Next generation inference tools for cosmology and beyond

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

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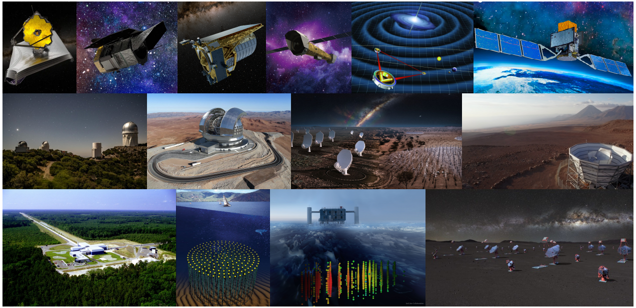
The golden age of cosmology data

- Over our research lifetimes we will see next-generation data rates across the electromagnetic spectrum & beyond:

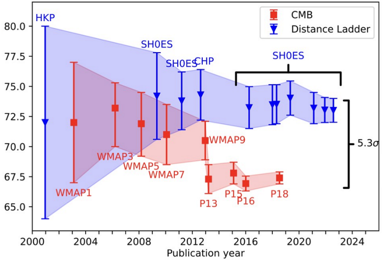
Radio	SKA *et al*
Micro	SO/CMB-S4
IR	JWST, Roman (WFIRST)
Optical	Euclid, DESI, Rubin (LSST), EELT
X-ray	Athena
Gamma-ray	e-ASTROGAM
Gravitational	LIGO/Virgo/Kagra + LISA
Particle	CTA, IceCube, KM3NeT

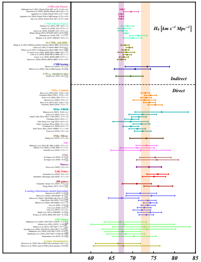


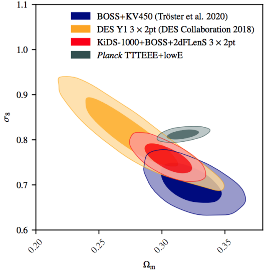
- We are moving from an age of **precision** cosmology to **accurate** cosmology.
- **Systematics** $\gtrsim$ **statistics**.
- Tools risk lagging behind hardware

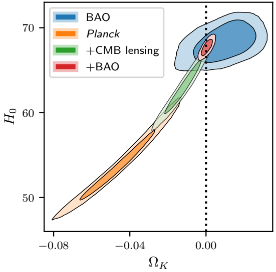
Tensions in cosmology

- **Data**: H_0, S_8, A_L/Ω_K, Li
- **Theory**: Initial conditions, Entropy, Dark energy, dark matter, quantum gravity
- **Analysis**:
- Disentangling systematics from new physics is challenging!
- Almost all cosmological analyses pragmatically assume a fiducial flat ΛCDM assumption during their analyses.
- Unless this is resolved, we risk confirmation bias in the analysis of next-generation data.









Structure of talk

1. Likelihood-based inference
2. Nested sampling
3. Marginal hierarchical inference
4. Simulation-based inference
5. Fully Bayesian Forecasts

Bayesian notation

- A "generative" model M, with tunable parameters θ, describing (compressed) data D.
  - e.g. $M = \Lambda\mathrm{CDM}$, $\theta = \{\Omega_b, \Omega_c, \tau, H_0, A_s, n_s\}$, $D = \{C_\ell\}$.
- Described by simulation process $\theta \to D$, or likelihood $P(D|\theta, M)$.
- Frequentists & Bayesians agree on the likelihood.
- Bayesians treat parameter space θ the same as data space D.
- Quantifying uncertainty with probability using Bayes theorem:

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

- Follows from the oft-forgotten Joint (the probability of everything):

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

- Also relevant (in many overlapping contexts) is the dimensionless ratio

$$r = \frac{\mathcal{J}}{\pi \times \mathcal{Z}} = \frac{\mathcal{L}}{\mathcal{Z}} = \frac{\mathcal{P}}{\pi}$$

The three pillars of Bayesian inference

Parameter estimation

What do the data tell us about the parameters of a model? *e.g. the size or age of a ΛCDM universe*

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

$$\mathcal{P} = \frac{\mathcal{L}\times\pi}{\mathcal{Z}}$$

$$\text{Posterior} = \frac{\text{Likelihood}\times\text{Prior}}{\text{Evidence}}$$

Model comparison

How much does the data support a particular model? *e.g. ΛCDM vs a dynamic dark energy cosmology*

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

$$\frac{\mathcal{Z}_\mathcal{M}\Pi_\mathcal{M}}{\sum_m Z_m\Pi_m}$$

$$\text{Posterior} = \frac{\text{Evidence}\times\text{Prior}}{\text{Normalisation}}$$

Tension quantification

Do different datasets make consistent predictions from the same model? *e.g. CMB vs Type IA supernovae data*

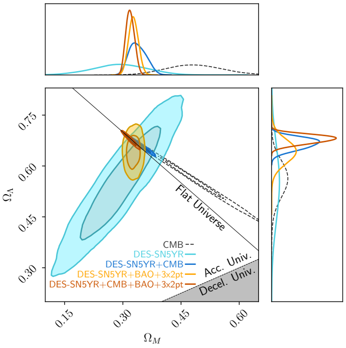
$$\mathcal{R} = \frac{\mathcal{Z}_{AB}}{\mathcal{Z}_A\mathcal{Z}_\mathcal{B}}$$

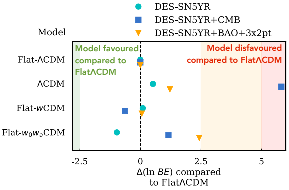
$$\log\mathcal{S} = \langle\log\mathcal{L}_{AB}\rangle_{\mathcal{P}_{AB}} - \langle\log\mathcal{L}_A\rangle_{\mathcal{P}_A} - \langle\log\mathcal{L}_B\rangle_{\mathcal{P}_B}$$

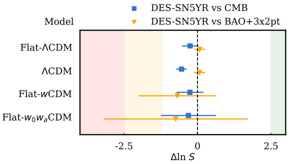
LBI: Likelihood-based inference

The standard approach if you are fortunate enough to have a likelihood function $\mathcal{L}(D|\theta)$: e.g recent DES analysis [2401.02929]

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)
4. Optionally talk about tensions
   - Bayes ratio (Nested Sampling)
   - Suspiciousness (MCMC) [2007.08496]





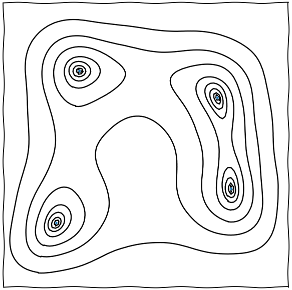


What is Nested Sampling?

- Nested sampling is a radical, multi-purpose numerical tool.
- Given a (scalar) function f with a vector of parameters θ, it can be used for:

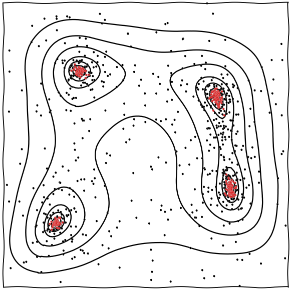
Optimisation

$$\theta_{\max} = \max_{\theta} f(\theta)$$



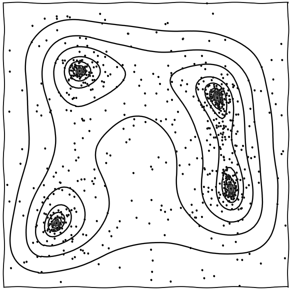
Exploration

$$\text{draw/sample} \quad \theta \sim f$$

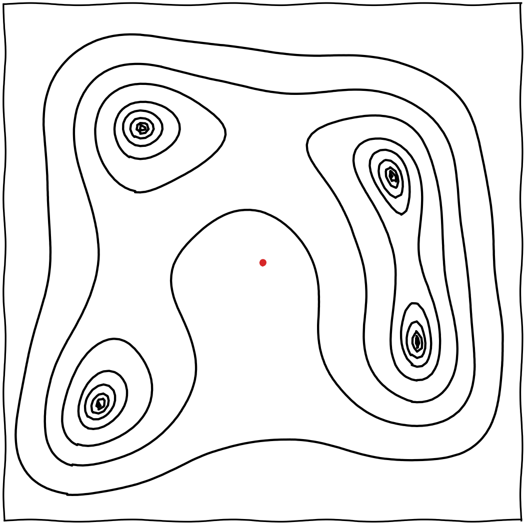


Integration

$$\int f(\theta) dV$$



MCMC



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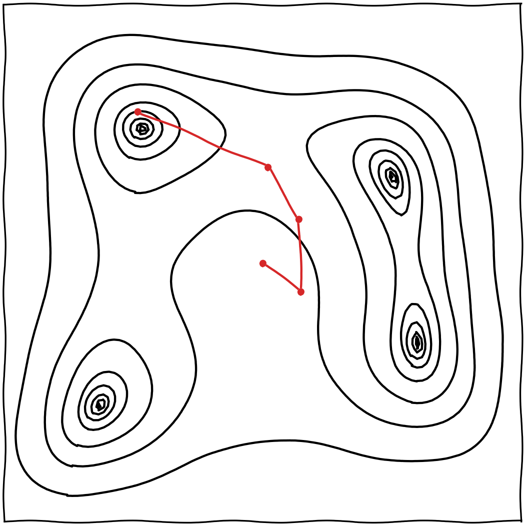

