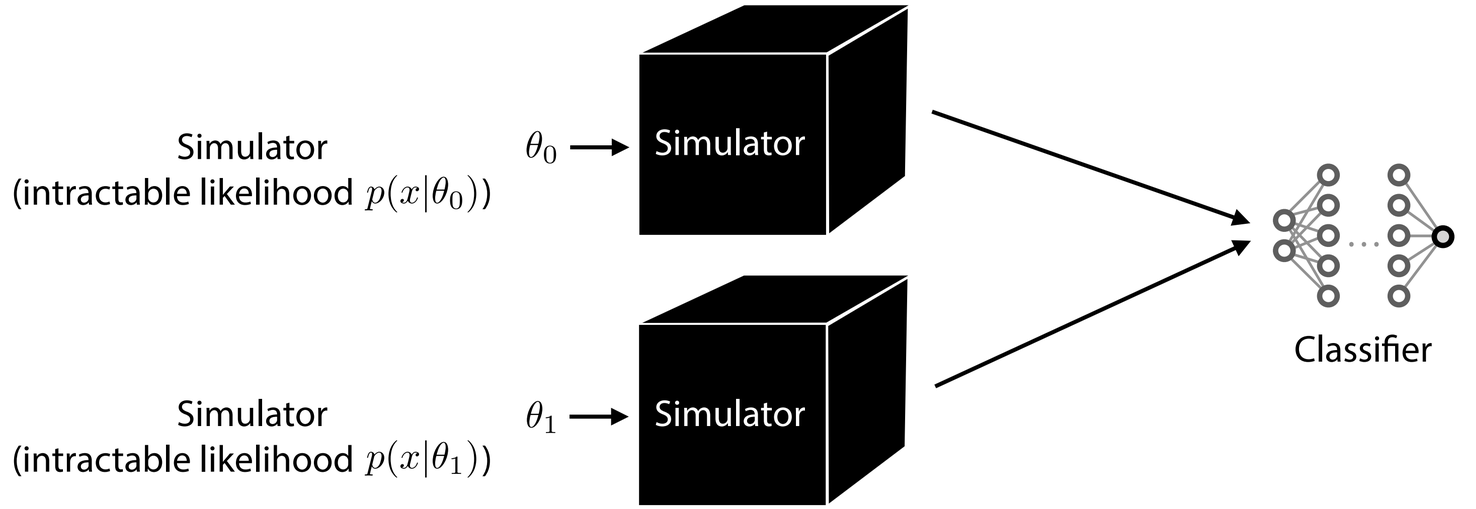
- Generative Adversarial Networks (GANs): [I. Goodfellow et al. 1406.2661]



Discriminator learns decision function

$$s(x) \to \frac{p_{\rm true}(x)}{p_{\rm gen}(x) + p_{\rm true}(x)}$$

- Similarly, we can train a classifier between two sets of simulated samples [K. Cranmer, J. Pavez, G. Louppe 1506.02169]



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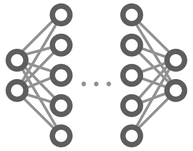
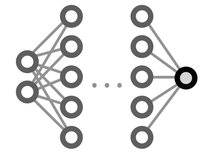


Examples
(intractable likelihood $p_{\rm true}(x)$)



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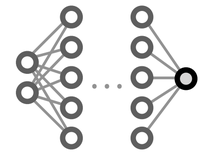
- Similarly, we can train a classifier between two sets of simulated samples [K. Cranmer, J. Pavez, G. Louppe 1506.02169]

Simulator
(intractable likelihood $p(x|\theta_0)$)

θ_0 → Simulator

Simulator
(intractable likelihood $p(x|\theta_1)$)

θ_1 → Simulator



Classifier

Classifier learns decision function

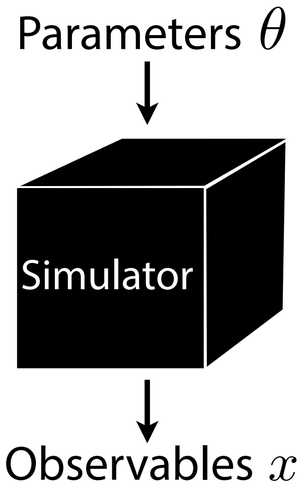
$$s(x) \to \frac{p(x|\theta_1)}{p(x|\theta_0) + p(x|\theta_1)}$$

⇒ Estimator for likelihood ratio

$$\hat{r}(x) = \frac{1 - s(x)}{s(x)} \to \frac{p(x|\theta_0)}{p(x|\theta_1)}$$

Inference by likelihood ratio trick

[K. Cranmer J. Pavez, G. Louppe 1506.02169]



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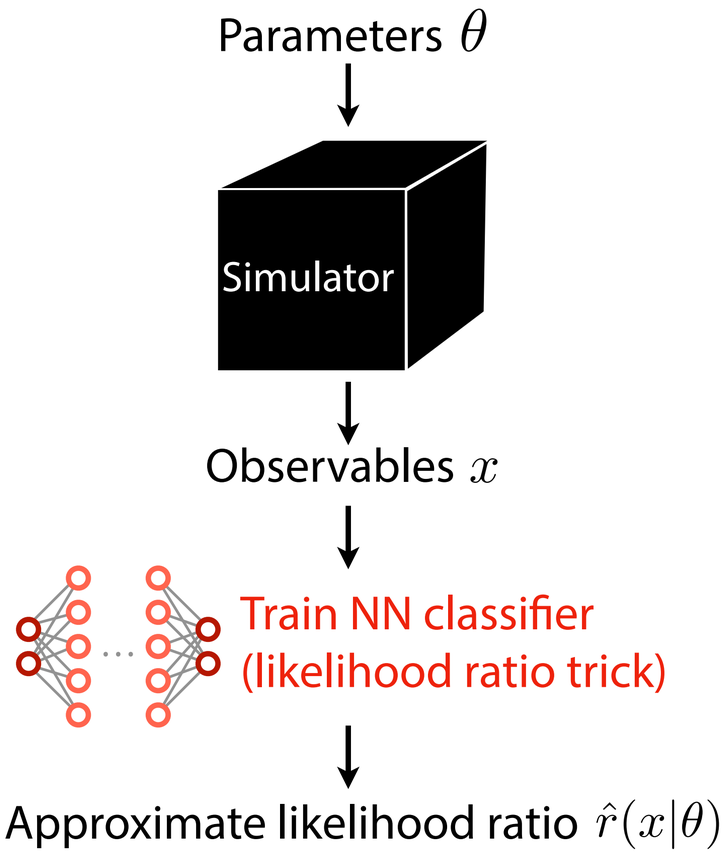

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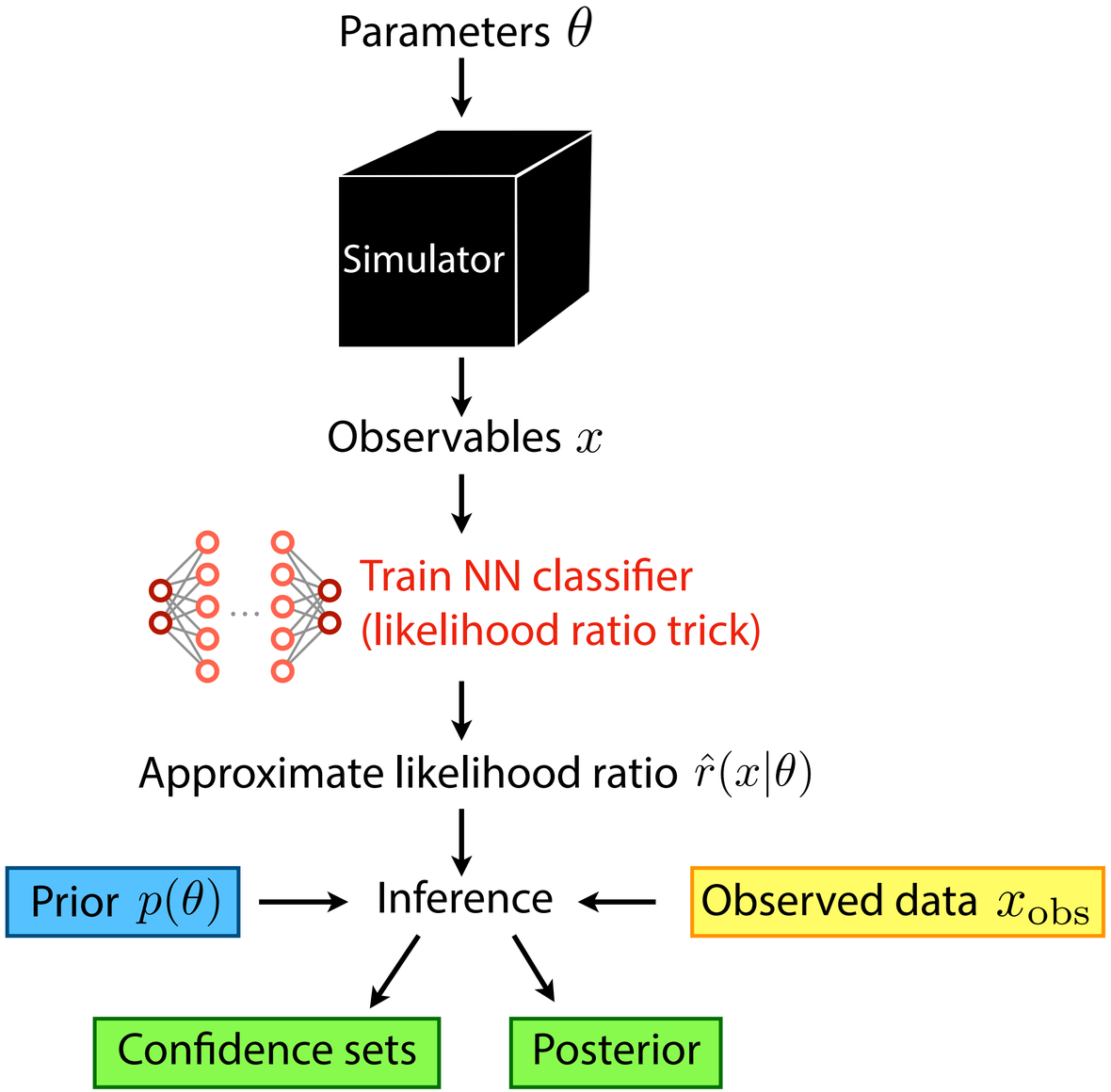

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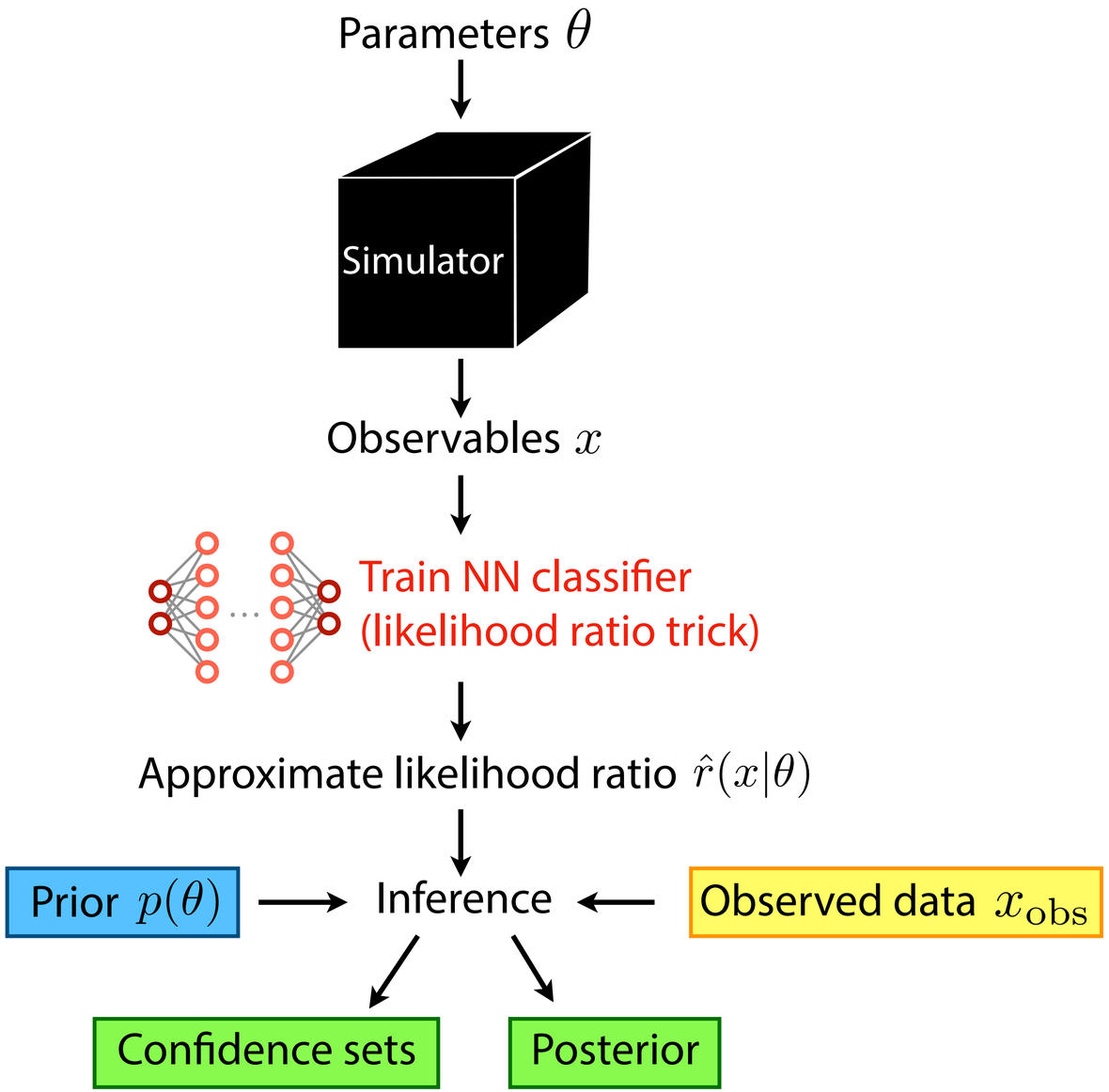
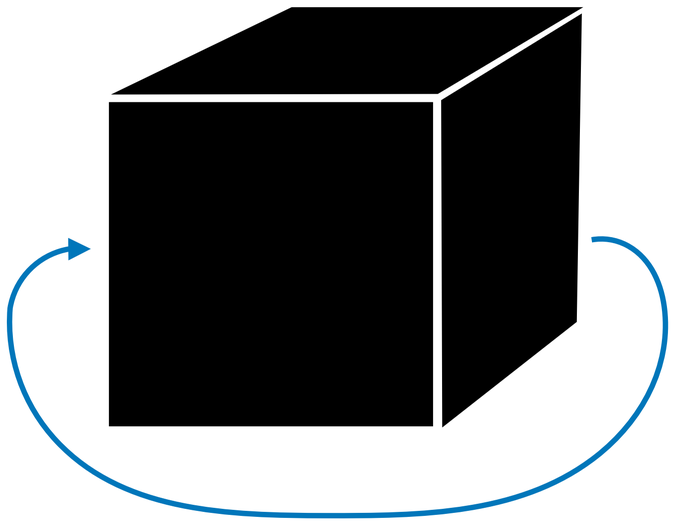


- Instead of the intractable likelihood of the simulator, we use the likelihood ratio learned by a NN from simulated data
- Scales well to high-dimensional data
  (no compression to summary stats necessary)
- Amortized: After upfront simulation + training phase, inference is efficient for new data or prior
- Alternative approaches: train NN to learn likelihood or posterior
  [review: K. Cranmer, JB, G. Louppe 1911.01429]

Improving sample efficiency

[K. Cranmer, JB, G. Louppe 1911.01429]



Active learning:
Iteratively guide simulator to important parameter regions based on past results

Improving sample efficiency

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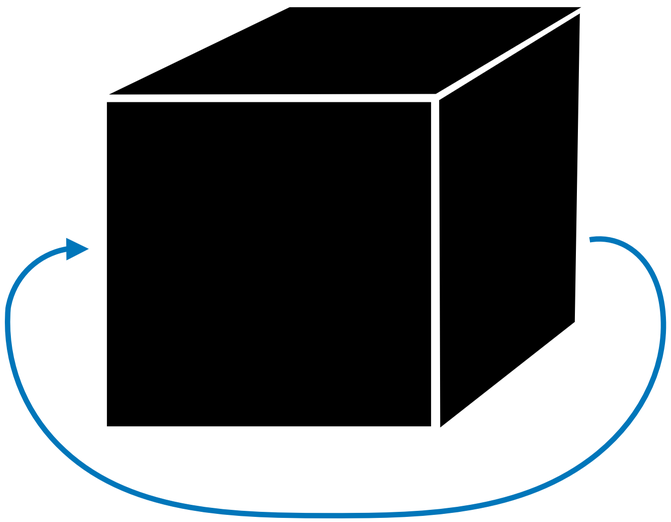

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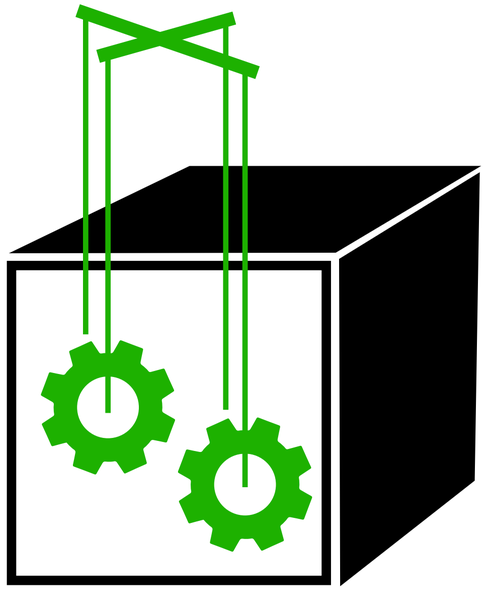

Probabilistic programming:
Explicitly write simulator as probabilistic program, with ability to condition execution trace on observations

Improving sample efficiency

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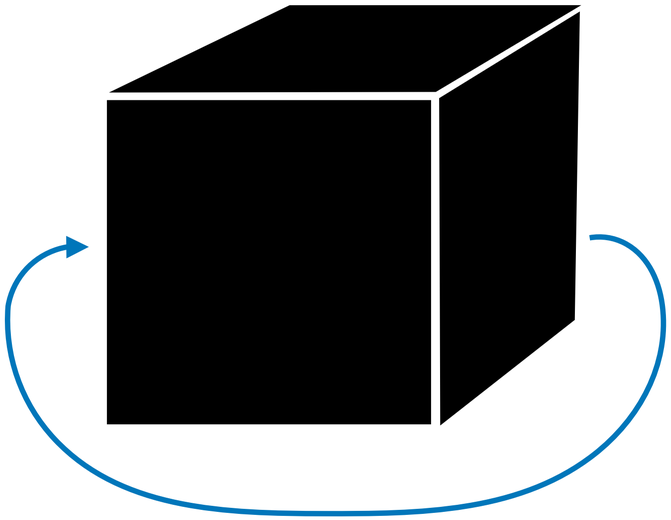

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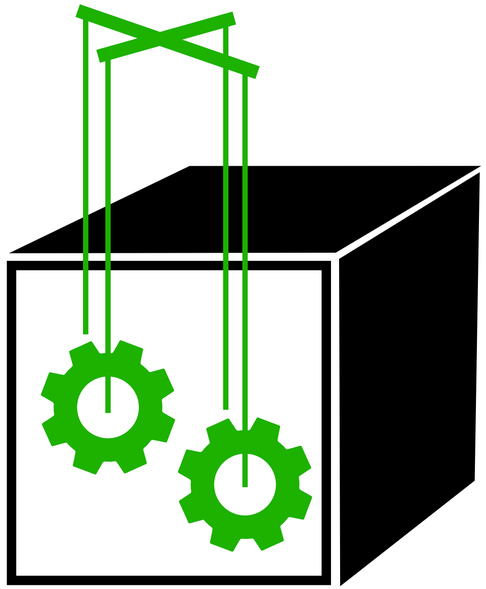
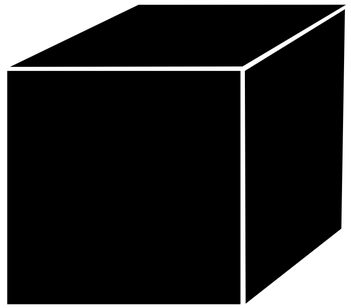


Probabilistic programming:
Explicitly write simulator as probabilistic program, with ability to condition execution trace on observations

Mining gold:
Extract and leverage information from the simulator that characterizes the latent process

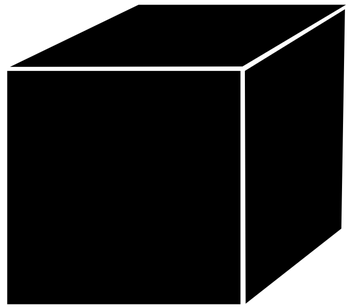
Improving robustness to mismodelling

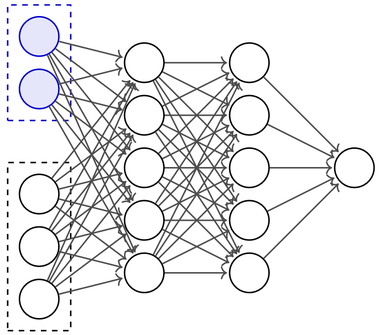


Don’t fully trust the simulator?

