PolySwyft

a sequential simulation-based nested sampler

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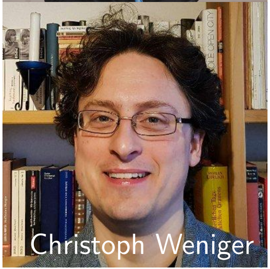
5. Future prospects

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



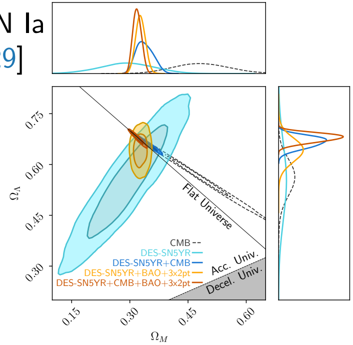
LBI: Likelihood-based inference

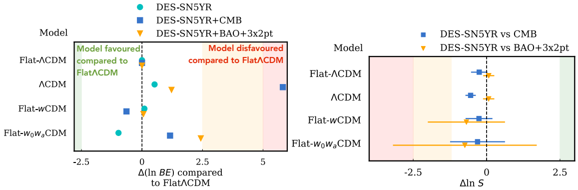
The standard approach if you are fortunate enough to have a likelihood function $P(D|\theta)$:

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

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]





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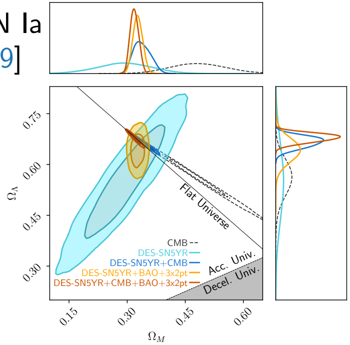

$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)} \qquad \text{Posterior} = \frac{\text{Likelihood} \times \text{Prior}}{\text{Evidence}}$$

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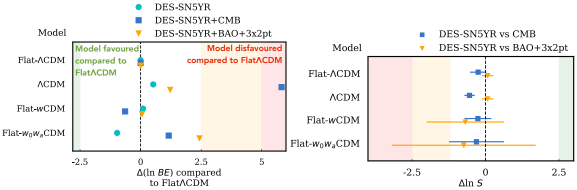

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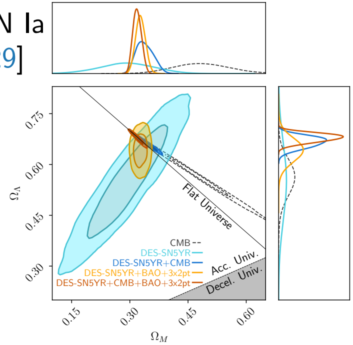

$$\mathcal{P}(\theta|D) = \frac{\mathcal{L}(D|\theta)\pi(\theta)}{\mathcal{Z}(D)} \qquad \text{Posterior} = \frac{\text{Likelihood} \times \text{Prior}}{\text{Evidence}}$$

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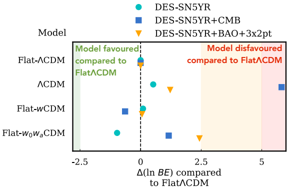

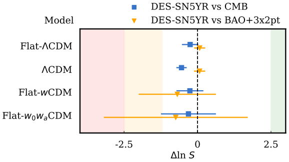

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$$P(\theta|D)P(D) = P(D,\theta) = P(D|\theta)P(\theta),$$

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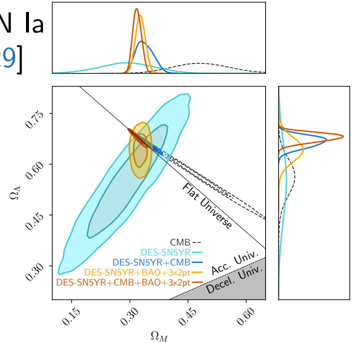

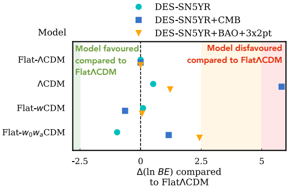

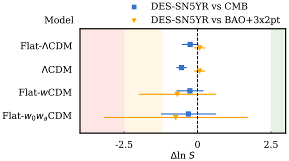

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$$\mathcal{P} \times \mathcal{Z} = \mathcal{J} = \mathcal{L} \times \pi, \qquad \text{Joint} = \mathcal{J} = P(D, \theta)$$

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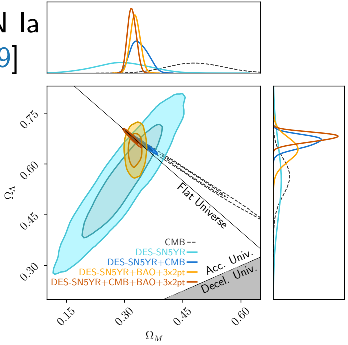

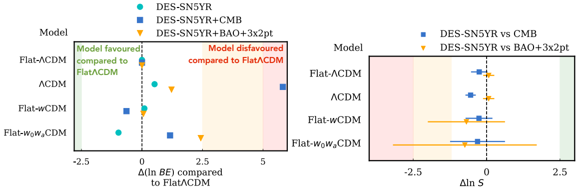

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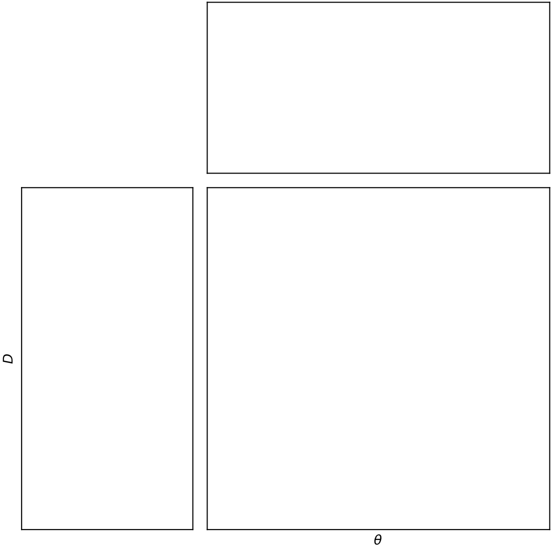

