

# Sampling methods for high energy physics & particle astrophysics

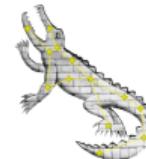
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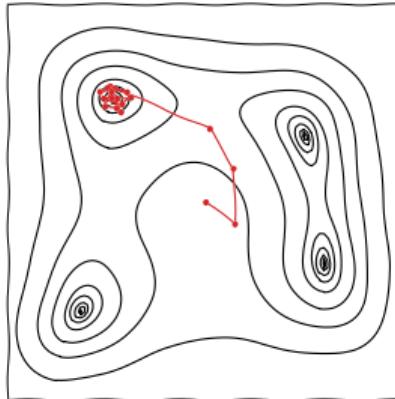


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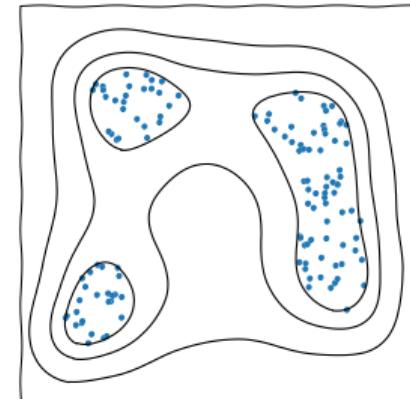
## MCMC