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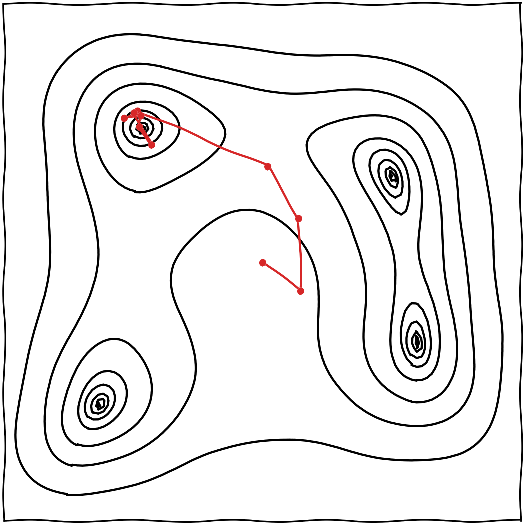

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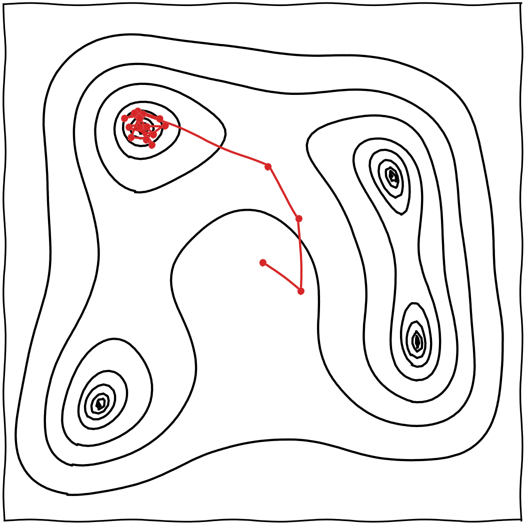

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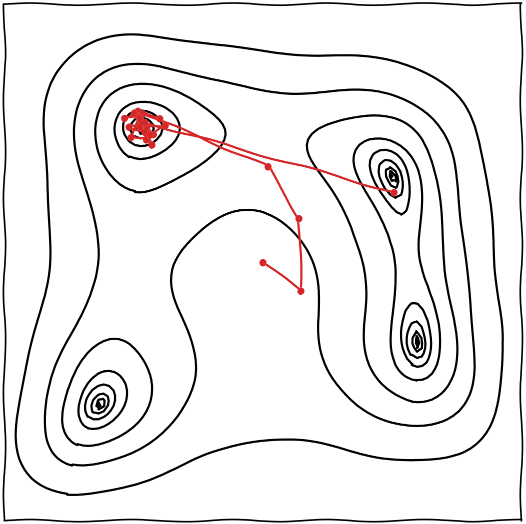

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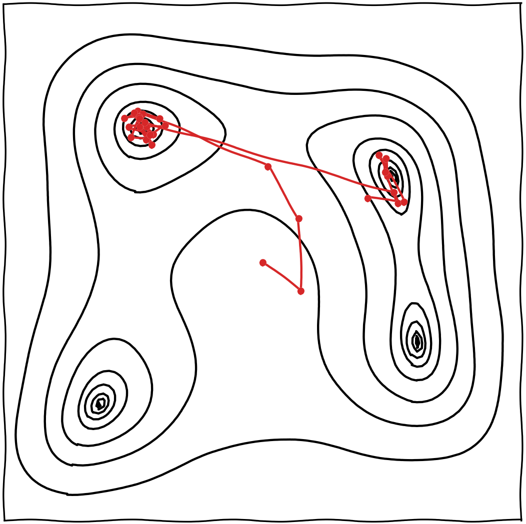

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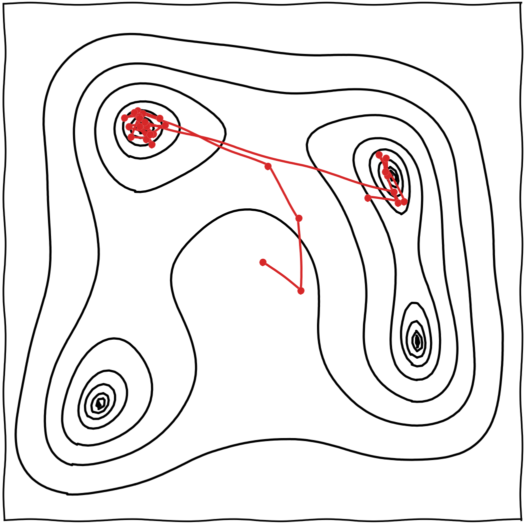
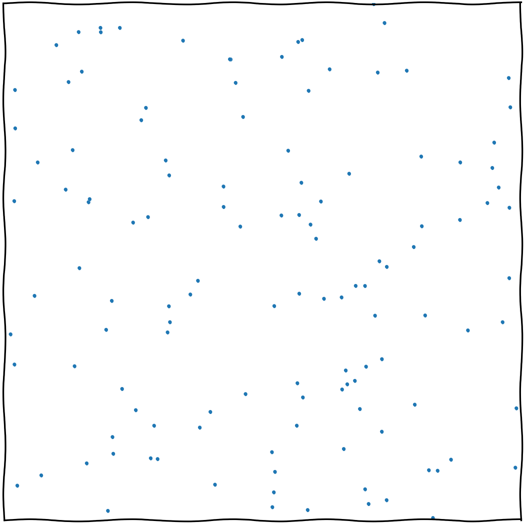
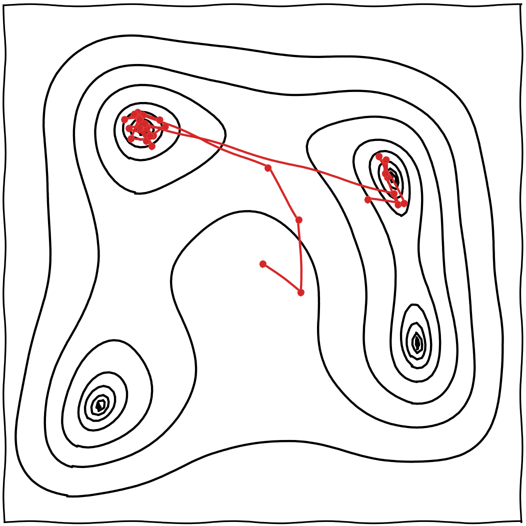


Nested sampling



MCMC



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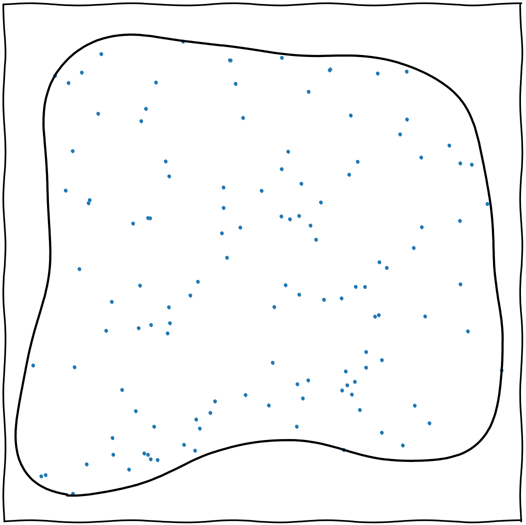

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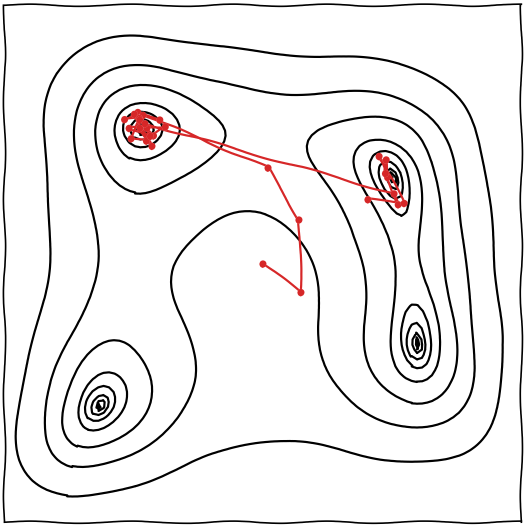

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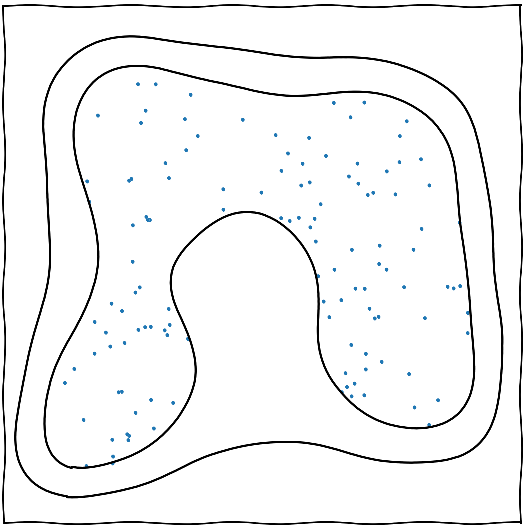