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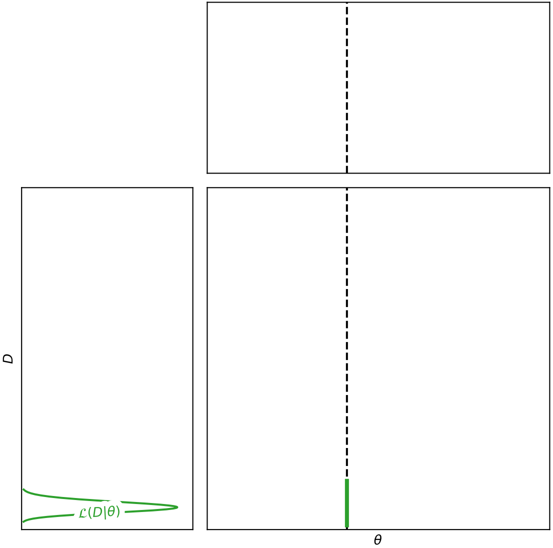

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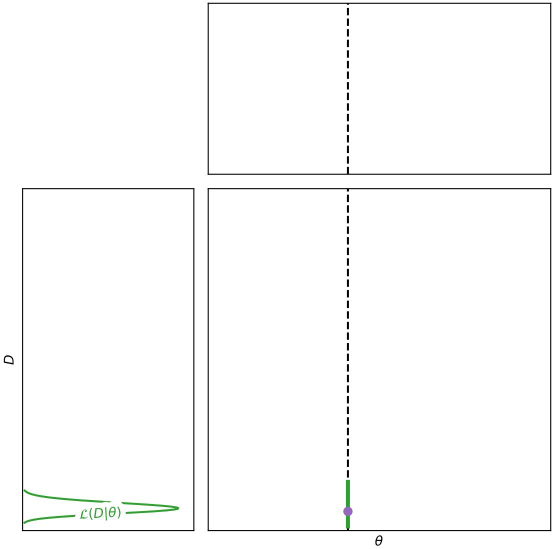

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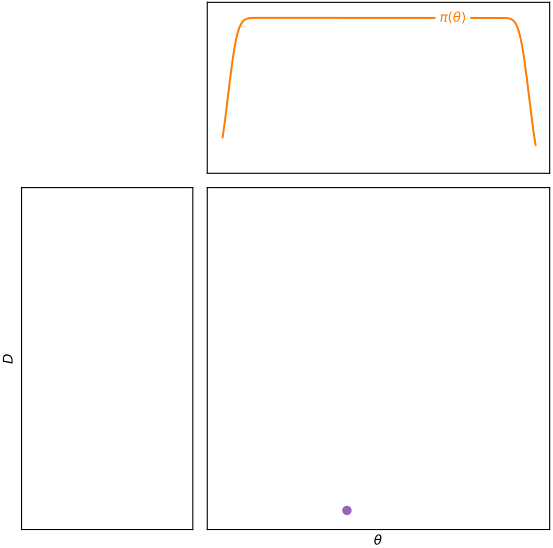

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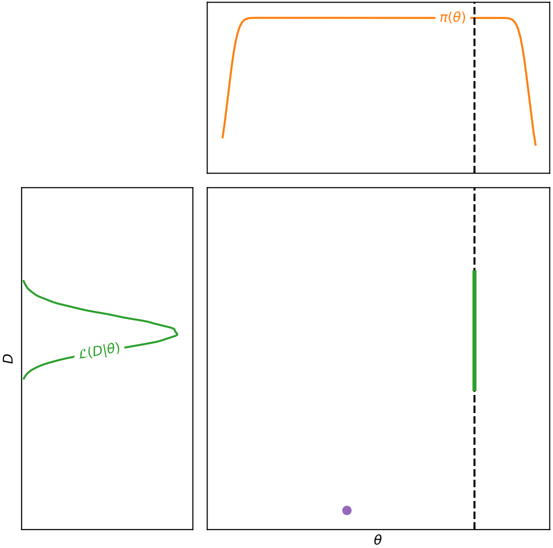

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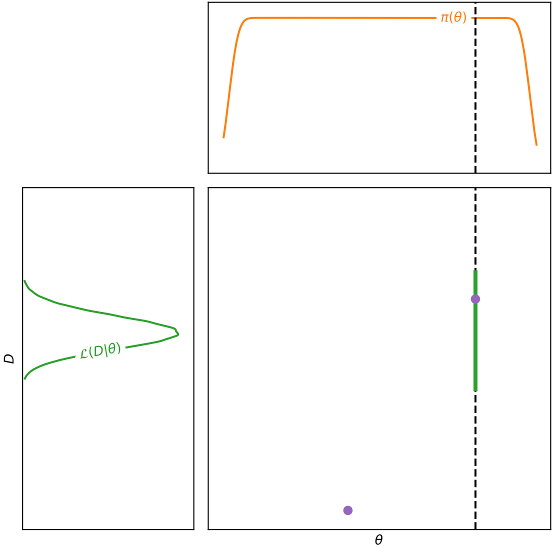

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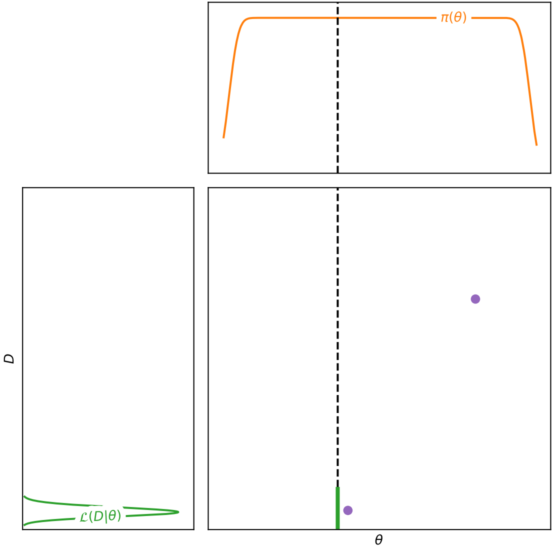