- Nuisance parameters to model systematic uncertainties
- Methods learn dependence both on parameters of interest and nuisance parameters
- Profile / marginalize over nuisance parameters
- Alternatively: Robustness to nuisance with adversarial training
  [G. Louppe, M. Kagan, K. Cranmer 1611.01046]

Improving robustness to mismodelling





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  [G. Louppe, M. Kagan, K. Cranmer 1611.01046]

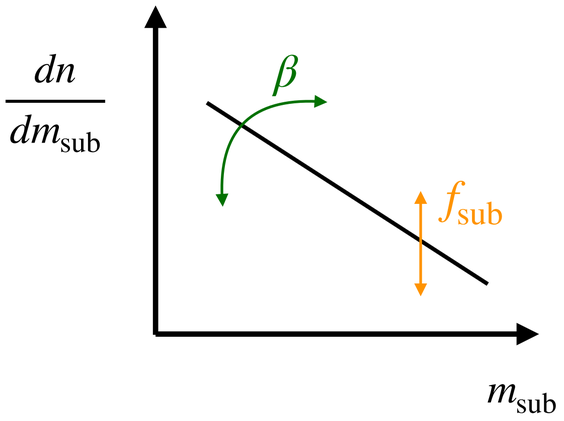
Don’t blindly trust the neural network?

- Sanity checks: expectation values, “critic” tests
- Calibration / Neyman construction with toys
  (badly trained network can lead to suboptimal limits, but not to wrong limits)

This method lets us infer Dark Matter substructure from strong lensing observations.

Overview

2 parameters $\theta = (\beta, f_{\rm sub})$



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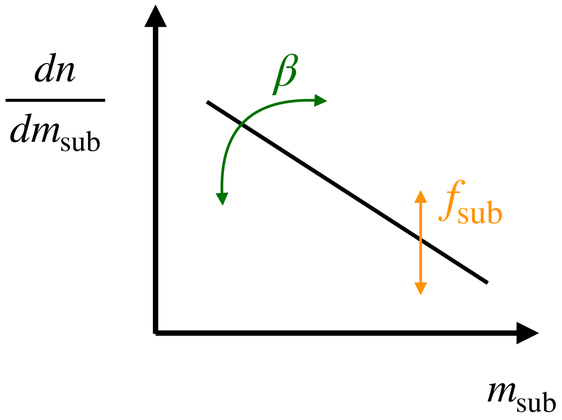

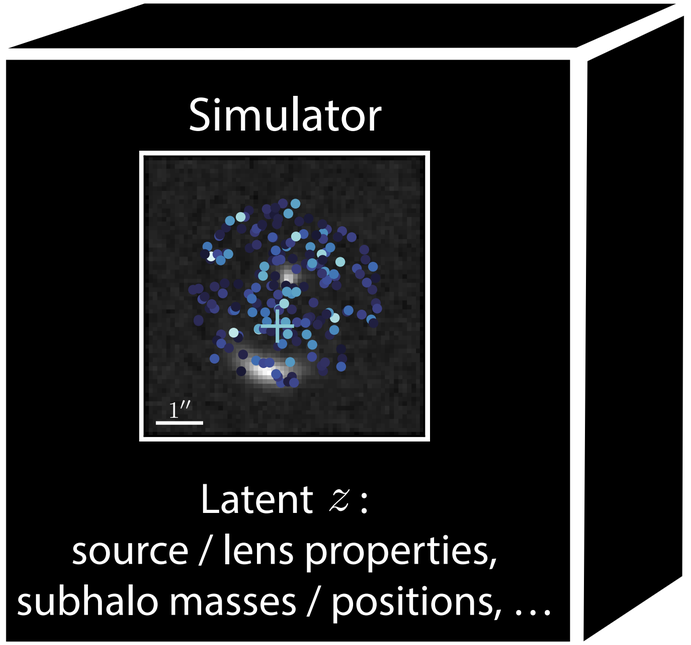

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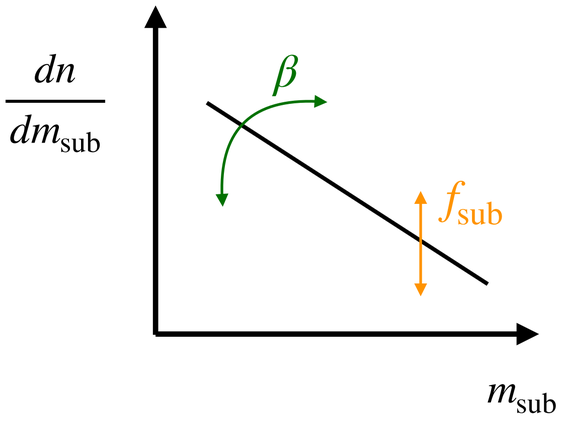
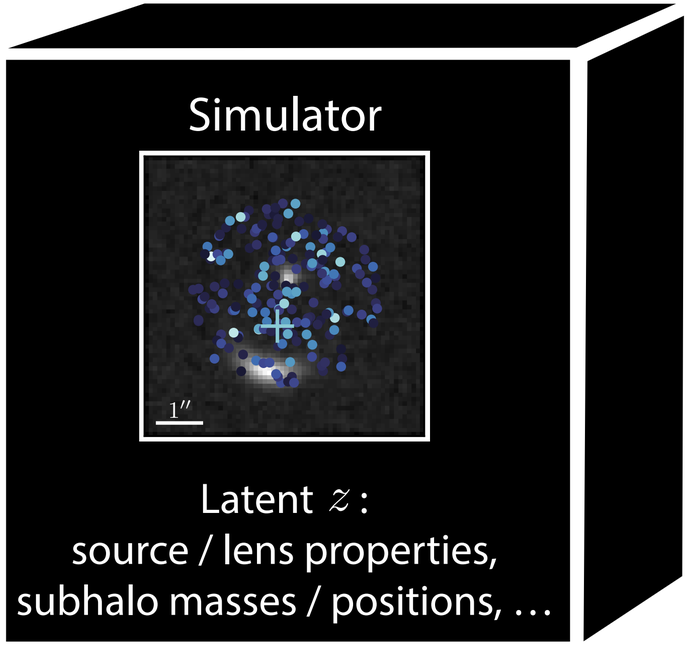
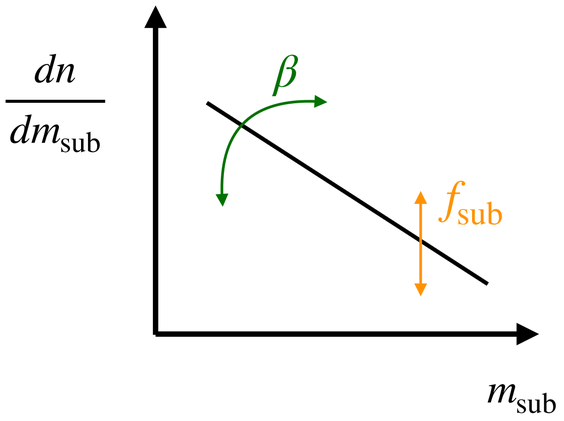


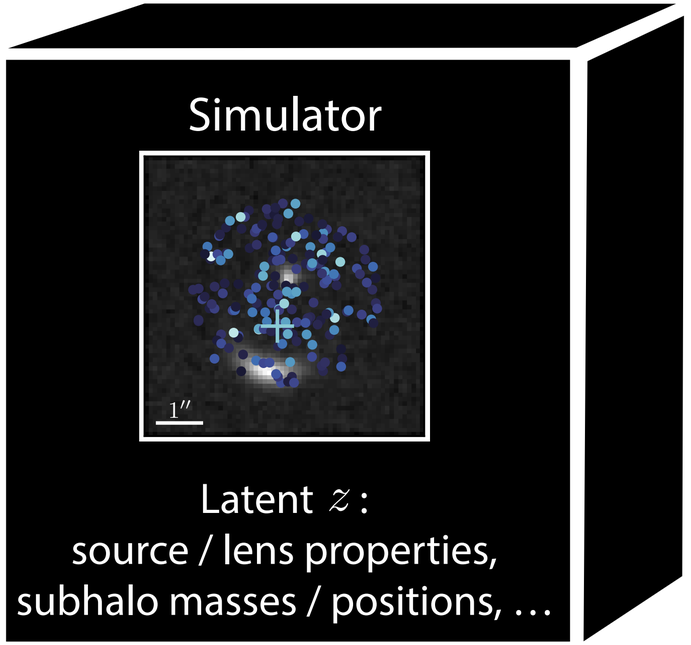


64^2 observables x

Overview

2 parameters $\theta = (\beta, f_{\rm sub})$





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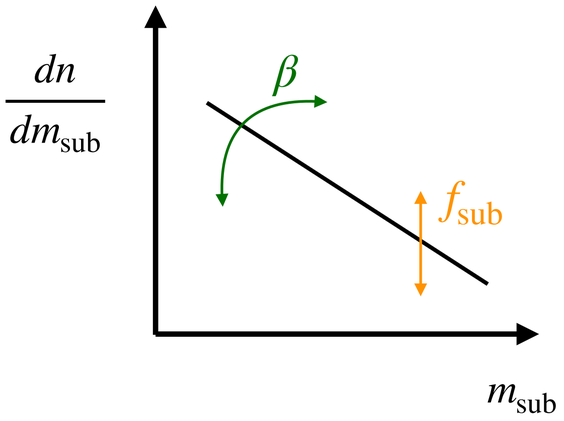
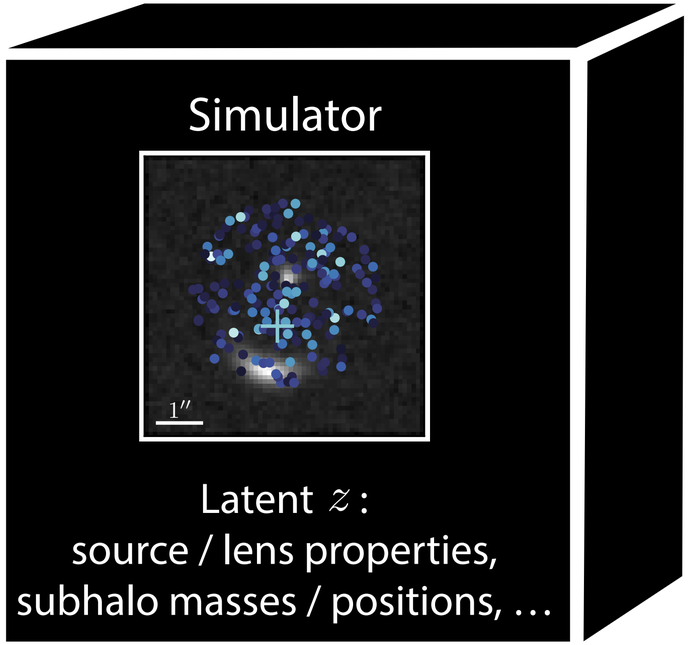
Prediction: We construct a simulator that can sample $x \sim p(x|\theta)$

Overview

2 parameters $\theta = (\beta, f_{\rm sub})$





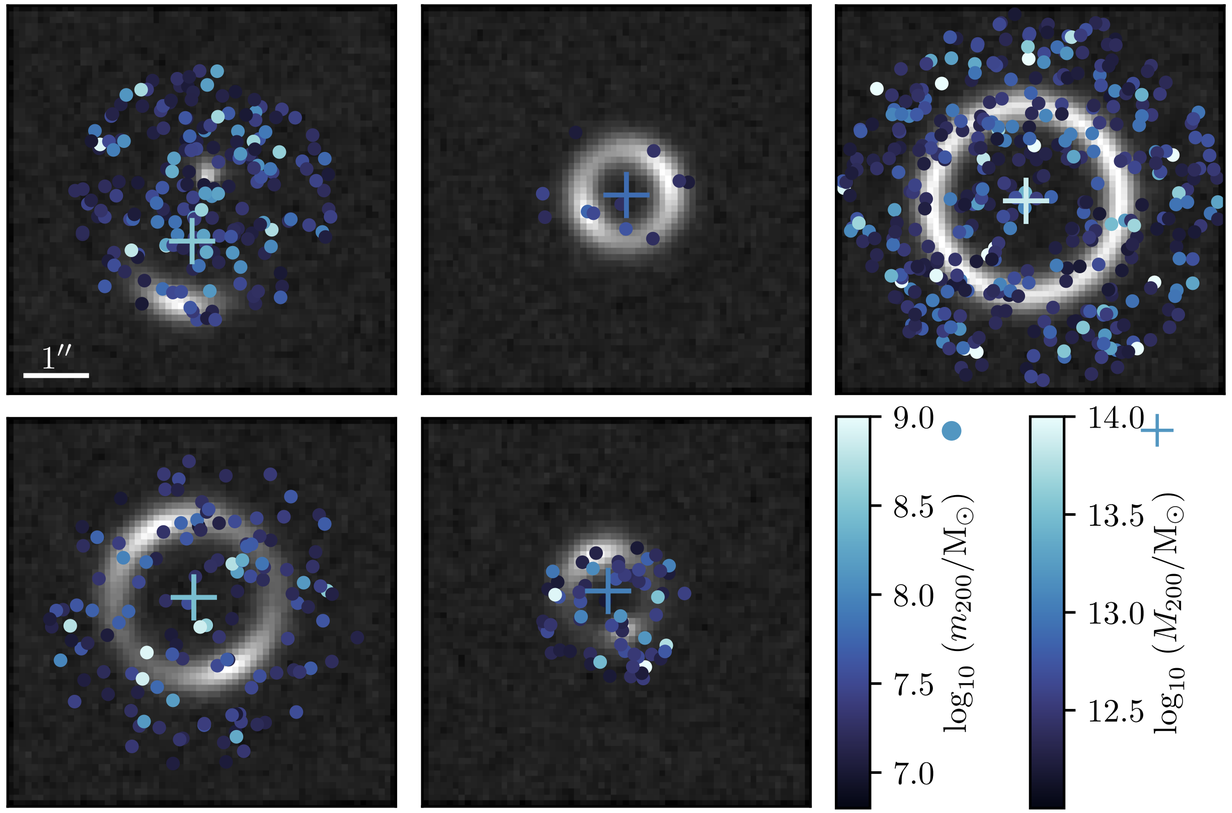
64^2 observables x

Prediction: We construct a simulator that can sample $x \sim p(x|\theta)$

Inference: We train neural likelihood ratio estimators $\hat{r}(x|\theta)$

Proof-of-principle simulator

[following T. Collett 1507.02657]

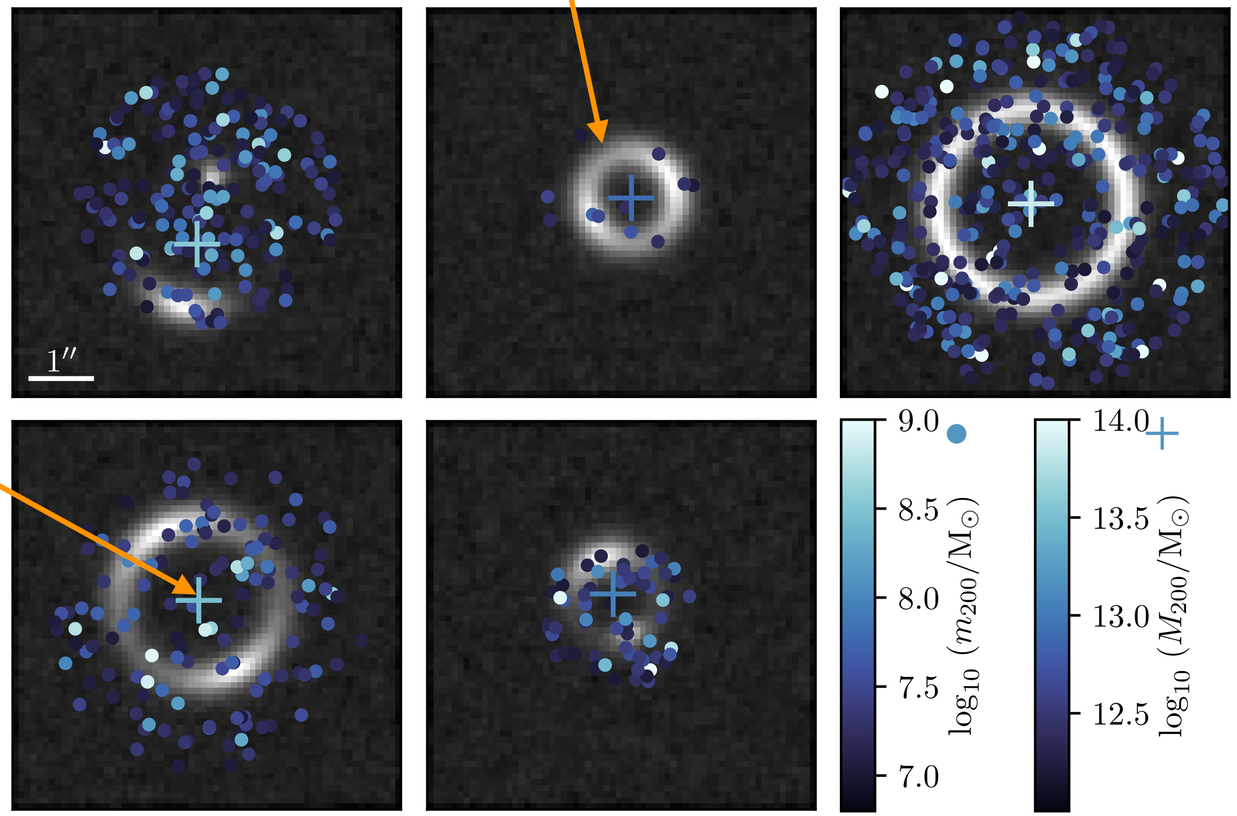


Proof-of-principle simulator

[following T. Collett 1507.02657]

Spherical lensing host galaxies
at redshift ~0.5…1

Extended galaxy sources
at redshift 1.5



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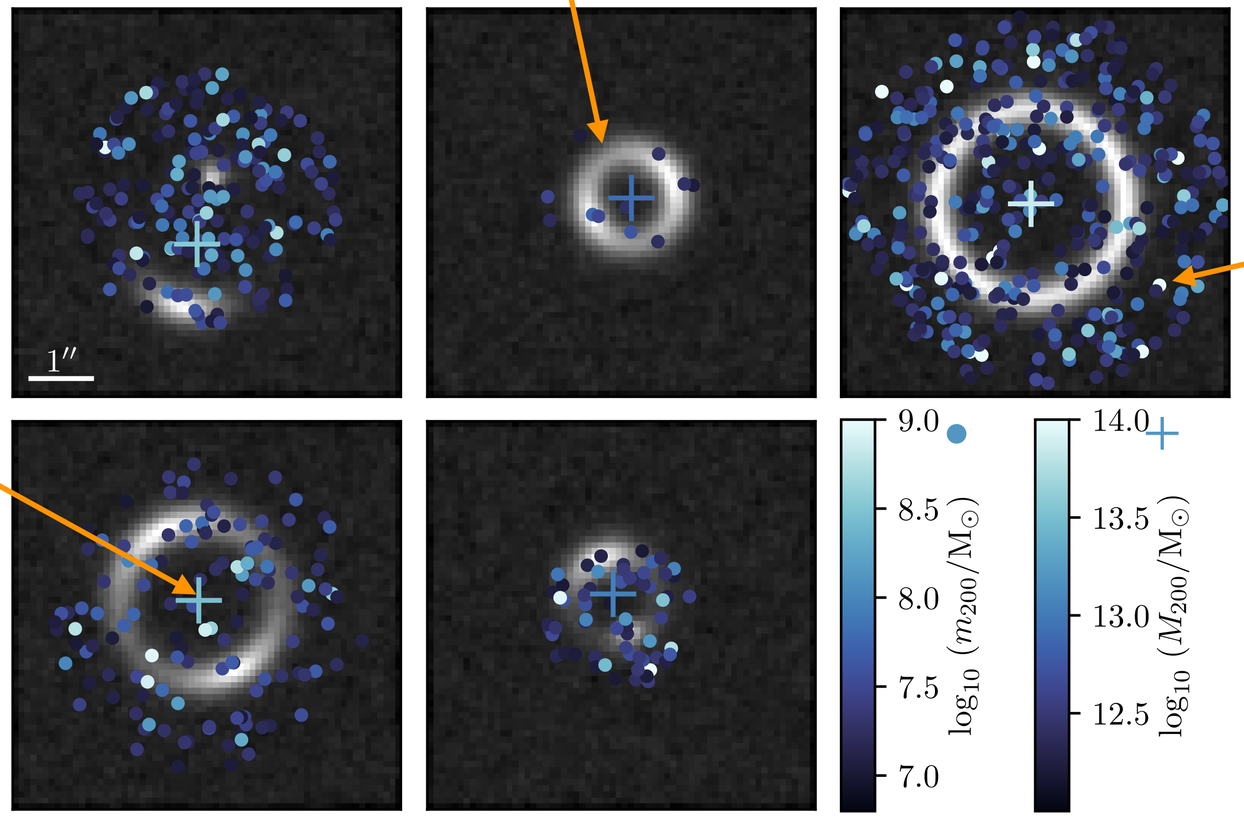
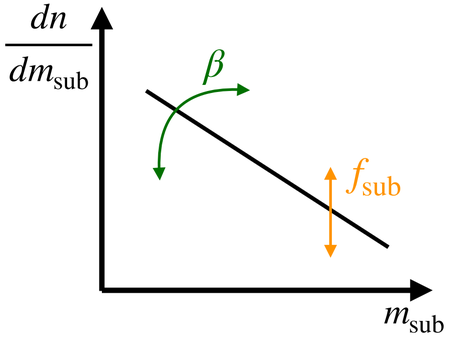


