PolySwyft

a sequential simulation-based nested sampler

Will Handley
<wh260@cam.ac.uk>

Royal Society University Research Fellow
Astrophysics Group, Cavendish Laboratory, University of Cambridge
Kavli Institute for Cosmology, Cambridge
Gonville & Caius College
willhandley.co.uk/talks

30th October 2024


UNIVERSITY OF CAMBRIDGE

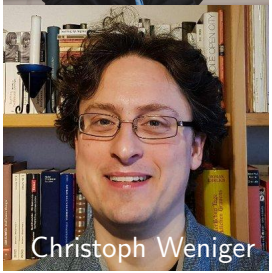


Contents

1. Likelihood- vs Simulation-based inference (LBI vs SBI)
2. Neural Ratio estimation (NRE)
3. Nested sampling (NS)
4. NS+NRE
5. Future prospects

Stems from over a year of discussion, with the majority of the work done by Kilian Scheutwinkel (PhD student).


Kilian Scheutwinkel


Christoph Weniger

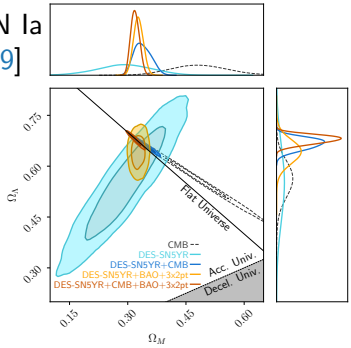
LBI: Likelihood-based inference

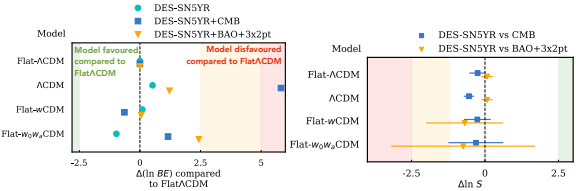
The standard approach if you are fortunate enough to have a likelihood function $P(D|\theta)$:

$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$$

1. Define prior $\pi(\theta)$
   - spend some time being philosophical
2. Sample posterior $\mathcal{P}(\theta|D)$
   - use out-of-the-box MCMC tools such as `emcee` or `MultiNest`
   - make some triangle plots
3. Optionally compute evidence $\mathcal{Z}(D)$
   - e.g. nested sampling or parallel tempering
   - do some model comparison (i.e. science)
   - talk about tensions

DES Y5 SN Ia [2401.02929]





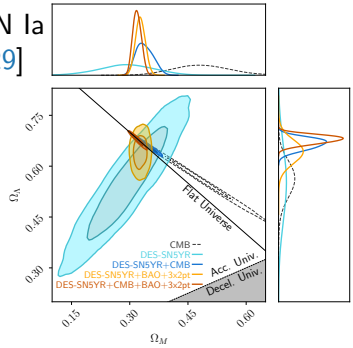
LBI: Likelihood-based inference

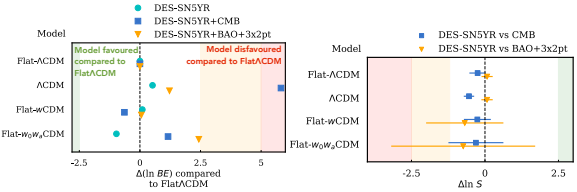
The standard approach if you are fortunate enough to have a likelihood function $P(D|\theta)$:

$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)} \qquad \text{Posterior} = \frac{\text{Likelihood} \times \text{Prior}}{\text{Evidence}}$$

1. Define prior $\pi(\theta)$
   - spend some time being philosophical
2. Sample posterior $\mathcal{P}(\theta|D)$
   - use out-of-the-box MCMC tools such as `emcee` or `MultiNest`
   - make some triangle plots
3. Optionally compute evidence $\mathcal{Z}(D)$
   - e.g. nested sampling or parallel tempering
   - do some model comparison (i.e. science)
   - talk about tensions

DES Y5 SN Ia [2401.02929]





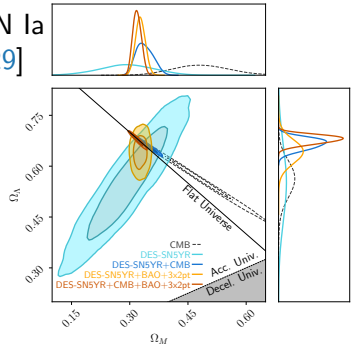
LBI: Likelihood-based inference

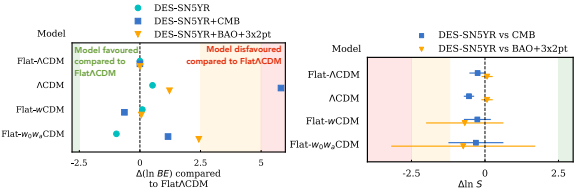
The standard approach if you are fortunate enough to have a likelihood function $\mathcal{L}(D|\theta)$:

$$\mathcal{P}(\theta|D) = \frac{\mathcal{L}(D|\theta)\pi(\theta)}{\mathcal{Z}(D)} \qquad \text{Posterior} = \frac{\text{Likelihood} \times \text{Prior}}{\text{Evidence}}$$

1. Define prior $\pi(\theta)$
   - spend some time being philosophical
2. Sample posterior $\mathcal{P}(\theta|D)$
   - use out-of-the-box MCMC tools such as `emcee` or `MultiNest`
   - make some triangle plots
3. Optionally compute evidence $\mathcal{Z}(D)$
   - e.g. nested sampling or parallel tempering
   - do some model comparison (i.e. science)
   - talk about tensions

DES Y5 SN Ia [2401.02929]





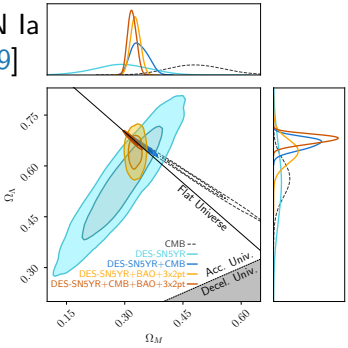
LBI: Likelihood-based inference

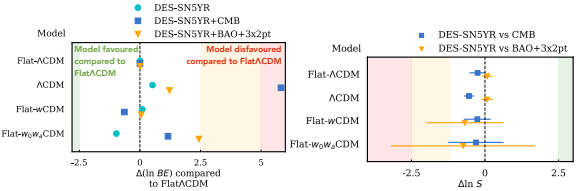
The standard approach if you are fortunate enough to have a likelihood function $\mathcal{L}(D|\theta)$:

$$P(\theta|D)P(D) = P(\theta, D) = P(D|\theta)P(\theta),$$

1. Define prior $\pi(\theta)$
   - spend some time being philosophical
2. Sample posterior $\mathcal{P}(\theta|D)$
   - use out-of-the-box MCMC tools such as `emcee` or `MultiNest`
   - make some triangle plots
3. Optionally compute evidence $\mathcal{Z}(D)$
   - e.g. nested sampling or parallel tempering
   - do some model comparison (i.e. science)
   - talk about tensions

DES Y5 SN Ia [2401.02929]





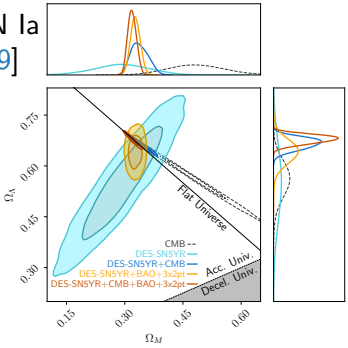
LBI: Likelihood-based inference

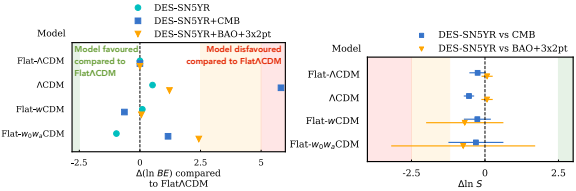
The standard approach if you are fortunate enough to have a likelihood function $\mathcal{L}(D|\theta)$:

$$\mathcal{P} \times \mathcal{Z} = \mathcal{J} = \mathcal{L} \times \pi, \qquad \text{Joint} = \mathcal{J} = P(\theta, D)$$

1. Define prior $\pi(\theta)$
   - spend some time being philosophical
2. Sample posterior $\mathcal{P}(\theta|D)$
   - use out-of-the-box MCMC tools such as `emcee` or `MultiNest`
   - make some triangle plots
3. Optionally compute evidence $\mathcal{Z}(D)$
   - e.g. nested sampling or parallel tempering
   - do some model comparison (i.e. science)
   - talk about tensions