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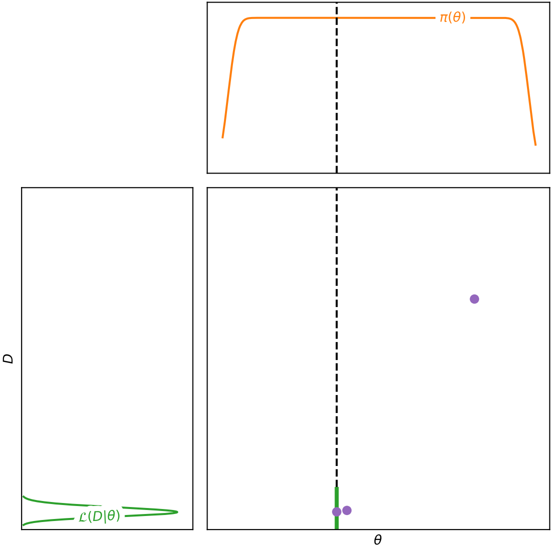

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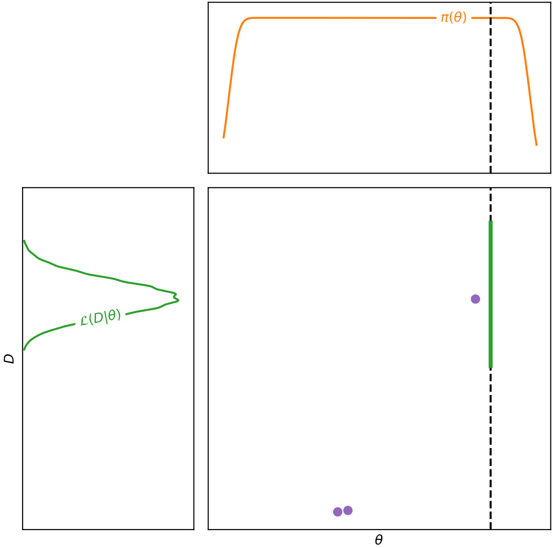

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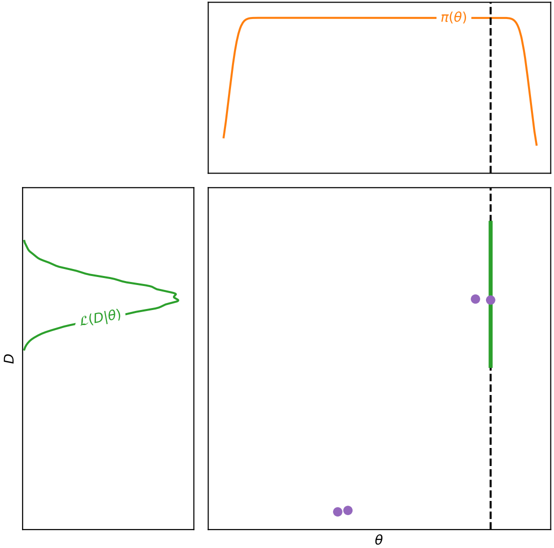

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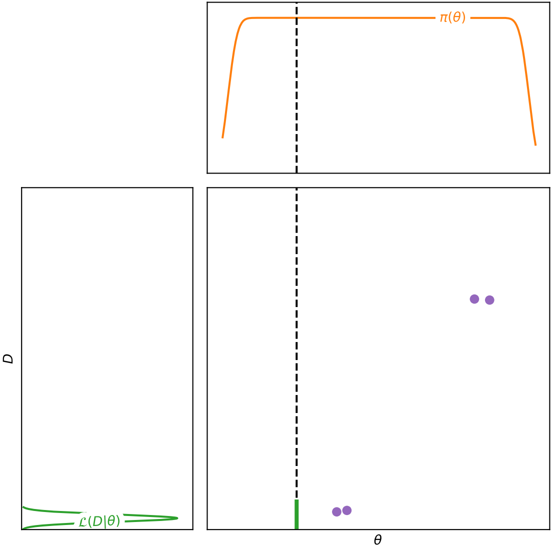

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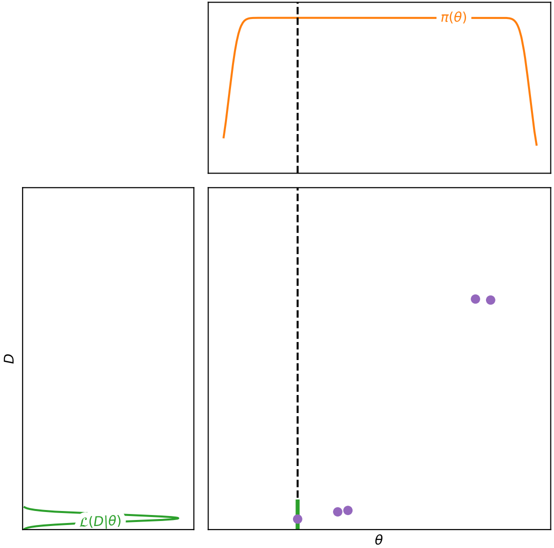

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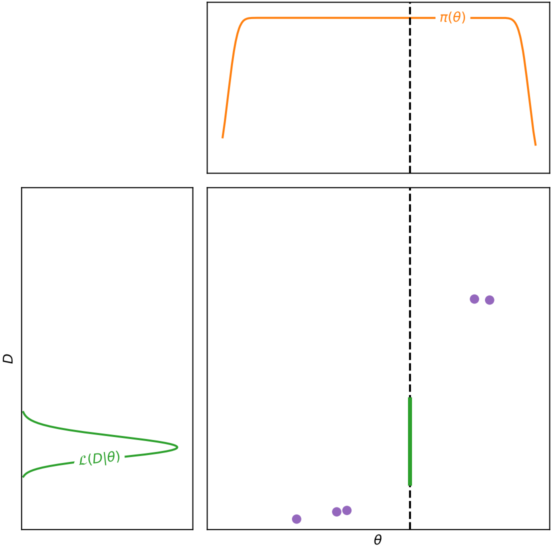