Subhalos follow mass distribution with two parameters



Proof-of-principle simulator

[following T. Collett 1507.02657]

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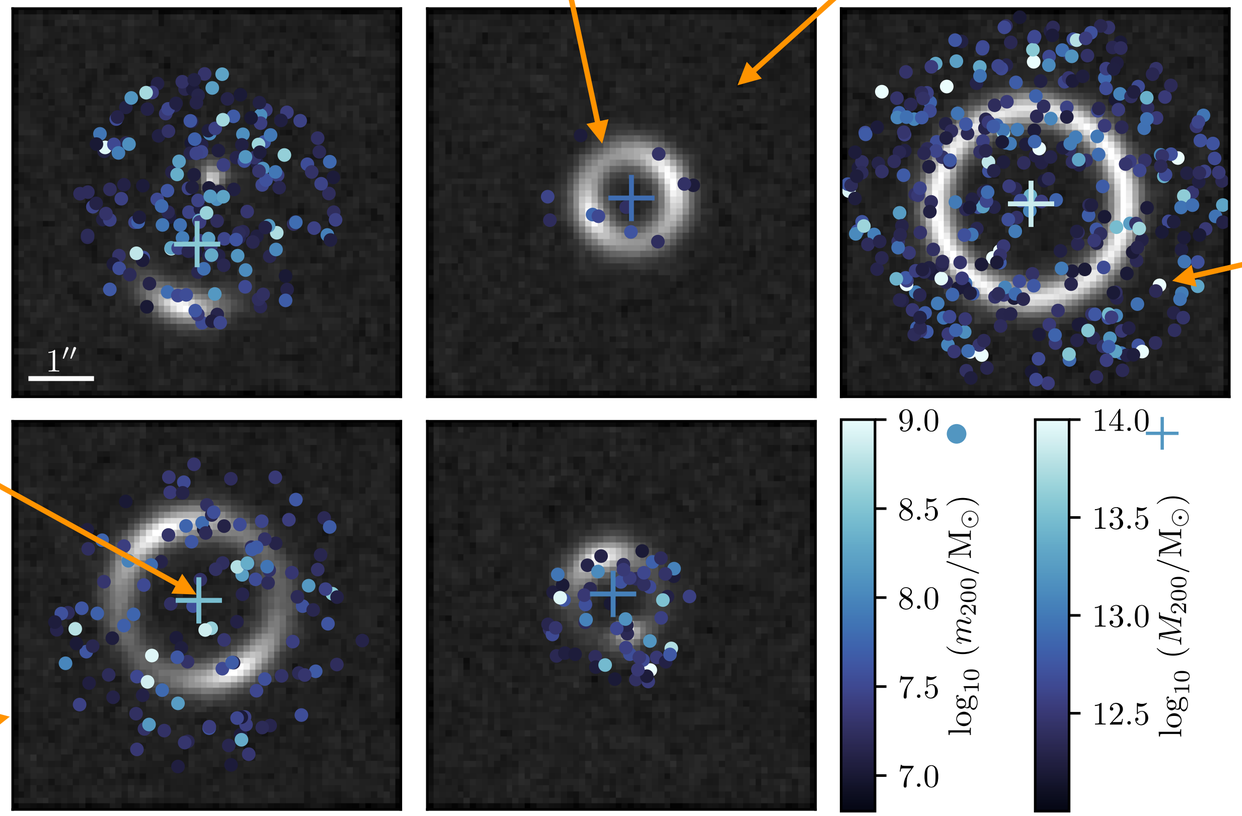
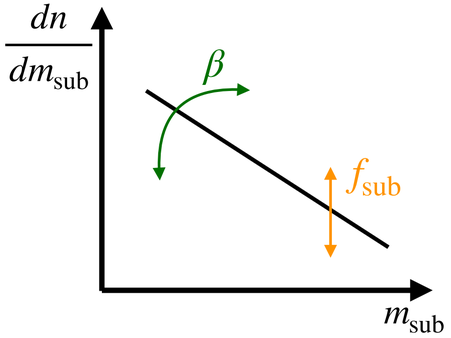
at redshift ~0.5…1

Poisson fluctuations

Extended galaxy sources
at redshift 1.5

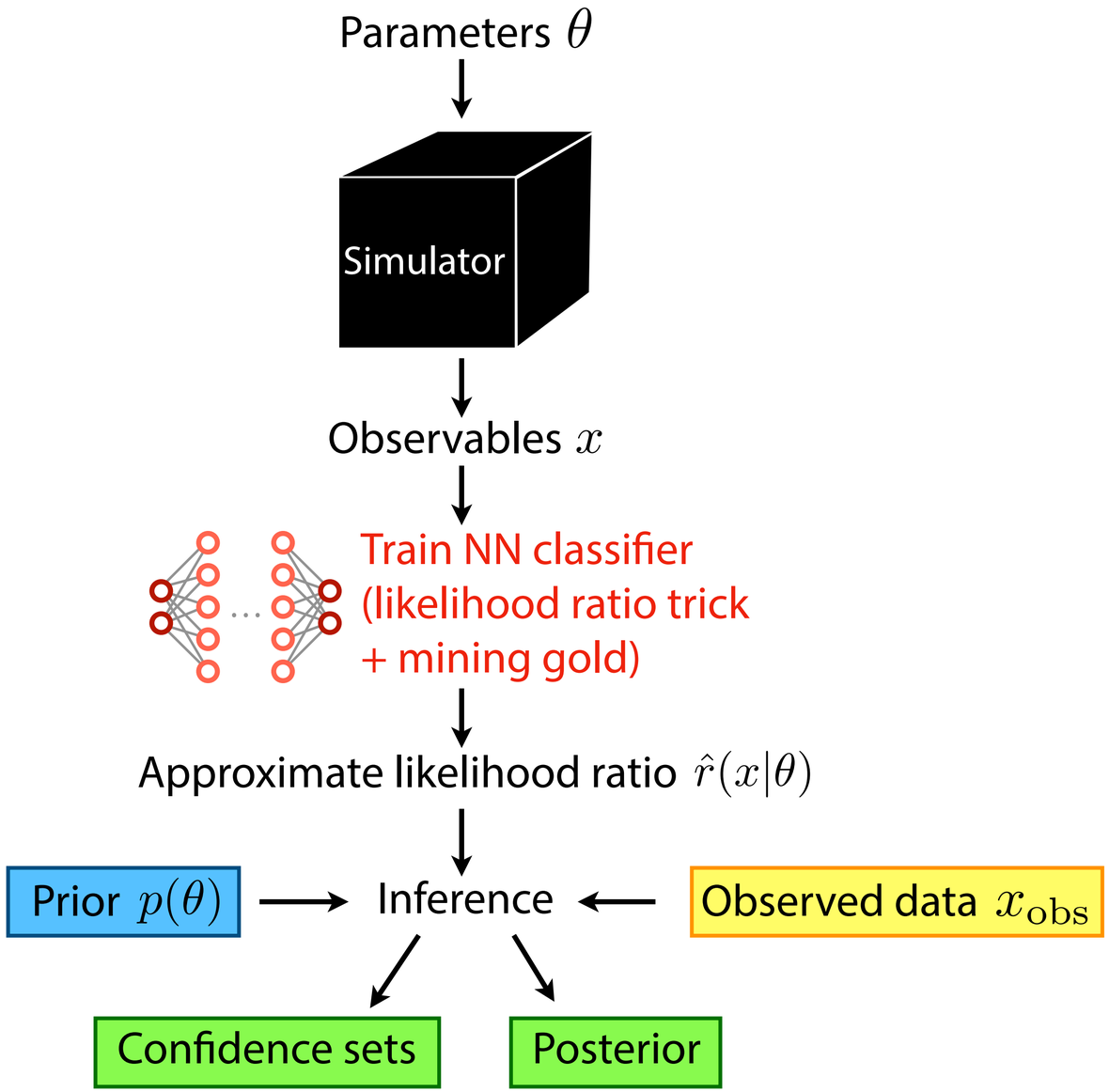
Subhalos follow mass distribution with two parameters





Euclid detector model
(single optical band,
64^2 pixel, Gaussian PSF)

Inference setup



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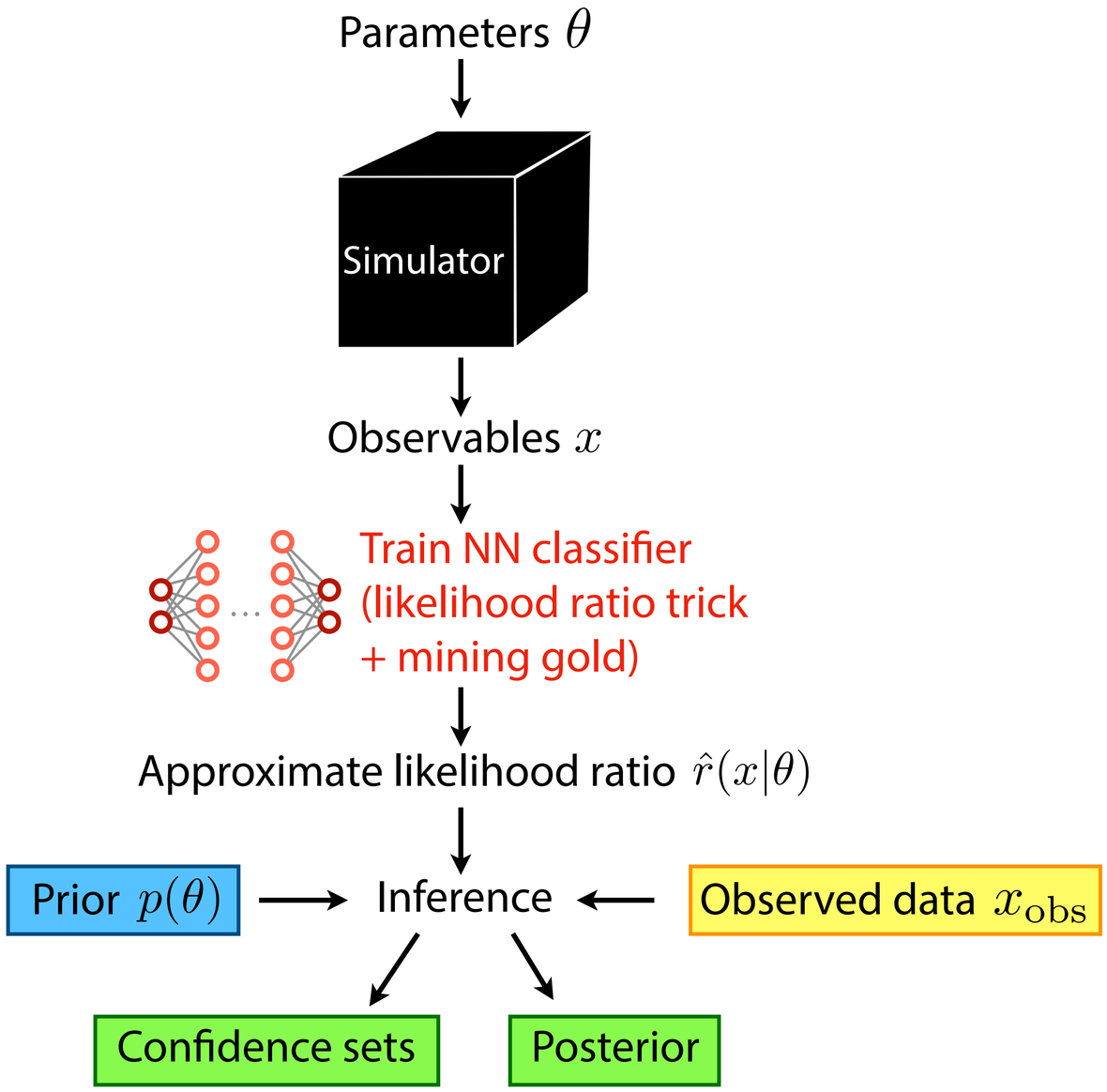
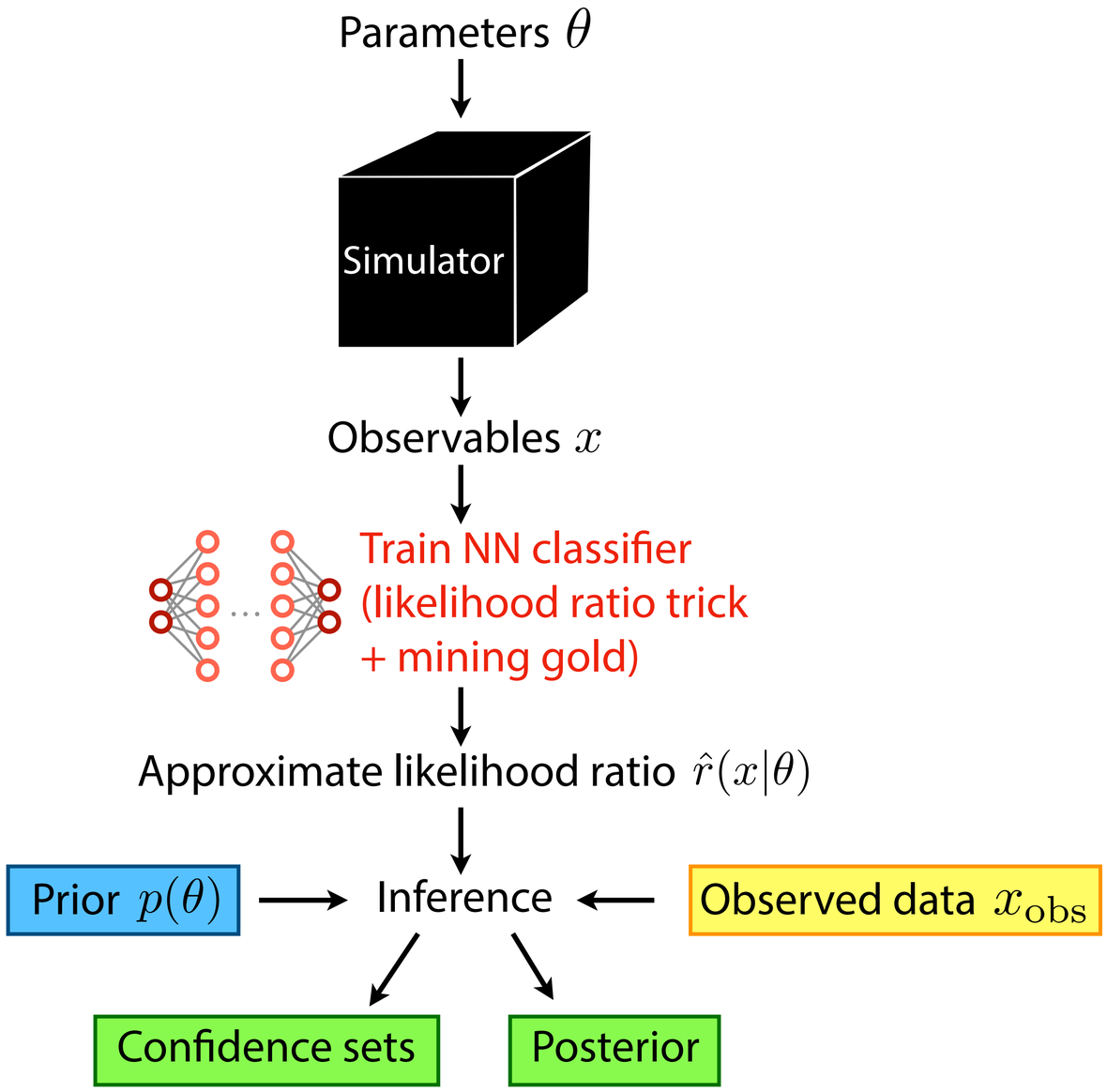


Training data: 10^6 lensed images with
$0 \leq f_{\rm sub} \leq 0.2, -1.5 \leq \beta \leq -0.5$

Inference setup



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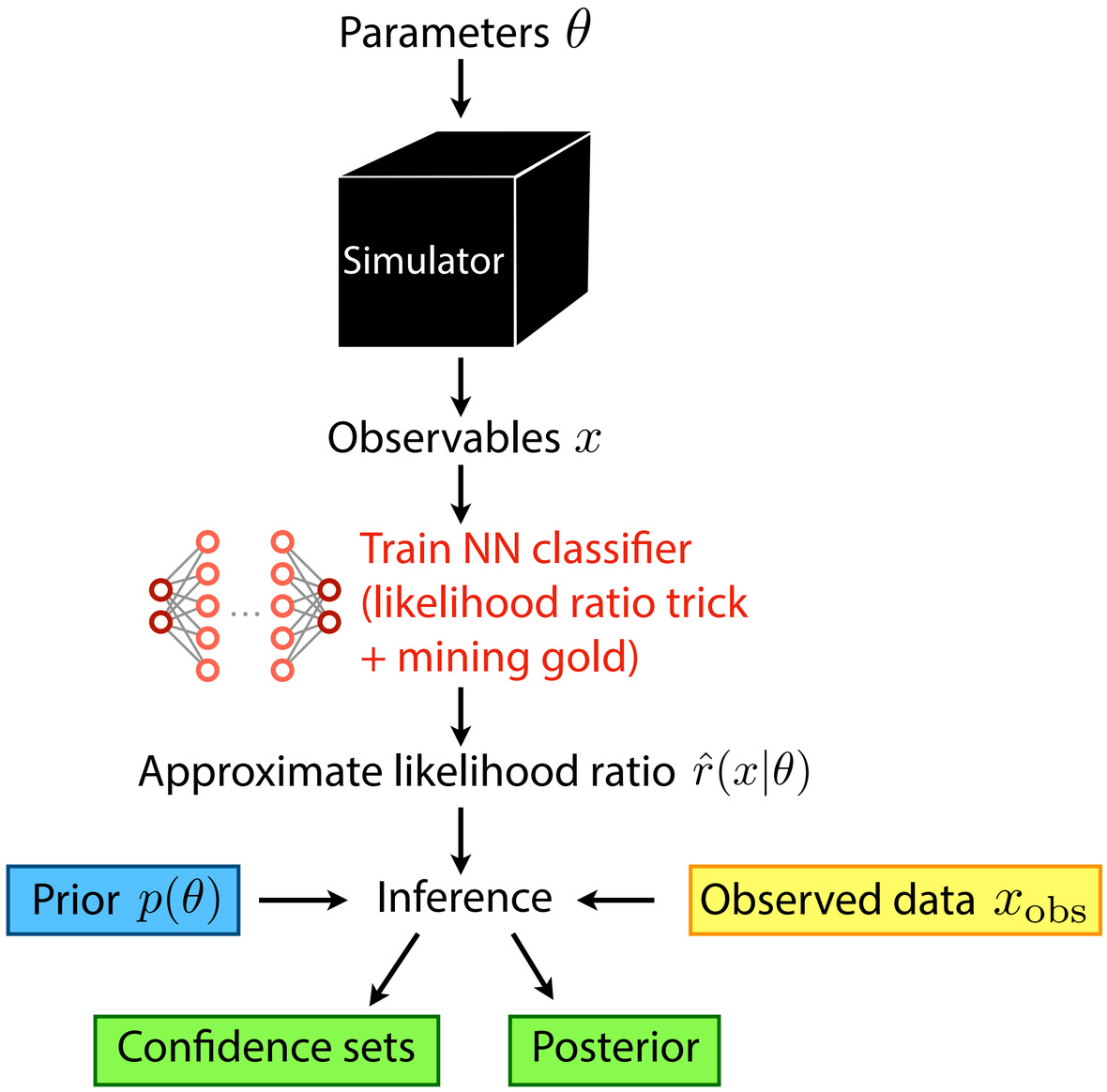
Convolutional neural network (modified ResNet-18) trained on ALICES loss

[M. Stoye, JB, J. Pavez, G, Louppe, K. Cranmer 1808.00973]