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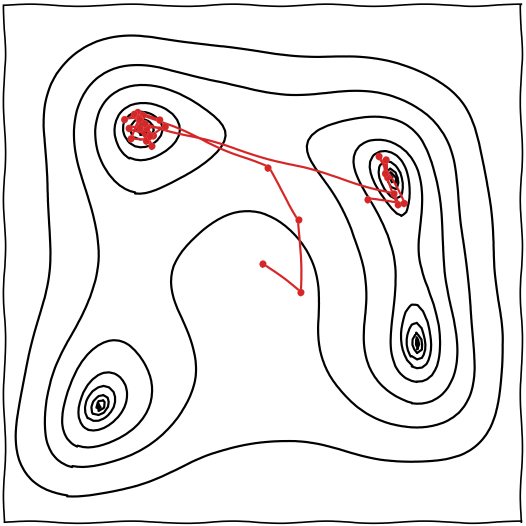

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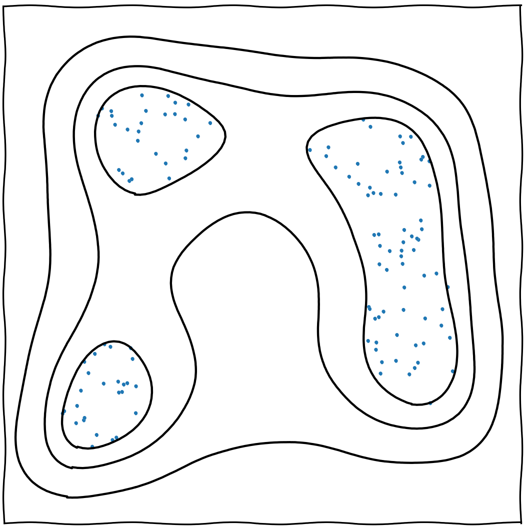

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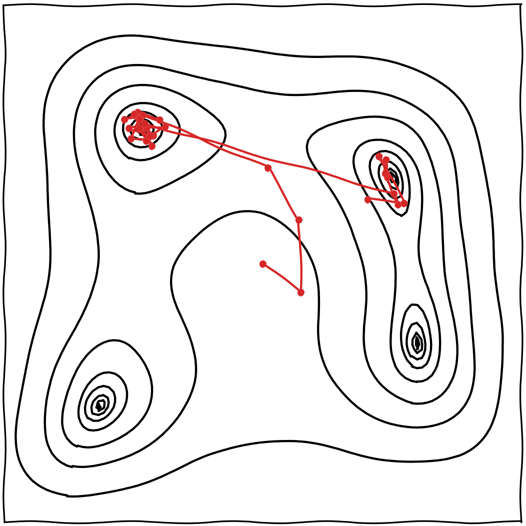

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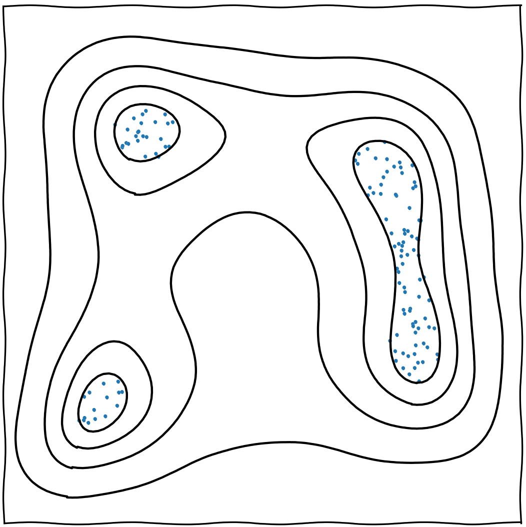

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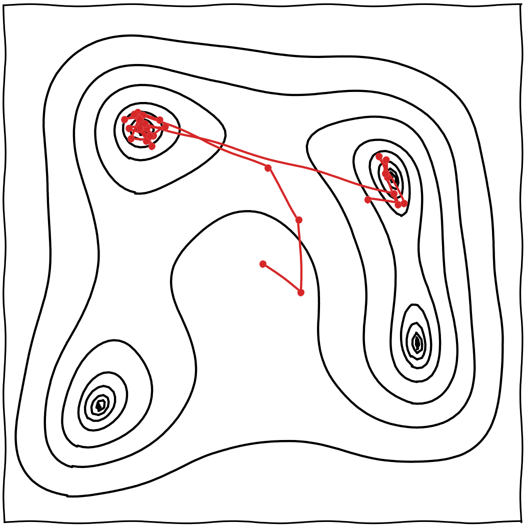

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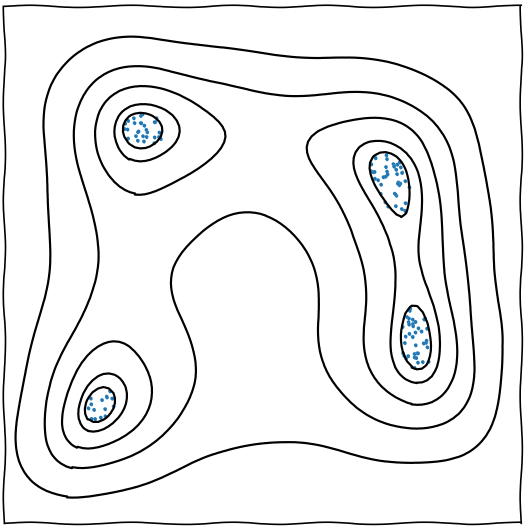

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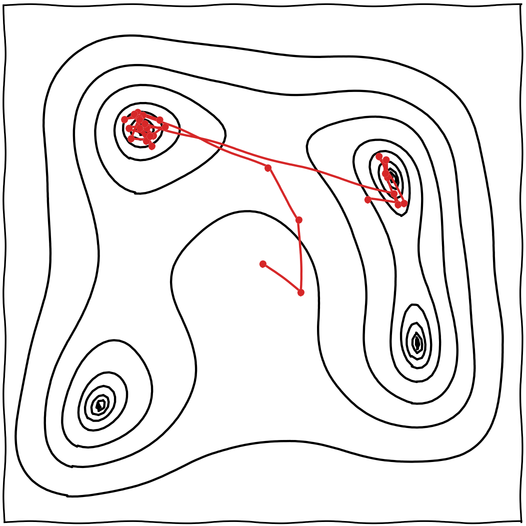

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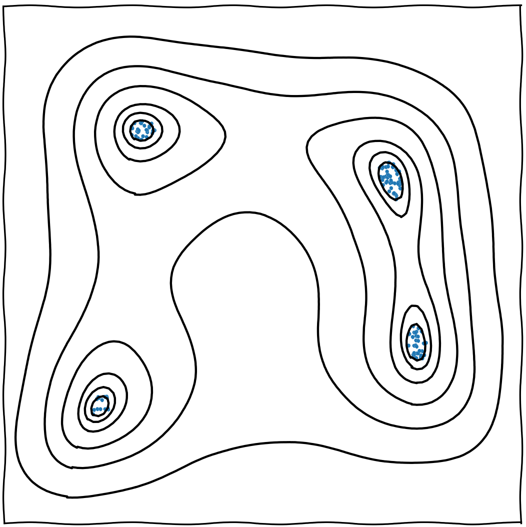

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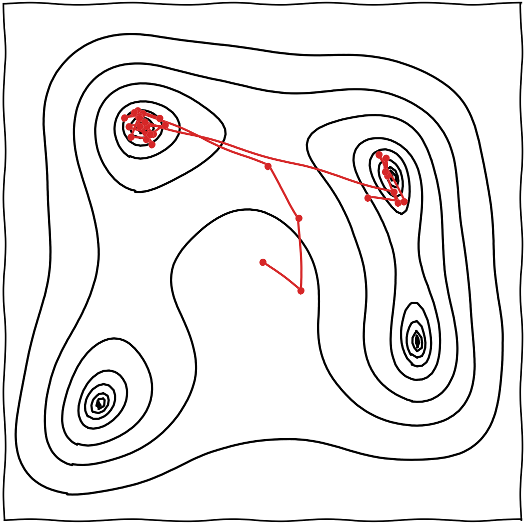
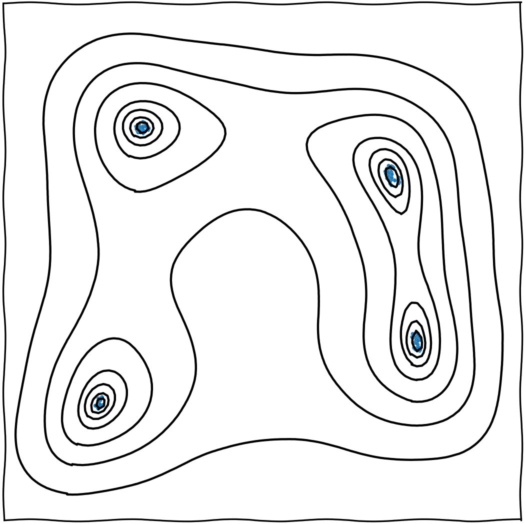


