Nested sampling: powering next-generation inference and machine learning tools for astrophysics, cosmology, particle physics and beyond

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UNIVERSITY OF CAMBRIDGE



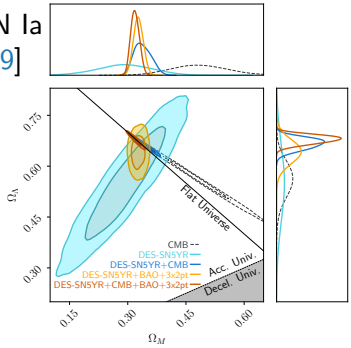
LBI: Likelihood-based inference

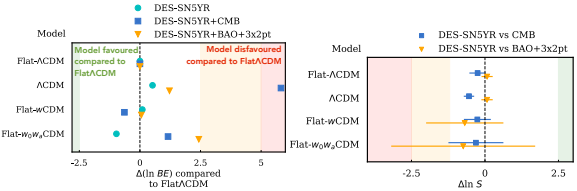
The standard approach if you are fortunate enough to have a likelihood function $P(D|\theta)$:

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

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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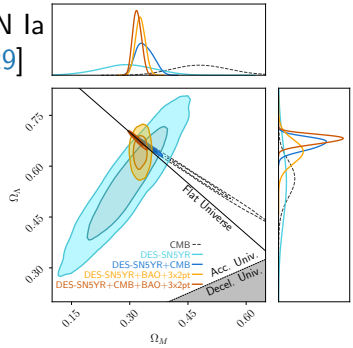

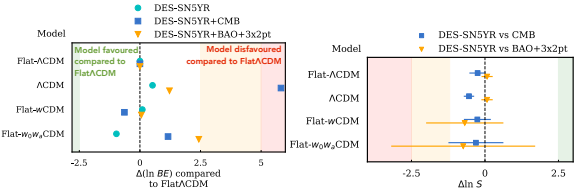

LBI: Likelihood-based inference

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

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

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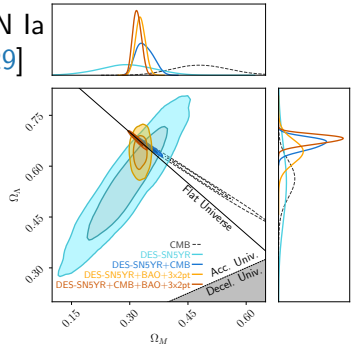

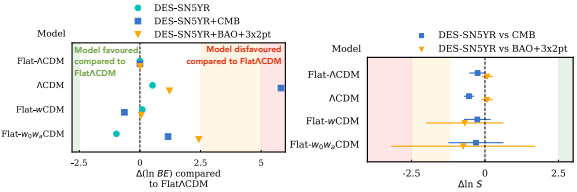

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$$P(\theta|D)P(D) = P(\theta, D) = P(D|\theta)P(\theta),$$

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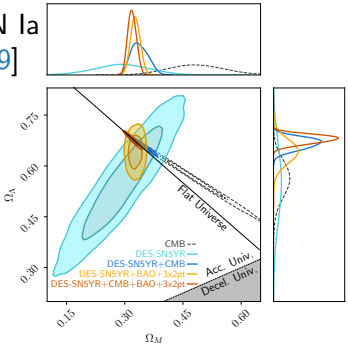

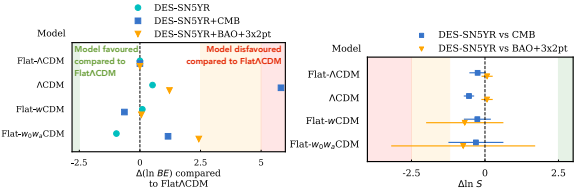

LBI: Likelihood-based inference

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

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

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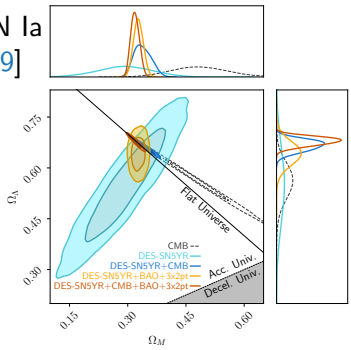
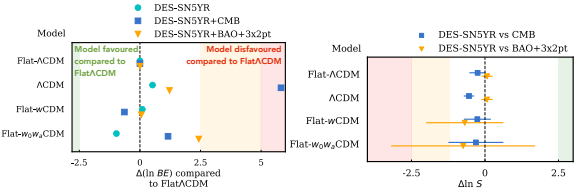


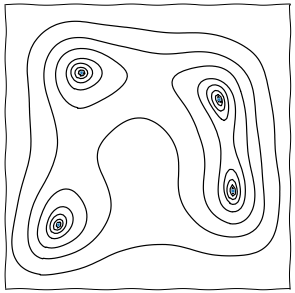


What is Nested Sampling?

- 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:

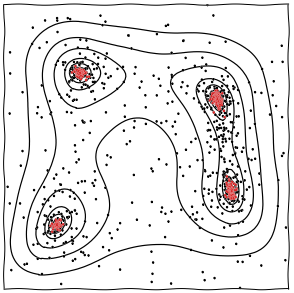
Optimisation

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



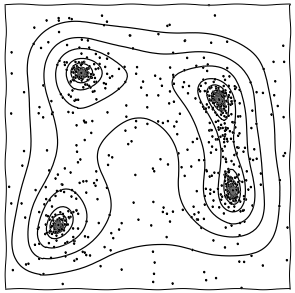
Exploration

draw/sample $\quad \theta \sim f$



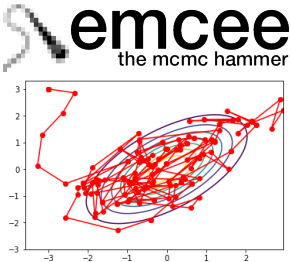
Integration

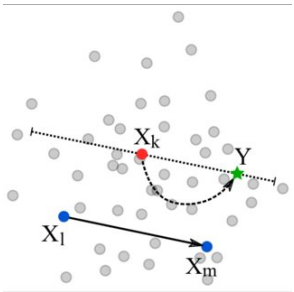
$$\int f(\theta) dV$$

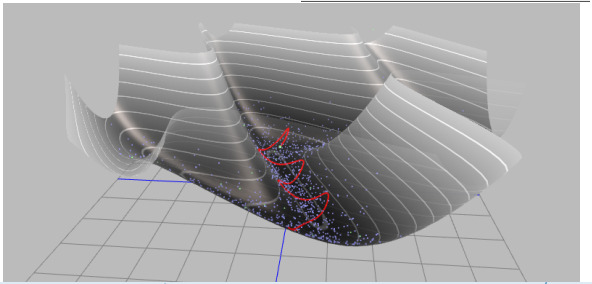


Where is Nested Sampling?

- For many purposes, in your Neural Net you should group Nested Sampling with (MCMC) techniques such as:
  - Metropolis-Hastings (PyMC, MontePython)
  - Hamiltonian Monte Carlo (Stan, blackjax)
  - Ensemble sampling (emcee, zeus).
  - Variational Inference (Pyro)
  - Sequential Monte Carlo
  - Thermodynamic integration
  - Genetic algorithms
- You may have heard of it branded form:
  - MultiNest
  - PolyChord
  - dynesty
  - ultranest







Integration in Physics

- Integration is a fundamental concept in physics, statistics and data science:

Partition functions

$$Z(\beta) = \int e^{-\beta H(q,p)} dq dp$$

Path integrals

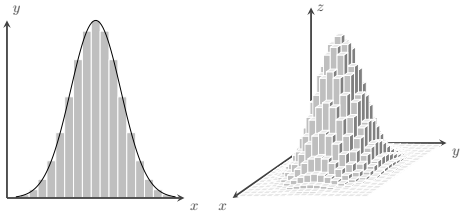
$$\Psi = \int e^{iS} \mathcal{D}x$$

Bayesian marginals

$$\mathcal{Z}(D) = \int \mathcal{L}(D|\theta)\pi(\theta) d\theta$$

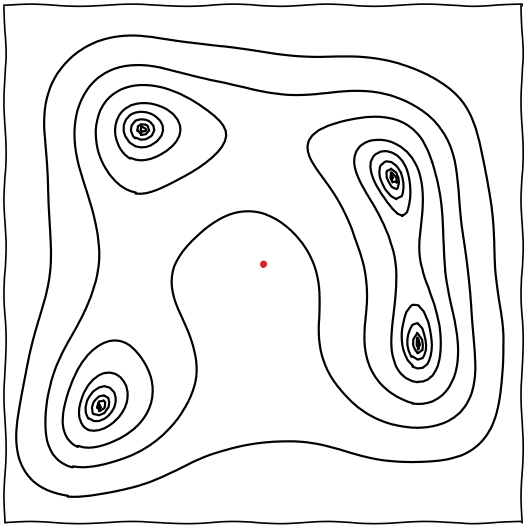
- Need numerical tools if analytic solution unavailable.
- High-dimensional numerical integration is hard.
- Riemannian strategy estimates volumes geometrically:

$$\int f(x) d^n x \approx \sum_i f(x_i) \Delta V_i \sim \mathcal{O}(e^n)$$



- Curse of dimensionality $\Rightarrow$ exponential scaling.