Calibration of network output

Inference setup



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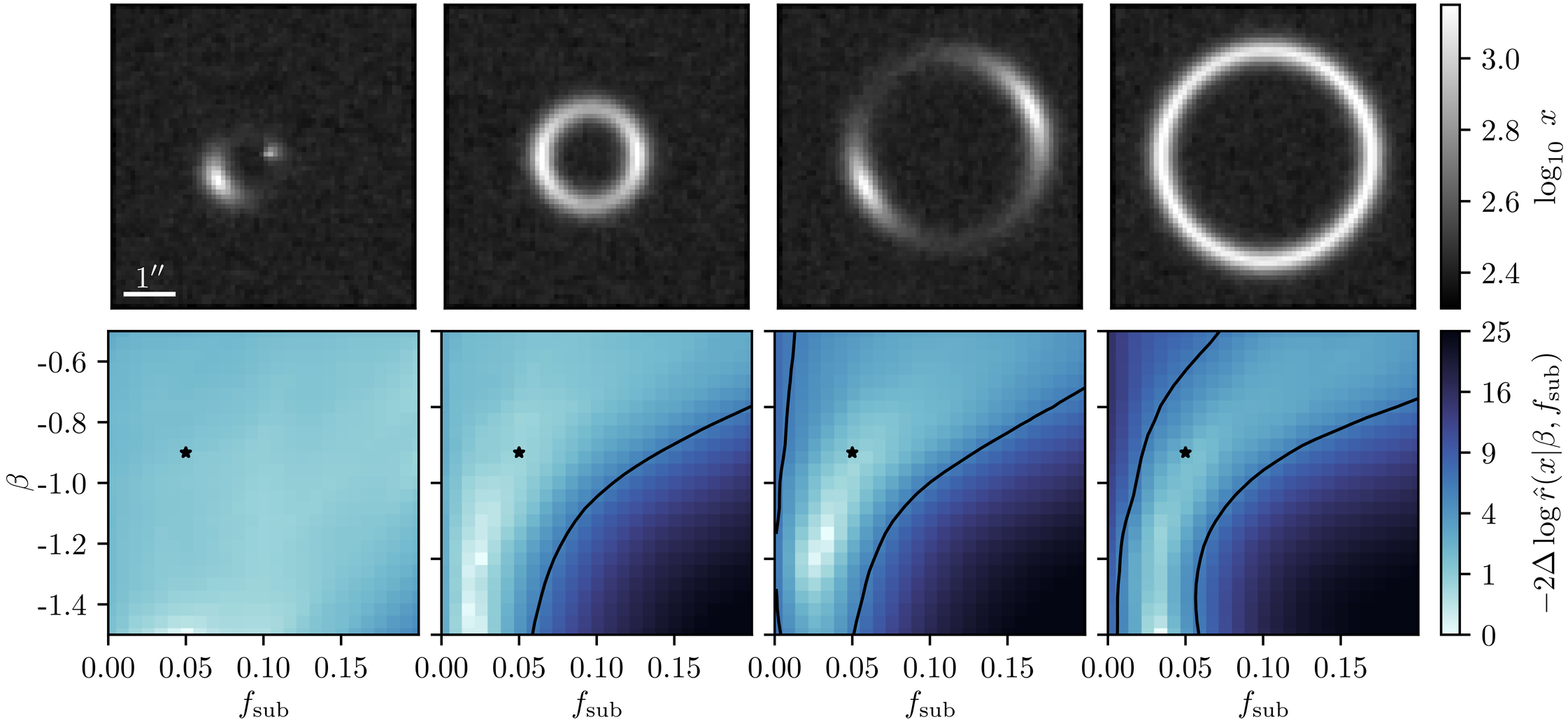
Calibration of network output

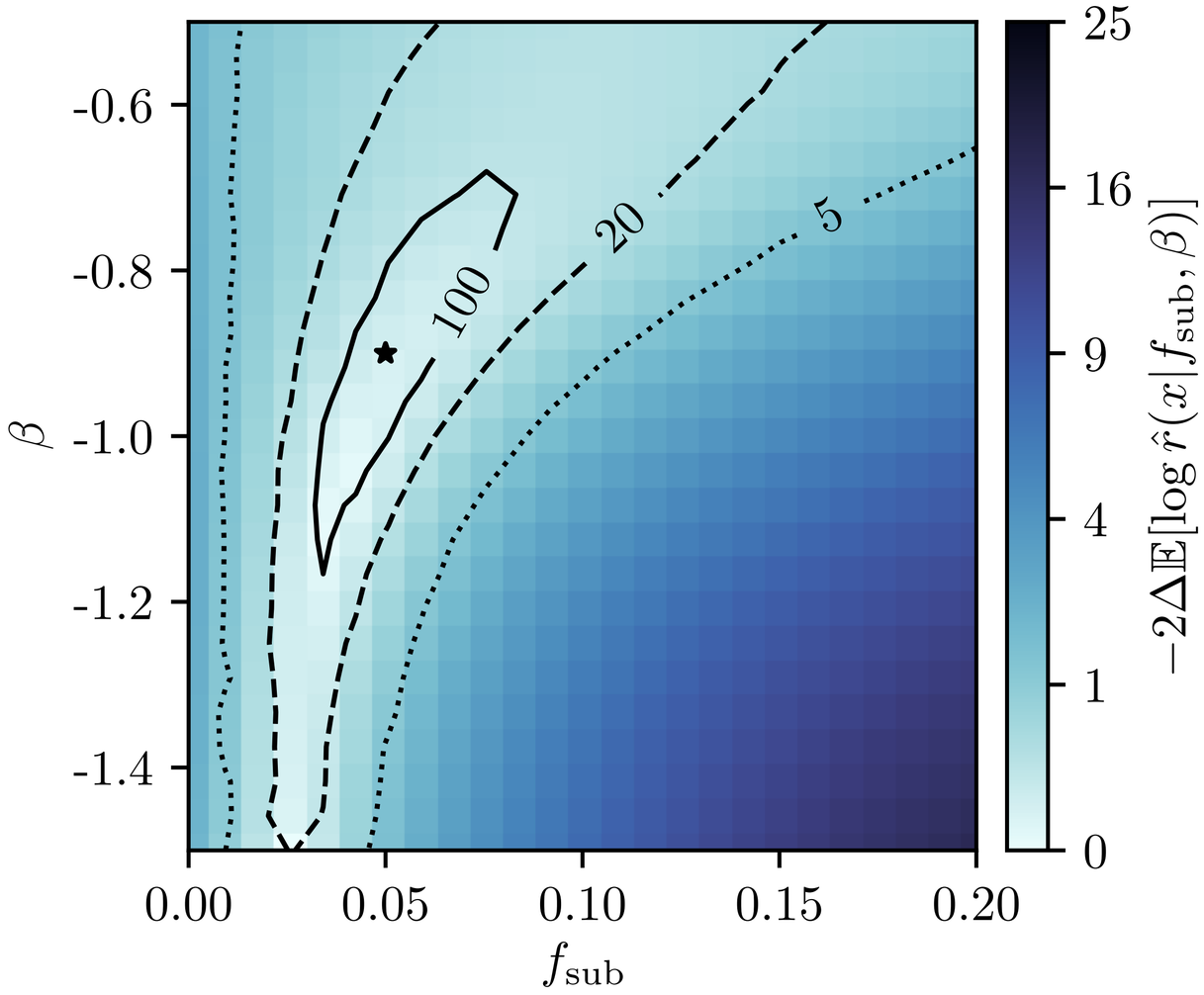
Synthetic "observed" data set: $f_{\rm sub} = 0.05, \beta = -0.9$

Bayesian & frequentist inference

Inferring parameters from individual images



Expected likelihood ratio map



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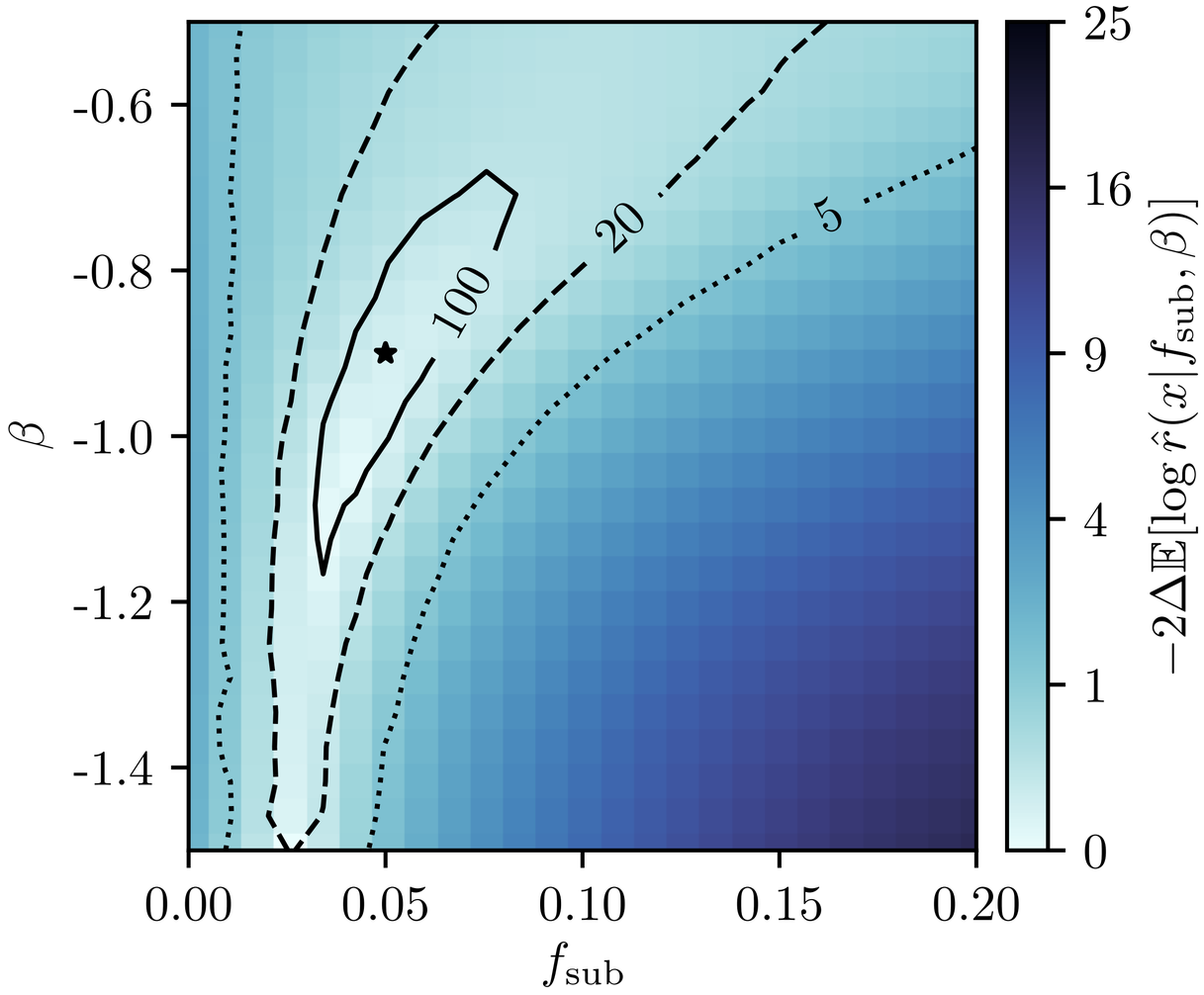
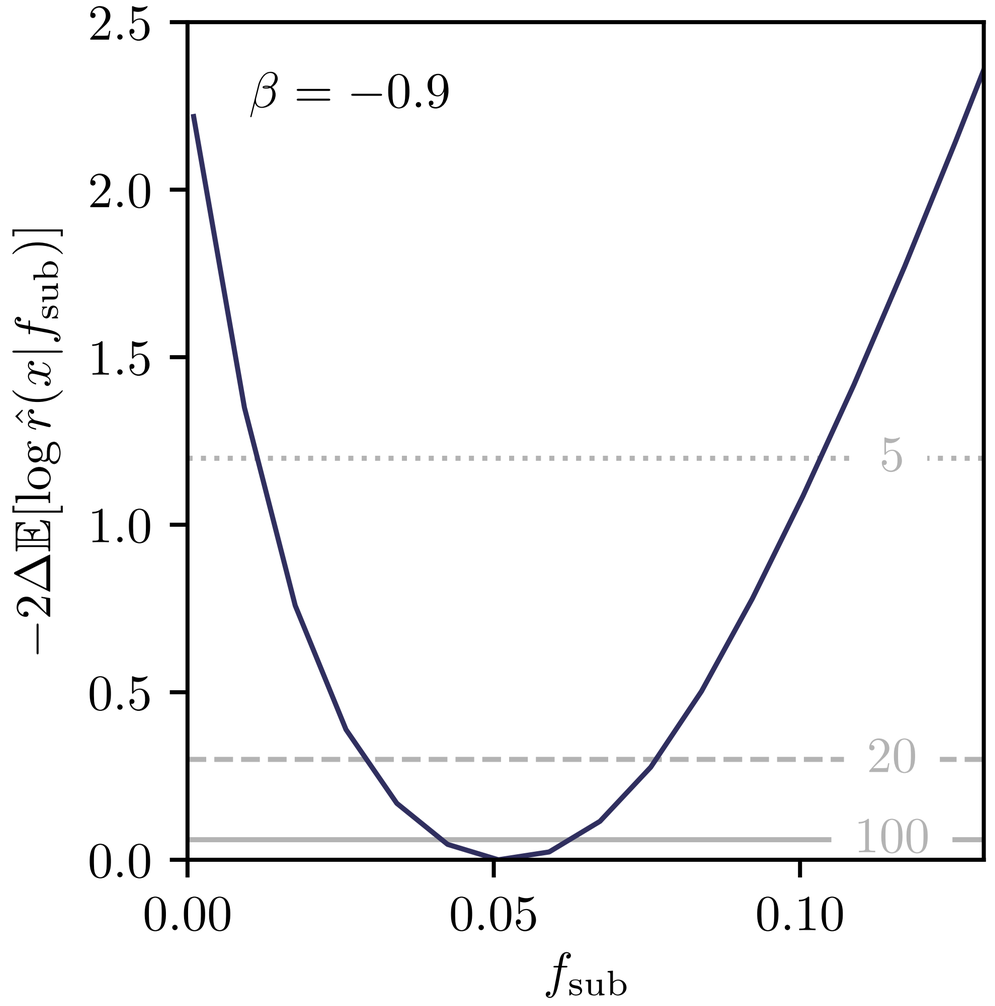
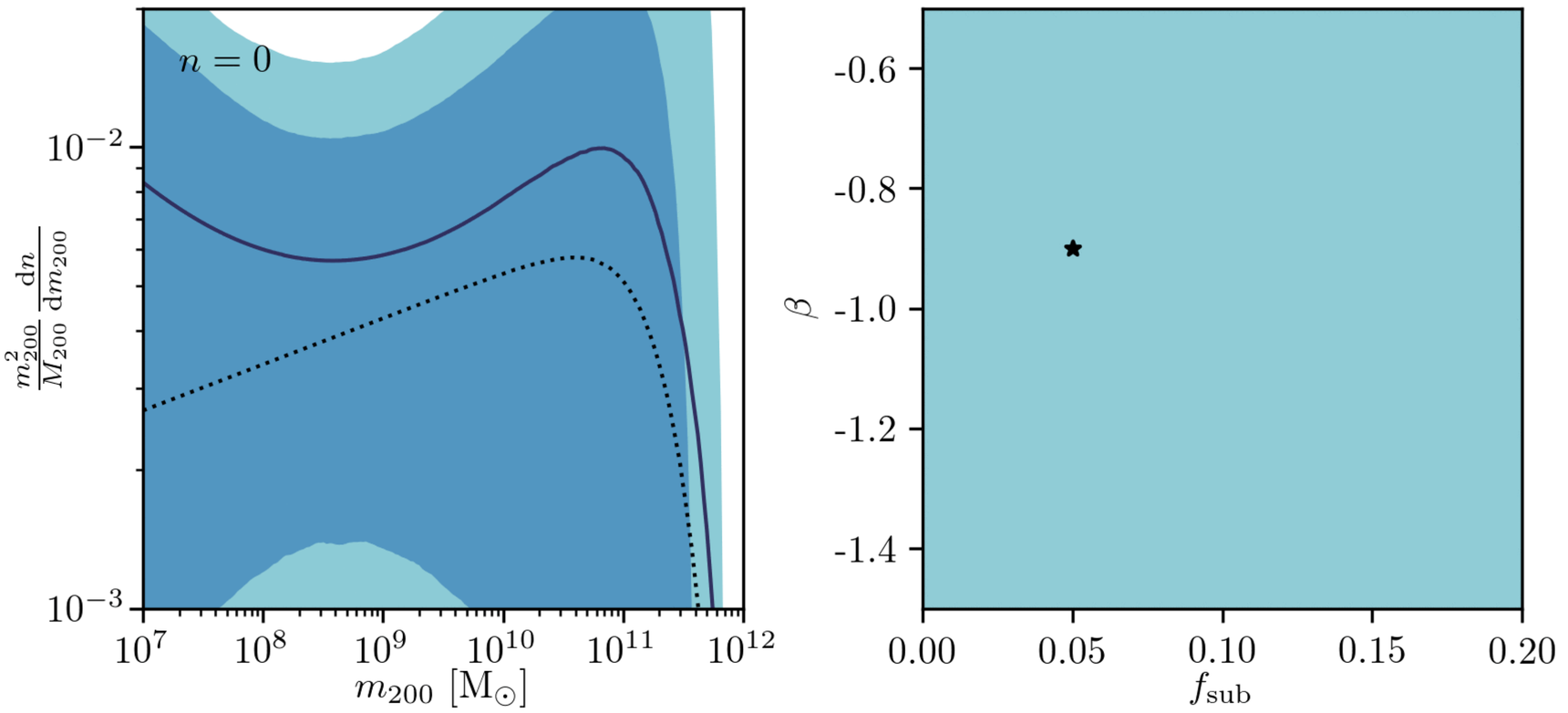




Bayesian inference



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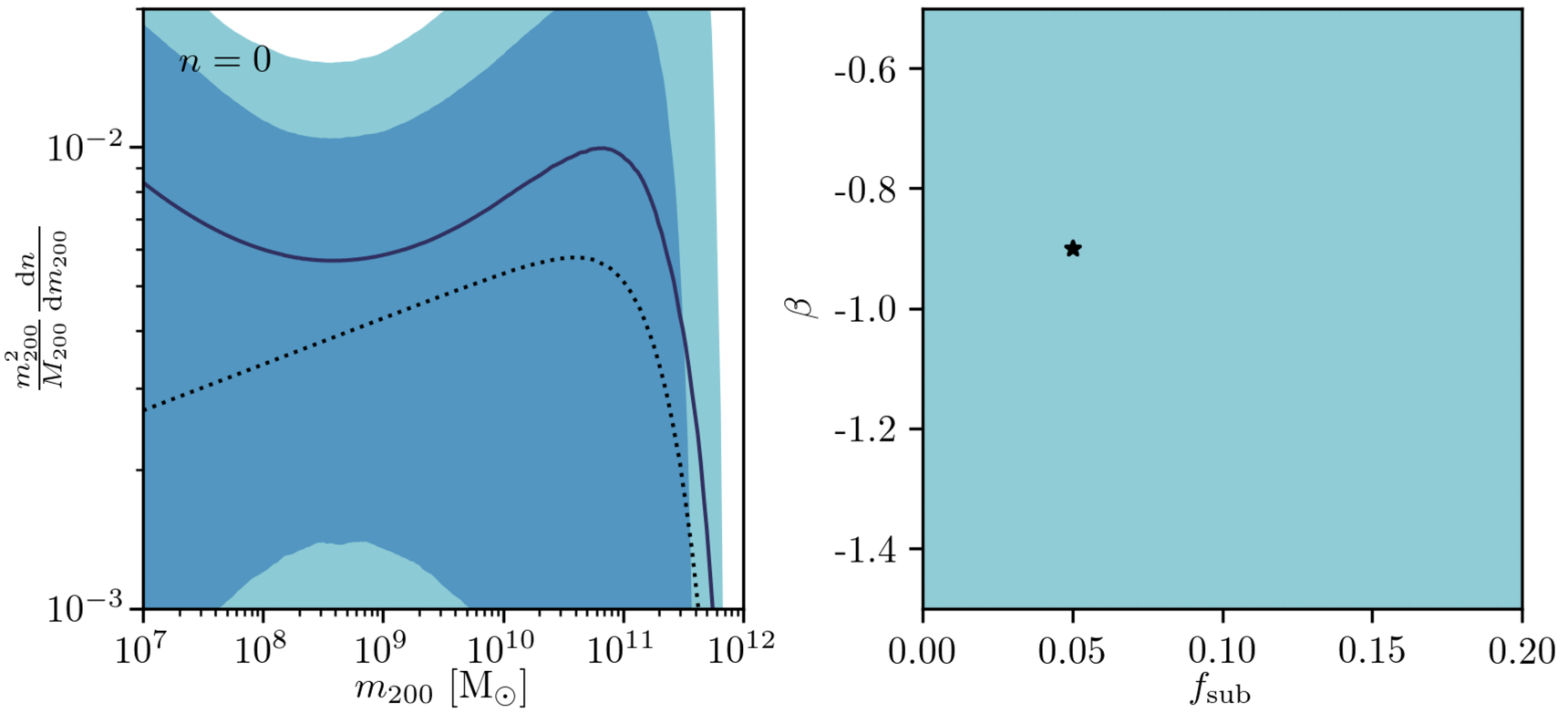
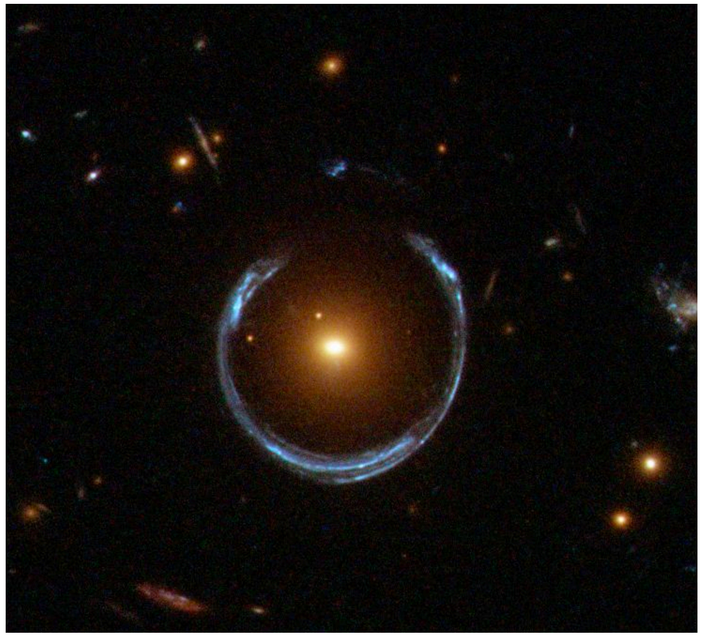