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



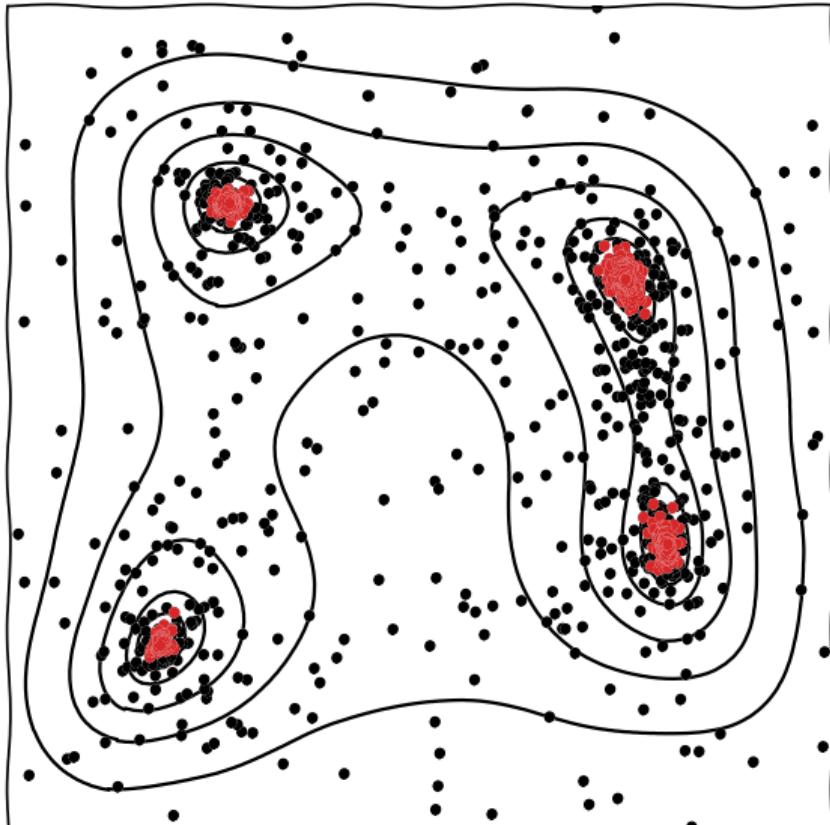
## Nested sampling

- ▶ 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



# Nested sampling: numerical Lebesgue integration

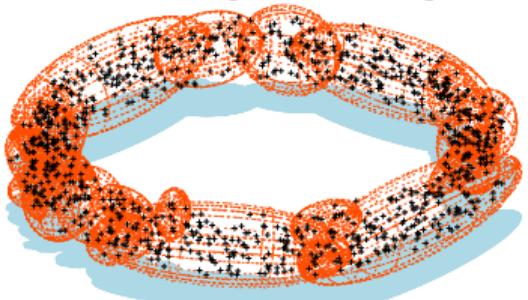
0. Start with  $N$  random samples over the space.
  - i. Delete outermost sample, and replace with a new random one at higher integrand value.
- ▶ The “live points” steadily contract around the peak(s) of the function.
- ▶ Discarded “dead points” can be weighted to form posterior, prior, or anything in between.
- ▶ Estimates the **density of states** and **partition function**  $\log \mathcal{Z}(\beta)$ .
- ▶ The evolving ensemble of live points allows:
  - ▶ implementations to self-tune,
  - ▶ exploration of multimodal functions,
  - ▶ global and local optimisation.



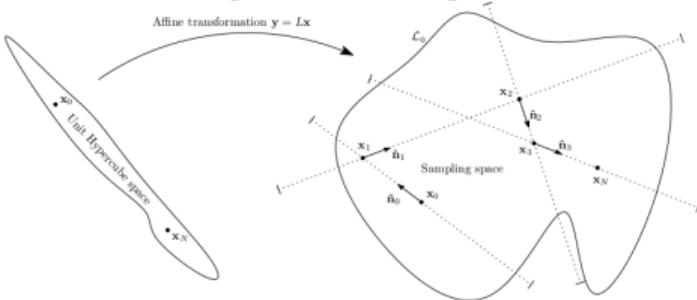
# The nested sampling zoo

[2205.15570]

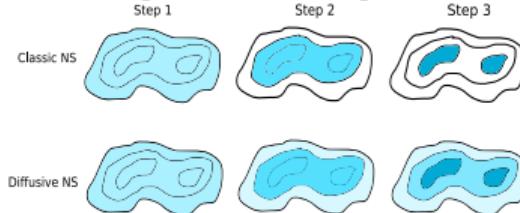
MultiNest [0809.3437]



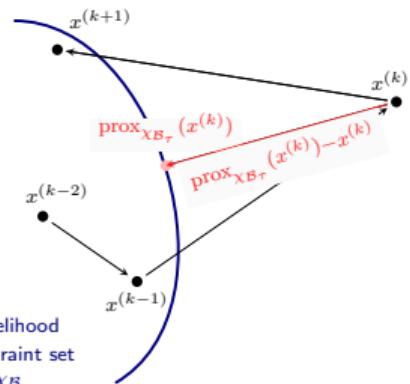
PolyChord [1506.00171]



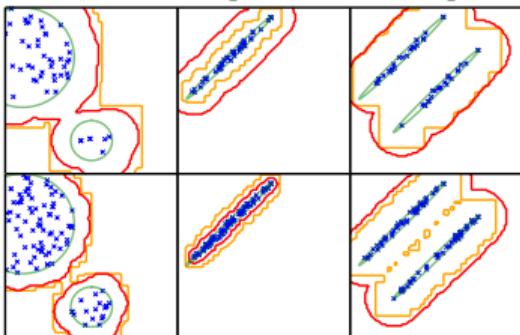
DNest [1606.03757]



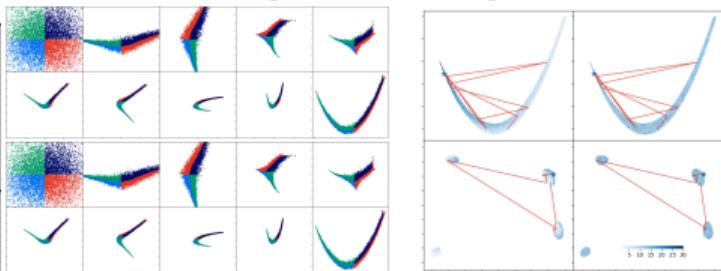
ProxNest [2106.03646]