MCMC



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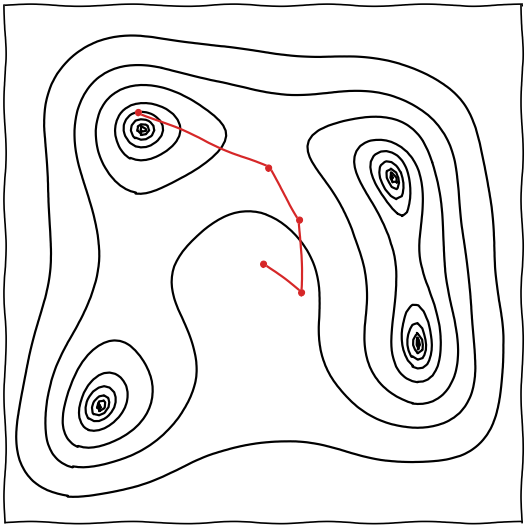

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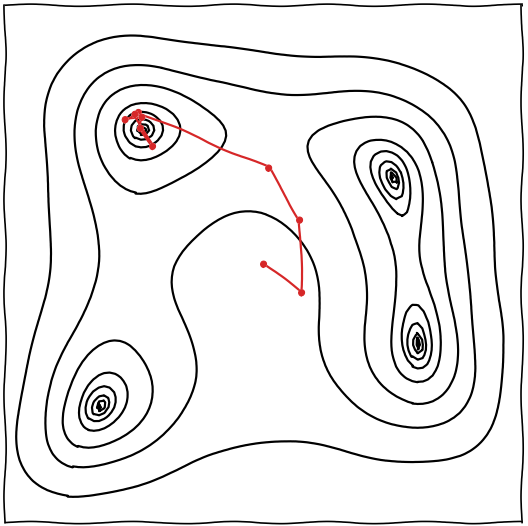

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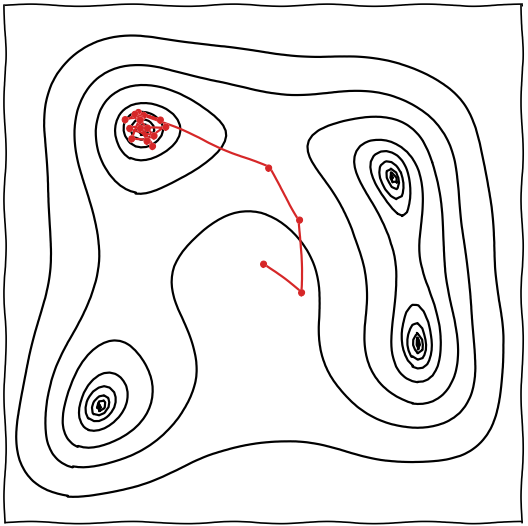

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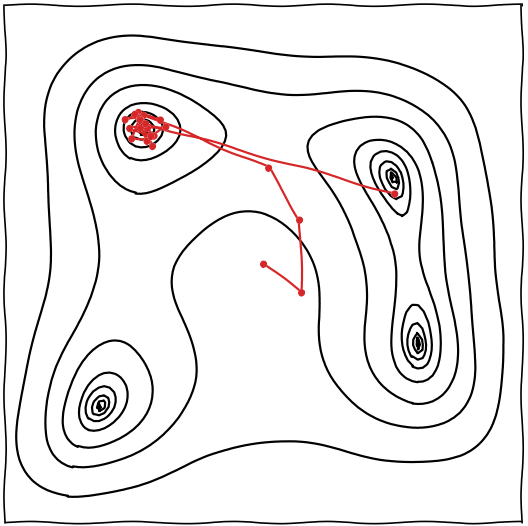

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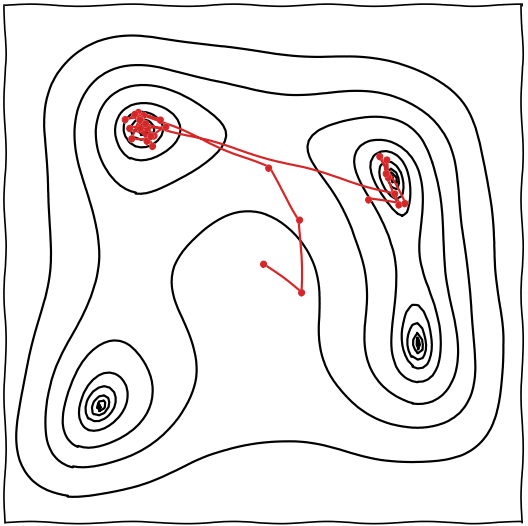

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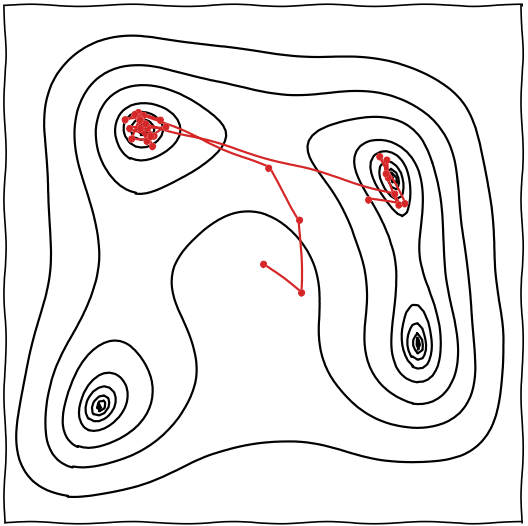

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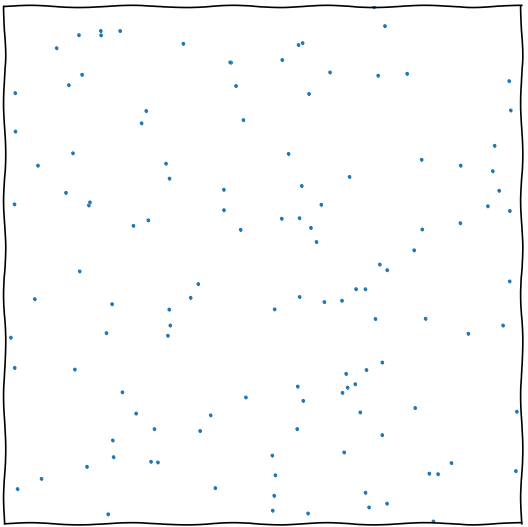

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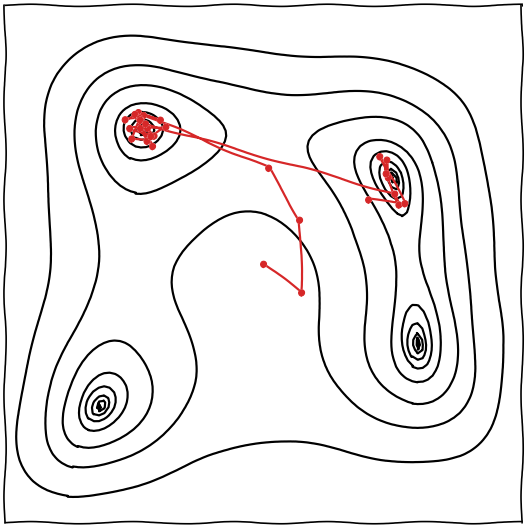

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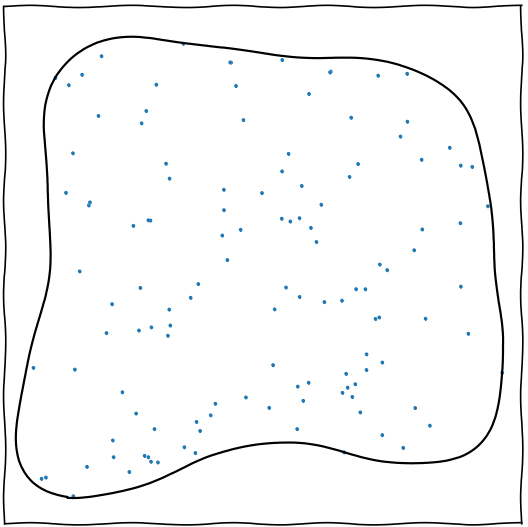

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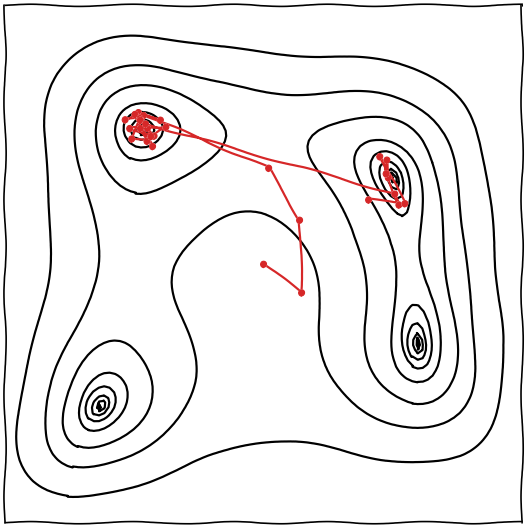

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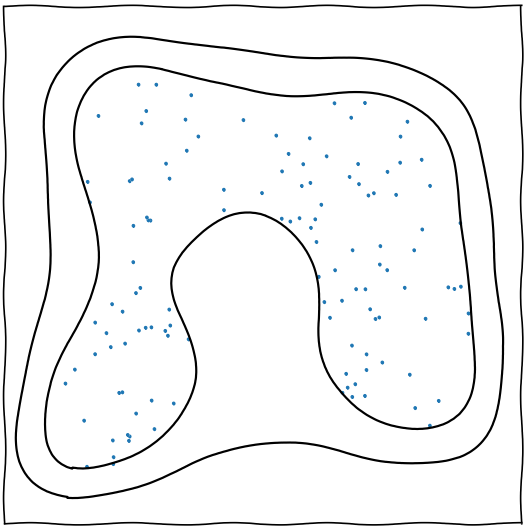

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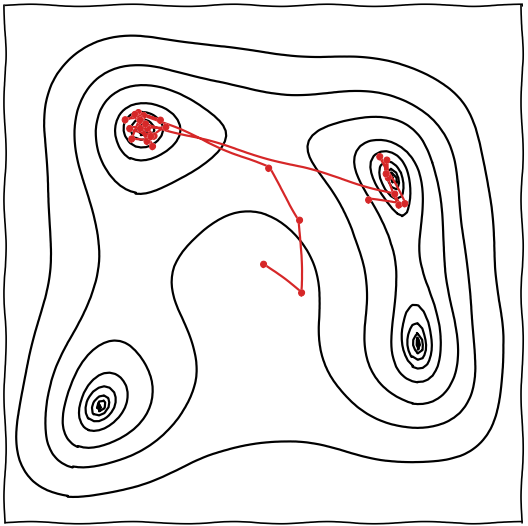

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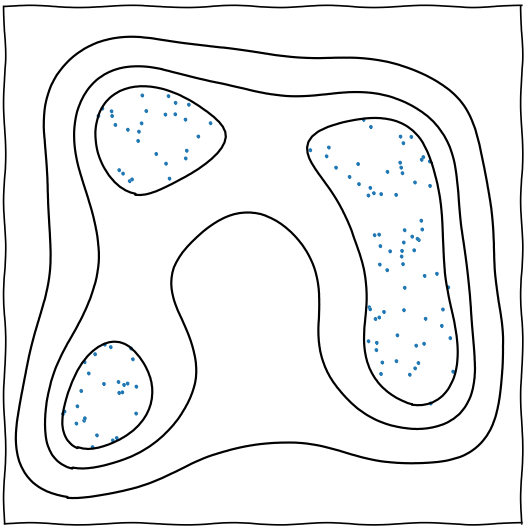

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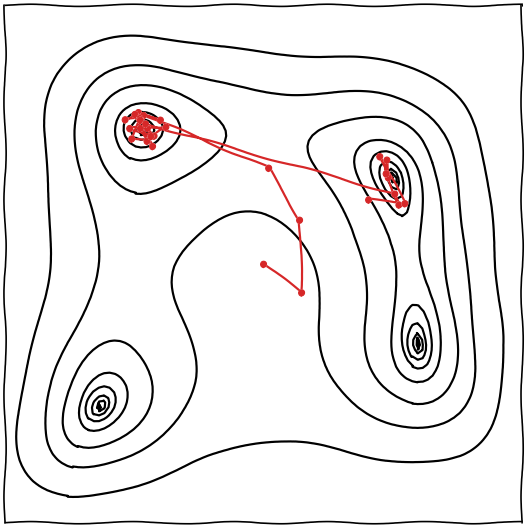