All the things we didn’t do

- More involved subhalo mass function
  - Warm DM with DM mass as parameter



[ESA/Hubble/NASA]

All the things we didn’t do

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- Realistic simulators
  - More diverse source and host galaxies (e.g. data-driven)
  - Realistic subhalo modelling (tidal disruption, redshift dependence…)
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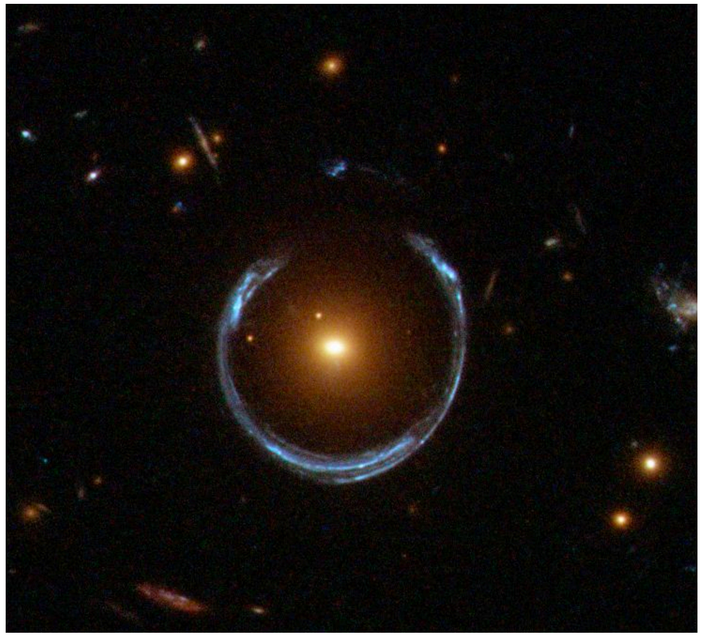
  - Realistic observation model (variable exposure / PSF, multiple bands…)



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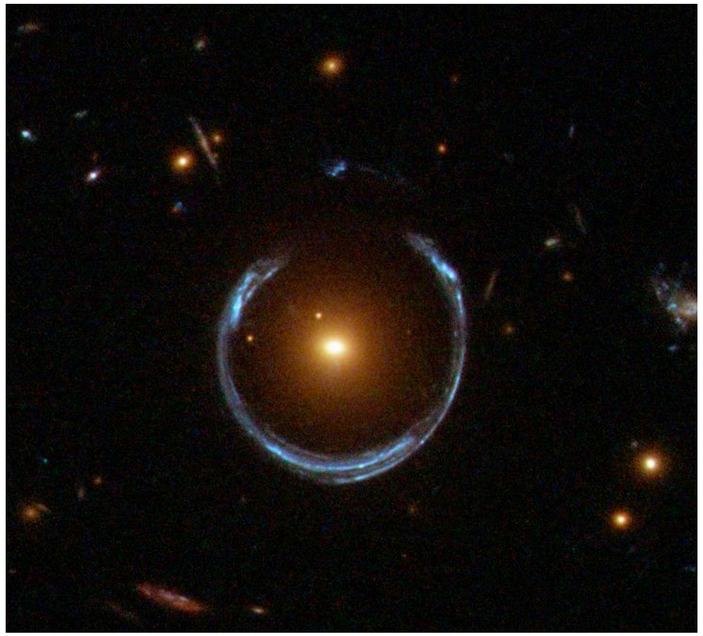

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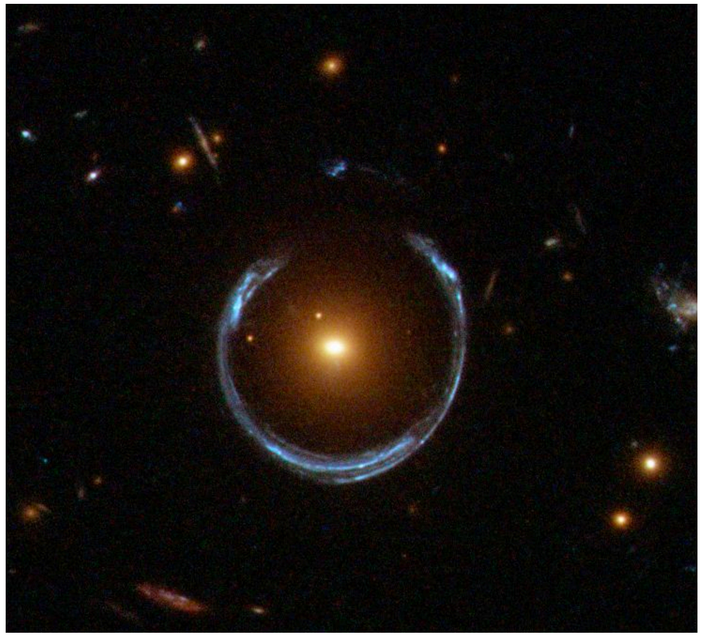

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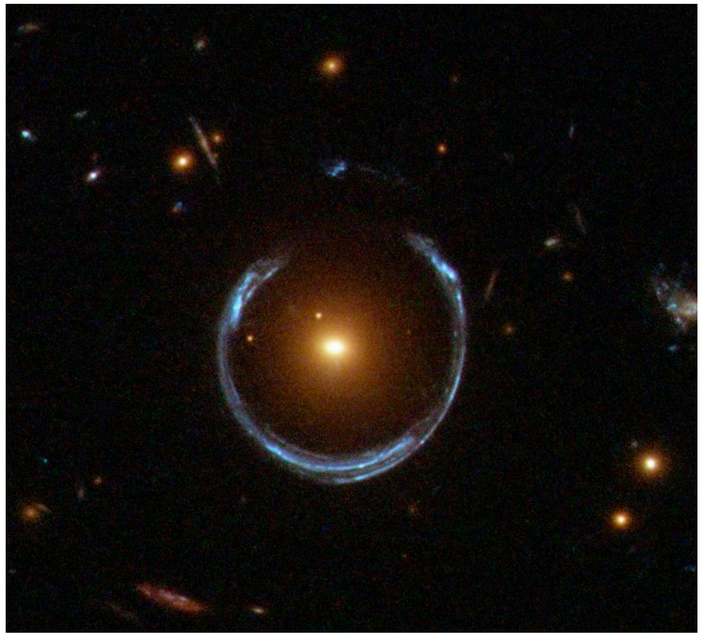
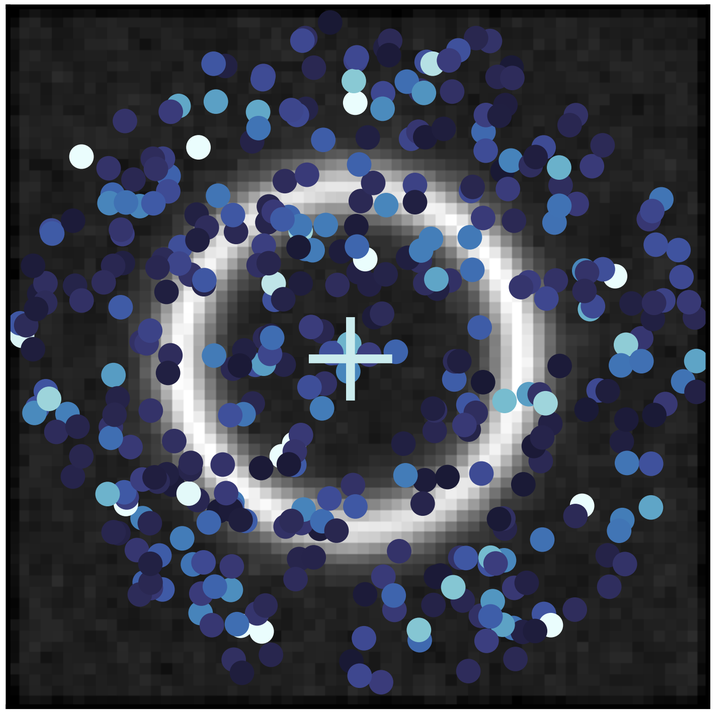
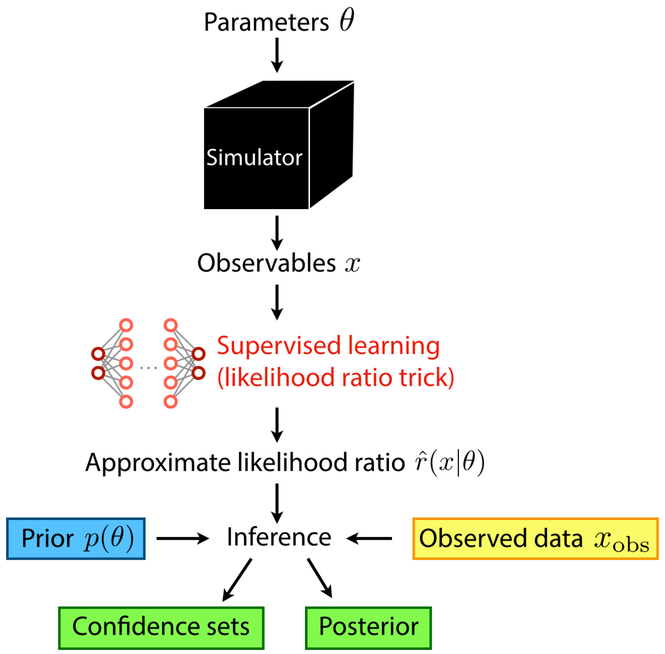


[ESA/Hubble/NASA]

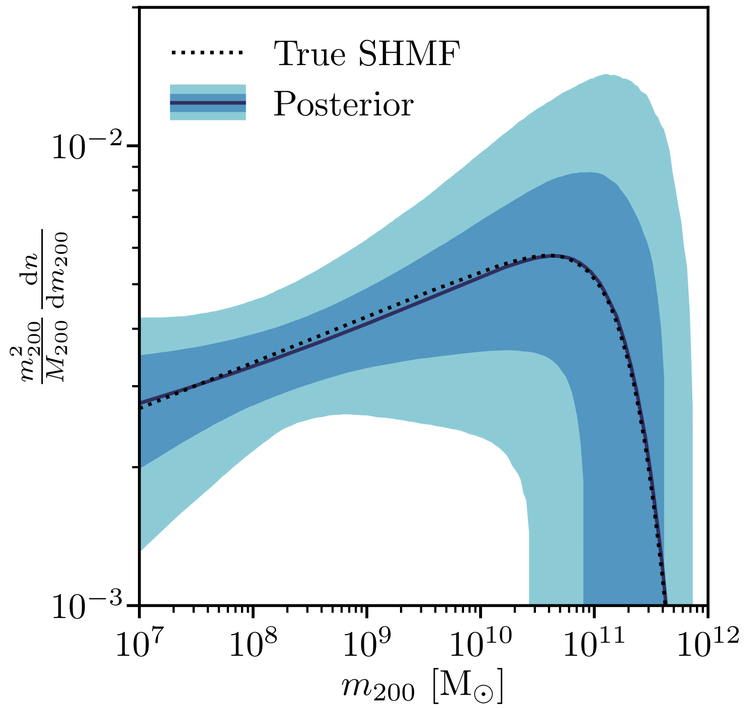
⇒ Our method should scale to a realistic setting, but will require more simulations and careful sanity checks



The small-scale structure of Dark Matter affects strong lensing, but teasing out this information is challenging.



New simulation-based inference algorithms based on machine learning can solve this problem in a scalable way.



In a proof-of-concept study, they allow us to constrain Dark Matter substructure from Euclid-like lensing observations.

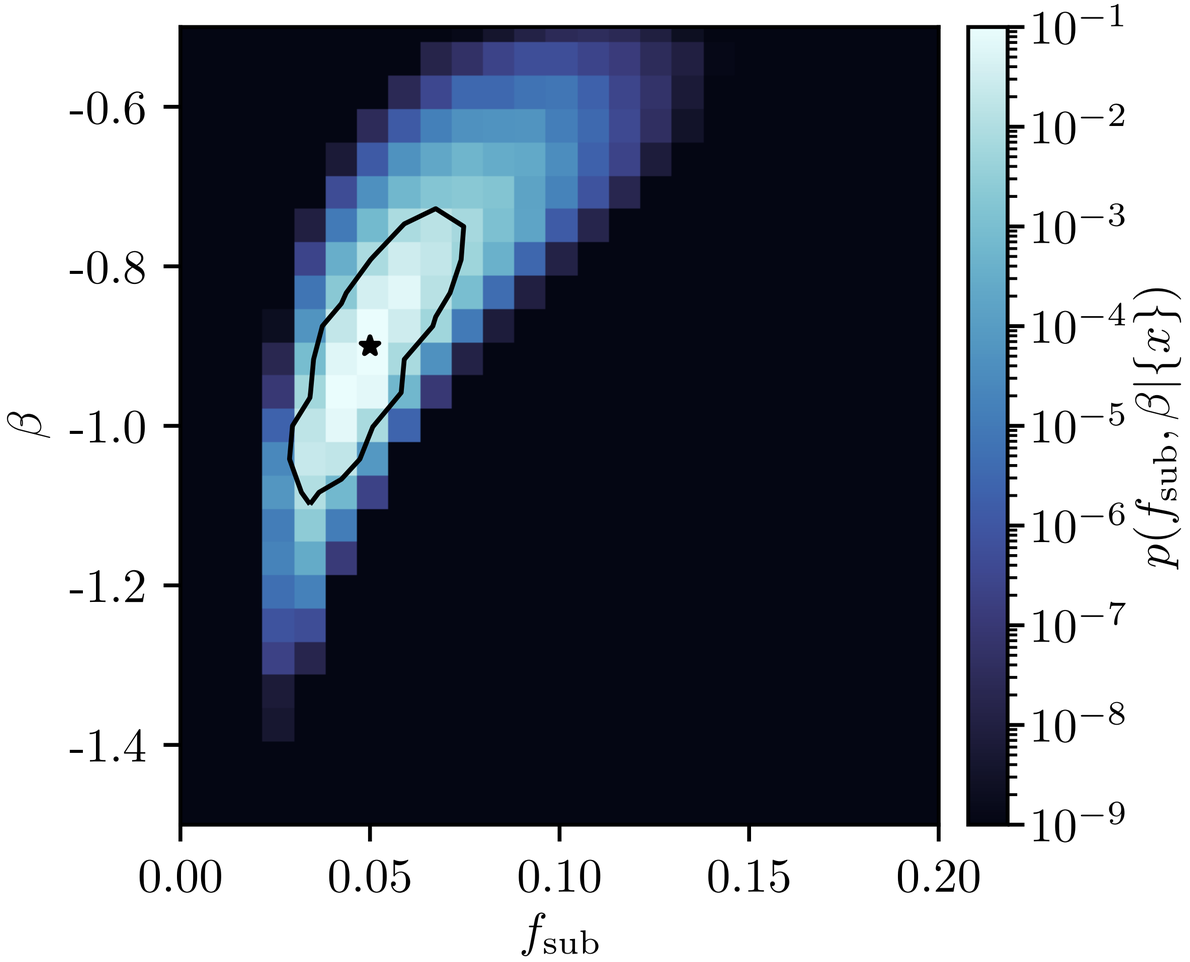
Strong lensing: **J**B, S. Mishra-Sharma, J. Hermans, G. Louppe, K. Cranmer 1909.02005

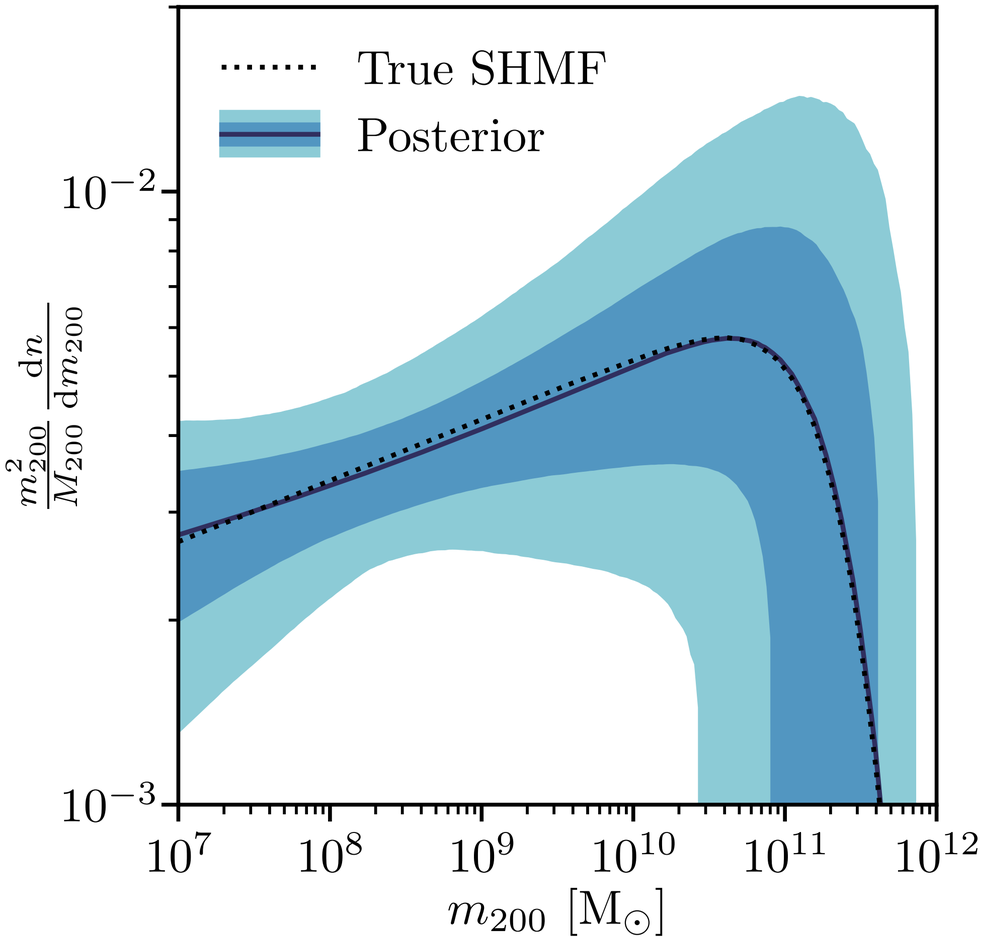
Broader review of simulation-based inference: K. Cranmer, JB, G. Louppe 1911.01429

“Hooray! Question mark?”