Nested sampling



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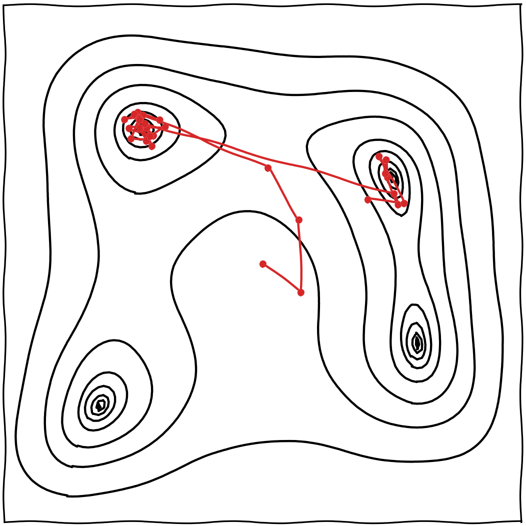

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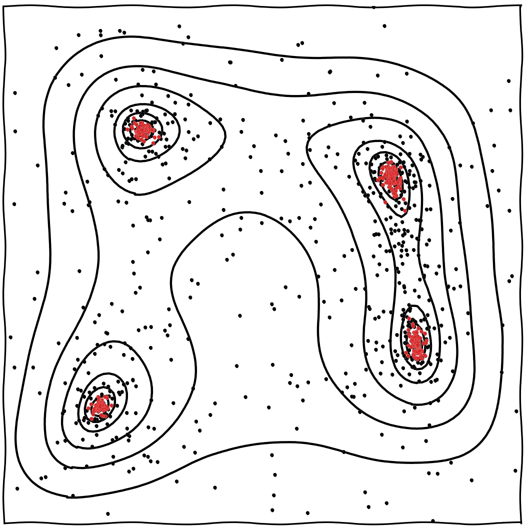
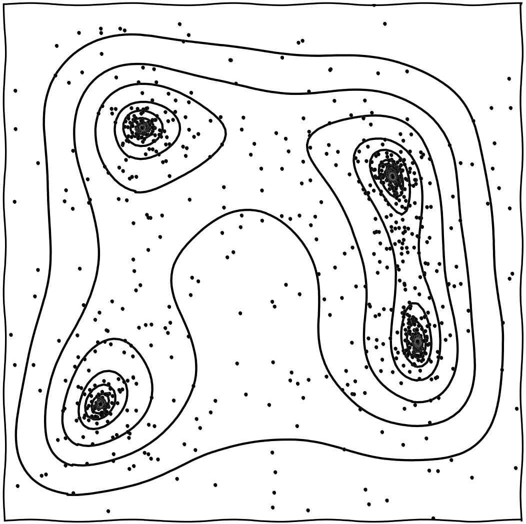


The nested sampling meta-algorithm: Lebesgue integration

- Full dead-point coverage of tails enables integration.
- Can be weighted to form posterior samples, prior samples, or anything in between.
- Nested sampling estimates the **density of states** and calculates partition functions

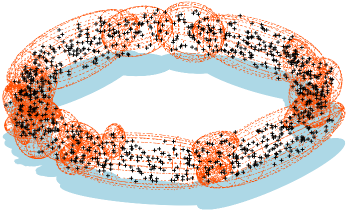
$$Z(\beta) = \sum_i f(x_i)^\beta \Delta V_i.$$

- The evolving ensemble of live points allows:
  - implementations to self-tune
  - exploration of multimodal functions
  - global and local optimisation

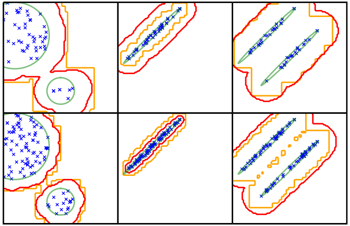


Implementations of Nested Sampling [2205.15570](NatReview)

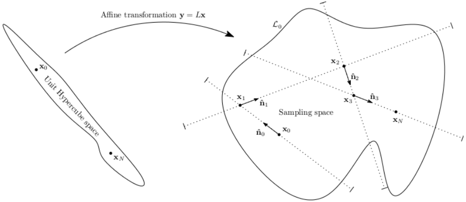
MultiNest [0809.3437]



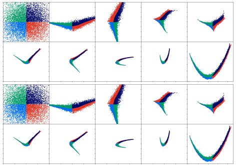
UltraNest [2101.09604]

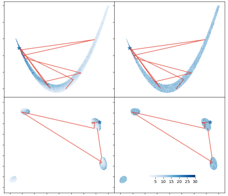


PolyChord [1506.00171]



NeuralNest [1903.10860]

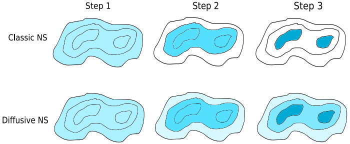




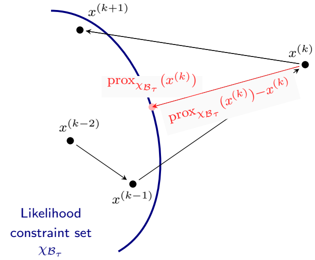
nessai [2102.11056]

nora [2305.19267]

DNest [1606.03757]



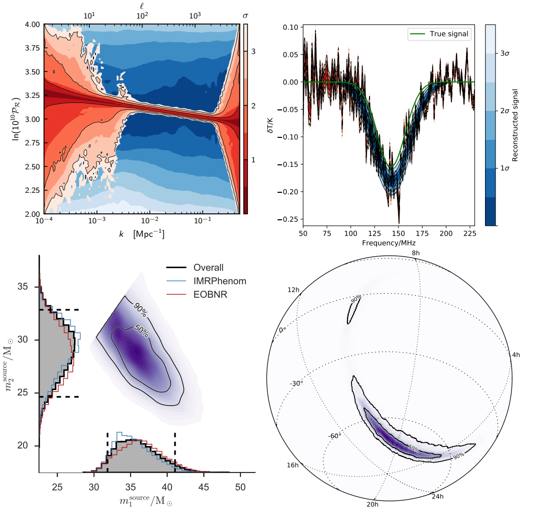
ProxNest [2106.03646]



dynesty [1904.02180]

Standard uses of nested sampling

- Battle-tested in Bayesian cosmology on
  - Parameter estimation: multimodal alternative to MCMC samplers.
  - Model comparison: using integration to compute the Bayesian evidence
  - Tension quantification: using deep tail sampling and suspiciousness computations.
- Plays a critical role in major cosmology pipelines: Planck, DES, KiDS, BAO, SNe.
- The default ΛCDM cosmology is well-tuned to have Gaussian-like posteriors for CMB data.
- Less true for alternative cosmologies/models and orthogonal datasets, so nested sampling crucial.
- Also used in Gravitational Waves & Exoplanets
- Often taken as “ground truth to beat”.



Marginal inference

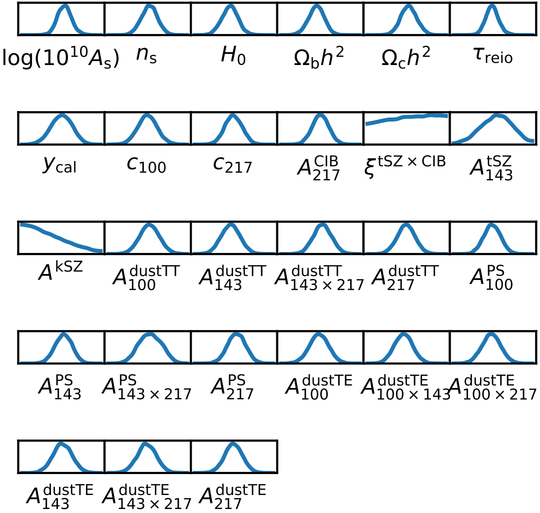
Harry Bevins

PhD→JRF

- Many cosmological likelihoods come with nuisance parameters that have limited relevance for onward inference.
- Notation: CMB cosmology

$\mathcal{L}$	Likelihood	(e.g. `plik`),
D	Data	(e.g. CMB),
θ	Cosmological parameters	(e.g. Ω_m, $H_0 \ldots$),
α	Nuisance parameters	(e.g. $A_{\mathrm{planck}} \ldots$),
M	Model	(e.g. ΛCDM).

- Some marginal statistics (e.g. marginal means, posteriors. . .) are easy to compute.
- More machinery is needed for e.g. nuisance marginalised likelihoods and marginal KL divergences $\mathcal{D}_{\mathrm{KL}}$.



Marginal inference

- Many cosmological likelihoods come with nuisance parameters that have limited relevance for onward inference.
- Notation: GW cosmology

$\mathcal{L}$	Likelihood	(e.g. LAL),
D	Data	(e.g. GW170817),
θ	Cosmological parameters	(e.g. , $H_0\ldots$),
α	Nuisance parameters	(e.g. m_1, $m_2\ldots$),
M	Model	(e.g. ΛCDM).

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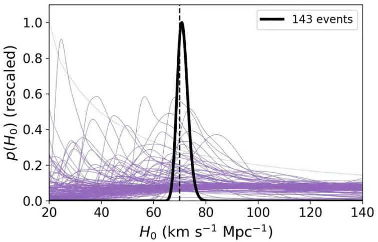

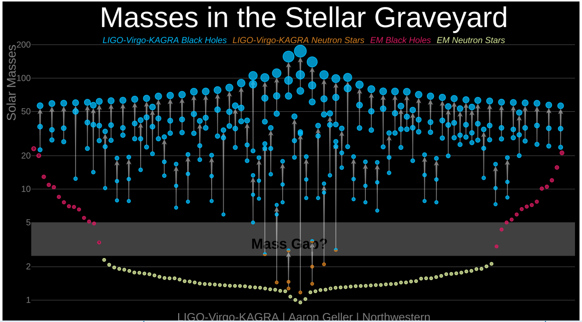

Nuisance marginalised likelihoods: Theory [2207.11457]

- Bayes theorem

$$\mathcal{L}(\theta,\alpha)\times\pi(\theta,\alpha)=\mathcal{P}(\theta,\alpha)\times\mathcal{Z} \qquad (1)$$

Likelihood × Prior = Posterior × Evidence

α: nuisance parameters, θ: cosmo parameters.