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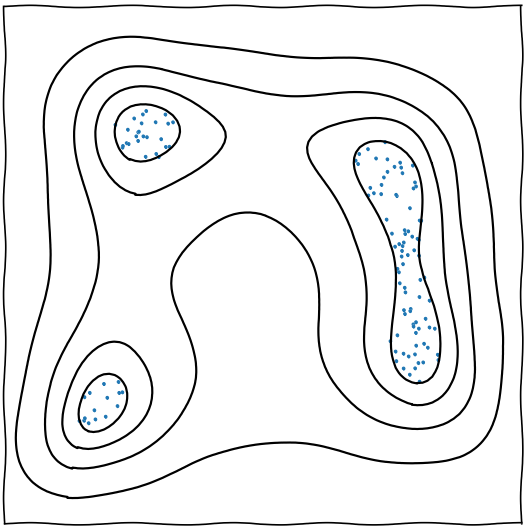

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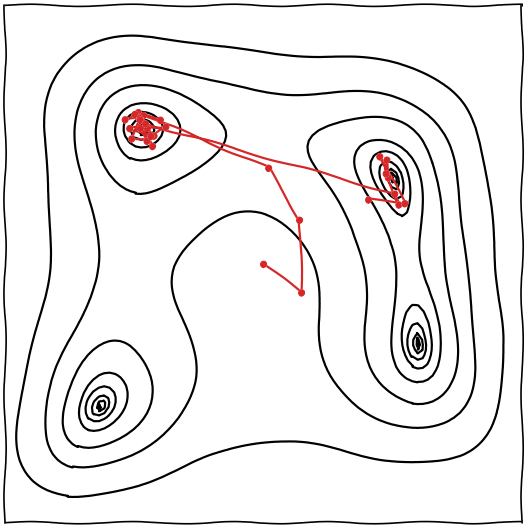

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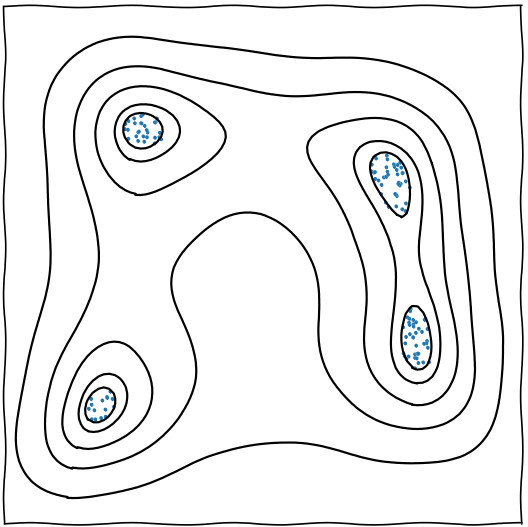

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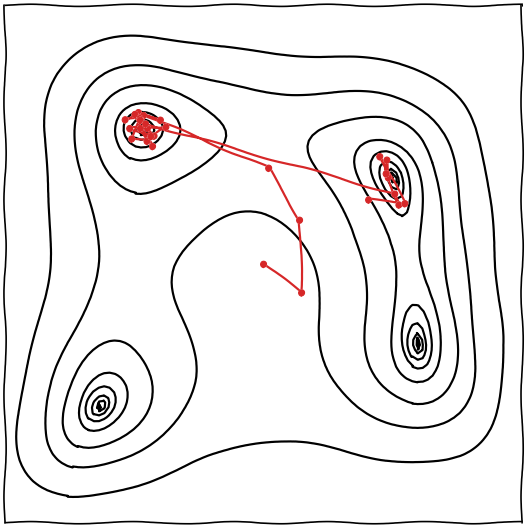

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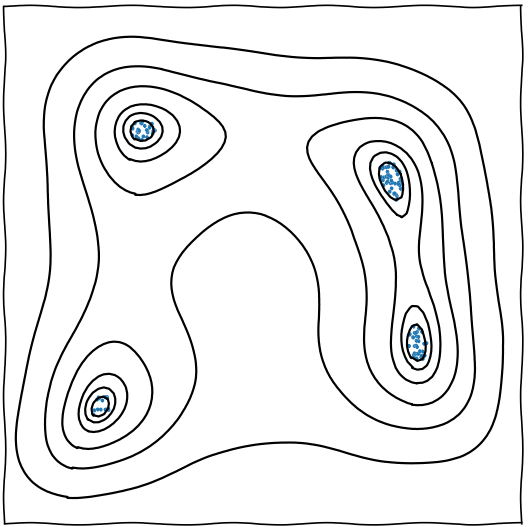

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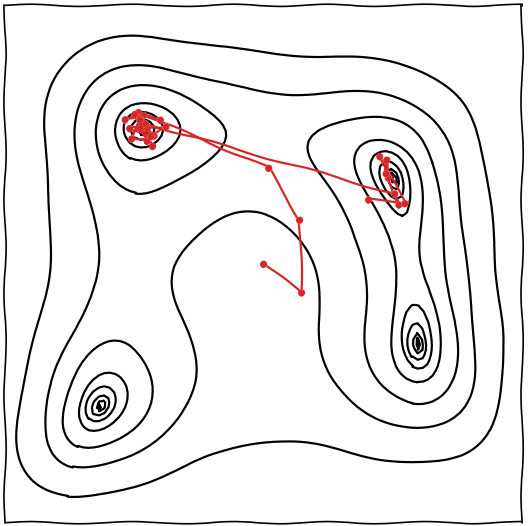

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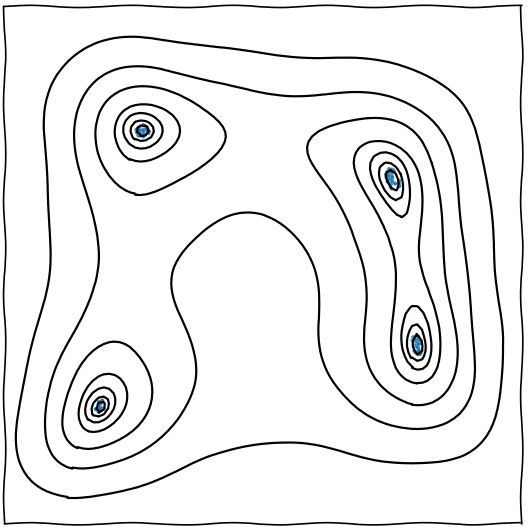

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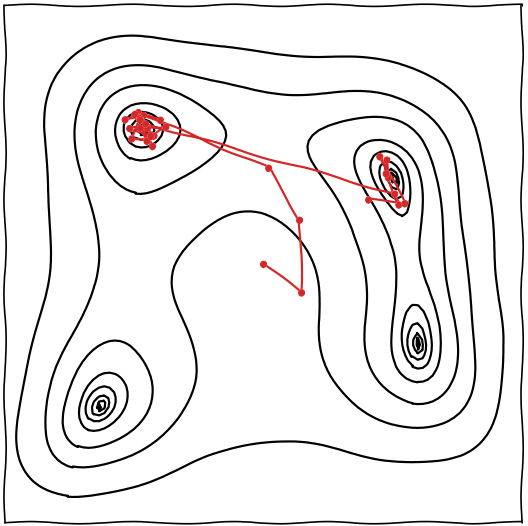

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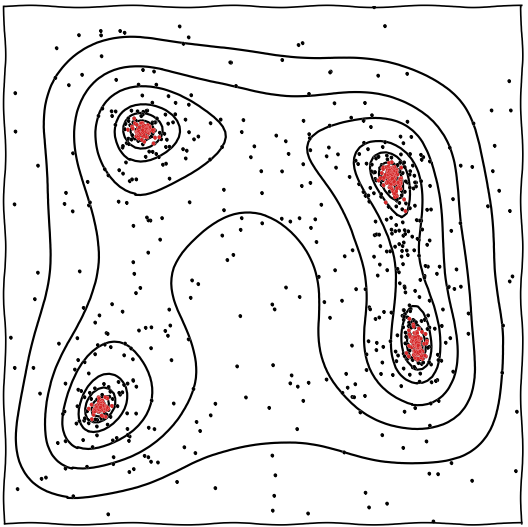
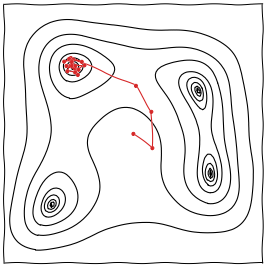


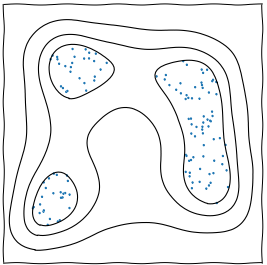
MCMC

- Single "walker"
- Explores posterior
- Fast, if proposal matrix is tuned
- Parameter estimation, suspiciousness calculation
- Channel capacity optimised for generating posterior samples



Nested sampling

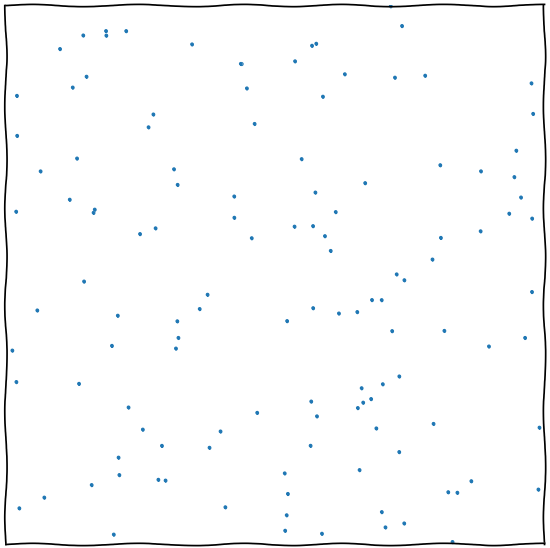
- Ensemble of "live points"
- Scans from prior to peak of likelihood
- Slower, no tuning required
- Parameter estimation, model comparison, tension quantification
- Channel capacity optimised for computing partition function



The nested sampling meta-algorithm: live points

- Start with n random samples over the space.
- 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.
- We can use this evolution to estimate volume *probabilistically*.
- At each iteration, the contours contract by $\sim \frac{1}{n}$ of their volume.
- This is an exponential contraction, so

$$\int f(x)dV \approx \sum_i f(x_i)\Delta V_i, \quad V_i = V_0 e^{-i/n}$$



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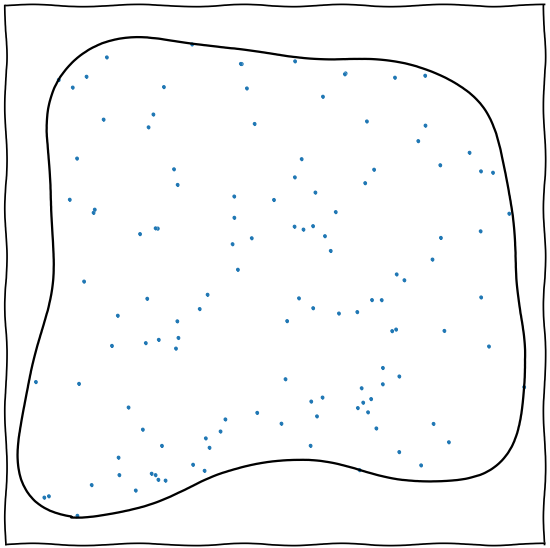