UltraNest [2101.09604]



NeuralNest [1903.10860]



nessai [2102.11056]

nora [2305.19267]

jaxnest [2012.15286]

nautilus [2306.16923]

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dynesty [1904.02180]

# Lattice field theory

## Applications of nested sampling

David Yallup

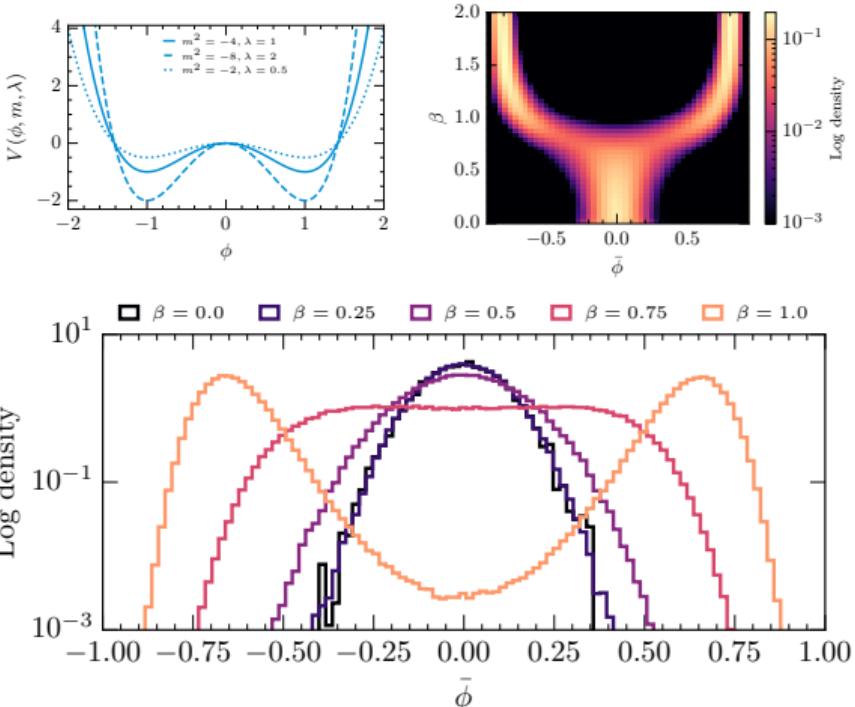


PDRA

- ▶ 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



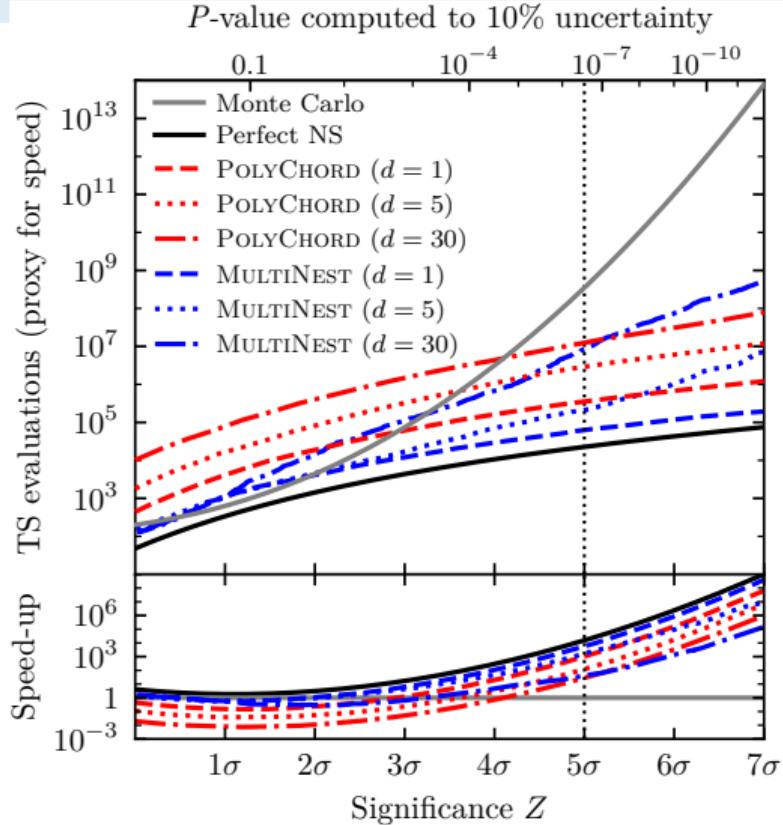
# Fast estimation of small $p$ -values [2106.02056](PRL)