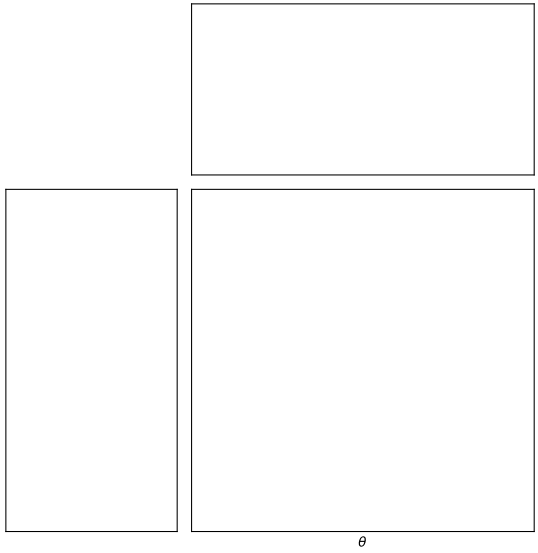
DES Y5 SN Ia [2401.02929]





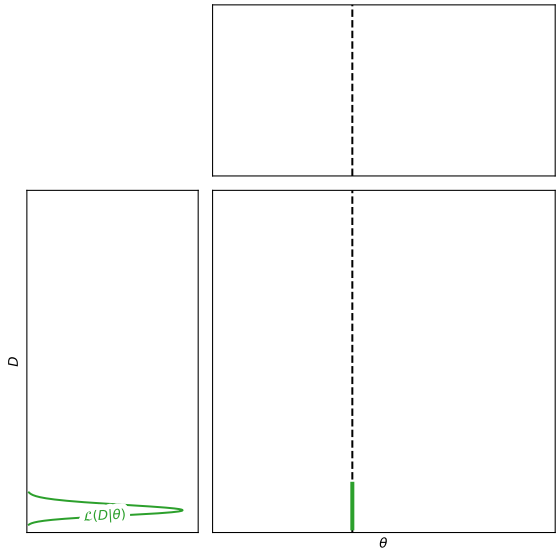
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$
  the "probability of everything".
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



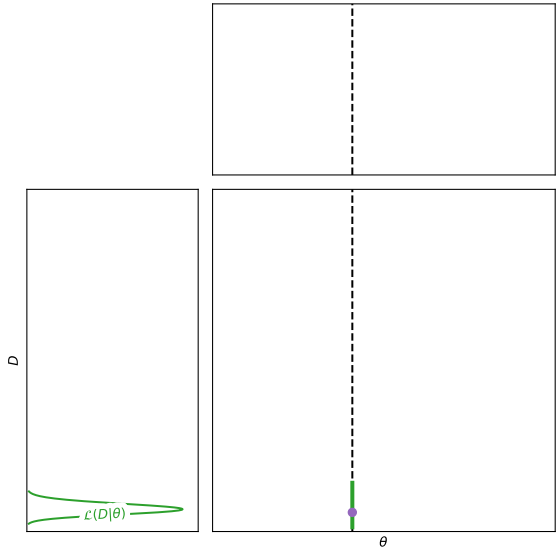
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$
  the "probability of everything".
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



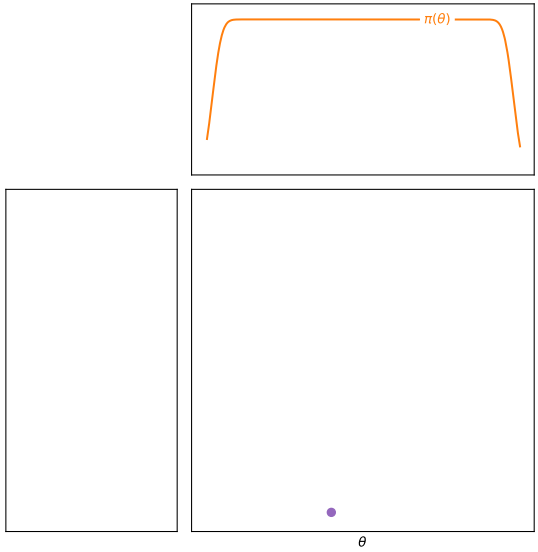
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$
  the "probability of everything".
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



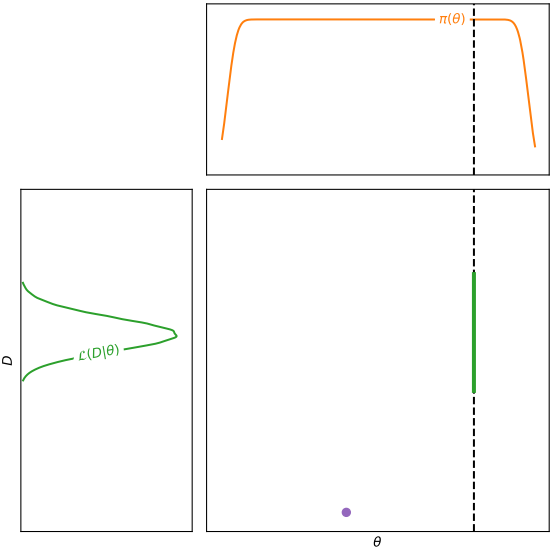
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$ *the "probability of everything".*
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



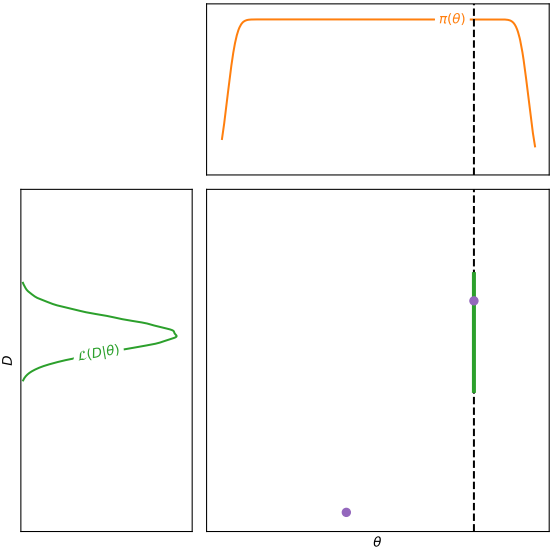
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$
  the "probability of everything".
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



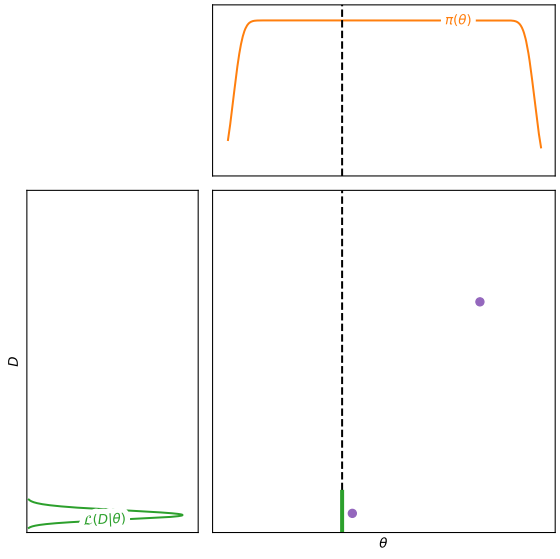
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$
  the "probability of everything".
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



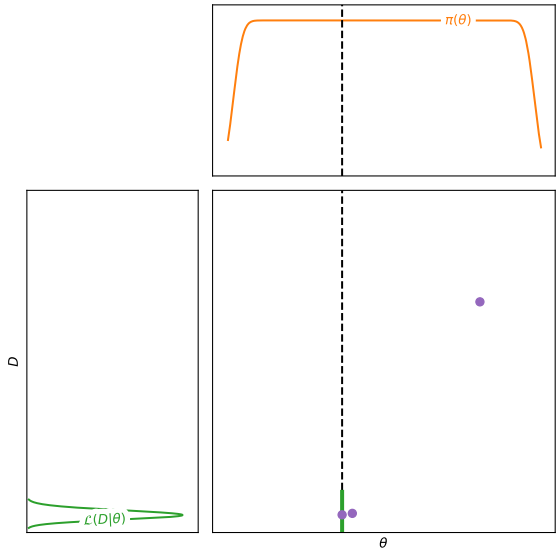
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$
  the "probability of everything".
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



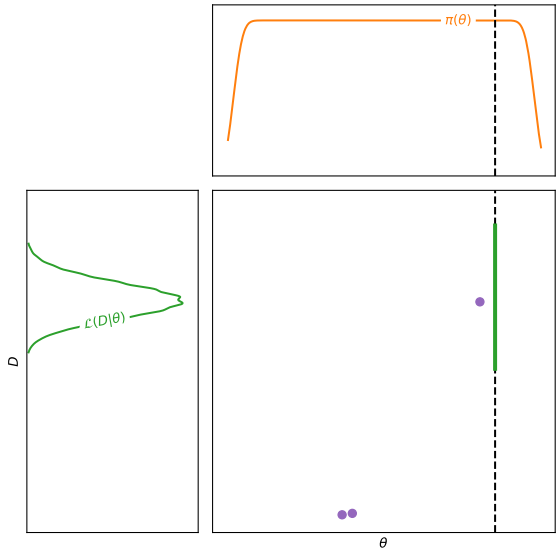
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$
  the "probability of everything".
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