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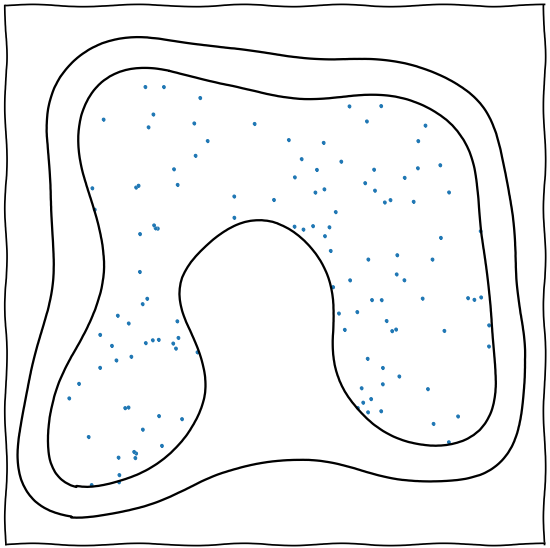

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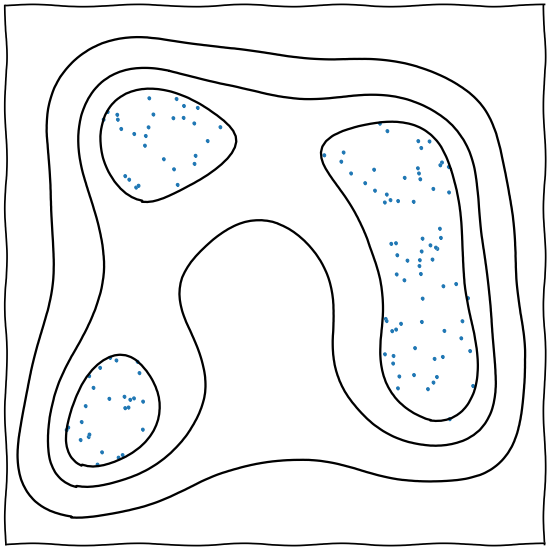

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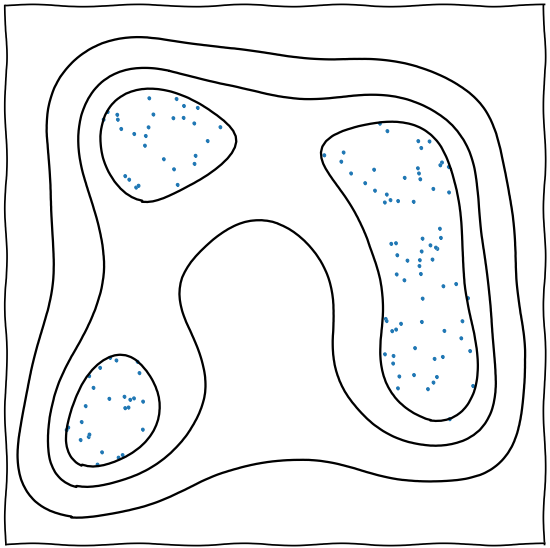
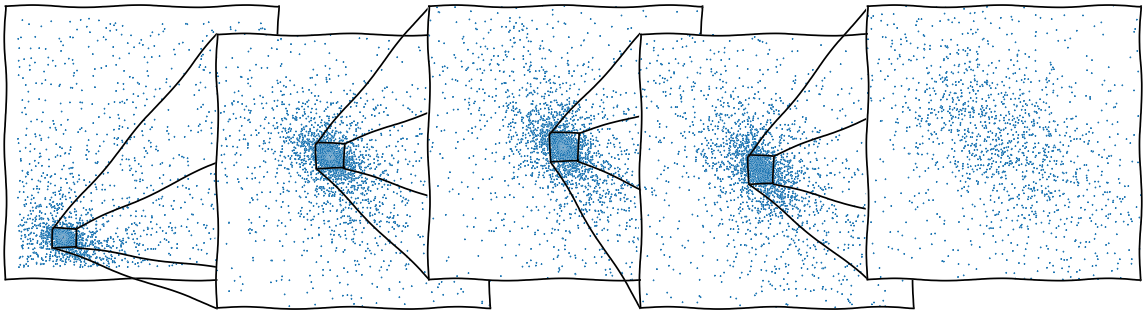
- At each iteration, the contours contract by $\sim \frac{1}{n} \pm \frac{1}{n}$ of their volume.
- This is an exponential contraction, so

$$\int f(x)dV \approx \sum_i f(x_i)\Delta V_i, \quad V_i = V_0 e^{-(i \pm \sqrt{i})/n}$$



The nested sampling meta-algorithm: dead points



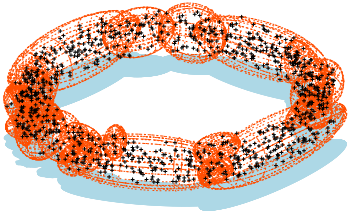
- At the end, one is left with a set of discarded "dead" points.
- Dead points have a unique scale-invariant distribution $\propto \frac{dV}{V}$.
- Uniform over original region, exponentially concentrating on region of interest (until termination volume).
- Good for training emulators (HERA [2108.07282]).

Applications

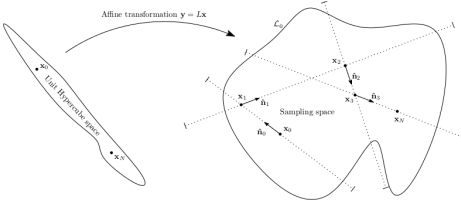
- training emulators.
- gridding simulations
- beta flows
- "dead measure"

Implementations of Nested Sampling [2205.15570](NatReview)

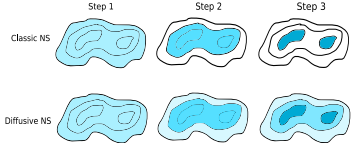
MultiNest [0809.3437]



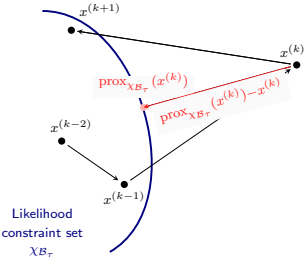
PolyChord [1506.00171]



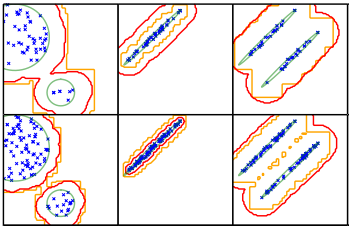
DNest [1606.03757]



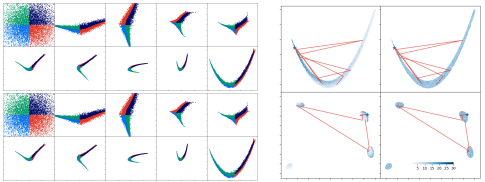
ProxNest [2106.03646]



UltraNest [2101.09604]



NeuralNest [1903.10860]



nessai [2102.11056]

nora [2305.19267]

jaxnest [2012.15286]

nautilus [2306.16923]

dynesty [1904.02180]

Types of nested sampler

- Broadly, most nested samplers can be split into how they create new live points.
- i.e. how they sample from the hard likelihood constraint $\{\theta \sim \pi : \mathcal{L}(\theta) > \mathcal{L}_*\}$.

Rejection samplers

- e.g. `MultiNest`, `UltraNest`.
- Constructs bounding region and draws many invalid points until $\mathcal{L}(\theta) > \mathcal{L}_*$.
- Efficient in low dimensions, exponentially inefficient $\sim \mathcal{O}(e^{d/d_0})$ in high $d > d_0 \sim 10$.

Chain-based samplers

- e.g. `PolyChord`, `ProxNest`.
- Run Markov chain starting at a live point, generating many valid (correlated) points.
- Linear $\sim \mathcal{O}(d)$ penalty in decorrelating new live point from the original seed point.

- Nested samplers usually come with:
  - *resolution* parameter n_{live} (which improve results as $\sim \mathcal{O}(n_{\text{live}}^{-1/2})$.
  - set of *reliability* parameters [2101.04525], which don't improve results if set arbitrarily high, but introduce systematic errors if set too low.
  - e.g. `Multinest` efficiency `eff` or `PolyChord` chain length n_{repeats}.

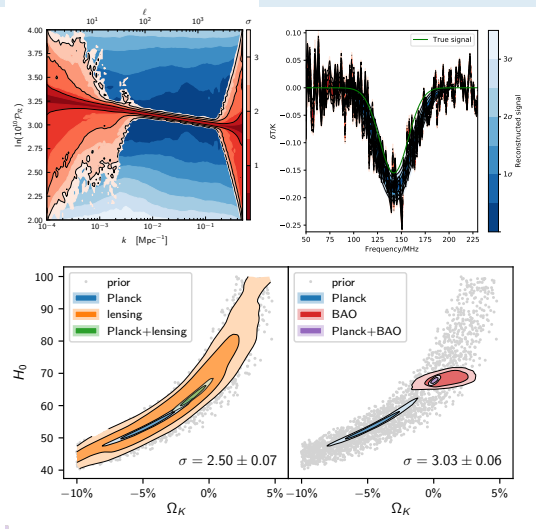
Applications of nested sampling

Cosmology

Adam Ormondroyd

PhD

- 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.