Andrew Fowlie



## Applications of nested sampling

- ▶ Nested sampling for frequentist computation!?
- ▶  $p$ -value:  $P(\lambda > \lambda^* | H_0)$  – probability that test statistic  $\lambda$  is at least as great as observed  $\lambda^*$ .
- ▶ Computation of a tail probability from sampling distribution of  $\lambda$  under  $H_0$ .
- ▶ For gold-standard  $5\sigma$ , this is very expensive to simulate directly ( $\sim 10^9$  by definition).
- ▶ Need insight/approximation to make efficient.
- ▶ Nested sampling is tailor-made for this, just make switch:  $X \leftrightarrow p$ ,  $\mathcal{L} \leftrightarrow \lambda$ ,  $\theta \leftrightarrow x$ .
- ▶ The only real conceptual shift is switching the integrator from parameter- to data-space.



# Cross section calculation

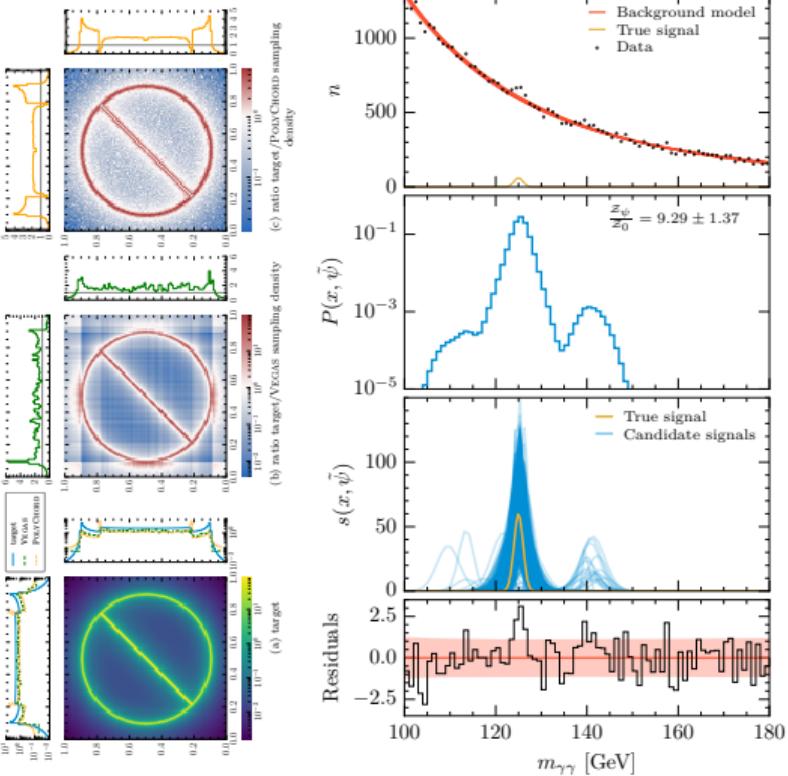
## Applications of nested sampling

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  $\Omega$  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