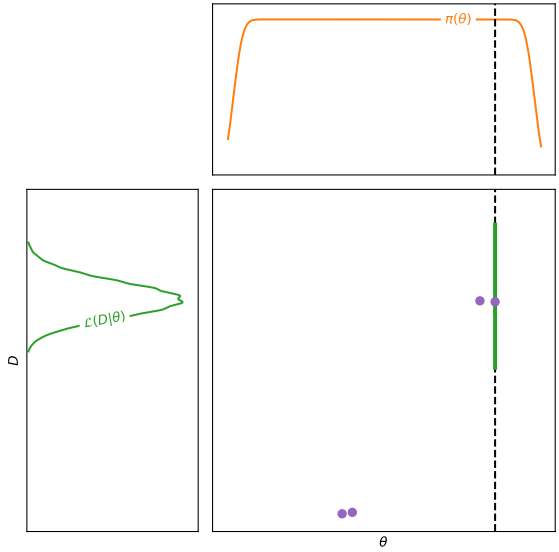
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$
  the "probability of everything".
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



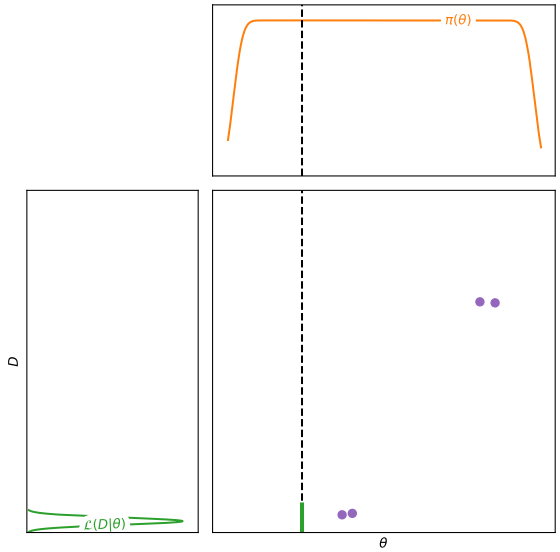
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$ *the "probability of everything".*
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



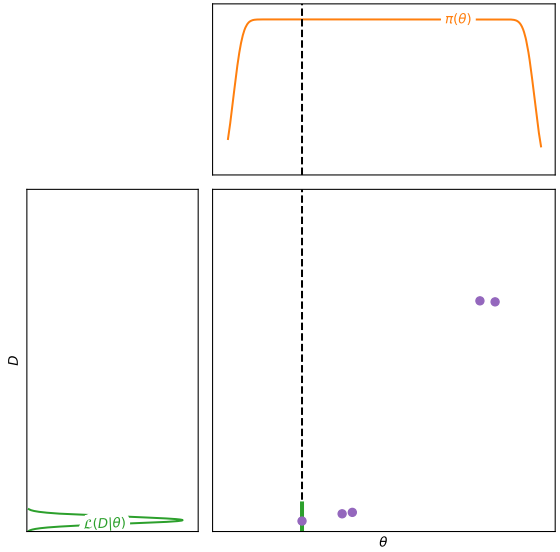
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$ *the "probability of everything".*
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



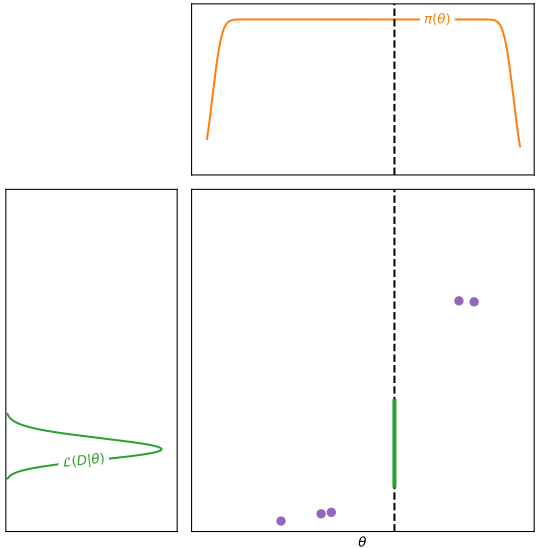
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$ *the "probability of everything".*
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



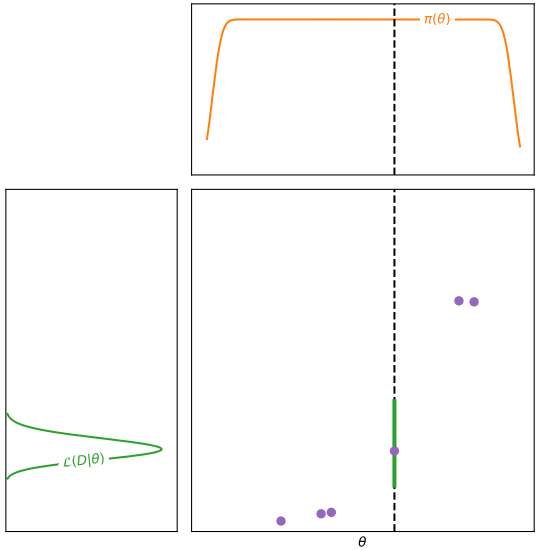
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$ *the "probability of everything".*
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



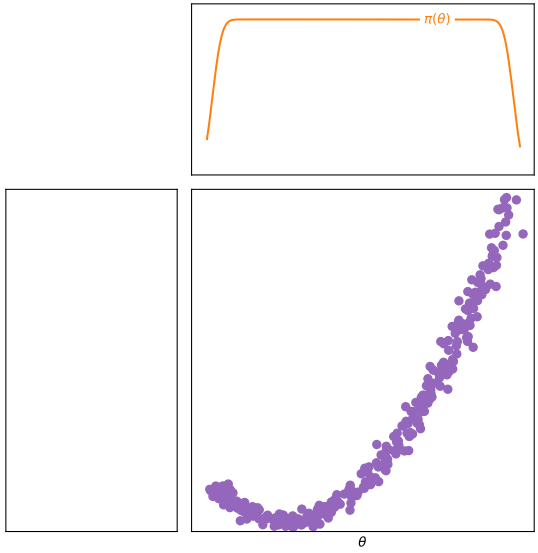
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$
  the "probability of everything".
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



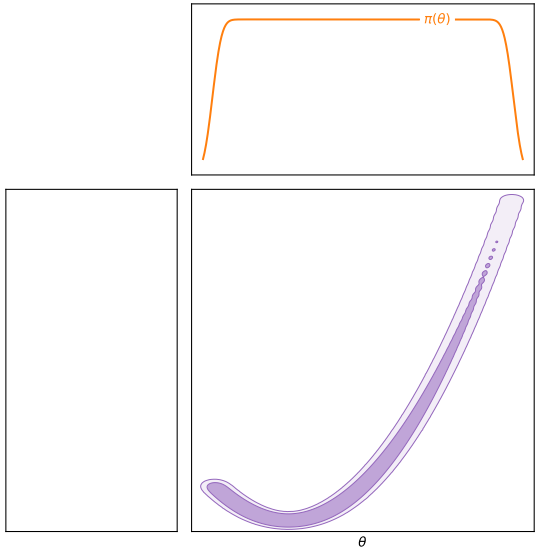
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$ *the "probability of everything".*
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



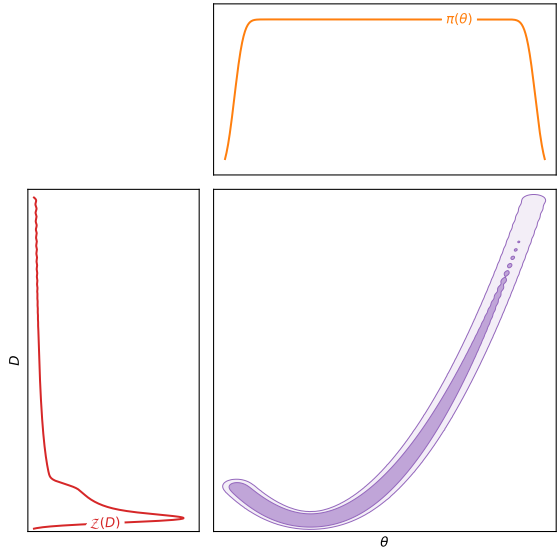
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$
  the "probability of everything".
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