- Marginal Bayes theorem

$$\mathcal{L}(\theta)\times\pi(\theta)=\mathcal{P}(\theta)\times\mathcal{Z} \qquad (2)$$

- Non-trivially gives **nuisance-free likelihood**

$$\boxed{\mathcal{L}(\theta)=\frac{\mathcal{P}(\theta)\mathcal{Z}}{\pi(\theta)}}=\frac{\int\mathcal{L}(\theta,\alpha)\pi(\theta,\alpha)d\alpha}{\int\pi(\theta,\alpha)d\alpha} \qquad (3)$$

Key properties

- Given datasets A and B, each with own nuisance parameters α_A and α_B:
- If you use $\mathcal{L}_A(\theta)$, you get the same (marginal) posterior and evidence if you had run with nuisance parameters α_A (ditto B).
- If you run inference on $\mathcal{L}_A(\theta)\times\mathcal{L}_B(\theta)$, you get the same (marginal) posterior and evidence if you had run with all nuisance parameters α_A, α_B on.

  (weak marginal consistency requirements on joint $\pi(\theta,\alpha_A,\alpha_B)$ and marginal priors)

Nuisance marginalised likelihoods: Practice [2205.12841]

Harry Bevins
PhD→JRF

$$\mathcal{L}(\theta) = \frac{\mathcal{P}(\theta)\mathcal{Z}}{\pi(\theta)}$$

- To compute the nuisance marginalised likelihood, need:
  1. Bayesian evidence $\mathcal{Z}$
  2. Marginal prior and posterior **densities**

$\boxed{\mathcal{L}(\theta,\alpha)}$ $\boxed{\pi(\theta,\alpha)}$

1. Bayesian evidence $\mathcal{Z}$: g
   - Nested sampling
   - Parallel tempering (pocomc, ptmcmc)
   - Sequential Monte Carlo (SMC)
   - MCEvidence
2. Marginal prior $\pi(\theta)$ and posterior $\mathcal{P}(\theta)$ densities:
   - Histograms of samples
   - Kernel density estimation
   - Normalising flows / Diffusion models
   - ...

- Emulators usually much faster than original likelihoods
- `margarine`: PyPI, github.com/htjb/margarine

Nuisance marginalised likelihoods: Practice [2205.12841]

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$$\mathcal{L}(\theta) = \frac{\mathcal{P}(\theta)\mathcal{Z}}{\pi(\theta)}$$

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↓ ↓

Nested Sampling

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Harry Bevins

PhD→JRF

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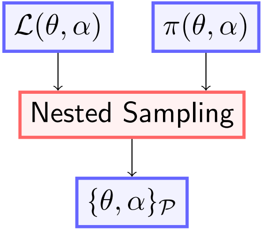

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Nuisance marginalised likelihoods: Practice [2205.12841]

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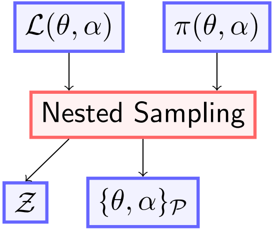

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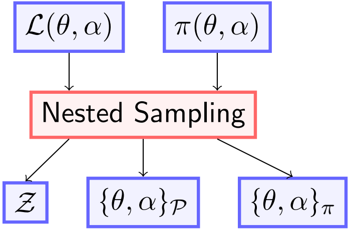

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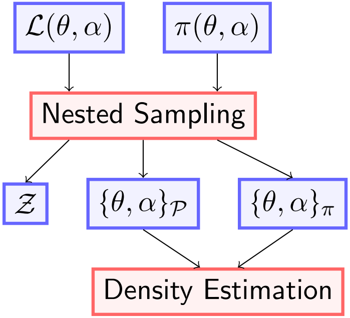

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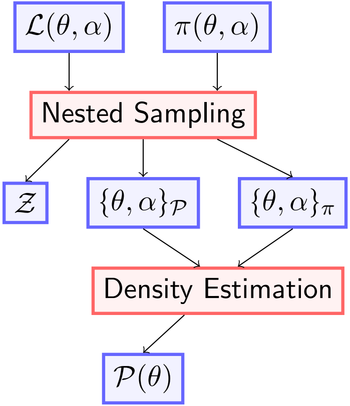

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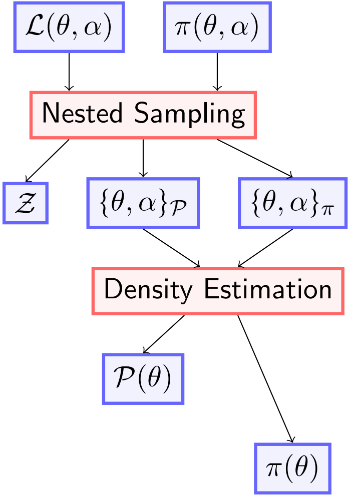

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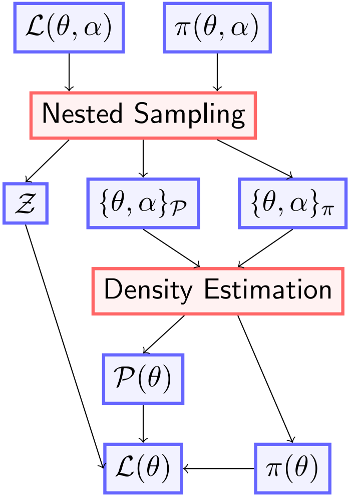

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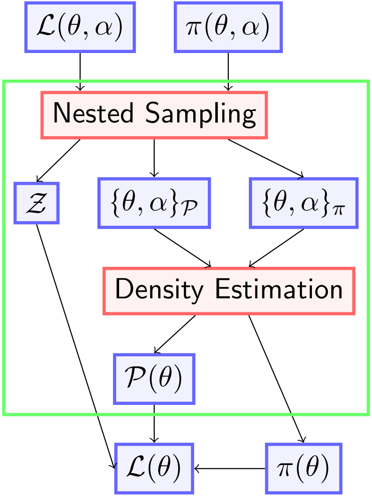

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Nuisance marginalised likelihoods: Example uses

- Library of pre-trained bijectors to be used as priors/emulators/nuisance marginalised likelihoods (DiRAC allocation `unimpeded`)
- e.g. easy to apply a *Planck*/DES/HERA/JWST prior or likelihood to your existing MCMC chains without needing to install the whole cosmology machinery.
- Hierarchical modelling:
  - Usually, have N objects, each with nuisance parameters α_i, and shared parameters of interest θ.
  - Likelihood $\mathcal{L}(\{D_i\}|\theta,\{\alpha_i\}) = \prod_i^N \mathcal{L}_i(D_i|\theta,\alpha_i)$ has $N\times \texttt{len}(\alpha_i) + \texttt{len}(\theta)$ parameters
  - Instead, break problem down into N runs on $\texttt{len}(\theta) + \texttt{len}(\alpha_i)$ parameters, and one final one on $\texttt{len}(\theta)$ parameters, using nuisance marginal likelihoods $\mathcal{L}_i(\theta)$.
  - In addition to computational tractability, also can perform model comparison with nuisance marginalised likelihoods.

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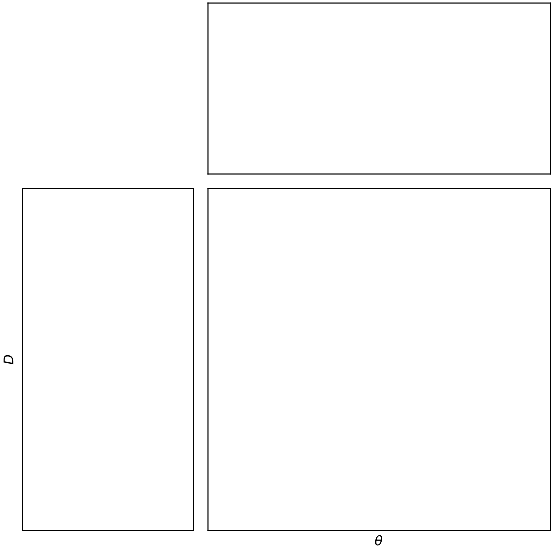

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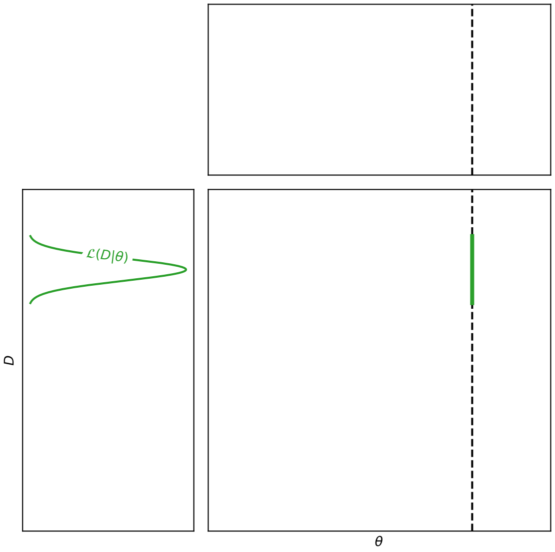