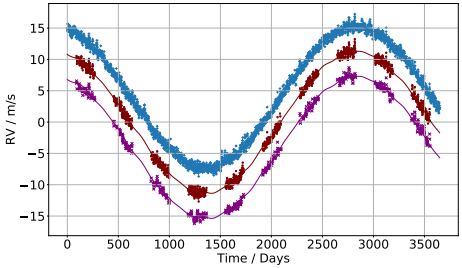


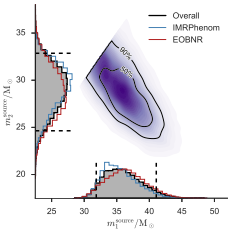
Applications of nested sampling

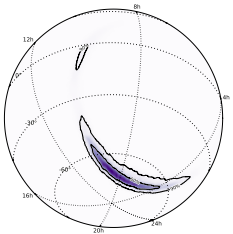
Astrophysics

Metha Prathaban
PhD

- In exoplanets [1806.00518]
  - Parameter estimation: determining properties of planets.
  - Model comparison: how many planets? Stellar modelling [2007.07278].
  - exoplanet problems regularly have posterior phase transitions [2102.03387]
- In gravitational waves
  - Parameter estimation: Binary merger properties
  - Model comparison: Modified theories of gravity, selecting phenomenological parameterisations [1803.10210]
  - Likelihood reweighting: fast slow properties





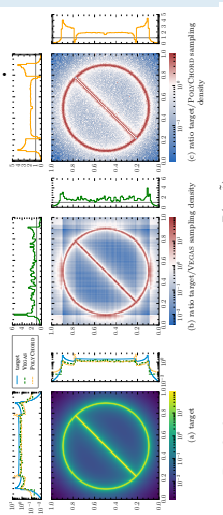


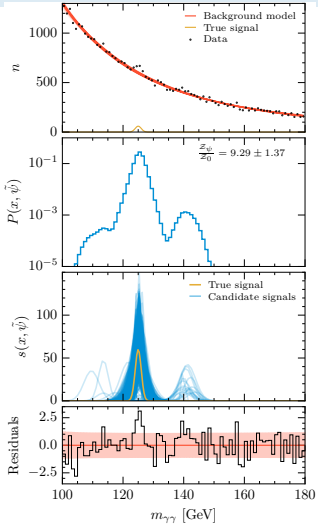
Applications of nested sampling

Particle physics

David Yallup
PDRA

- Nested sampling for cross section computation/event generation $\sigma = \int_\Omega d\Phi |\mathcal{M}|^2$.
- Nested sampling can explore the phase space Ω and compute integral blind with comparable efficiency to HAAG/RAMBO [2205.02030].
- Bayesian sparse reconstruction [1809.04598] applied to bump hunting allows evidence-based detection of signals in phenomenological backgrounds [2211.10391].
- Fine tuning quantification
- Fast estimation of small p-values [2106.02056](PRL), just make switch: $X \leftrightarrow p$, $\mathcal{L} \leftrightarrow \lambda$, $\theta \leftrightarrow x$.





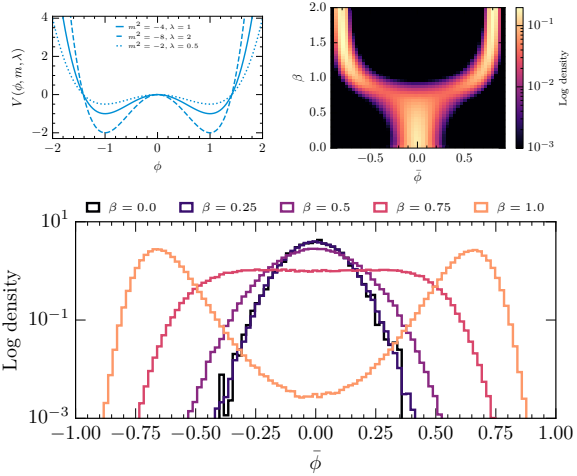
David Yallup

PDRA

- Consider standard field theory Lagrangian:

$$Z(\beta) = \int D\phi e^{-\beta S(\phi)}, \quad S(\phi) = \int dx^{\mu} \mathcal{L}(\phi)$$

- Discretize onto spacetime grid.
- Compute partition function
- NS unique traits:
  - Get full partition function for free
  - allows for critical tuning
  - avoids critical slowing down
- Applications in lattice gravity, QCD, condensed matter physics

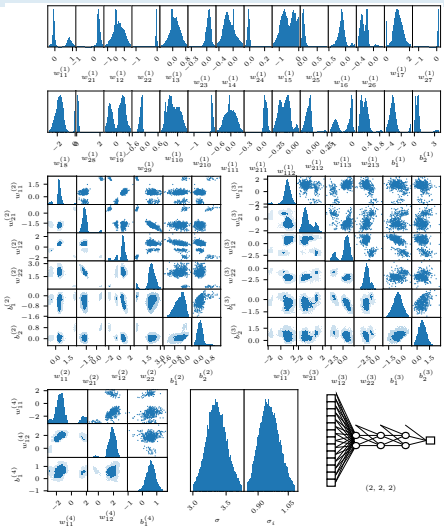


Applications of nested sampling

Machine learning

Kamran Javid
PDRA

- Machine learning requires:
  - Training to find weights
  - Choice of architecture/topology/hyperparameters
- Bayesian NNs treat training as a model fitting problem
- Compute posterior of weights (parameter estimation), rather than optimisation (gradient descent)
- Use evidence to determine best architecture (model comparison), correlates with out-of-sample performance!
- Solving the full "shallow learning" problem without compromise [2004.12211][2211.10391].
  - Promising work ongoing to extend this to transfer learning and deep nets.
- More generally, dead points are optimally spaced for training traditional ML approaches e.g. [2309.05697]

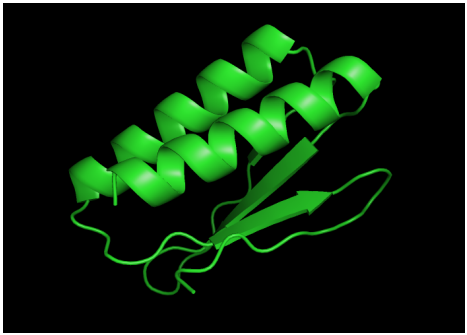


Applications of nested sampling

And beyond...

Catherine Watkinson
Senior Data Scientist

- Techniques have been spun-out (PolyChord Ltd) to:
- Protein folding
  - Navigating free energy surface.
  - Computing misfolds.
  - Thermal motion.
- Nuclear fusion reactor optimisation
  - multi-objective.
  - uncertainty propagation.
- Telecoms & DSTL research (MIDAS)
  - Optimising placement of transmitters/sensors.
  - Maximum information data acquisition strategies.



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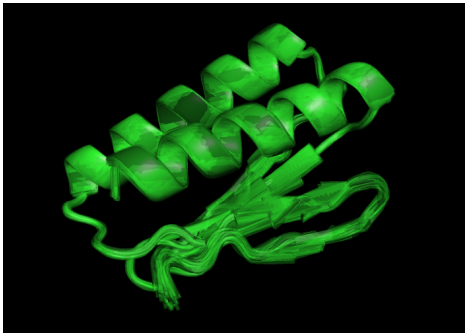

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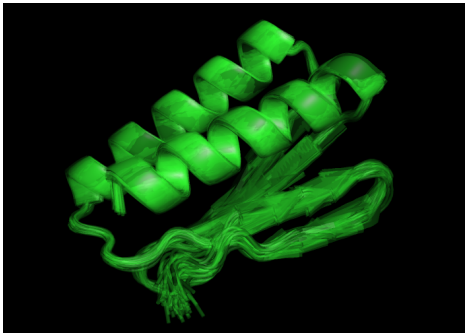

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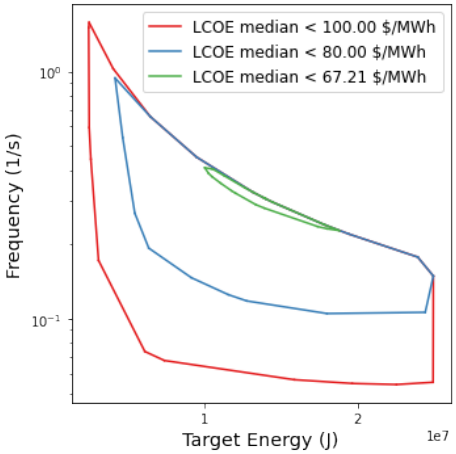

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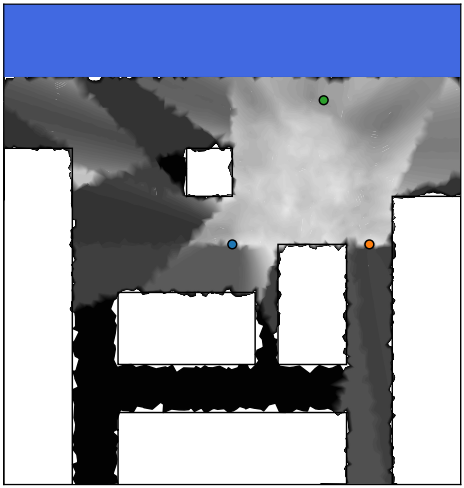

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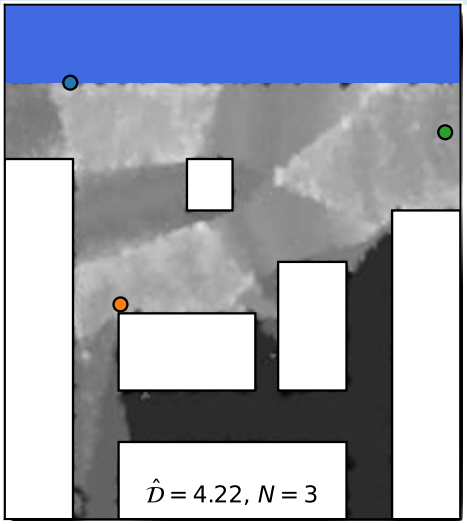

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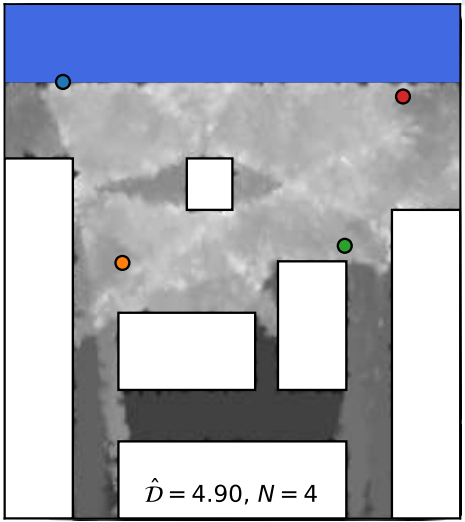

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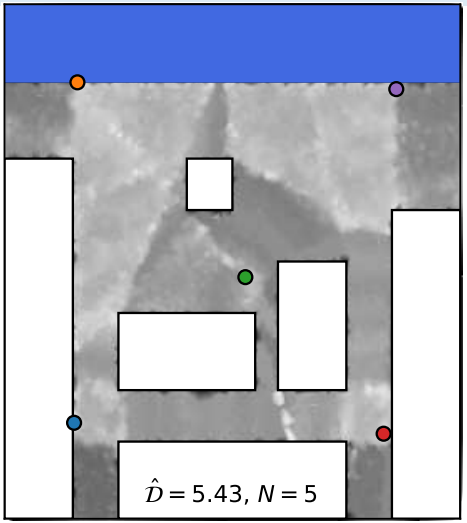
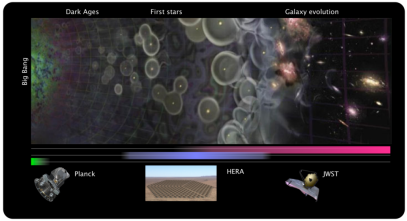
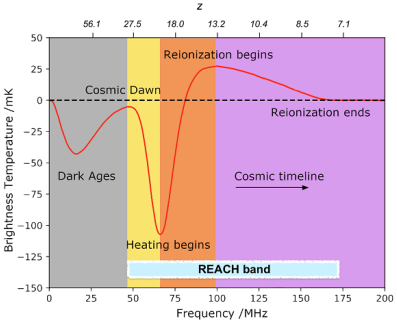


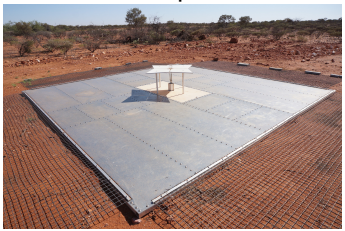
REACH: Global 21cm cosmology [2210.07409](NatAstro)

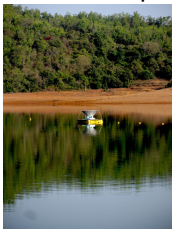
Ian Roque
PhD

- Imaging the universal dark ages using CMB backlight.
- 21cm hyperfine line emission from neutral hydrogen.
- Global experiments measure monopole across frequency.
- Challenge: science hidden in foregrounds $\sim 10^4 \times$signal.
- Lead data analysis team (REACH first light in January)
- Nested sampling woven in from the ground up (calibrator, beam modelling, signal fitting, likelihood selection).
- All treated as parameterised model comparison problems.