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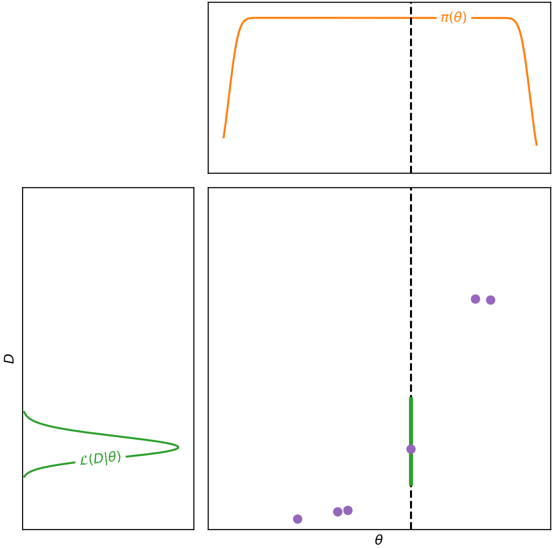

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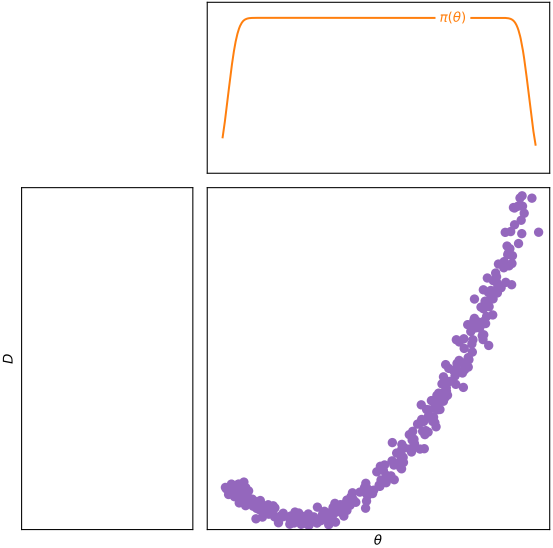

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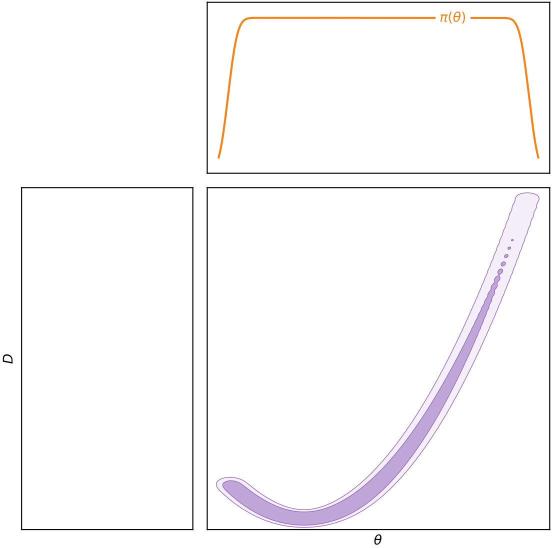

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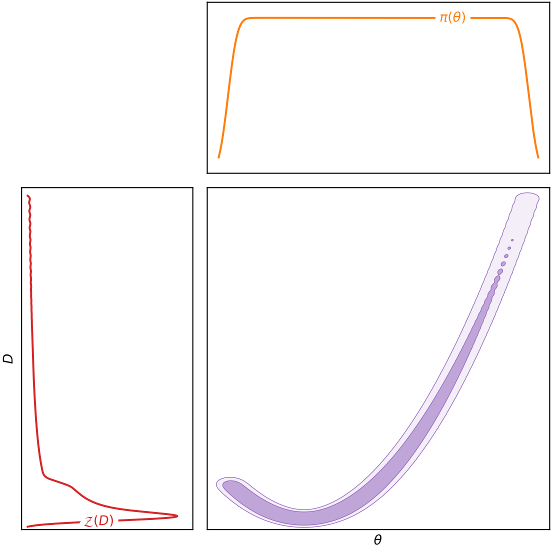

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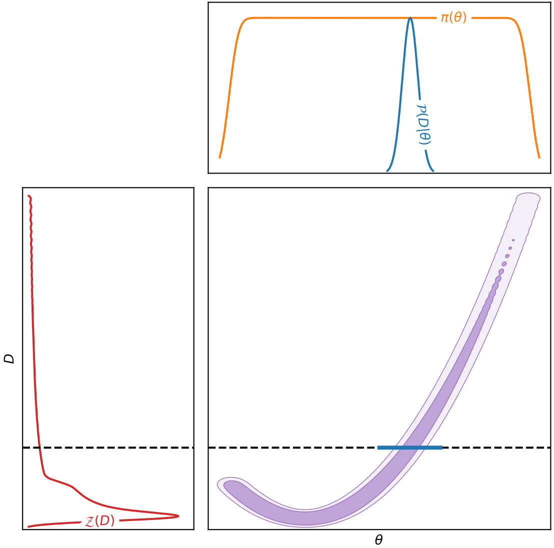
- If you have a simulator/forward model $\theta \rightarrow D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$ *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`.