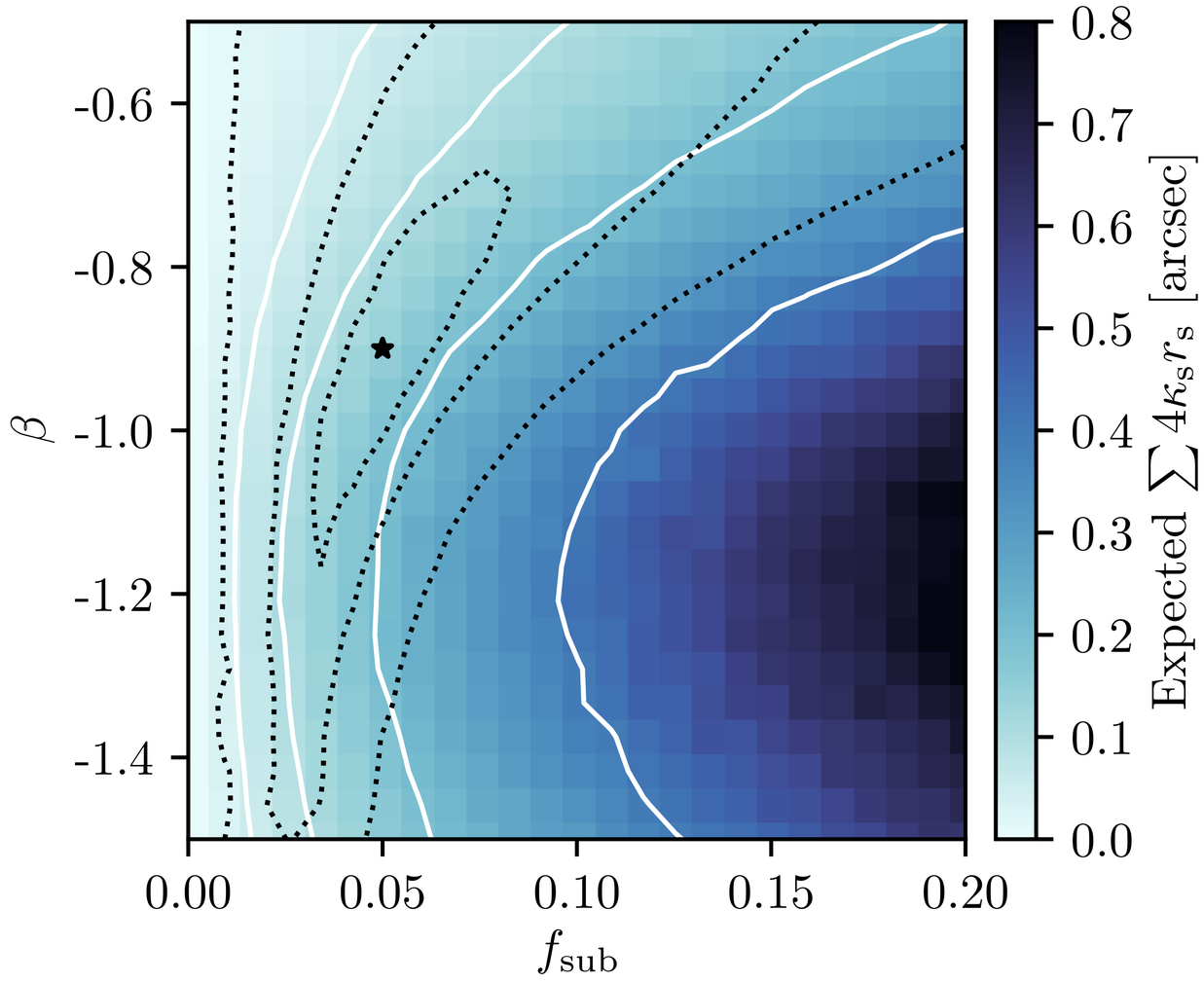
— Todd Chavez

Expected posterior

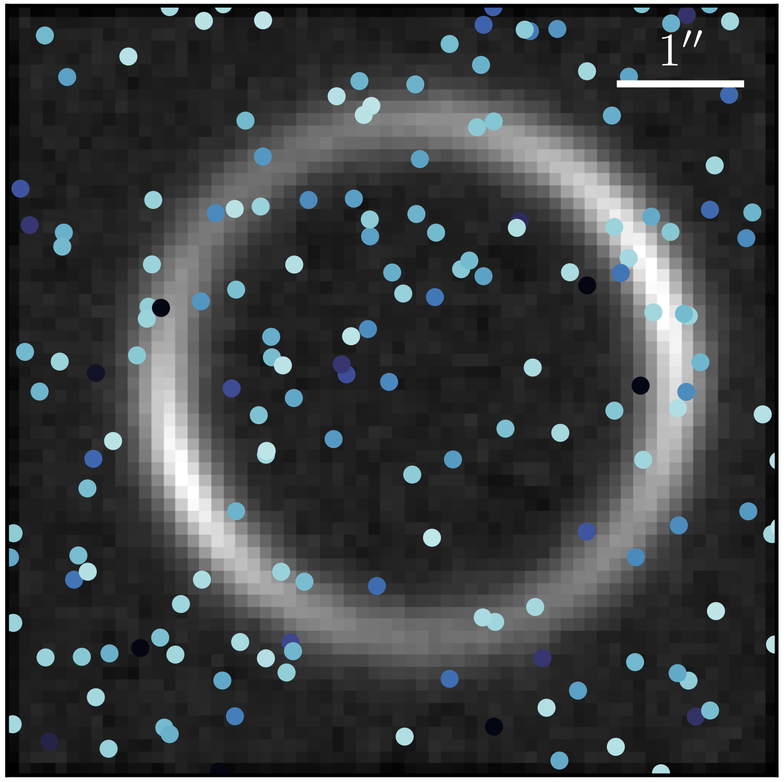


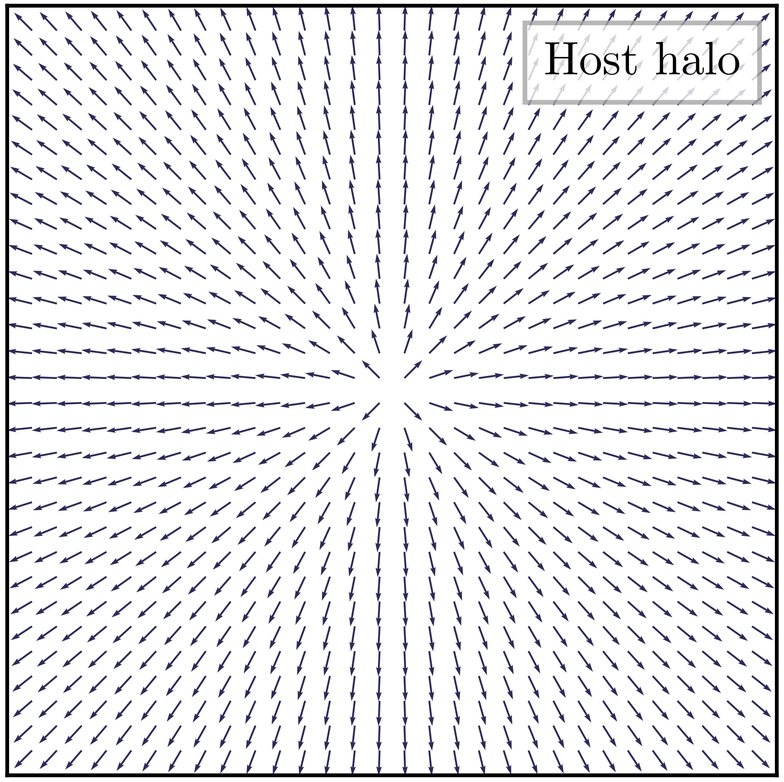


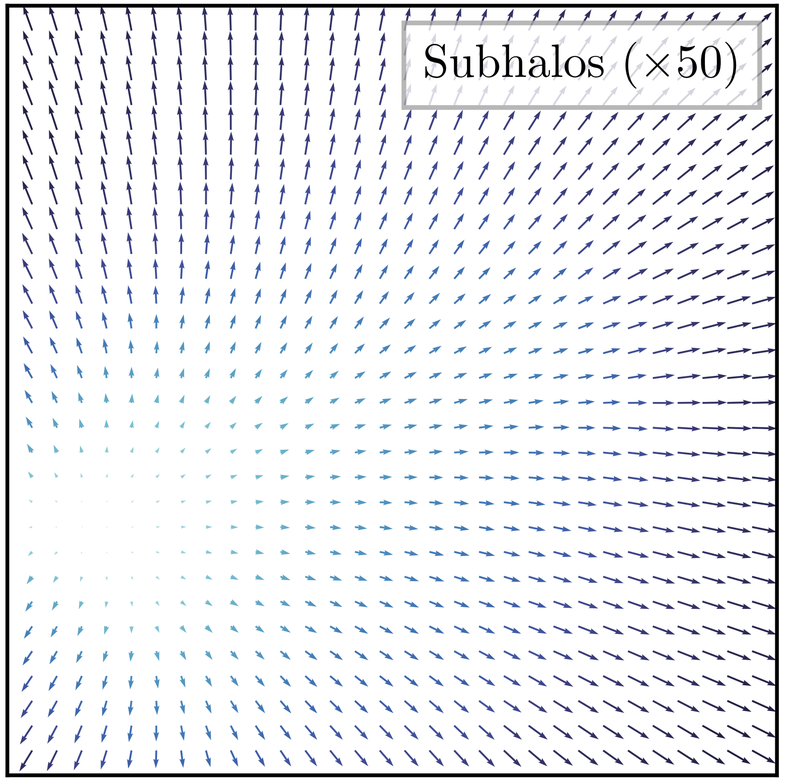
Likelihood vs total subhalo deflection



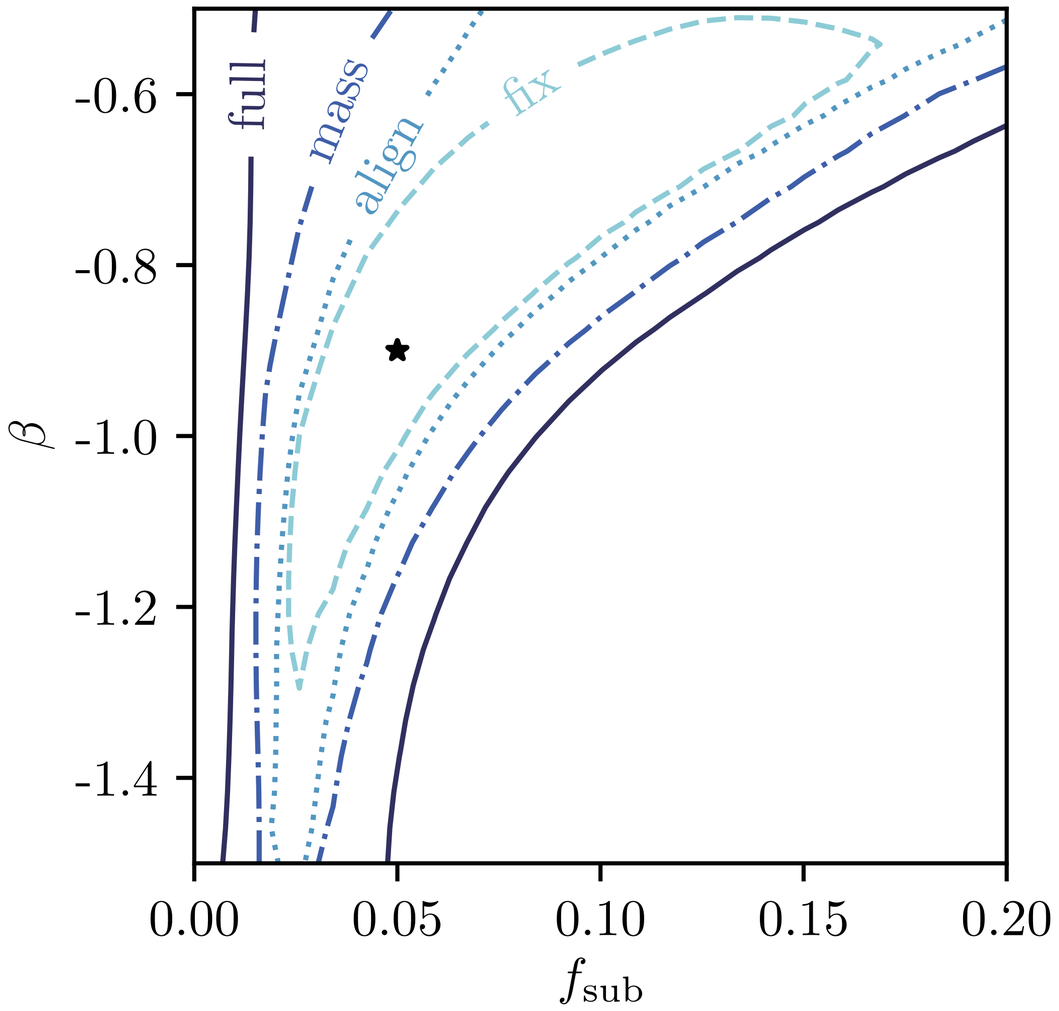
Deflection maps

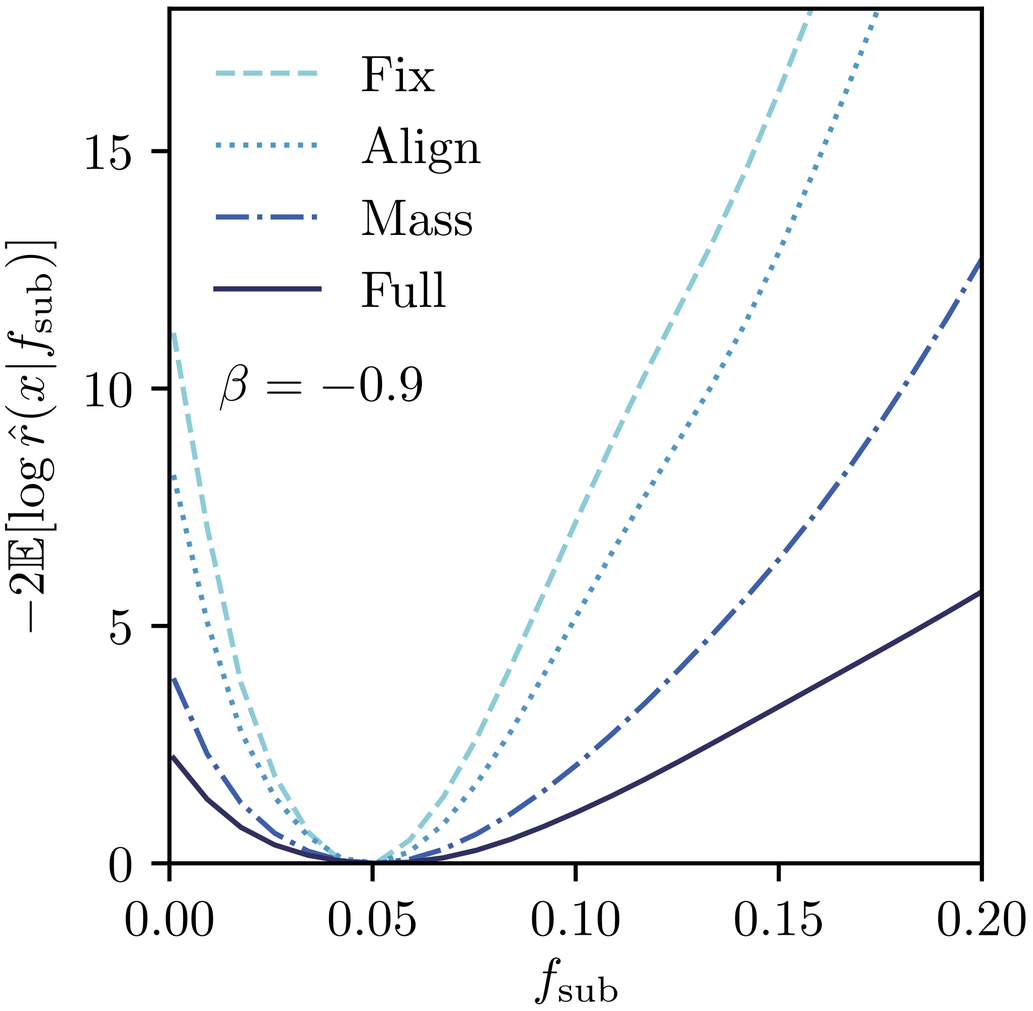






Simplified scenarios

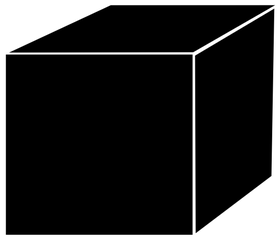




Formalizing the problem

You are given

- a simulator that lets you generate N samples $x_i \sim p(x_i|\theta_i)$ for parameter points θ_i of your choice



- observed data $x_{\mathrm{obs}} \sim p(x_{\mathrm{obs}}|\theta_{\mathrm{true}})$
- prior belief $p(\theta)$

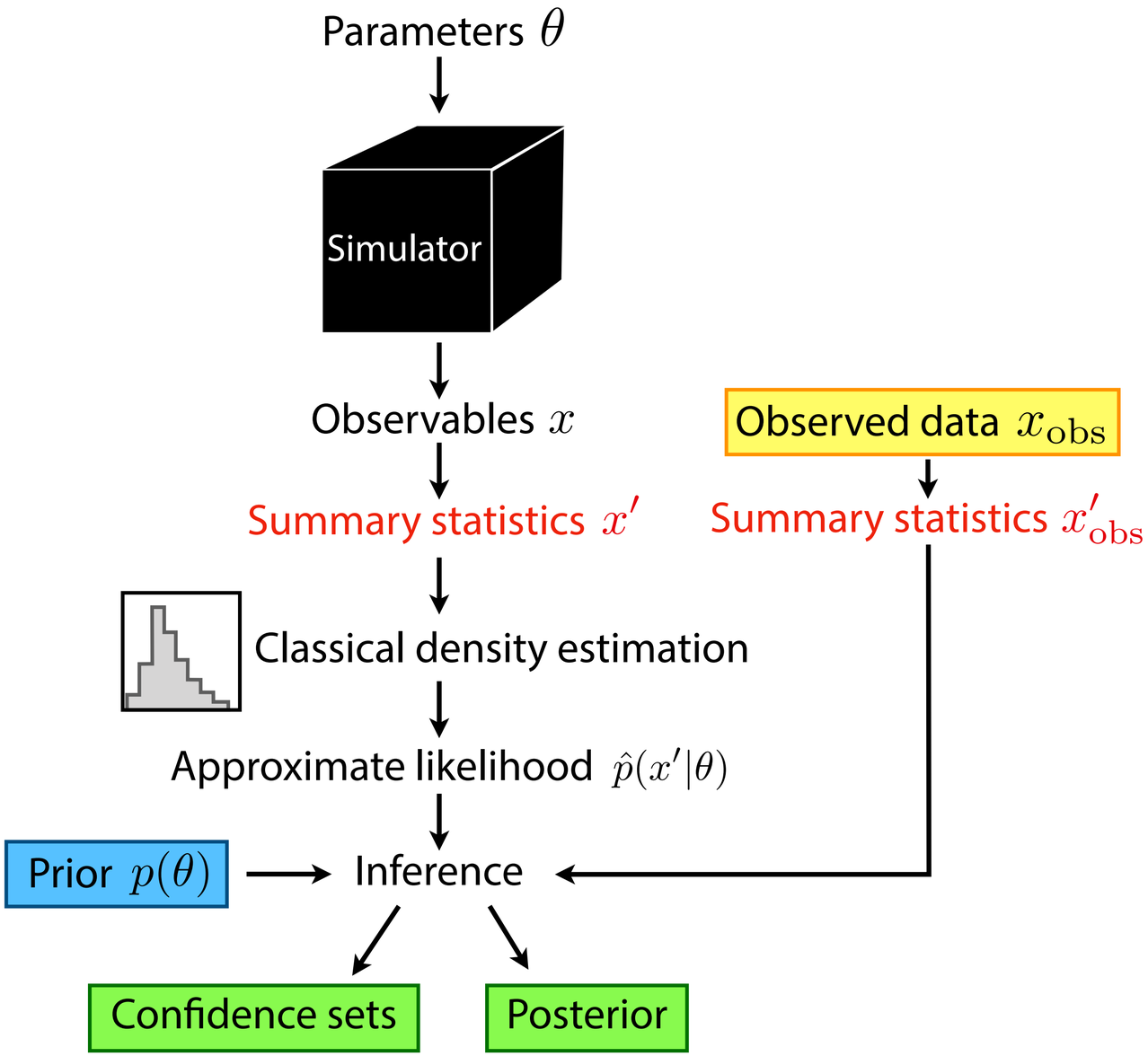
Goals: estimate either…

- true parameters $\hat{\theta}_{\mathrm{true}}$
- confidence sets based on likelihood $\hat{p}(x_{\mathrm{obs}}|\theta)$
- posterior $\hat{p}(\theta|x_{\mathrm{obs}}) = \dfrac{\hat{p}(x_{\mathrm{obs}}|\theta)\, p(\theta)}{\int \mathrm{d}\theta'\, \hat{p}(x_{\mathrm{obs}}|\theta')\, p(\theta')}$
  or samples from posterior $\theta \sim \hat{p}(\theta|x_{\mathrm{obs}})$

… depending on domain conventions

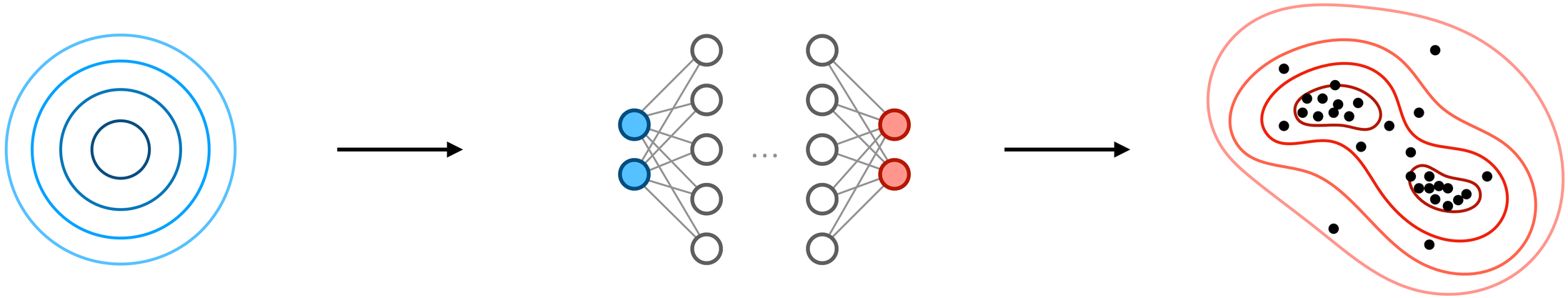
Inference by estimating the likelihood

[e.g. P. Diggle, R. Gratton 1984]



- Compression to summary statistics reduces quality of inference
- Curse of dimensionality: does not scale to more than a few summary statistics