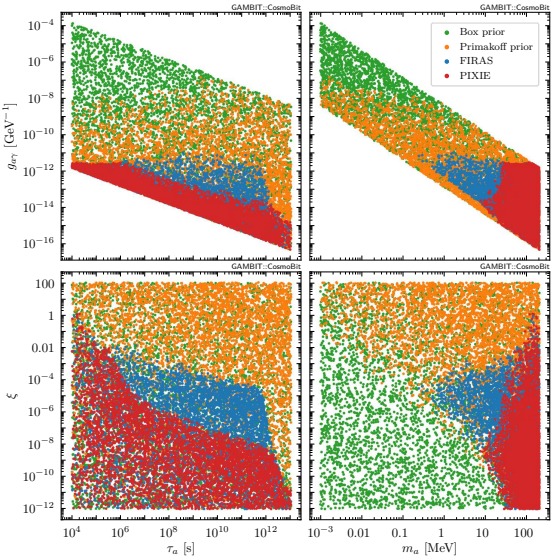






GAMBIT: combining particle physics & cosmological data

- Multinational team of particle physicists, cosmologists and statisticians.
- Combine cosmological data, particle colliders, direct detection, & neutrino detectors in a statistically principled manner [2205.13549].
- Lead Cosmo/Dark Matter working group [2009.03286].
- Nested sampling used for global fitting, and fine-tuning quantification [2101.00428]



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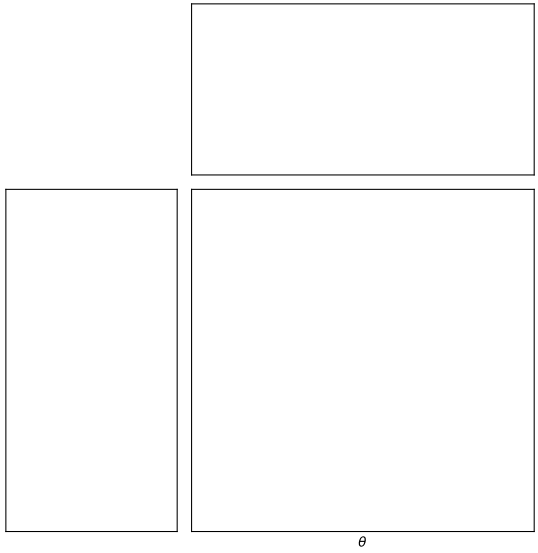

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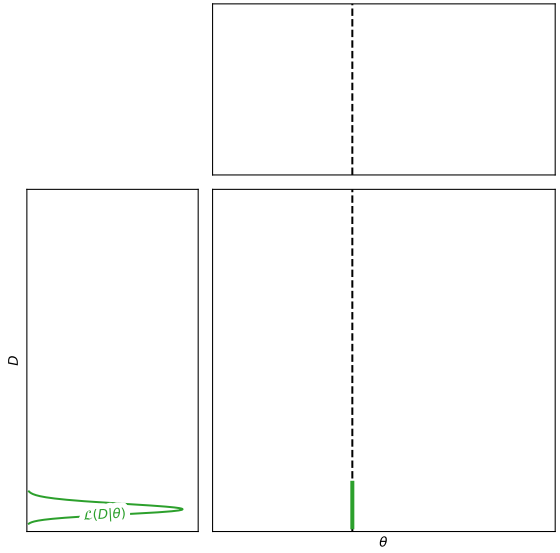

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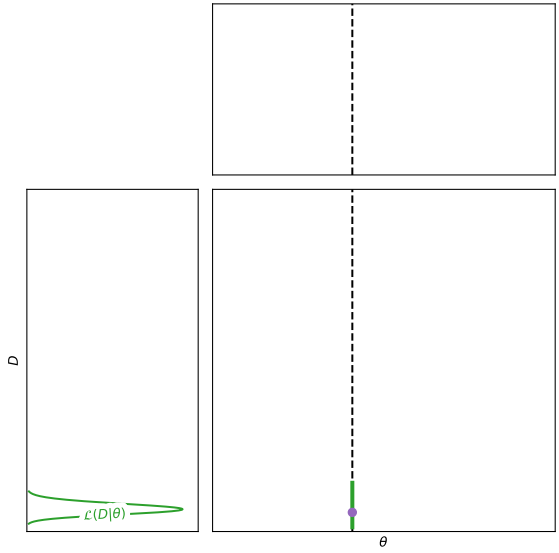

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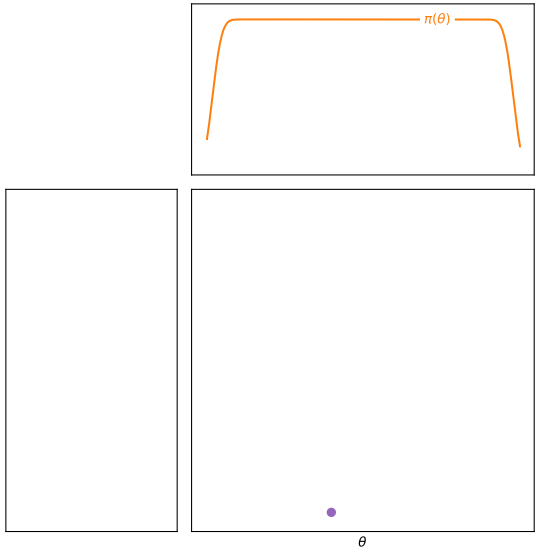

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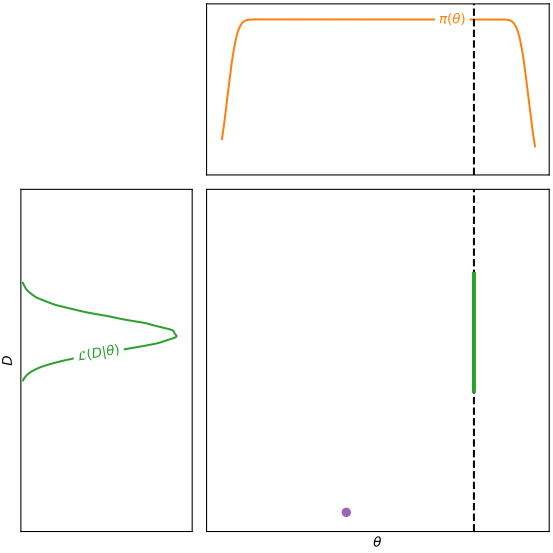

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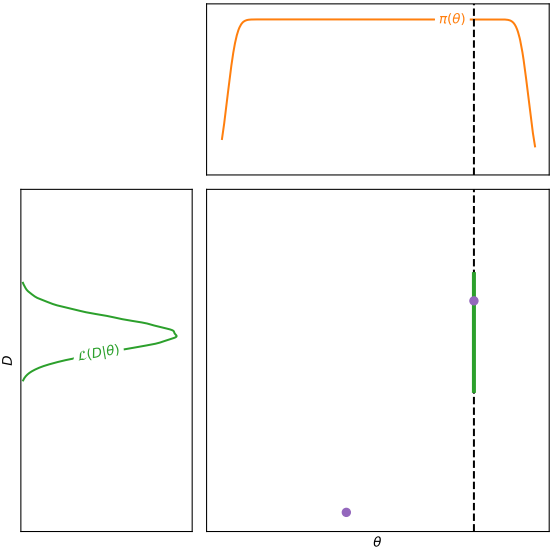

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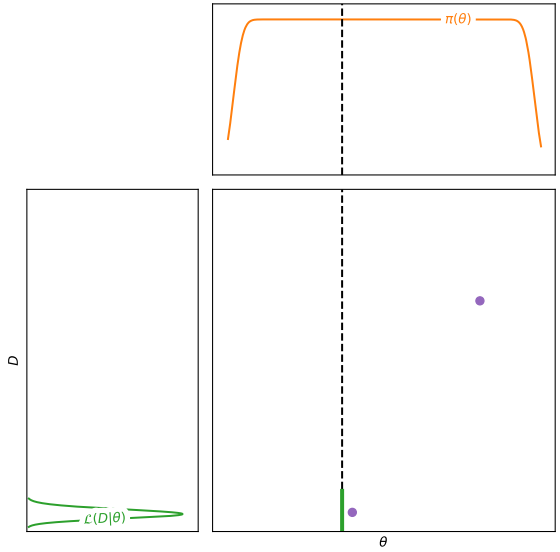

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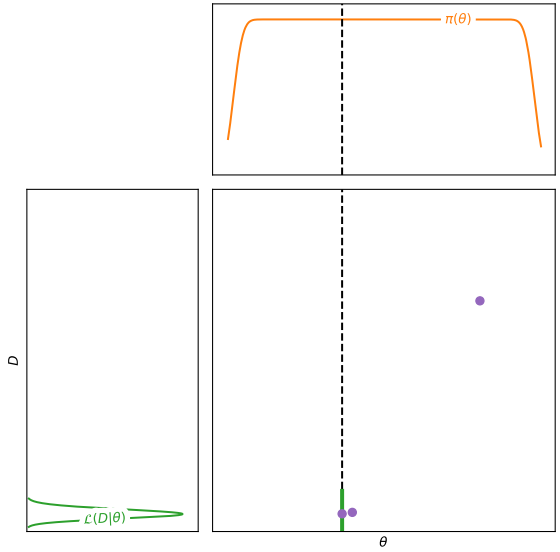