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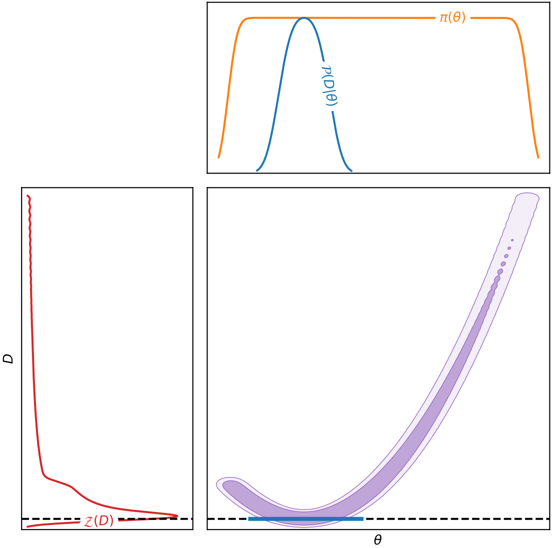

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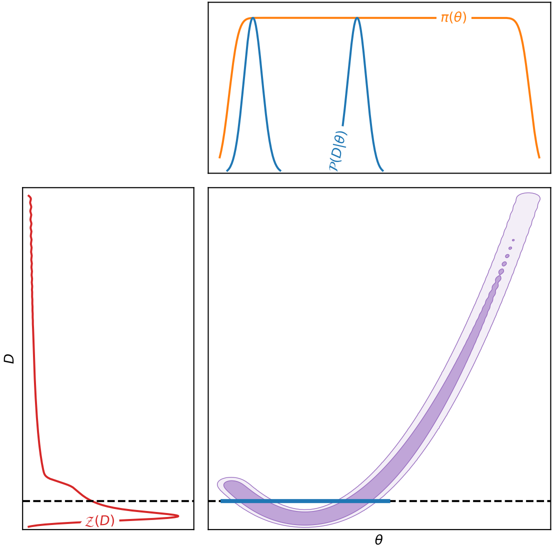

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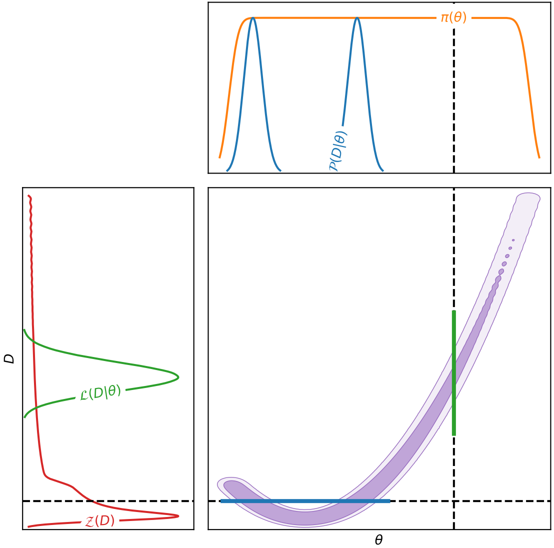
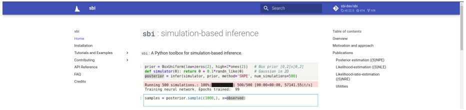


Why SBI?

SBI is useful because:

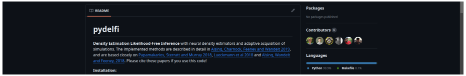
1. If you don't have a likelihood, you can still do inference
   - This is the usual case beyond CMB cosmology
2. Faster than LBI
   - emulation – also applies to LBI in principle
3. No need to pragmatically encode fiducial cosmologies
   - Covariance computation implicitly encoded in simulations
   - 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. Dupourqué[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[5], 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

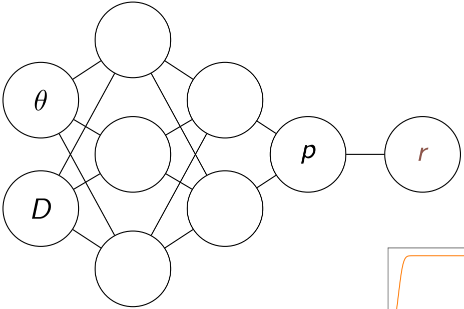
Elena Massara,[1,2,*] ChangHoon Hahn,[3] Michael Eickenberg,[4] Shirley Ho,[5] Jiamin Hou,[6,7] Pablo Lemos,[8,9,5] Chirag Modi,[4,5] Azadeh Moradinezhad Dizgah,[10,11] Liam Parker,[5,12] and Bruno Régaldo-Saint Blancard[4]

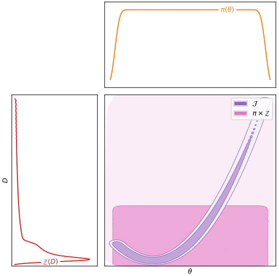
Neural Ratio Estimation

- 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 $\mathcal{P} = r \times \pi$





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

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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

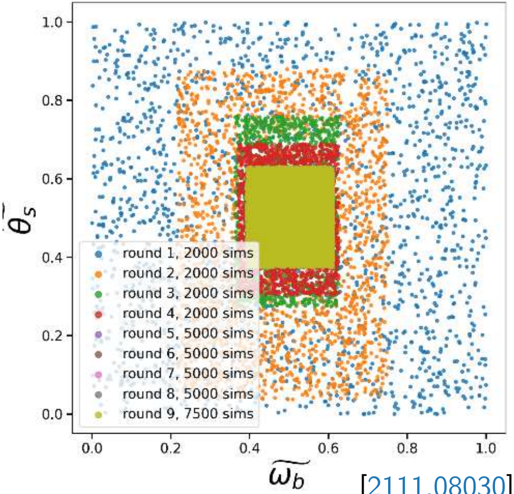
- Two tricks for practical NRE:

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

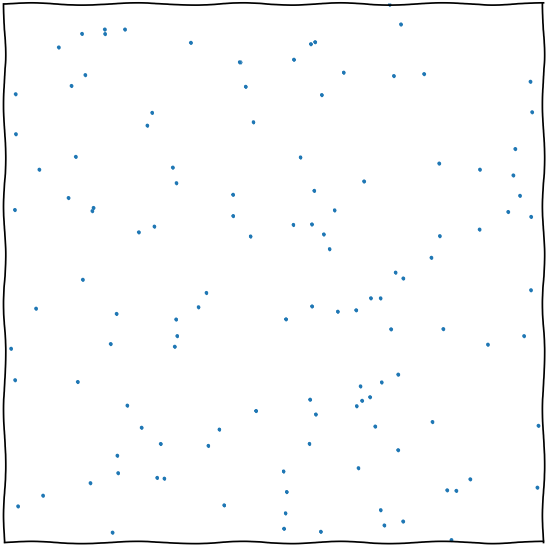


[2111.08030]

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.