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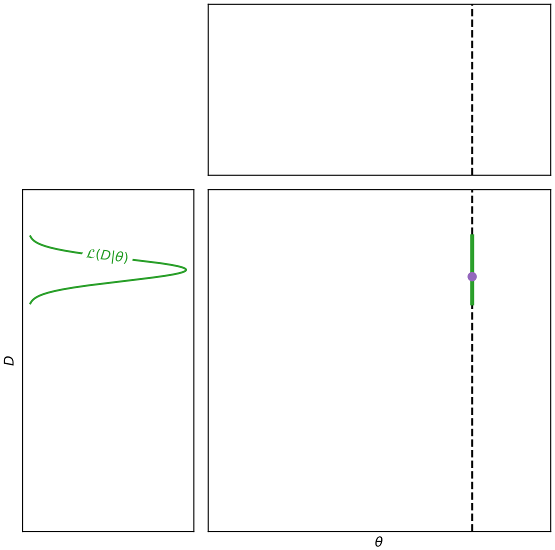

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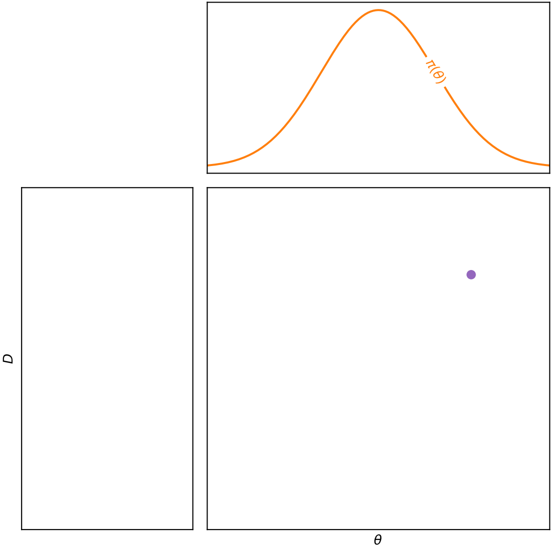

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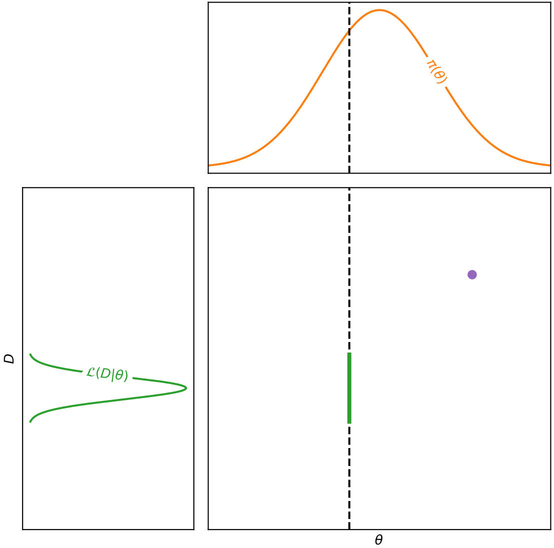

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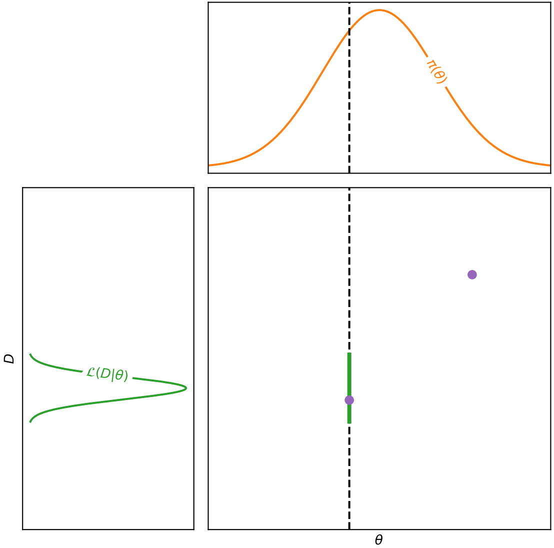

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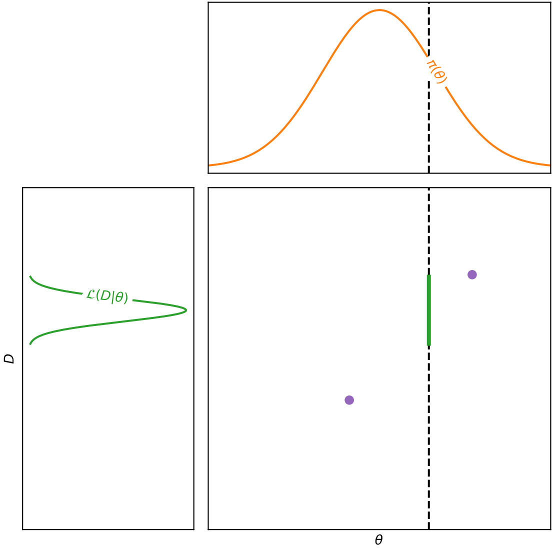

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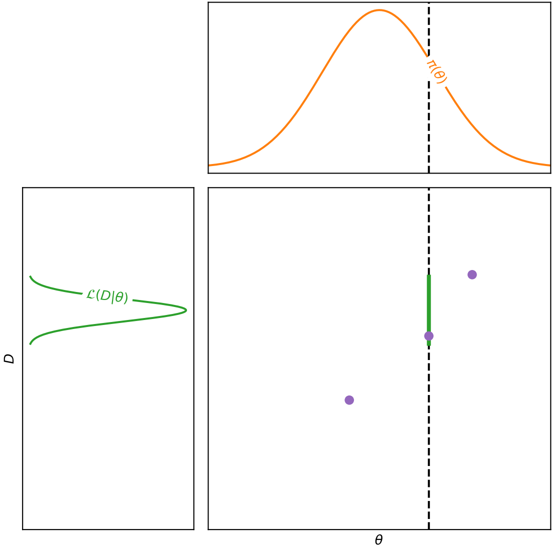

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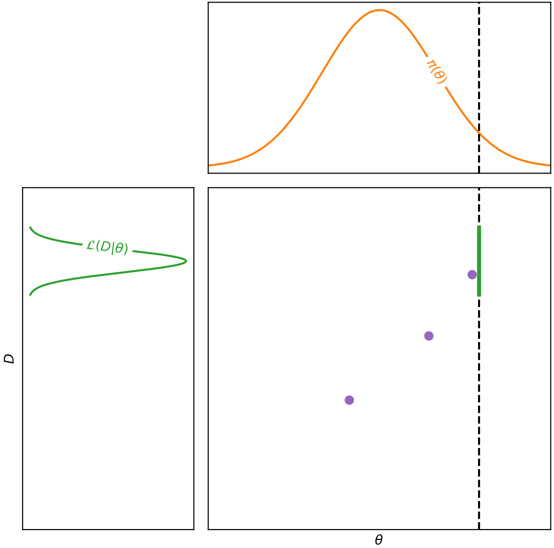

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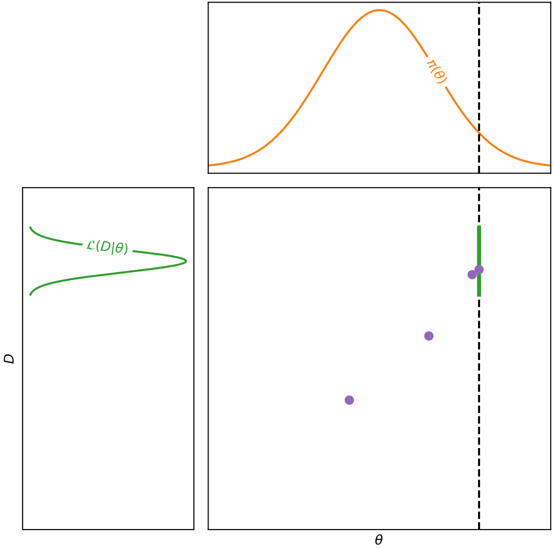

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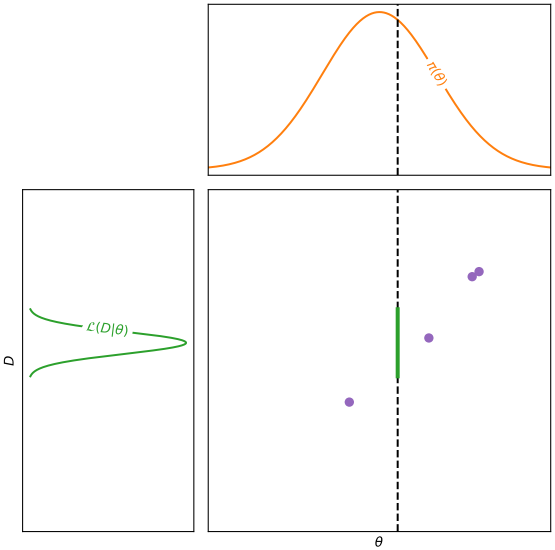