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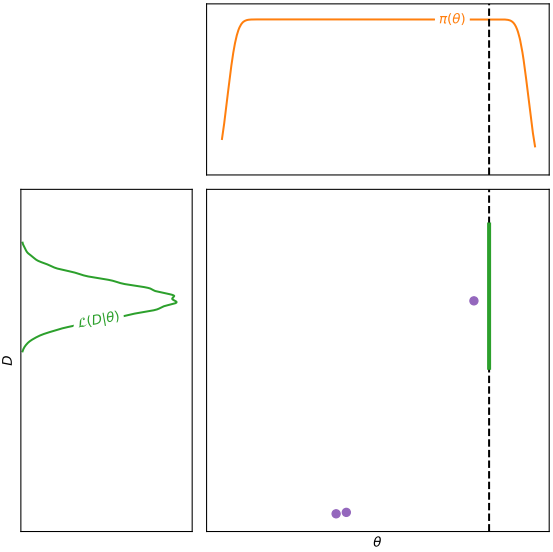

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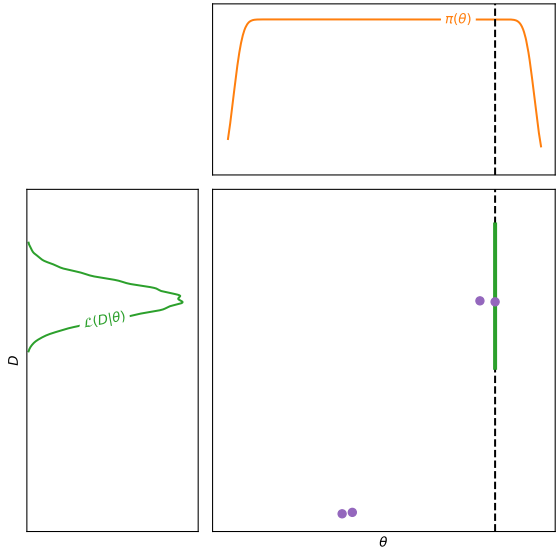

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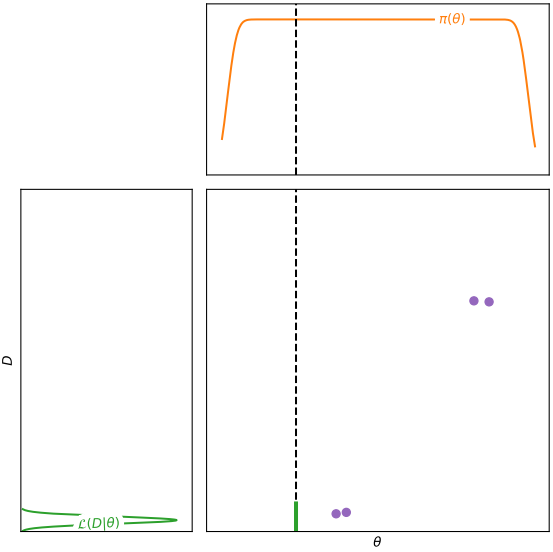

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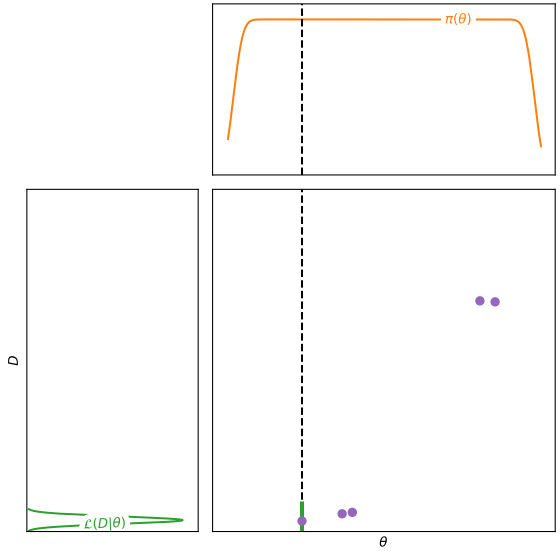

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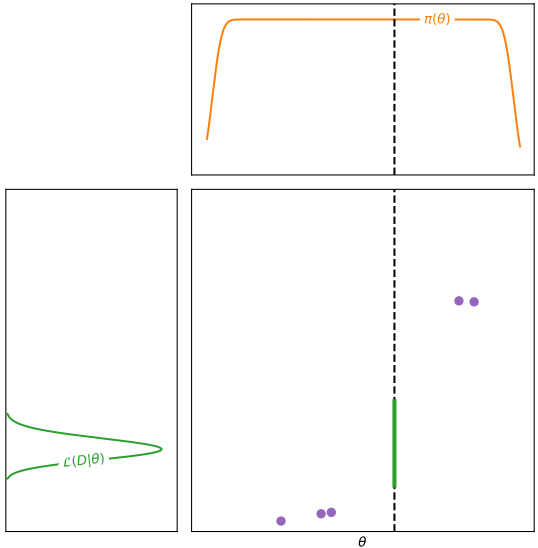

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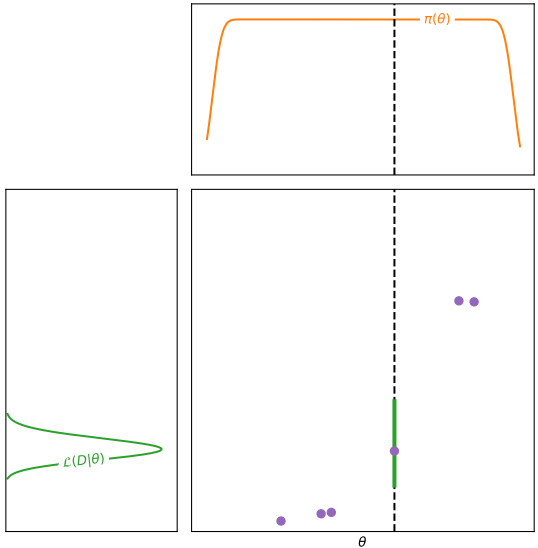

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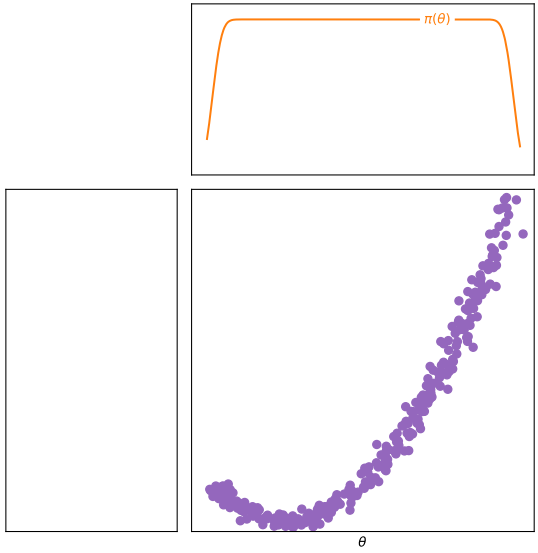

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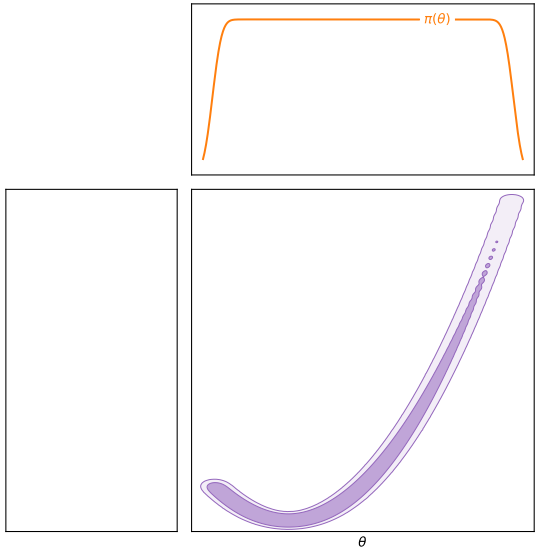

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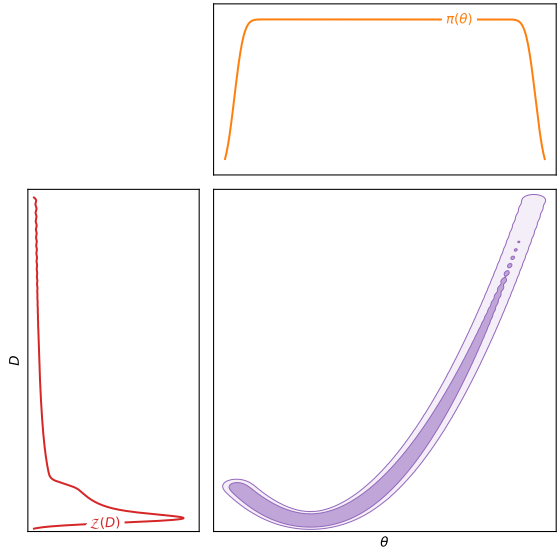

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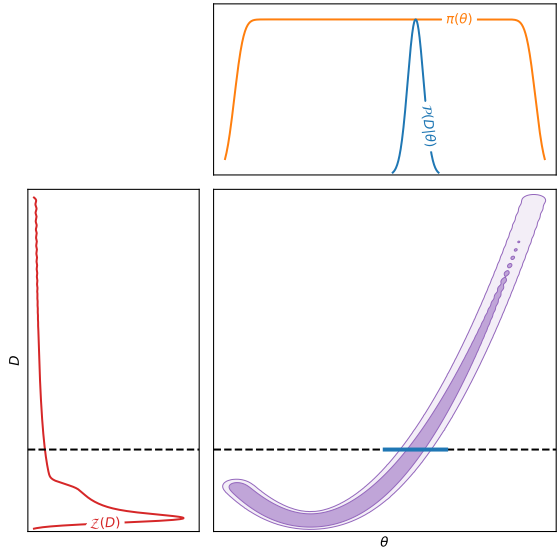

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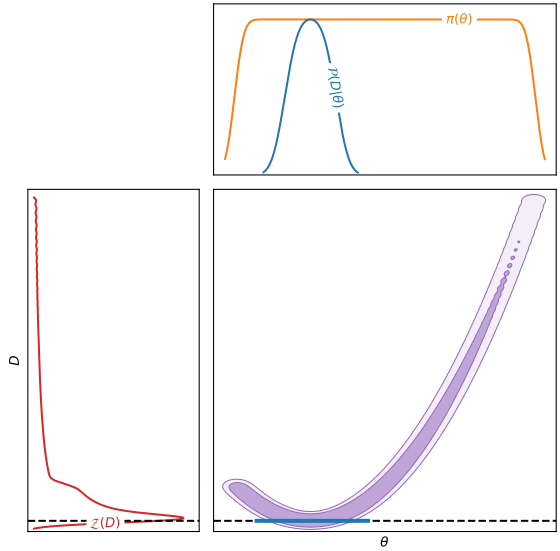