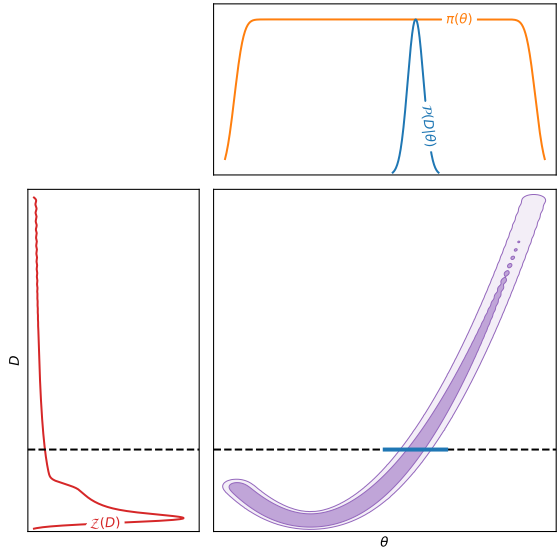
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$
  the "probability of everything".
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



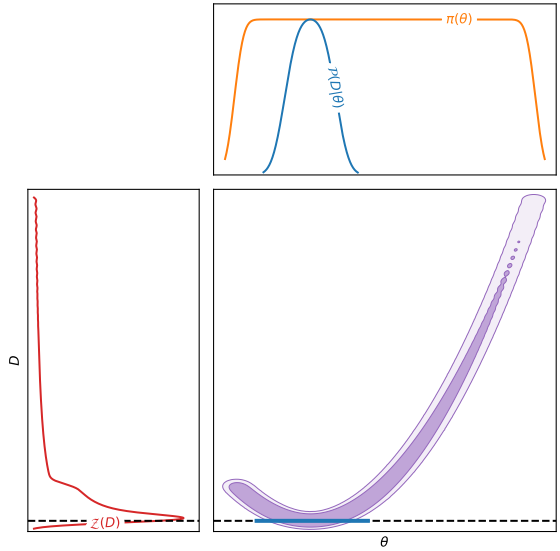
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$ *the "probability of everything".*
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



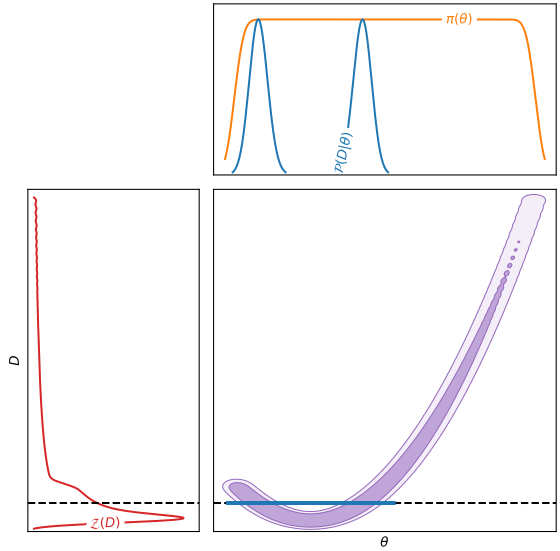
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$
  the "probability of everything".
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



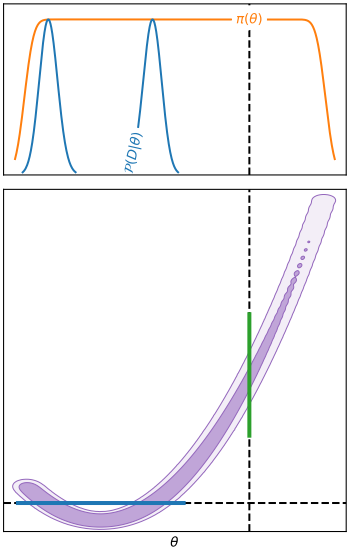
SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$ *the "probability of everything".*
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \to D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$
  the "probability of everything".
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



Why SBI?

SBI is useful because:

1. If you don't have a likelihood, you can still do inference
   - This is the usual case beyond CMB cosmology
2. Faster than LBI
   - emulation – also applies to LBI in principle
3. No need to pragmatically encode fiducial cosmologies
   - Covariance computation implicitly encoded in simulations
   - Highly relevant for disentangling tensions & systematics
4. Equips AI/ML with Bayesian interpretability
5. Lower barrier to entry than LBI
   - Much easier to forward model a systematic
   - Emerging set of plug-and-play packages
   - For this reason alone, it will come to dominate scientific inference

github.com/sbi-dev

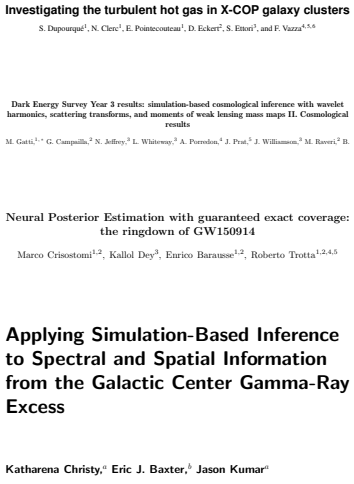
github.com/undark-lab/swyft

github.com/florent-leclercq/pyselfi

github.com/justinalsing/pydelfi

Why aren't we currently using SBI in cosmology?

- Short answer: we are!
  - Mostly for weak lensing
  - 2024 has been the year it has started to be applied to real data.
- Longer answer: SBI requires mock data generation code
- Most data analysis codes were built before the generative paradigm.
- It's still a lot of work to upgrade cosmological likelihoods to be able to do this (e.g. `plik` & `camspec`).



Investigating the turbulent hot gas in X-COP galaxy clusters

S. Dupourque[1], N. Clerc[1], E. Pointecouteau[1], D. Eckert[2], S. Ettori[3], and F. Vazza[4,5,6]

Dark Energy Survey Year 3 results: simulation-based cosmological inference with wavelet harmonics, scattering transforms, and moments of weak lensing mass maps II. Cosmological results

M. Gatti,[1,*] G. Campailla,[2] N. Jeffrey,[3] L. Whiteway,[3] A. Porredon,[4] J. Prat,[5] J. Williamson,[3] M. Raveri,[2] B.

Neural Posterior Estimation with guaranteed exact coverage: the ringdown of GW150914

Marco Crisostomi[1,2], Kallol Dey[3], Enrico Barausse[1,2], Roberto Trotta[1,2,4,5]

Applying Simulation-Based Inference to Spectral and Spatial Information from the Galactic Center Gamma-Ray Excess

Katharena Christy,[a] Eric J. Baxter,[b] Jason Kumar[a]

KiDS-1000 and DES-Y1 combined: Cosmology from peak count statistics

Joachim Harnois-Déraps[1]*, Sven Heydenreich[2], Benjamin Giblin[3], Nicolas Martinet[4], Tilman Tröster[3], Marika Asgari[1,6,7], Pierre Burger[8,9,10],Tiago Castro[11,12,13,14], Klaus Dolag[15], Catherine Heymans[3,16], Hendrik Hildebrandt[16], Benjamin Joachimi[17] & Angus H. Wright[16]

KiDS-SBI: Simulation-Based Inference Analysis of KiDS-1000 Cosmic Shear

Maximilian von Wietersheim-Kramsta[1,2,3], Kiyam Lin[1], Nicolas Tessore[1], Benjamin Joachimi[1], Arthur Loureiro[4,5], Robert Reischke[6,7], and Angus H. Wright[7]

Simulation-based inference of deep fields: galaxy population model and redshift distributions

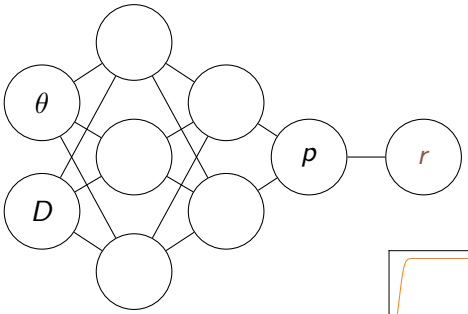
Beatrice Moser,[a,1] Tomasz Kacprzak,[a,b] Silvan Fischbacher,[a] Alexandre Refregier,[a] Dominic Grimm,[a] Luca Tortorelli[c]

SimBIG: Cosmological Constraints using Simulation-Based Inference of Galaxy Clustering with Marked Power Spectra

Elena Massara, Chang'Hoon Hahn, Michael Eickenberg, Shirley Ho, Jiamin Hou, Pablo Lemos, Chirag Modi, Azadeh Moradinezhad Dizgah, Liam Parker, and Bruno Régaldo-Saint Blancard