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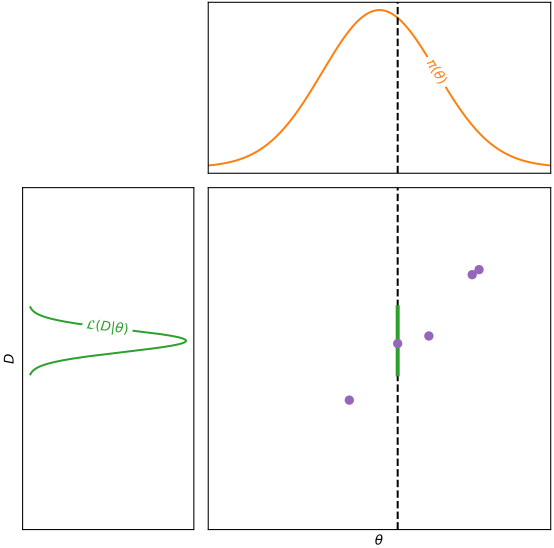

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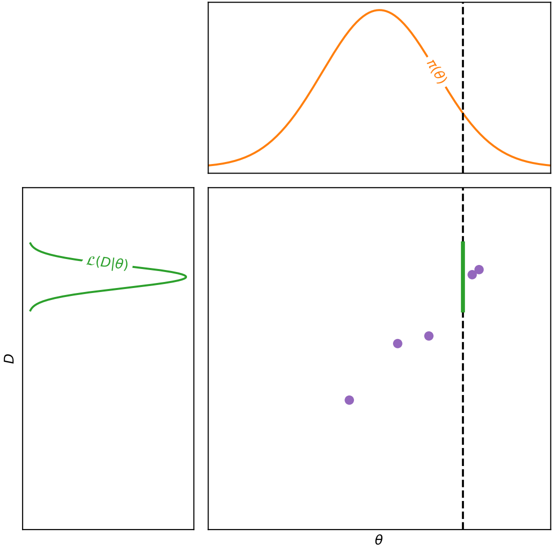

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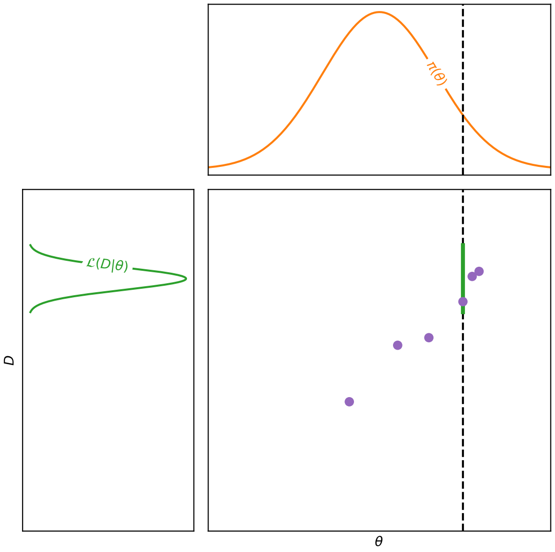

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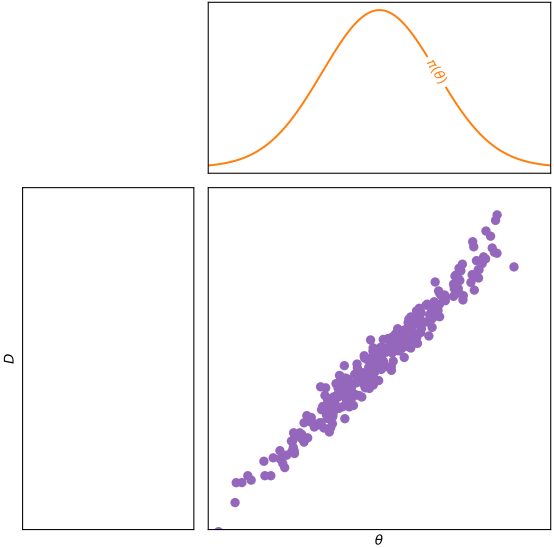

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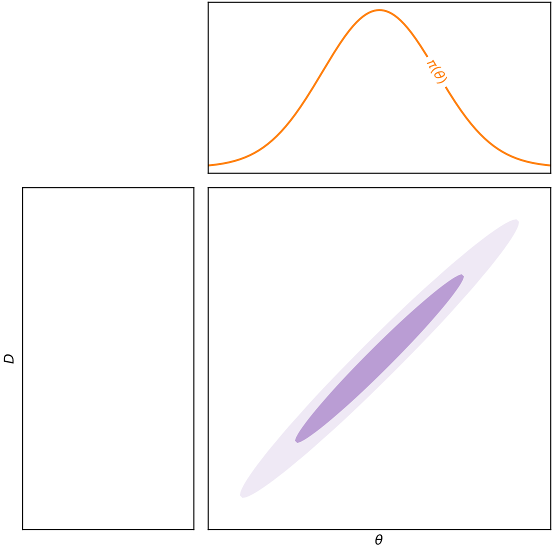

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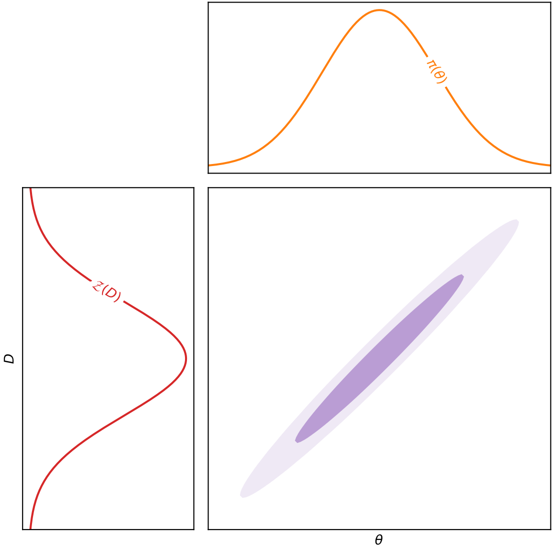
- Only have access to a forward model $\theta \to D$.
- (θ, D) plane gives a more expansive theoretical view of inference.
- Forward model defines *implicit* likelihood $\mathcal{L}$:
- Simulator generates samples from $\mathcal{L}(D|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$ *the "probability of everything"*.
- Task of SBI is then to go from joint $\mathcal{J}$ samples to posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ – and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present SotA: NPE, NLE, NJE, NRE
- SBI & forward modelling force us to think about data space D & parameter space θ.



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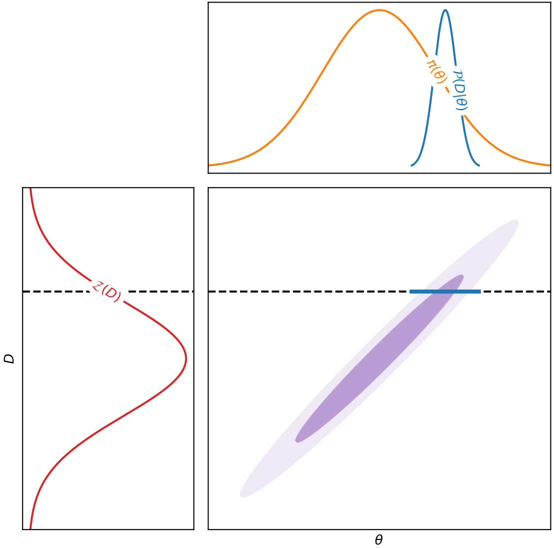

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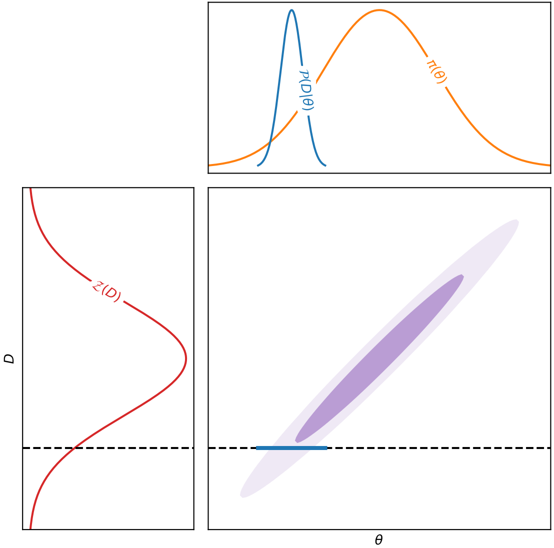

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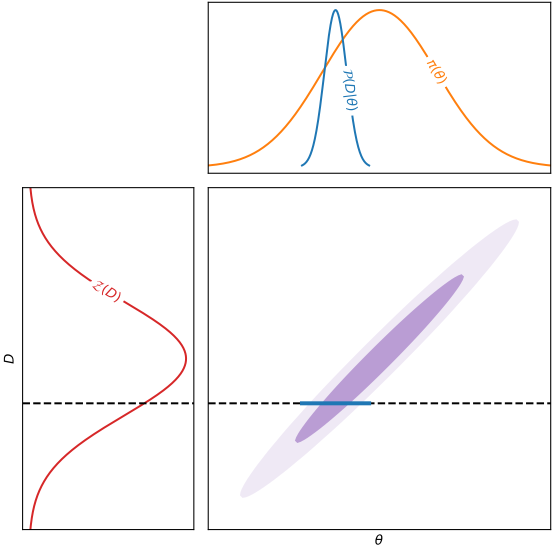