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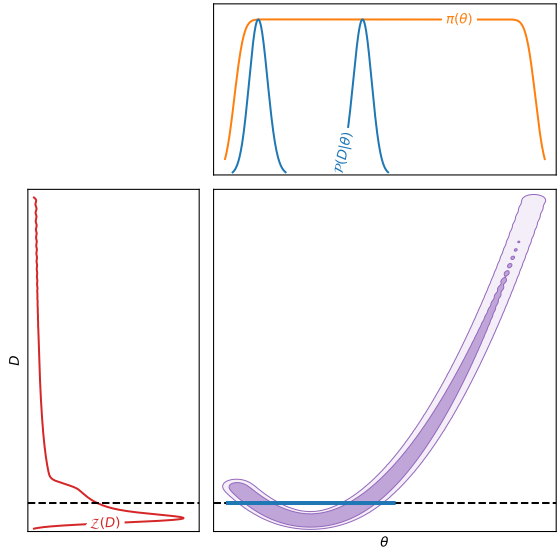

SBI: Simulation-based inference

- 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).
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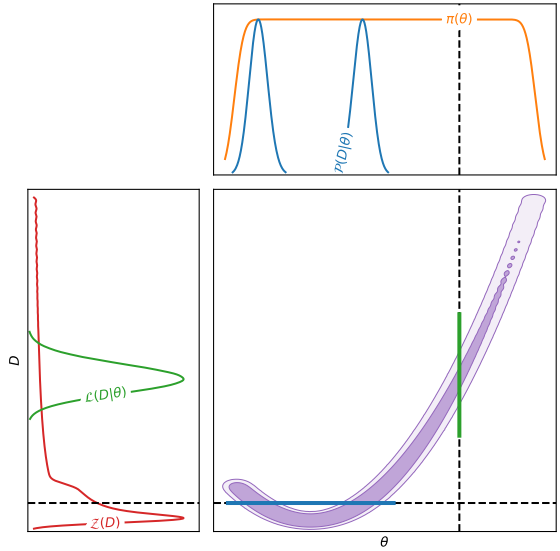
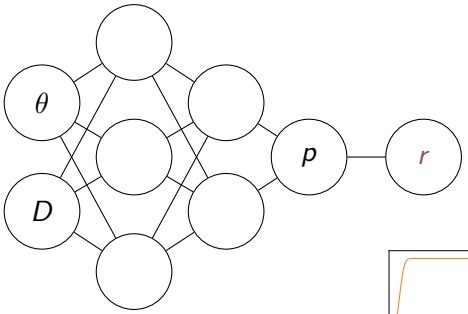


Neural Ratio Estimation

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

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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

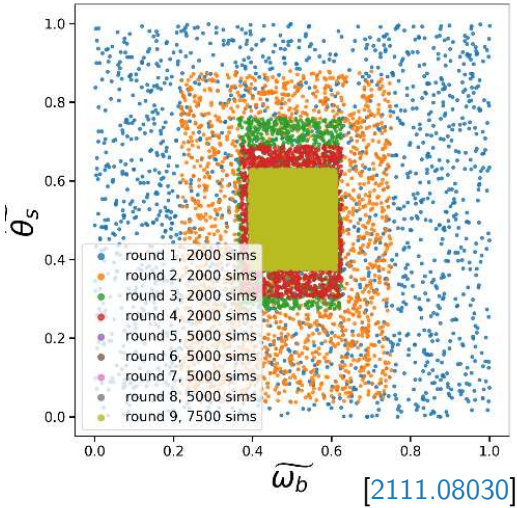
- Two tricks for practical NRE:

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.

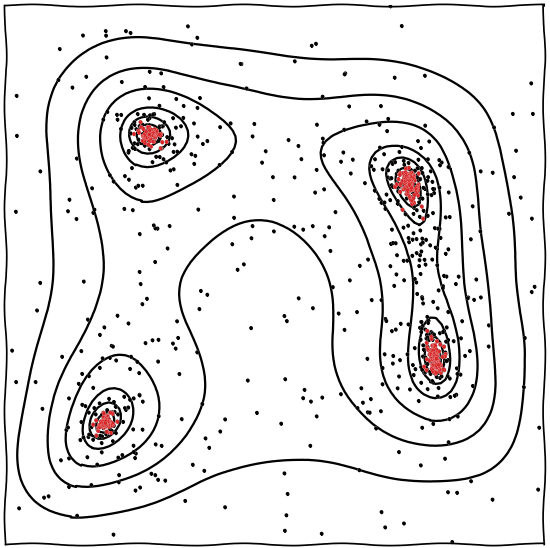
Truncation

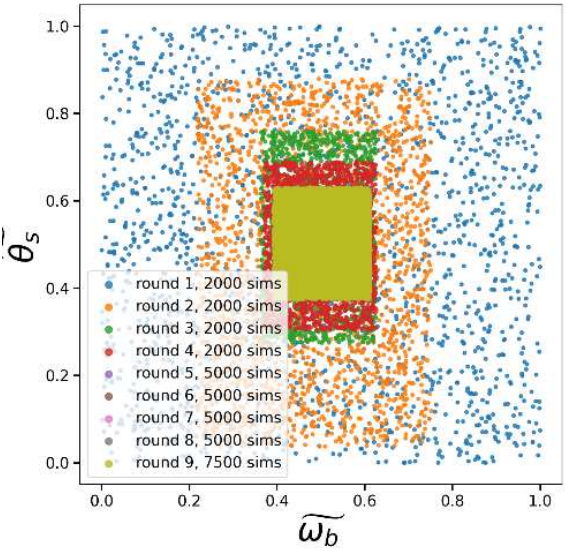
- focus parameters θ on a subset of the prior which reproduces observed data D_{obs}
- region is somewhat arbitrary (usually a box)
- not amortised, sounds a bit like ABC



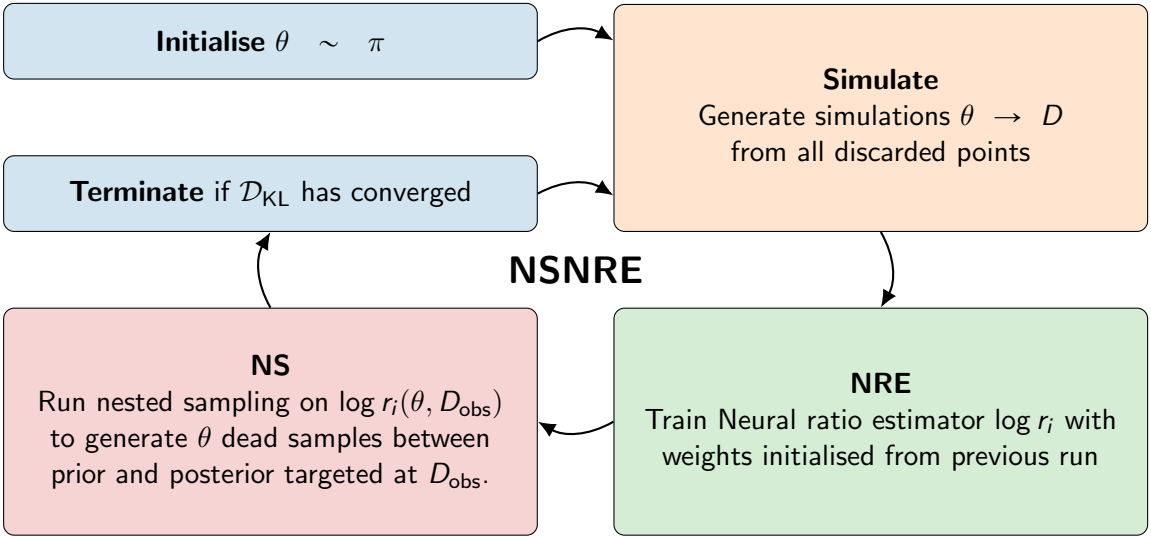
[2111.08030]

Similarities





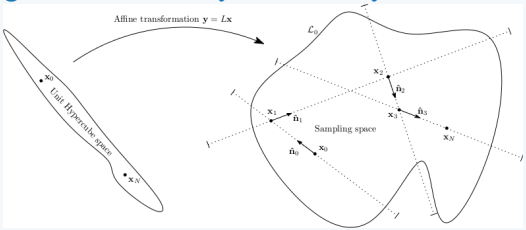
Sequential NRE with nested sampling



PolySwyft

PolyChord

github.com/PolyChord/PolyChordLite



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

Swyft

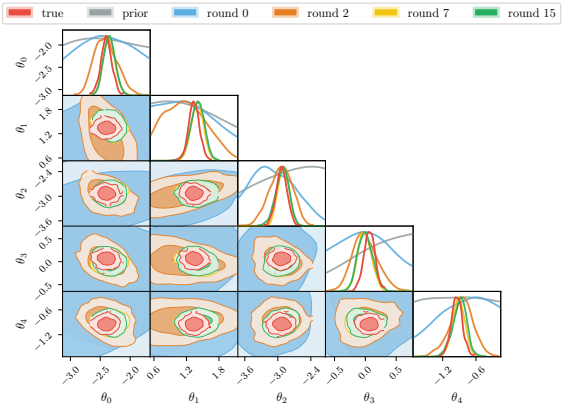
github.com/undark-lab/swyft

- 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).



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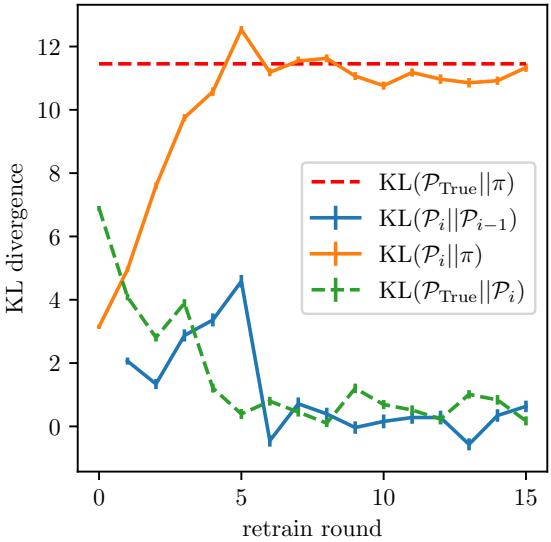

Conclusions

github.com/handley-lab

- Nested sampling is a multi-purpose numerical tool for:
  - Numerical integration $\int f(x)dV$,
  - Exploring/scanning/optimising *a priori* unknown functions,
  - Performing Bayesian inference and model comparison.
- It is applied widely across cosmology, particle physics & machine learning.
- It's unique traits as the only numerical Lebesgue integrator mean with compute it will continue to grow in importance.