Neural Ratio Estimation

- SBI flavours: `github.com/sbi-dev/sbi`
  - NPE Neural posterior estimation
  - NLE Neural likelihood estimation
  - NJE Neural joint estimation
  - NRE Neural ratio estimation
- NRE recap:
  1. Generate joint samples $(\theta, D) \sim \mathcal{J}$
     - *straightforward if you have a simulator:* $\theta \sim \pi(\cdot)$, $D \sim \mathcal{L}(\cdot|\theta)$
  2. Generate separated samples $\theta \sim \pi$, $D \sim \mathcal{Z}$
     - *aside: can shortcut step 2 by scrambling the* (θ, D) *pairings from step 1*
  3. Train probabilistic classifier p to distinguish whether (θ, D) came from $\mathcal{J}$ or $\pi \times \mathcal{Z}$.
  4. $\frac{p}{1-p} = r = \frac{P(\theta,D)}{P(\theta)P(D)} = \frac{\mathcal{J}}{\pi \times \mathcal{Z}} = \frac{\mathcal{L}}{\mathcal{Z}} = \frac{\mathcal{P}}{\pi}$.
  5. Use ratio r for parameter estimation $\mathcal{P} = r \times \pi$



Neural Ratio Estimation

- SBI flavours: `github.com/sbi-dev/sbi`
  - NPE Neural posterior estimation
  - NLE Neural likelihood estimation
  - NJE Neural joint estimation
  - NRE Neural ratio estimation
- NRE recap:
  1. Generate joint samples $(\theta, D) \sim \mathcal{J}$
     - *straightforward if you have a simulator:* $\theta \sim \pi(\cdot)$, $D \sim \mathcal{L}(\cdot|\theta)$
  2. Generate separated samples $\theta \sim \pi$, $D \sim \mathcal{Z}$
     - *aside: can shortcut step 2 by scrambling the* (θ, D) *pairings from step 1*
  3. Train probabilistic classifier p to distinguish whether (θ, D) came from $\mathcal{J}$ or $\pi \times \mathcal{Z}$.
  4. $\frac{p}{1-p} = r = \frac{P(\theta,D)}{P(\theta)P(D)} = \frac{\mathcal{J}}{\pi \times \mathcal{Z}} = \frac{\mathcal{L}}{\mathcal{Z}} = \frac{\mathcal{P}}{\pi}$.
  5. Use ratio r for parameter estimation $\mathcal{P} = r \times \pi$

Bayesian proof

- Let $M_{\mathcal{J}}$: $(\theta, D) \sim \mathcal{J}$, $M_{\pi\mathcal{Z}}$: $(\theta, D) \sim \pi \times \mathcal{Z}$
- Classifier gives $p(\theta, D) = P(M_{\mathcal{J}}|\theta, D) = 1 - P(M_{\pi\mathcal{Z}}|\theta, D)$
- Bayes theorem then shows $\frac{p}{1-p} = \frac{P(M_{\mathcal{J}}|\theta,D)}{P(M_{\pi\mathcal{Z}}|\theta,D)} = \frac{P(\theta,D|M_{\mathcal{J}})P(M_{\mathcal{J}})}{P(\theta,D|M_{\pi\mathcal{Z}})P(M_{\pi\mathcal{Z}})} = \frac{\mathcal{J}}{\pi\mathcal{Z}}$, where we have assumed
  - $P(M_{\mathcal{J}}) = P(M_{\pi\mathcal{Z}})$,

  and by definition
  - $\mathcal{J}(\theta, D) = P(\theta, D|M_{\mathcal{J}})$
  - $\pi(\theta)\mathcal{Z}(D) = P(\theta, D|M_{\pi\mathcal{Z}})$.

Neural Ratio Estimation

- SBI flavours: github.com/sbi-dev/sbi
  - NPE Neural posterior estimation
  - NLE Neural likelihood estimation
  - NJE Neural joint estimation
  - NRE Neural ratio estimation
- NRE recap:
  1. Generate joint samples $(\theta, D) \sim \mathcal{J}$
     - *straightforward if you have a simulator:* $\theta \sim \pi(\cdot)$, $D \sim \mathcal{L}(\cdot|\theta)$
  2. Generate separated samples $\theta \sim \pi$, $D \sim \mathcal{Z}$
     - *aside: can shortcut step 2 by scrambling the* (θ, D) *pairings from step 1*
  3. Train probabilistic classifier p to distinguish whether (θ, D) came from $\mathcal{J}$ or $\pi \times \mathcal{Z}$.
  4. $\frac{p}{1-p} = r = \frac{P(\theta,D)}{P(\theta)P(D)} = \frac{\mathcal{J}}{\pi \times \mathcal{Z}} = \frac{\mathcal{L}}{\mathcal{Z}} = \frac{\mathcal{P}}{\pi}$.
  5. Use ratio r for parameter estimation $\mathcal{P} = r \times \pi$

Why I like NRE

- The link between classification and inference is profound.
- Density estimation is hard – Dimensionless r divides out the hard-to-calculate parts.

Why I don't like NRE

- Practical implementations require marginalisation [2107.01214], or autoregression [2308.08597].
- Model comparison and parameter estimation are separate [2305.11241].

TMNRE: Truncated Marginal Neural Ratio Estimation

swyft: github.com/undark-lab/swyft

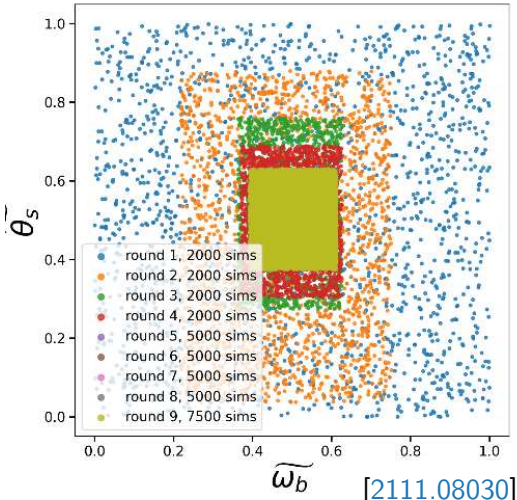
- Two tricks for practical NRE:

Marginalisation

- Only consider one or two parameters at a time.
- Fine if your goal is to produce triangle plots.
- Problematic if information is contained jointly in more than two parameters.

Truncation

- focus parameters θ on a subset of the prior which reproduces observed data D_{obs}
- region is somewhat arbitrary (usually a box)
- not amortised, sounds a bit like ABC

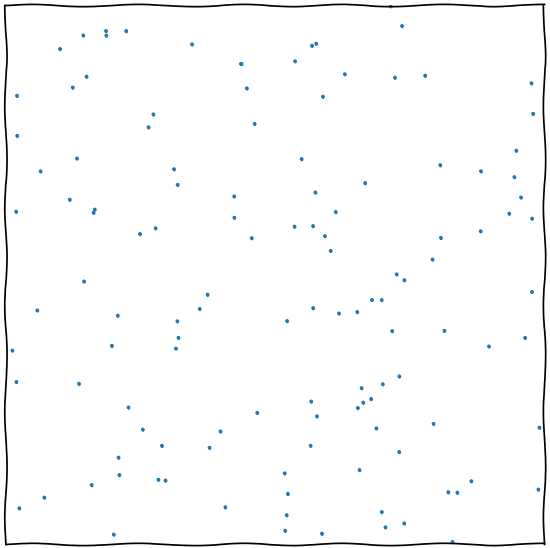


[2111.08030]

Nested sampling: numerical Lebesgue integration

0. Start with N random samples over the space.
i. Delete outermost sample, and replace with a new random one at higher integrand value.

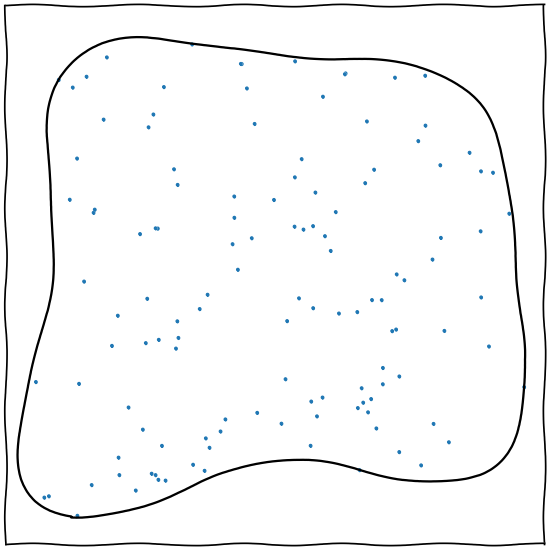
- The "live points" steadily contract around the peak(s) of the function.
- Discarded "dead points" can be weighted to form posterior, prior, or anything in between.
- Estimates the **density of states** and calculates evidences & partition functions.
- The evolving ensemble of live points allows:
  - implementations to self-tune,
  - exploration of multimodal functions,
  - global and local optimisation.



Nested sampling: numerical Lebesgue integration

0. Start with N random samples over the space.
i. Delete outermost sample, and replace with a new random one at higher integrand value.