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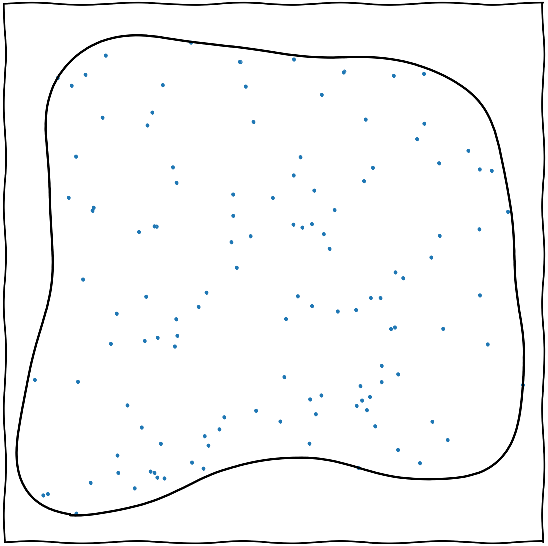

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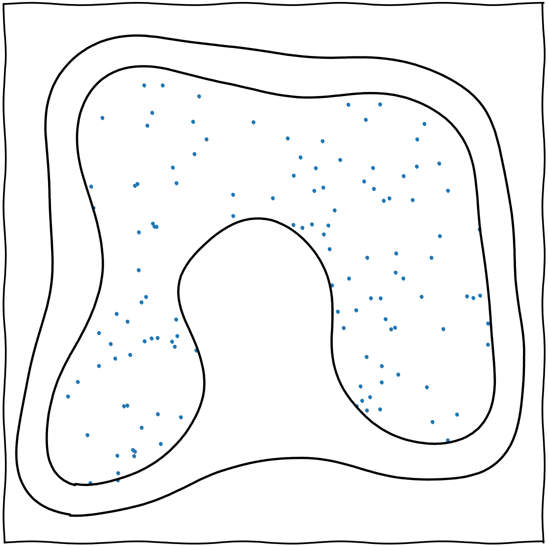

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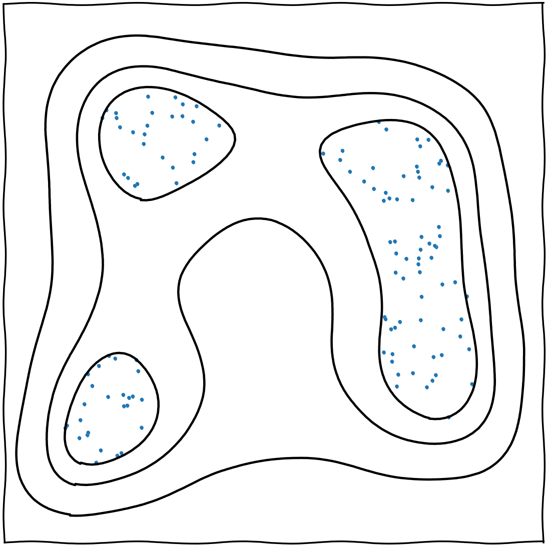

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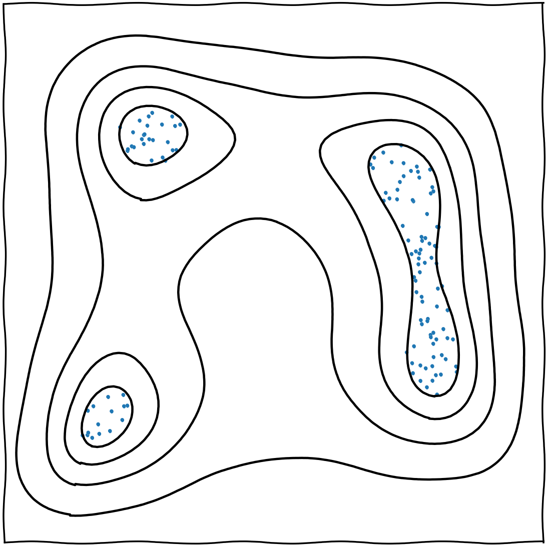

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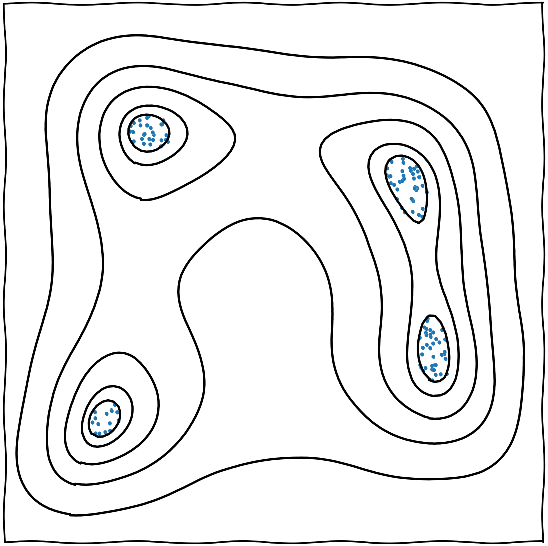

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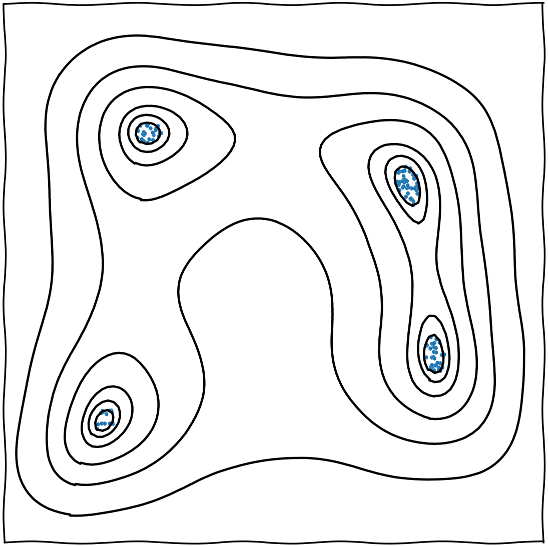