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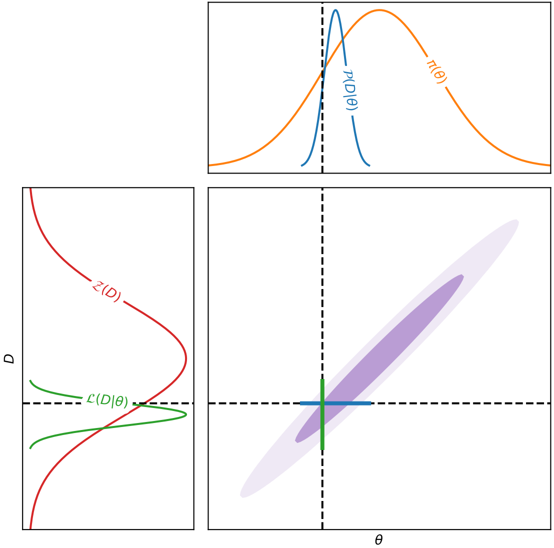
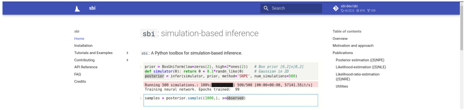


Why SBI?

SBI is useful because:

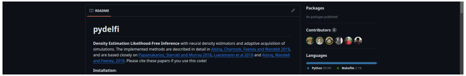
1. If you don't have a likelihood, you can still do inference
    - The usual case beyond CMB cosmology
2. Faster than LBI
    - emulation – also applies to LBI in principle
3. No need to pragmatically encode fiducial cosmologies
    - Covariance computation implicitly encoded in simulations
4. Equips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

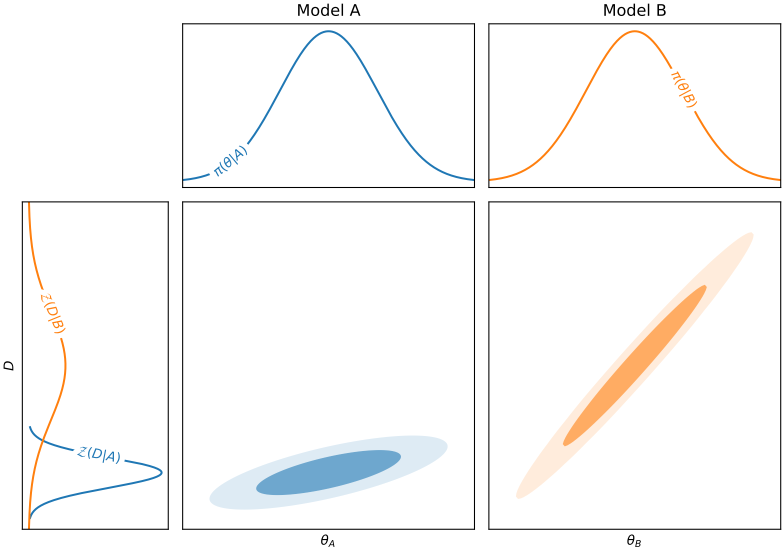
github.com/florent-leclercq/pyselfi



github.com/justinalsing/pydelfi

SBI & model comparison

- Extend: models A and B.
- Each with own separate parameters θ_A and θ_B (can be same).
- The evidence $\mathcal{Z}(D|M)$ compares models
- Occams razor: more predictive $\equiv$ more probable (due to normalisation).



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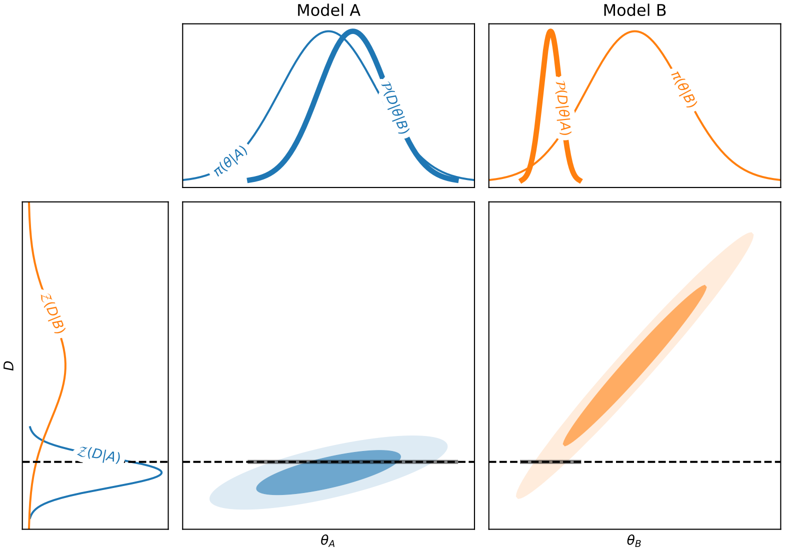

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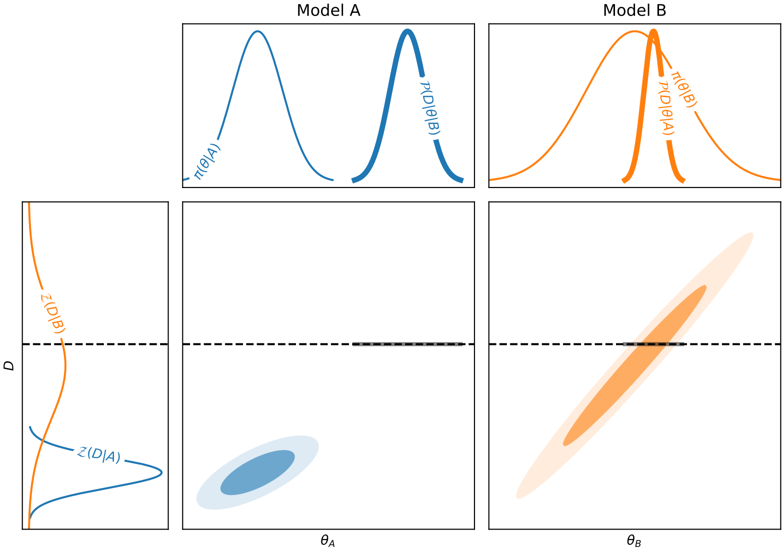


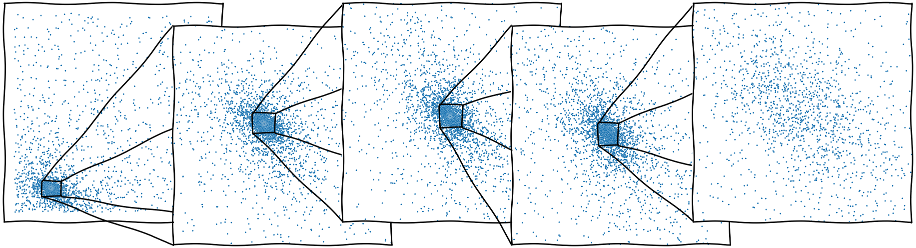
Kilian Scheutwinkel
PhD

Weak SBI

- Use model comparison to choose between likelihoods
- Use flexible likelihood (e.g. unknown noise scale σ, non-gaussian shape, mixture components [1809.04598])
- 21cm [2204.04491], SNe [2312.02075]

Strong SBI

- Develop "likelihood-free nested sampling"
- Use dead points to train NRE
- Replaces/enhances current SotA of truncation techniques



Cosmological forecasting

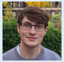
Have you ever done a Fisher forecast, and then felt Bayesian guilt?

- 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.

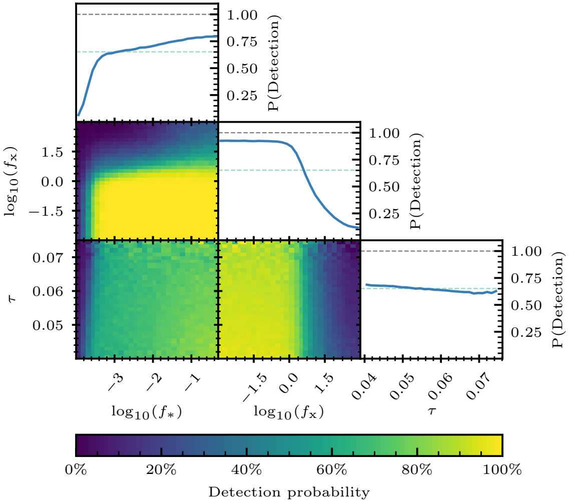
Fully Bayesian Forecasting [2309.06942]

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.
- 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`



Conclusions

github.com/handley-lab

Covered a suite of tools for next-generation "generative cosmology"

- Nested sampling for cosmological...
  - model comparison
  - parameter estimation
  - tension quantification
- Nuisance-marginalised cosmology $\boxed{\mathcal{L}(\theta) = \frac{\mathcal{P}(\theta)\mathcal{Z}}{\pi(\theta)}}$
- Simulation-based inference
- Fully Bayesian forecasting