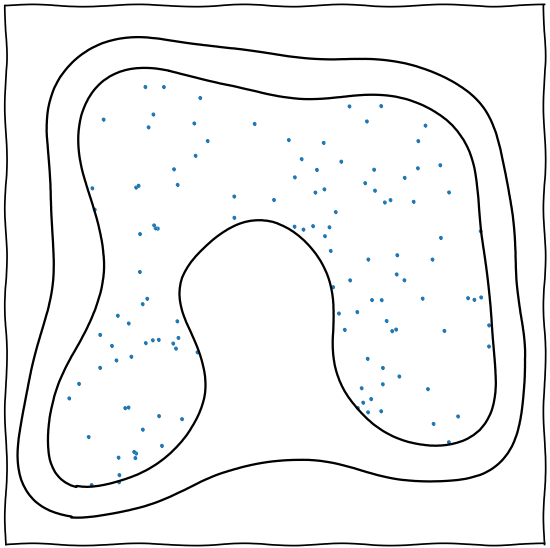
- The "live points" steadily contract around the peak(s) of the function.
- Discarded "dead points" can be weighted to form posterior, prior, or anything in between.
- Estimates the **density of states** and calculates evidences & partition functions.
- The evolving ensemble of live points allows:
  - implementations to self-tune,
  - exploration of multimodal functions,
  - global and local optimisation.



Nested sampling: numerical Lebesgue integration

0. Start with N random samples over the space.
i. Delete outermost sample, and replace with a new random one at higher integrand value.

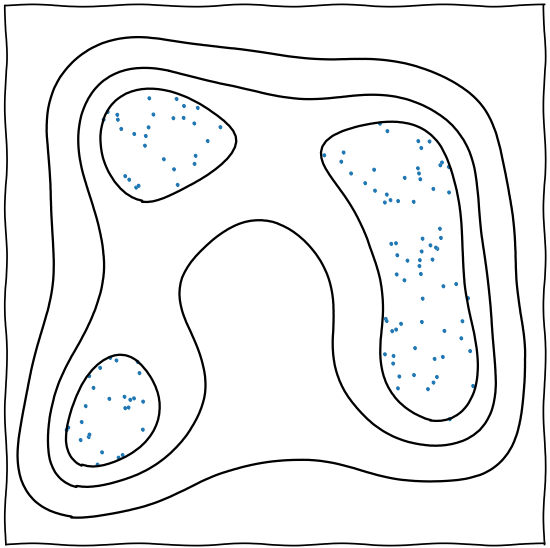
- The "live points" steadily contract around the peak(s) of the function.
- Discarded "dead points" can be weighted to form posterior, prior, or anything in between.
- Estimates the **density of states** and calculates evidences & partition functions.
- The evolving ensemble of live points allows:
  - implementations to self-tune,
  - exploration of multimodal functions,
  - global and local optimisation.



Nested sampling: numerical Lebesgue integration

0. Start with N random samples over the space.
i. Delete outermost sample, and replace with a new random one at higher integrand value.

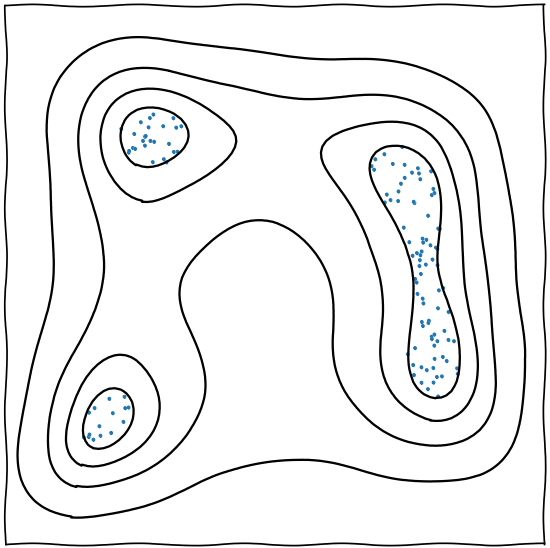
- The "live points" steadily contract around the peak(s) of the function.
- Discarded "dead points" can be weighted to form posterior, prior, or anything in between.
- Estimates the **density of states** and calculates evidences & partition functions.
- The evolving ensemble of live points allows:
  - implementations to self-tune,
  - exploration of multimodal functions,
  - global and local optimisation.



Nested sampling: numerical Lebesgue integration

0. Start with N random samples over the space.
i. Delete outermost sample, and replace with a new random one at higher integrand value.

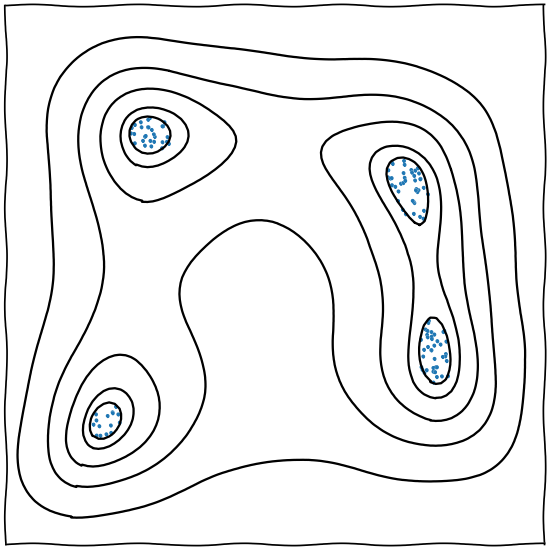
- The "live points" steadily contract around the peak(s) of the function.
- Discarded "dead points" can be weighted to form posterior, prior, or anything in between.
- Estimates the **density of states** and calculates evidences & partition functions.
- The evolving ensemble of live points allows:
  - implementations to self-tune,
  - exploration of multimodal functions,
  - global and local optimisation.



Nested sampling: numerical Lebesgue integration

0. Start with N random samples over the space.
i. Delete outermost sample, and replace with a new random one at higher integrand value.

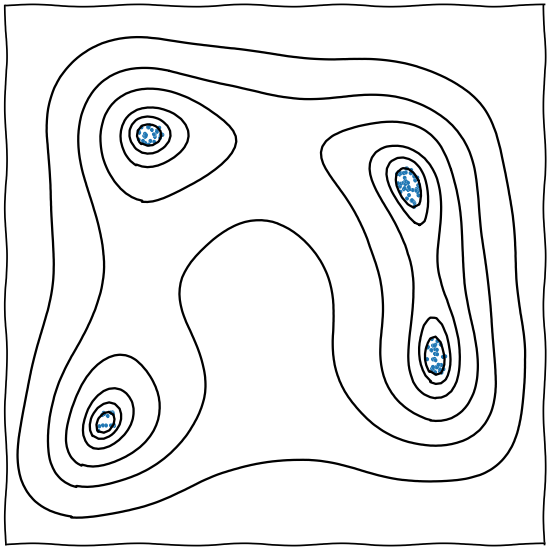
- The "live points" steadily contract around the peak(s) of the function.
- Discarded "dead points" can be weighted to form posterior, prior, or anything in between.
- Estimates the **density of states** and calculates evidences & partition functions.
- The evolving ensemble of live points allows:
  - implementations to self-tune,
  - exploration of multimodal functions,
  - global and local optimisation.



Nested sampling: numerical Lebesgue integration

0. Start with N random samples over the space.
i. Delete outermost sample, and replace with a new random one at higher integrand value.

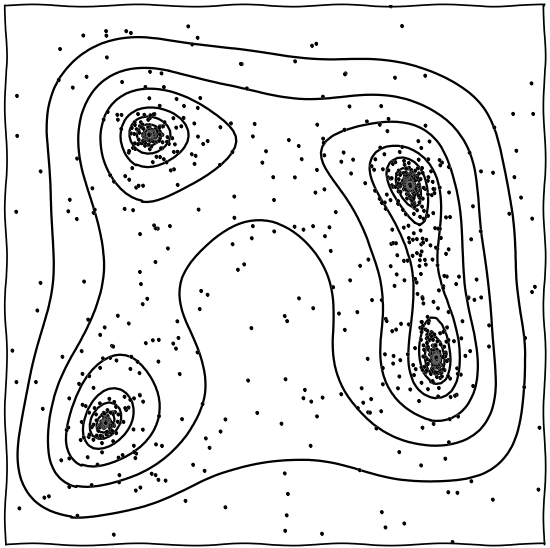
- The "live points" steadily contract around the peak(s) of the function.
- Discarded "dead points" can be weighted to form posterior, prior, or anything in between.
- Estimates the **density of states** and calculates evidences & partition functions.
- The evolving ensemble of live points allows:
  - implementations to self-tune,
  - exploration of multimodal functions,
  - global and local optimisation.



Nested sampling: numerical Lebesgue integration

0. Start with N random samples over the space.
i. Delete outermost sample, and replace with a new random one at higher integrand value.