High-dimensional density estimation with normalizing flows



Simple base density

$u \sim \pi(u)$

NN: transformation $x = f(u)$

- one-to-one and invertible
- differentiable
- f^{-1} and $\det \nabla f$ are tractable

Target density is given by

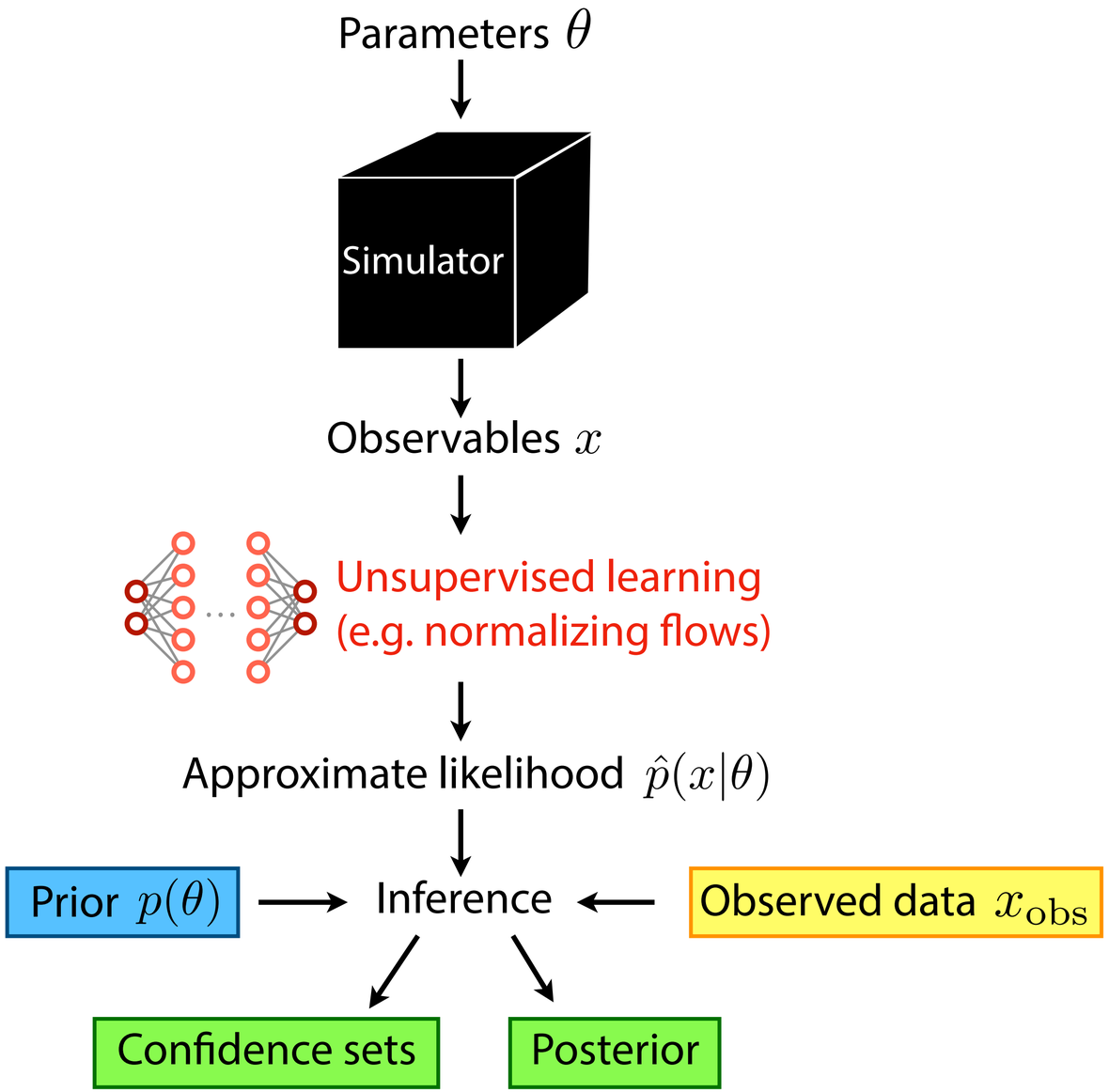
$\hat{p}(x) = \pi(f^{-1}(x)) \, |\det \nabla f|^{-1}$

Train transformation by maximizing $\log \hat{p}(x)$

Transformation can depend on θ to model conditional density $\log \hat{p}(x|\theta)$

[lots of great work recently; see G. Papamakarios et al 1912.02762 for a review]

Inference with neural likelihood estimation

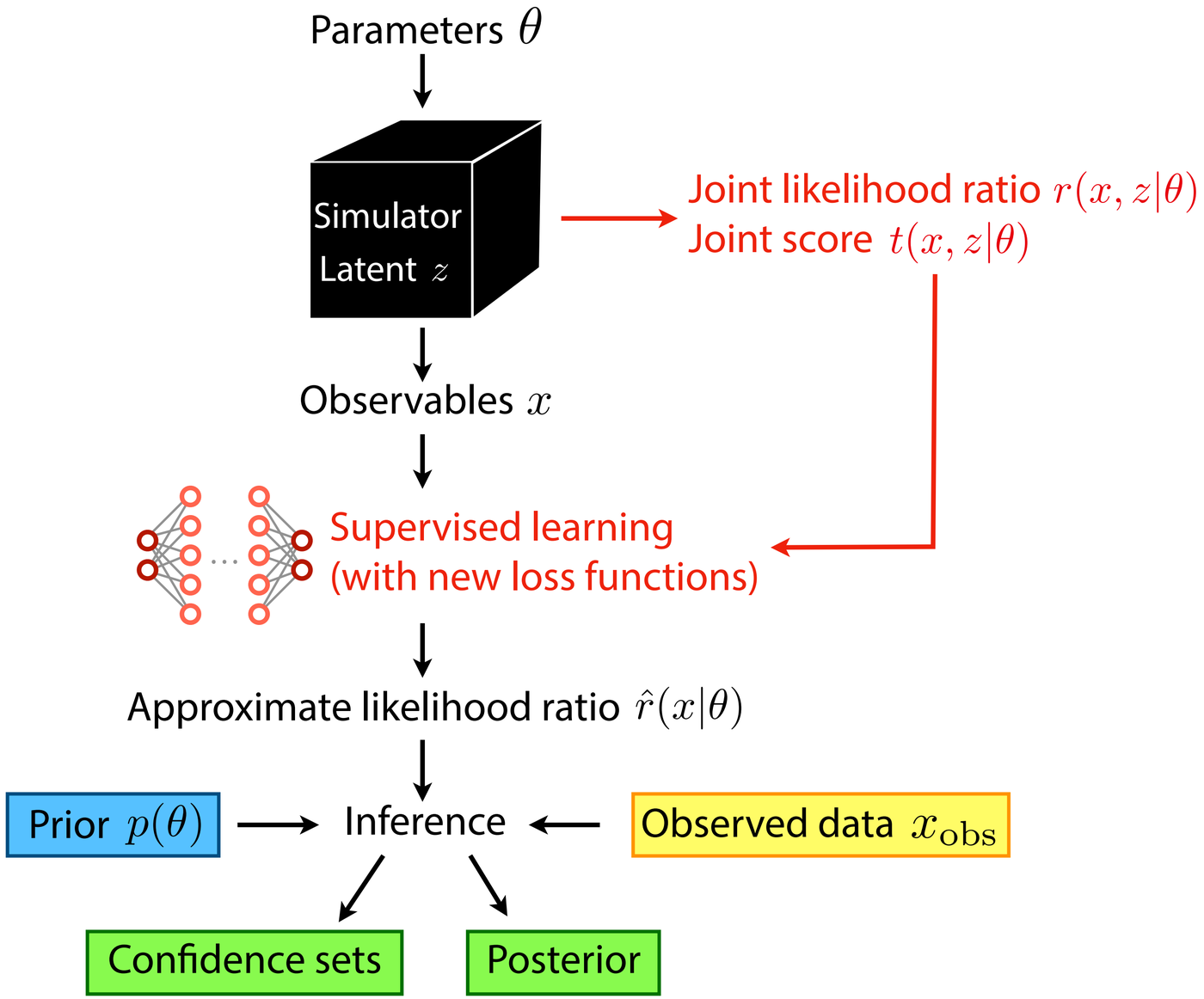


[G. Papamakarios, D. Sterrart, I. Murray 1805.07226;
J.-M. Lueckmann, G. Bassetto, T. Karaletsos, J. Macke 1805.09294]

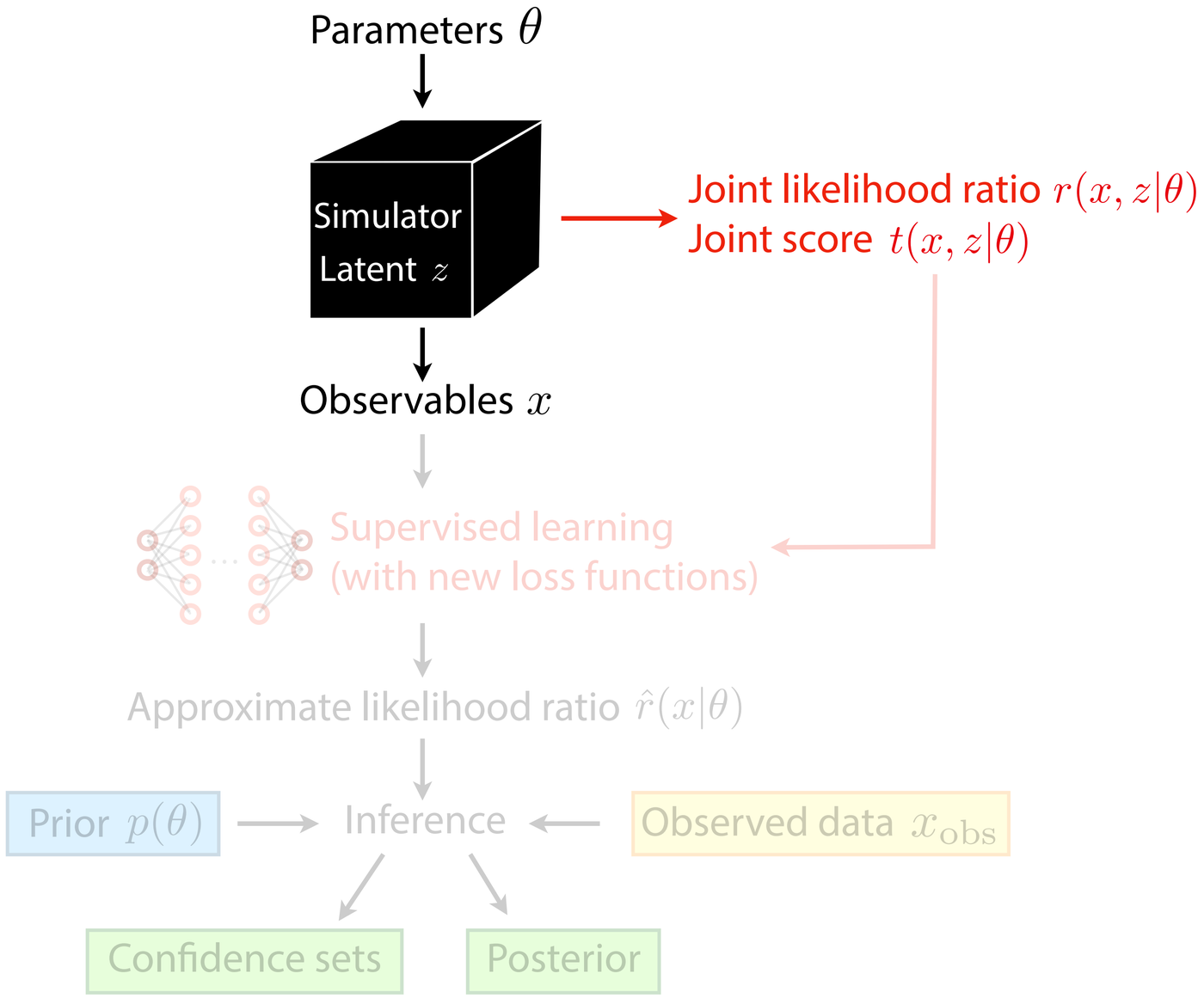
- Conditional neural density estimator (e.g. normalizing flow) as tractable surrogate for simulator likelihood
- Scales well to high-dimensional data (no compression to summary stats necessary)
- Amortized: After upfront simulation + training phase, inference is efficient for new data or prior
- Related alternative: learn posterior $\hat{p}(\theta|x_{\rm obs})$

[G. Papamakarios et al 1605.06376;
J.-M. Lueckmann et al 1711.01861]

Mining gold


Parameters θ
Simulator
Latent z
Joint likelihood ratio $r(x, z|\theta)$
Joint score $t(x, z|\theta)$
Observables x
Supervised learning
(with new loss functions)
Approximate likelihood ratio $\hat{r}(x|\theta)$
Prior $p(\theta)$
Inference
Observed data $x_{\rm obs}$
Confidence sets
Posterior

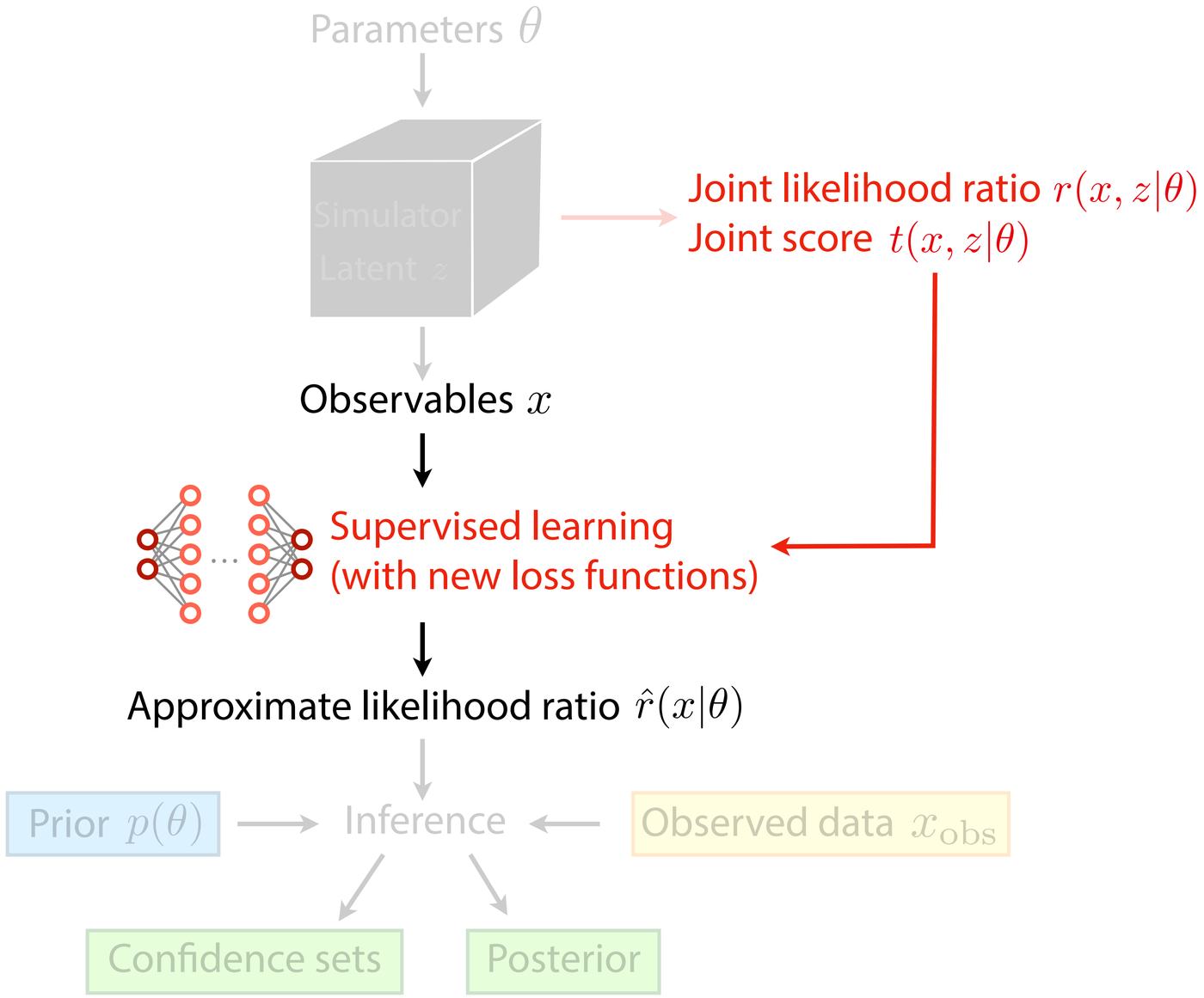
Step 1: Extracting more information from simulations



- For each simulated event, calculate
  - joint likelihood ratio $r(x, z|\theta) = \dfrac{p(x, z|\theta)}{p_{\rm ref}(x, z)}$
  - joint score $t(x, z|\theta) = \nabla_\theta \log p(x, z|\theta)$

(How much more or less likely would this simulated event (fixing all latent variables) be when changing the theory parameters?)

Step 2: Machine learning



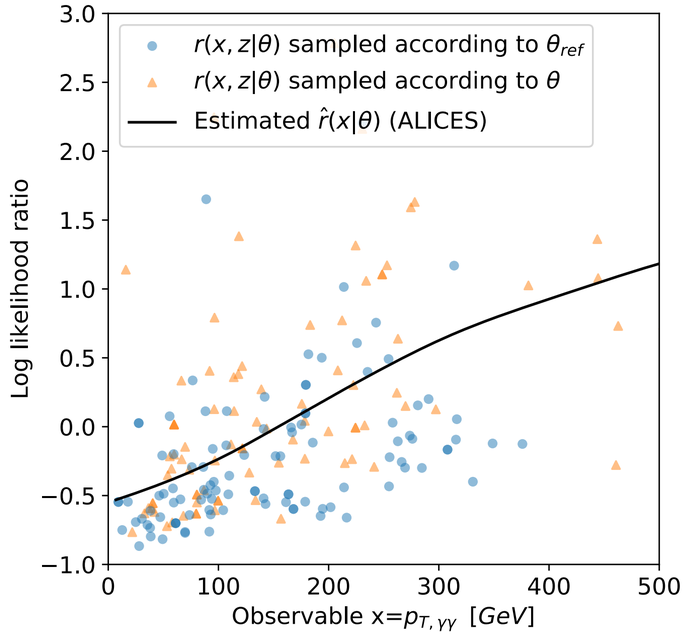
- Train a neural network $g(x, \theta)$ on loss functionals like

$$L[g] = \frac{1}{N} \sum_i |g(x_i, \theta_i) - r(x_i, z_i|\theta_i)|^2$$

- The network will converge to

$$g(x, \theta) \to \arg\min L[g] = r(x|\theta) = \frac{p(x|\theta)}{p_{\rm ref}(x)} \quad !$$

(for sufficient training data, NN capacity, efficient optimization)



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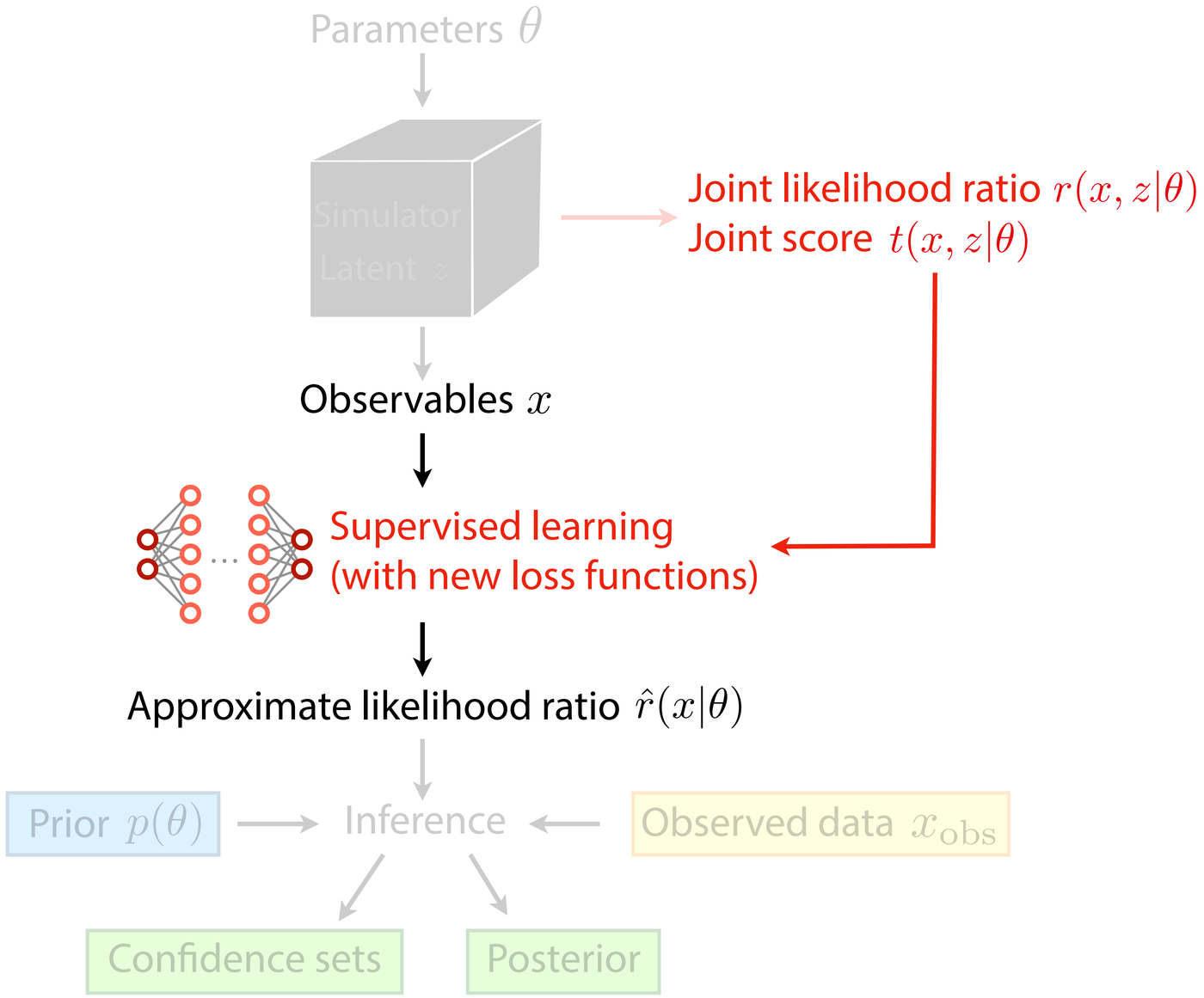