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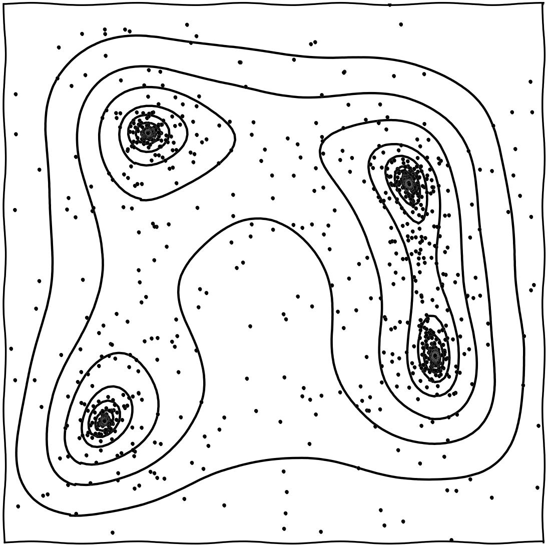

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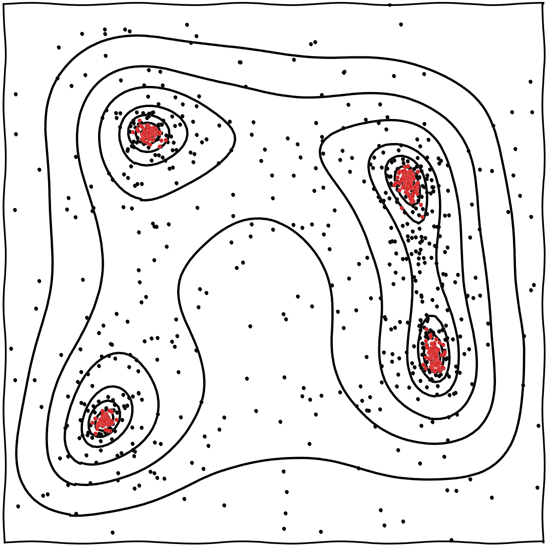
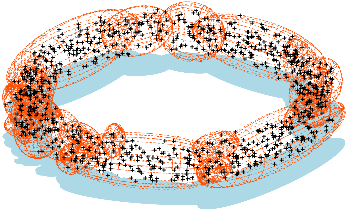
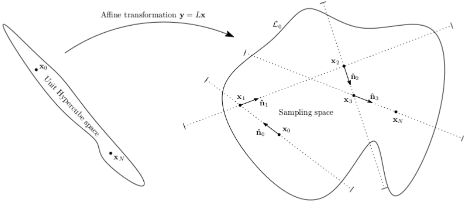


Implementations of Nested Sampling [2205.15570](NatReview)

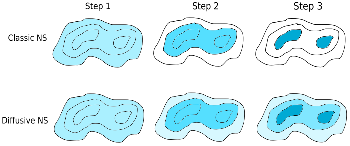
MultiNest [0809.3437]



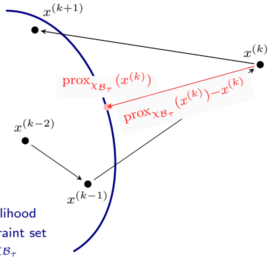
PolyChord [1506.00171]



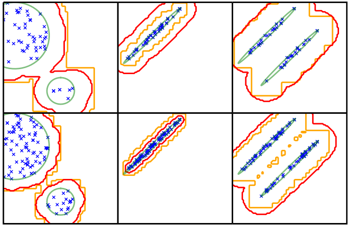
DNest [1606.03757]



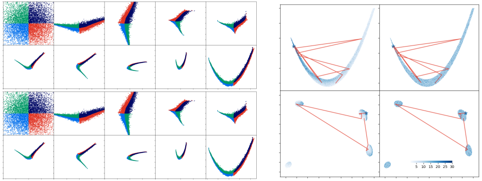
ProxNest [2106.03646]



UltraNest [2101.09604]



NeuralNest [1903.10860]



nessai [2102.11056]

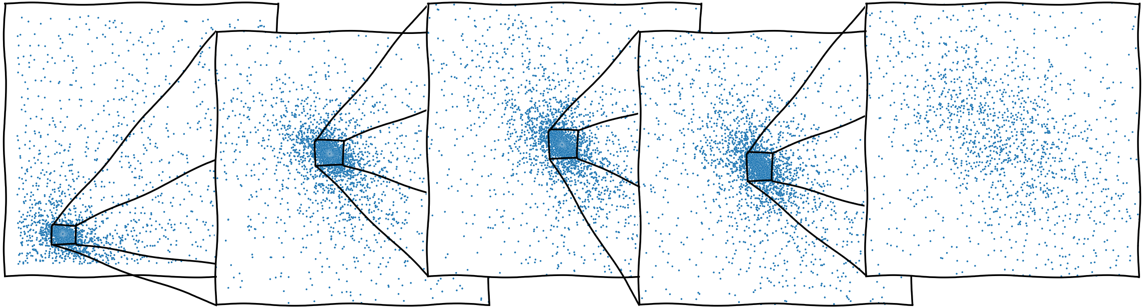
nora [2305.19267]

jaxnest [2012.15286]

nautilus [2306.16923]

dynesty [1904.02180]