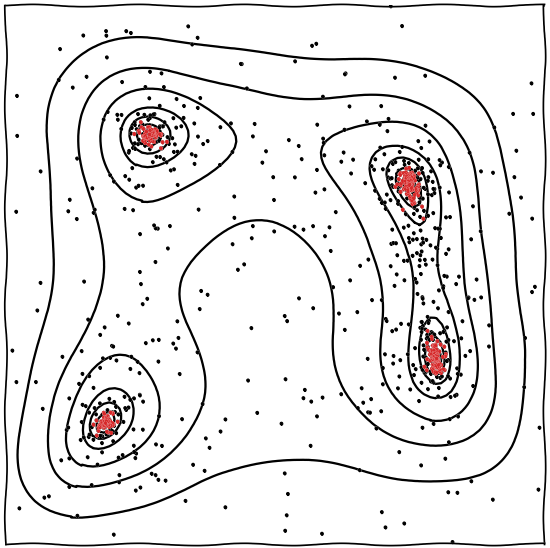
- The "live points" steadily contract around the peak(s) of the function.
- Discarded "dead points" can be weighted to form posterior, prior, or anything in between.
- Estimates the **density of states** and calculates evidences & partition functions.
- The evolving ensemble of live points allows:
  - implementations to self-tune,
  - exploration of multimodal functions,
  - global and local optimisation.



Nested sampling: numerical Lebesgue integration

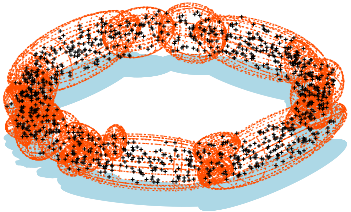
0. Start with N random samples over the space.
i. Delete outermost sample, and replace with a new random one at higher integrand value.

- The "live points" steadily contract around the peak(s) of the function.
- Discarded "dead points" can be weighted to form posterior, prior, or anything in between.
- Estimates the **density of states** and calculates evidences & partition functions.
- The evolving ensemble of live points allows:
  - implementations to self-tune,
  - exploration of multimodal functions,
  - global and local optimisation.

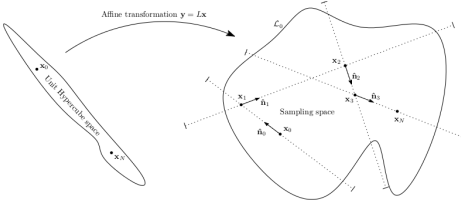


Implementations of Nested Sampling [2205.15570](NatReview)

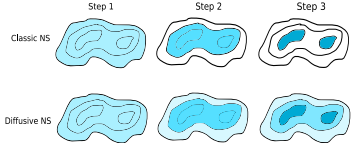
MultiNest [0809.3437]



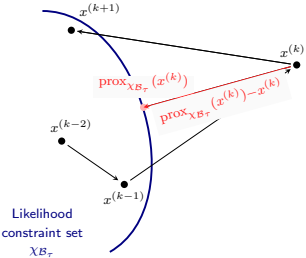
PolyChord [1506.00171]



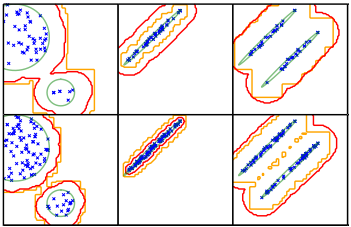
DNest [1606.03757]



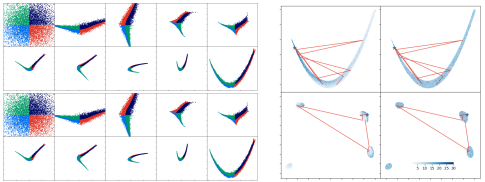
ProxNest [2106.03646]



UltraNest [2101.09604]



NeuralNest [1903.10860]



nessai [2102.11056]

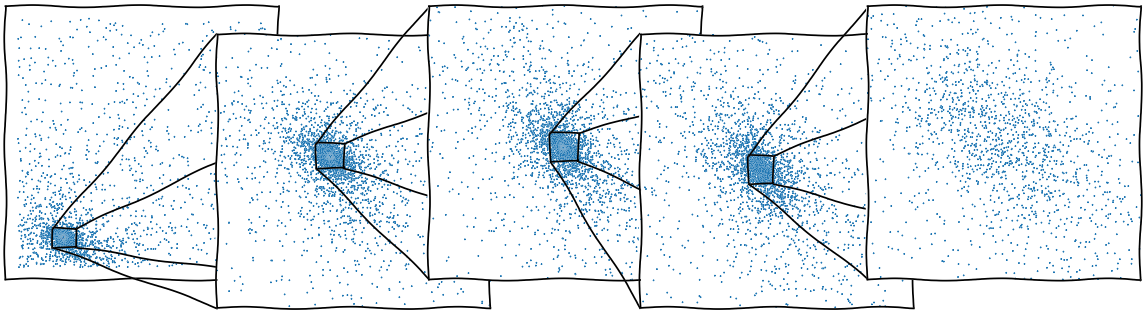
nora [2305.19267]

jaxnest [2012.15286]

nautilus [2306.16923]

dynesty [1904.02180]

The nested sampling meta-algorithm: dead points

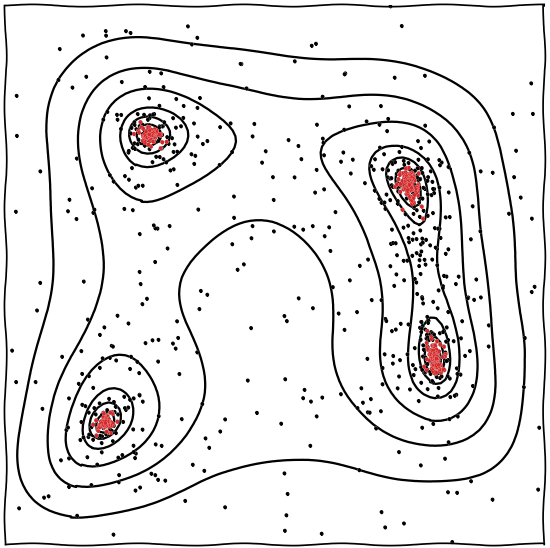


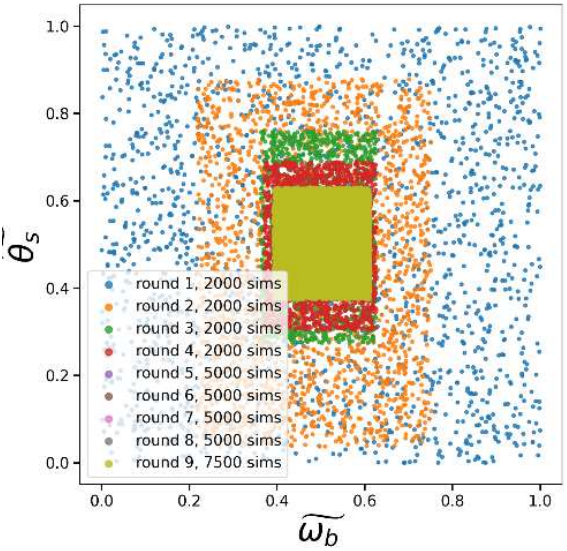
- At the end, one is left with a set of discarded "dead" points.
- Dead points have a unique scale-invariant distribution $\propto \frac{dV}{V}$.
- Uniform over original region, exponentially concentrating on region of interest (until termination volume).
- Good for training emulators (HERA [2108.07282]).