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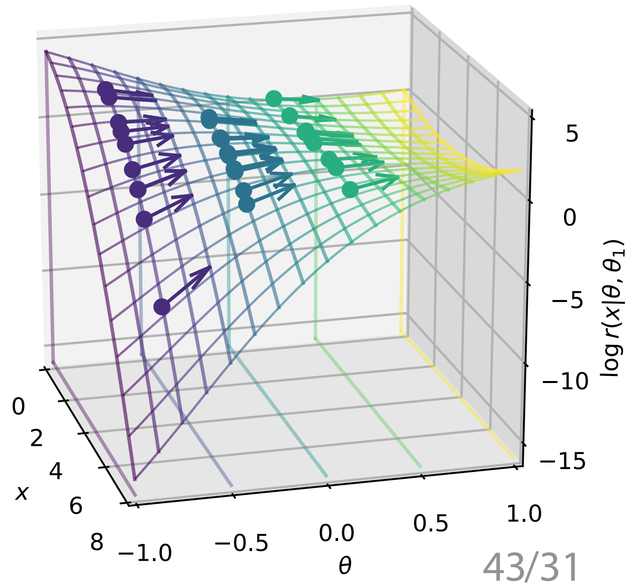
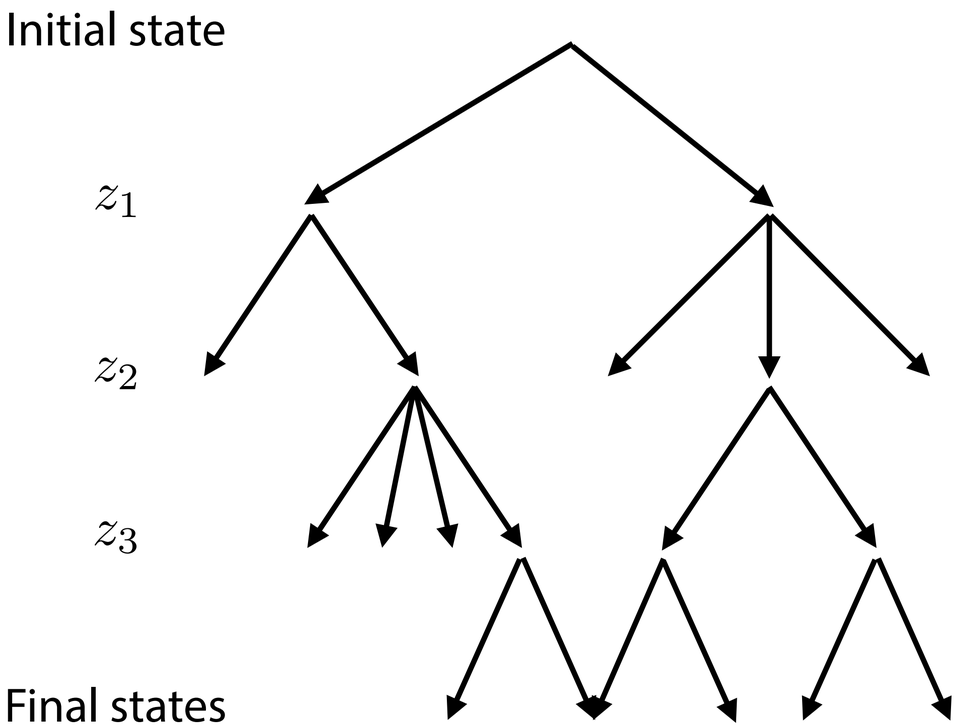
- RASCAL: Joint score adds gradient information ⇒ three orthogonal pieces of information



Mining gold from any simulation

- Computer simulation typically evolve along a tree-like structure of successive random branchings
- The probabilities of each branching $p_i(z_i|z_{i-1},\theta)$ are often clearly defined in the code:

```
if random() > 0.1 + 2.5 * model_parameter:
    do_one_thing()
else:
    do_another_thing()
```



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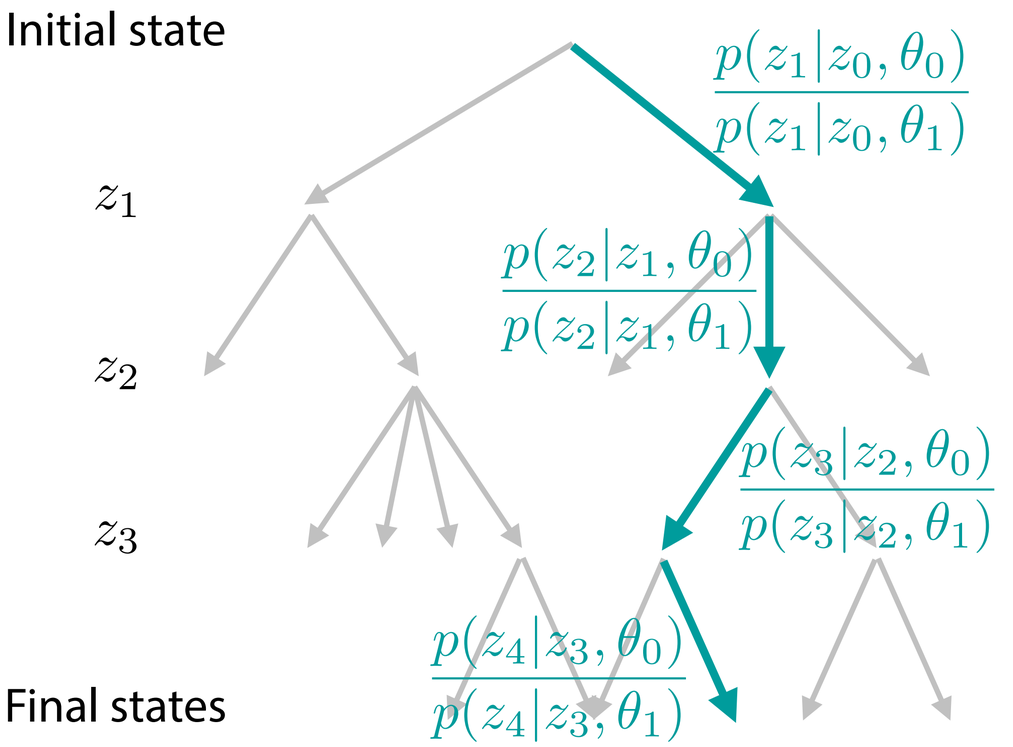
```

- For each run of the simulator, we can calculate the probability of the chosen path for different values of the parameters, and the "joint likelihood ratio":

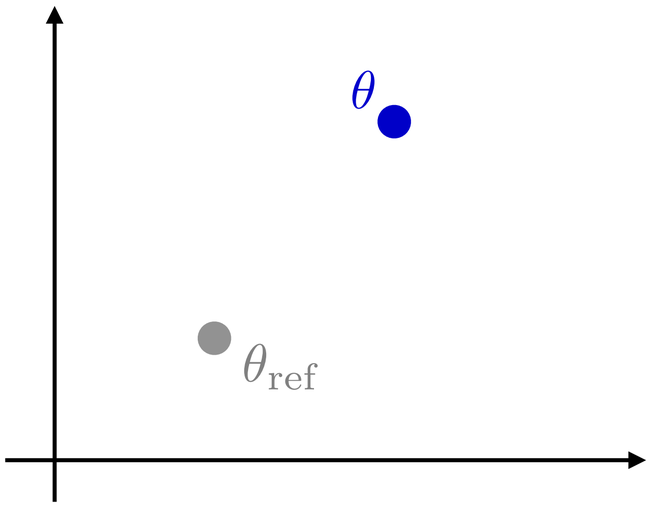
$$r(x,z|\theta_0,\theta_1) = \frac{p(x,z|\theta_0)}{p(x,z|\theta_1)} = \prod_i \frac{p(z_i|z_{i-1},\theta_0)}{p(z_i|z_{i-1},\theta_1)}$$



Frequentist inference

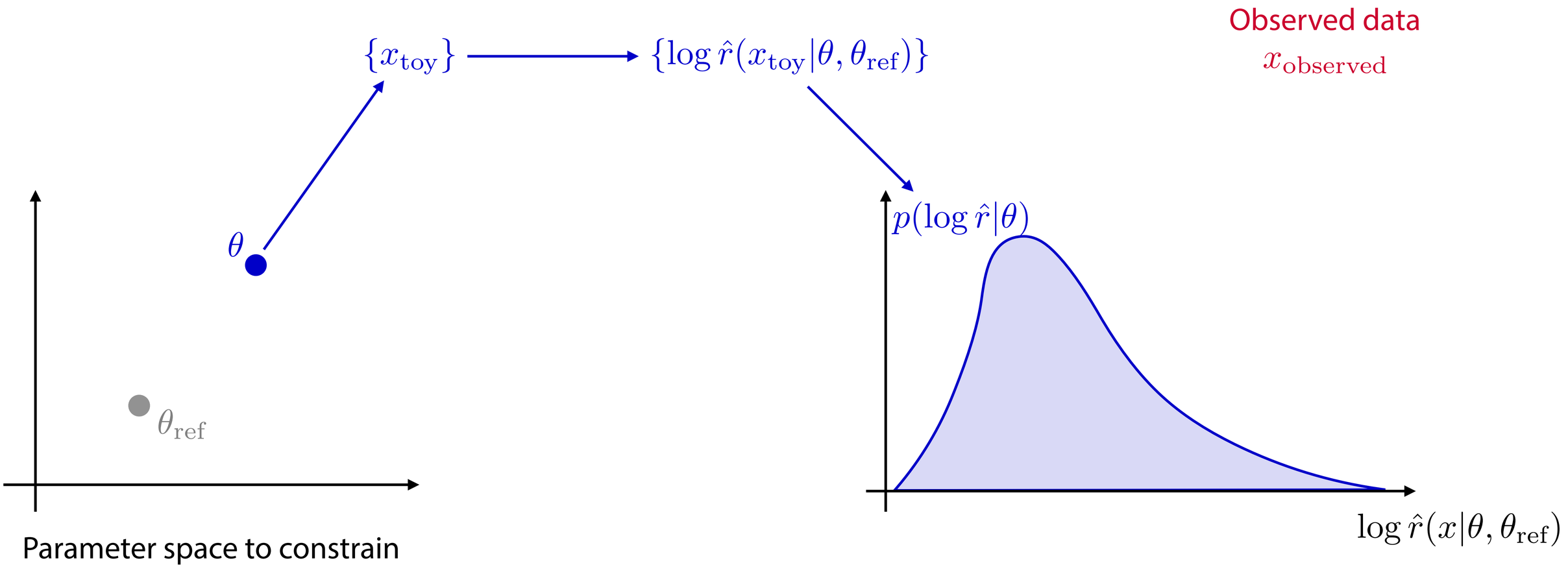
Observed data

x_{observed}

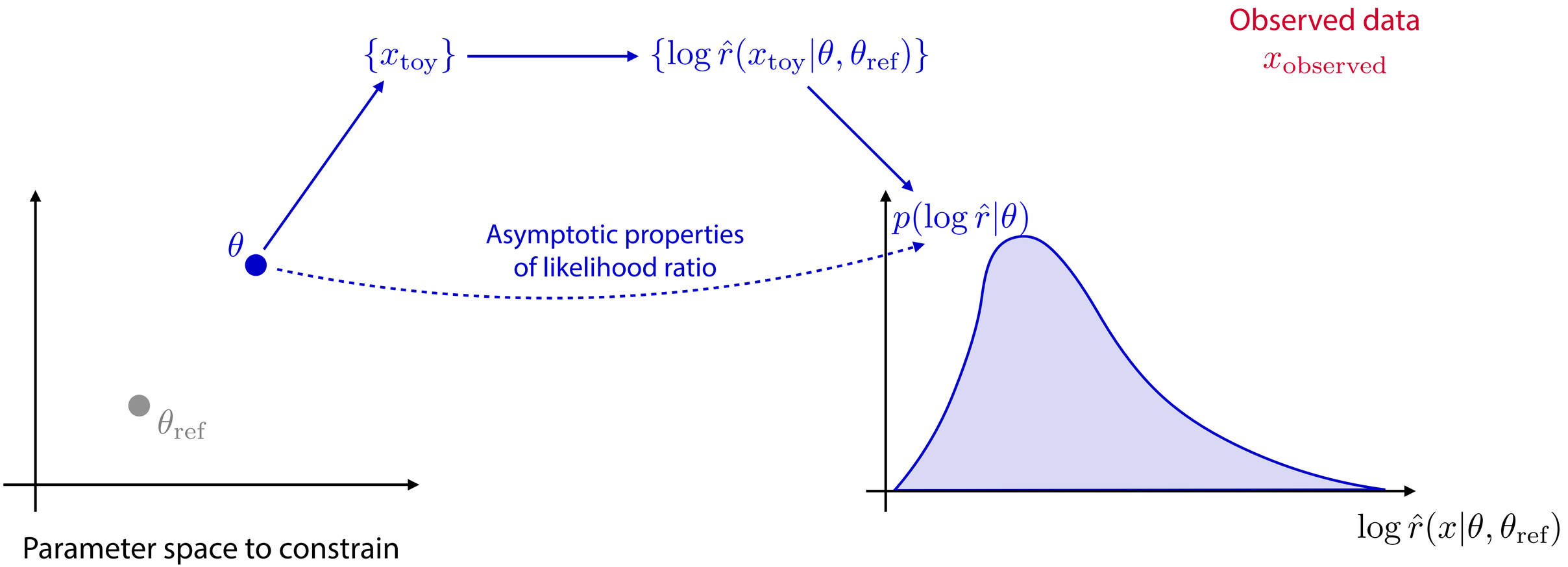


Parameter space to constrain

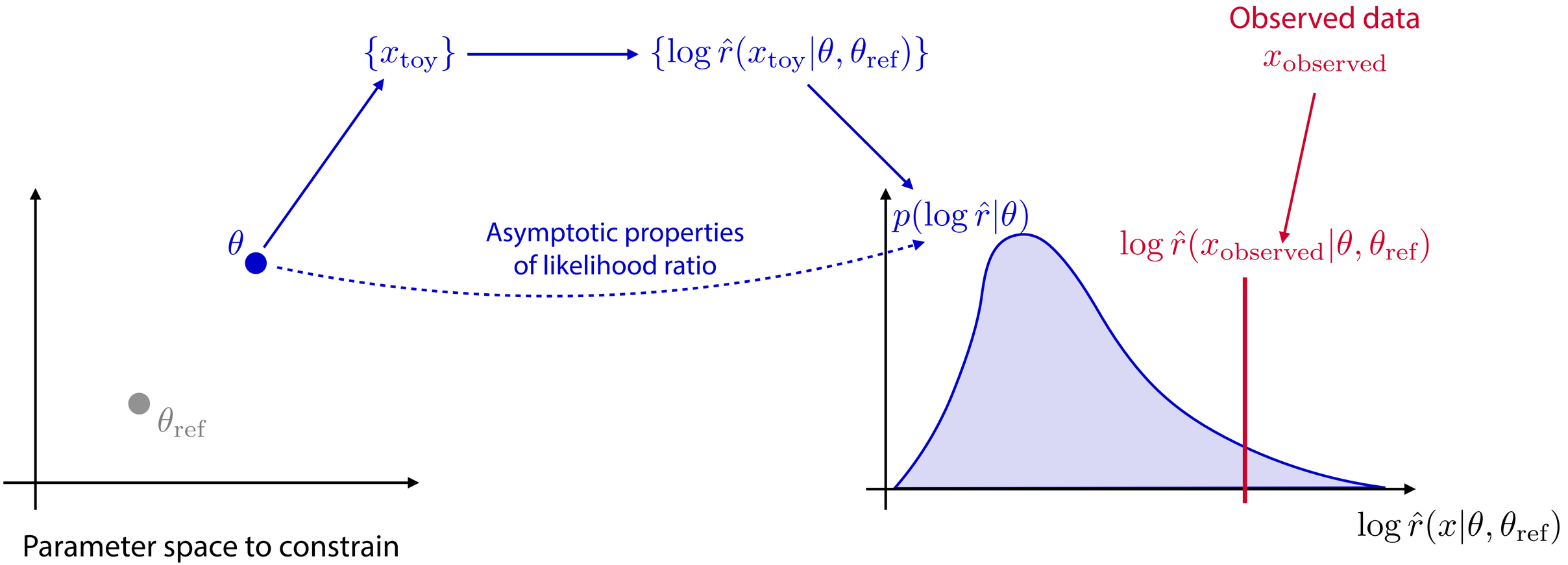
Frequentist inference



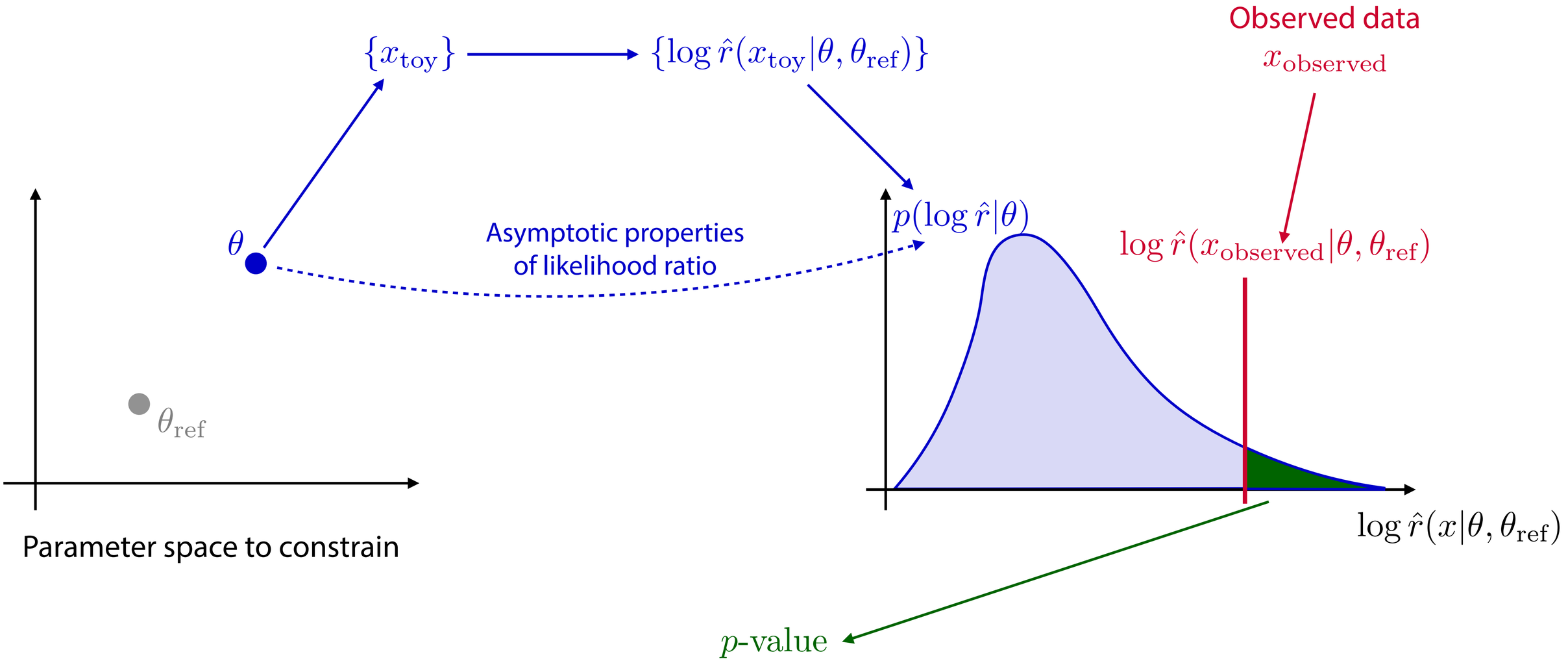
Frequentist inference



Frequentist inference



Frequentist inference



Frequentist inference