The nested sampling meta-algorithm: dead points

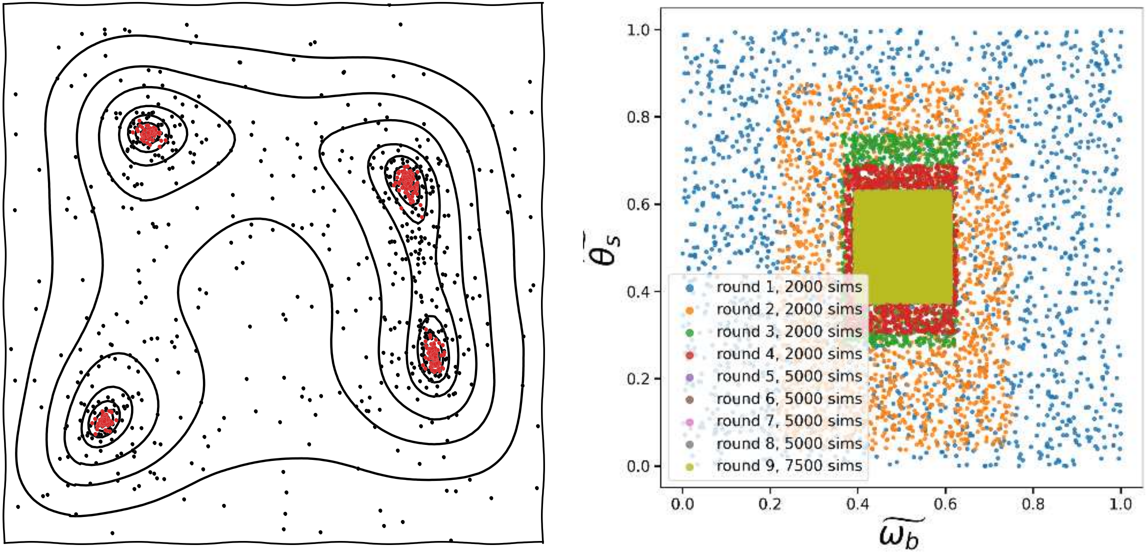


- At the end, one is left with a set of discarded "dead" points.
- Dead points have a unique scale-invariant distribution $\propto \frac{dV}{V}$.
- Uniform over original region, exponentially concentrating on region of interest (until termination volume).
- Good for training emulators (HERA [2108.07282]).

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

Initialise $\theta \sim \pi$

Simulate
Generate simulations $\theta \to D$
from all discarded points

NRE
Train Neural ratio estimator $\log r_i$ with weights initialised from previous run

NS
Run nested sampling on $\log r_i(\theta, D_{\mathrm{obs}})$ to generate θ dead samples between prior and posterior targeted at D_{obs}.

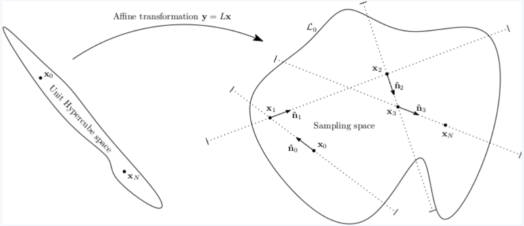
Terminate if $\mathcal{D}_{\mathrm{KL}}$ has converged

NSNRE

PolySwyft

PolyChord

github.com/PolyChord/PolyChordLite



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

Swyft

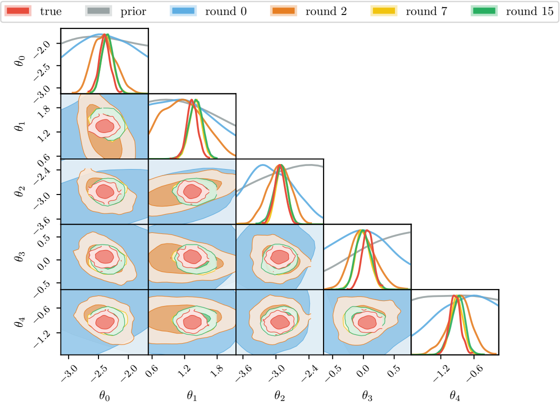
github.com/undark-lab/swyft

- 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).



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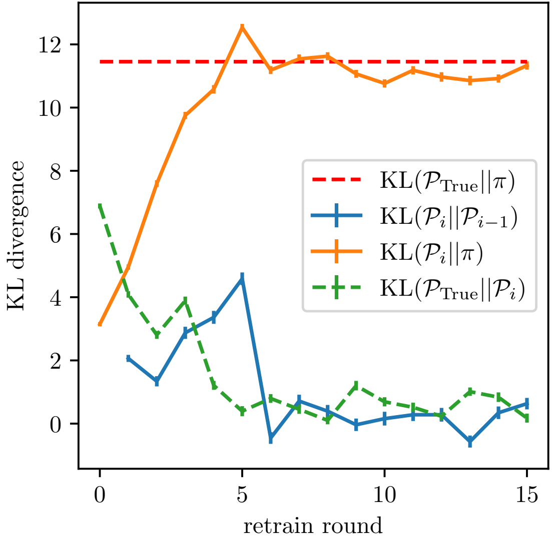


Conclusions

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

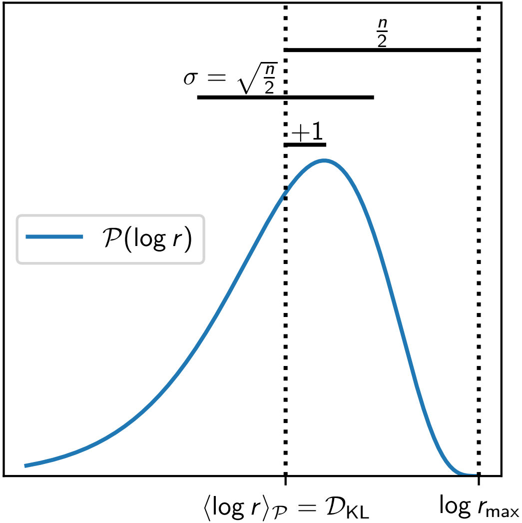
Zixiao Hu
MPhil

- 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:

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

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

- 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

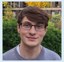
Have you ever done a Fisher forecast, and then felt Bayesian guilt?

- 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`