Applications

- training emulators.
- gridding simulations
- beta flows
- "dead measure"

Similarities





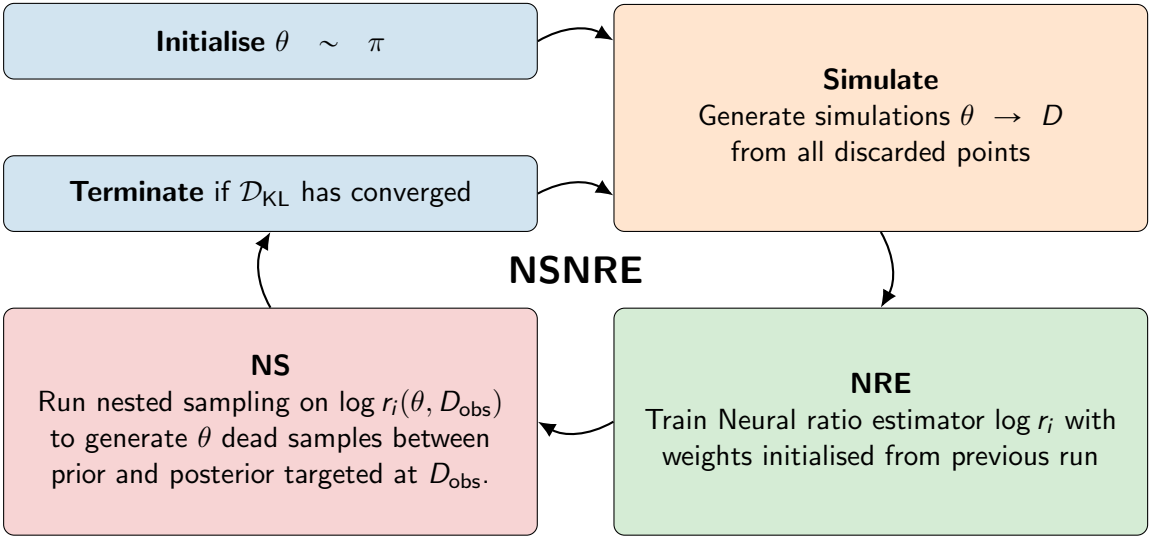
Why it's hard to do SBI with nested sampling

- At each iteration i, nested sampling requires you to be able to generate a new live point from the prior, subject to a hard likelihood constraint

$$\theta \sim \pi : \mathcal{L}(\theta) > \mathcal{L}_i$$

- This is hard if you don't have a likelihood!
- In addition, nested sampling does not do well if the likelihood is non-deterministic
- Previous attempts:
  - DNest paper [1606.03757](Section 10: Nested sampling for ABC)
  - ANRE [2308.08597] using non-box priors driven by current ratio estimate with slice sampling re-population.

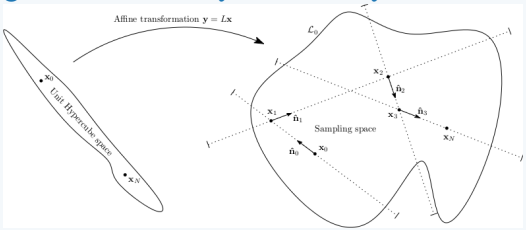
Sequential NRE with nested sampling



PolySwyft

PolyChord

github.com/PolyChord/PolyChordLite



- Widely used high-performance nested sampling tool (implementing slice sampling & clustering in MPI Fortran)

Swyft

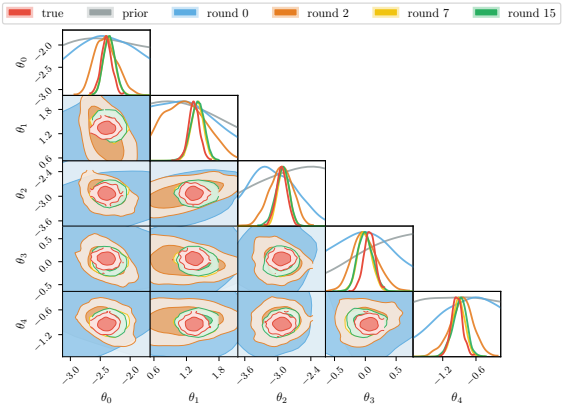
github.com/undark-lab/swyft

- Widely used TMNRE tool in cosmology/astrophysics.

However, NSNRE is general, and not specific to these choices.

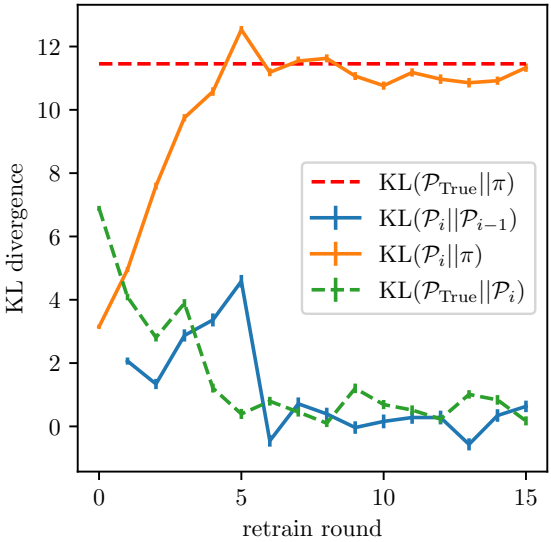
Convergence diagnostics

- Example for a $n = 5$ dimensional parameter space, with $d = 100$ data points, (`lsbi` gaussian mixture model).
- This is the regime for cosmological scale problems.
- To determine convergence we track:
  - The change in KL divergence between rounds (blue), and check when this goes to zero.
  - The total KL divergence between prior and posterior estimate (orange), and check when this levels off (ground truth in red).
  - Also shown is the KL divergence between the estimate and the ground truth (green).



Convergence diagnostics

- Example for a $n = 5$ dimensional parameter space, with $d = 100$ data points, (`lsbi` gaussian mixture model).
- This is the regime for cosmological scale problems.
- To determine convergence we track:
  - The change in KL divergence between rounds (blue), and check when this goes to zero.
  - The total KL divergence between prior and posterior estimate (orange), and check when this levels off (ground truth in red).
  - Also shown is the KL divergence between the estimate and the ground truth (green).



Conclusions

github.com/handley-lab

- `PolySwyft` can perform NRE on $n \sim 6$ parameter spaces and $d \sim 100$ data spaces.
- This makes it relevant for cosmological applications.
- Look out for imminent paper (post Kilian's thesis hand-in in $\sim \mathcal{O}(1\text{month})$)
- Examples produced using `lsbi` package: github.com/handley-lab/lsbi

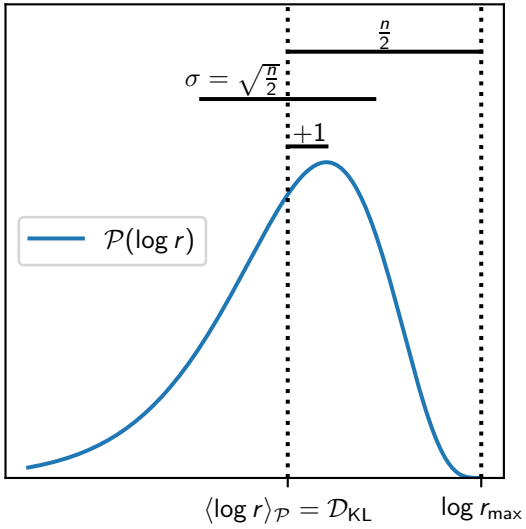
Considerations of ratio estimation

- Neural REs can in practice only estimate in a band of $\log r$ before the activation function saturates (typically $-5 < \log r < 5$).
- Consider a posterior $\mathcal{P}$ well approximated by a Gaussian profile in an n-dimensional parameter space [2312.00294]
- If $\mathcal{D}_{\mathrm{KL}} \gg 1$ between prior and posterior:

$$\log r = \frac{n}{2} + \mathcal{D}_{\mathrm{KL}} + \chi^2_n$$

$$\langle \log r \rangle_{\mathcal{P}} = \mathcal{D}_{\mathrm{KL}}, \qquad \sigma(\log r)_{\mathcal{P}} = \sqrt{\frac{n}{2}}$$

- Truncation (**T**MNRE) reduces $\mathcal{D}_{\mathrm{KL}}$, focusing the distribution into the $[-5, 5]$ band.
- Marginalisation (T**M**NRE) reduces n & σ.



Cosmological forecasting

Have you ever done a Fisher forecast, and then felt Bayesian guilt?

- Cosmologists are interested in forecasting what a Bayesian analysis of future data might produce.
- Useful for:
  - white papers/grants,
  - optimising existing instruments/strategies,
  - picking theory/observation to explore next.
- To do this properly:
  1. start from current knowledge $\pi(\theta)$, derived from current data
  2. Pick potential dataset D that might be collected from $P(D)$ $(= \mathcal{Z})$
  3. Derive posterior $P(\theta|D)$
  4. Summarise science (e.g. constraint on θ, ability to perform model comparison)

- This procedure should be marginalised over:
  1. All possible parameters θ (consistent with prior knowledge)
  2. All possible data D
- i.e. marginalised over the joint $P(\theta, D) = P(D|\theta)P(\theta)$.
- Historically this has proven very challenging.
- Most analyses assume a fiducial cosmology θ_*, and/or a Gaussian likelihood/posterior (c.f. Fisher forecasting).
- This runs the risk of biasing forecasts by baking in a given theory/data realisation.

Fully Bayesian Forecasting [2309.06942]

Thomas Gessey-Jones
PhD

- Simulation based inference gives us the language to marginalise over parameters θ and possible future data D.
- Evidence networks give us the ability to do this at scale for forecasting [2305.11241].
- Demonstrated in 21cm global experiments, marginalising over:
  - theoretical uncertainty
  - foreground uncertainty
  - systematic uncertainty
- Able to say "at 67mK radiometer noise", have a 50% chance of 5σ Bayes factor detection.
- Can use to optimise instrument design
- Re-usable package: `prescience`