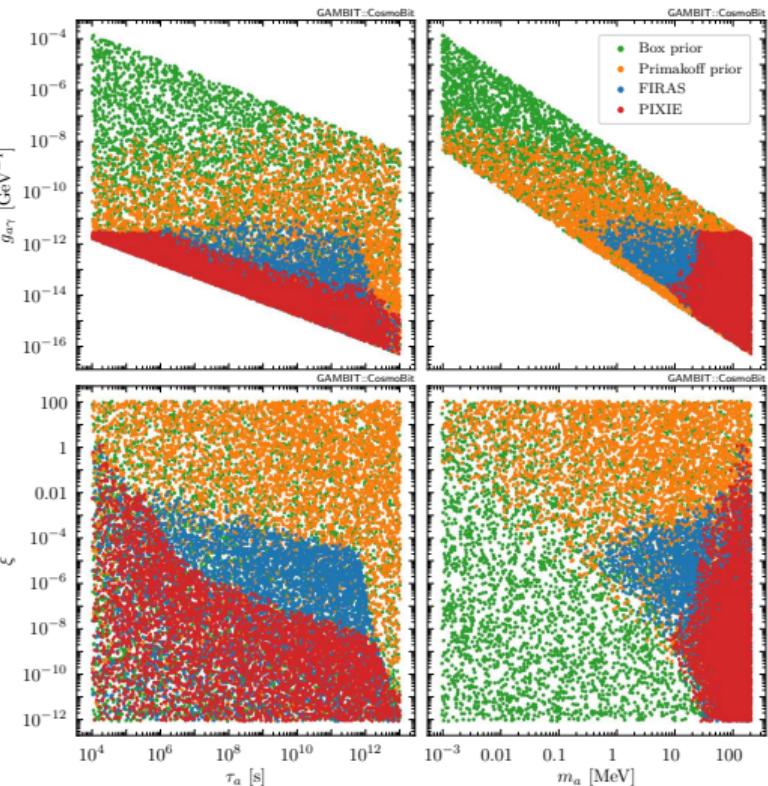
# Quantification of fine tuning [2101.00428] [2205.13549]

GAMBIT  
dm-cosmo WG



## Applications of nested sampling

- ▶ Example: Cosmological constraints on decaying axion-like particles [2205.13549]. (Also vary cosmology,  $\tau_a$  and nuisance params)
- ▶ Data: CMB, BBN, FIRAS, SMM, BAO.
- ▶ Standard profile likelihood fit shows ruled out regions and best-fit point.
- ▶ Nested sampling scan:
  - ▶ Quantifies amount of parameter space ruled out with Kullback-Liebler divergence  $\mathcal{D}_{\text{KL}}$ .
  - ▶ Identifies best fit region as statistically irrelevant from information theory/Bayesian.
  - ▶ No evidence for decaying ALPs. Fit the data equally well: but more constrained parameters create Occam penalty.



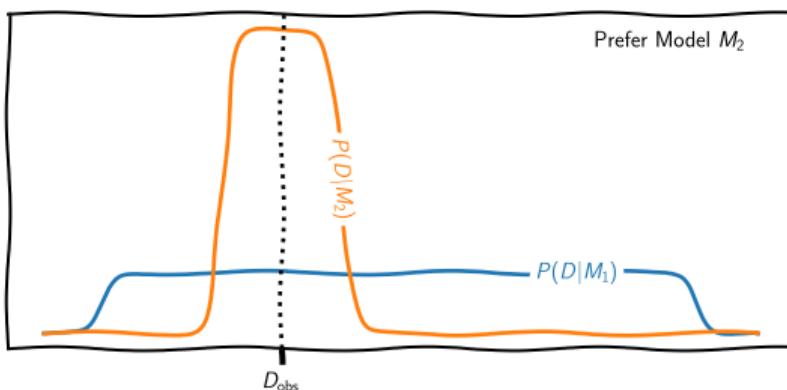
# Model comparison $\mathcal{Z} = P(D|M)$

- ▶ Bayesian model comparison allows mathematical derivation of key philosophical principles.

Viewed from data-space  $D$ :

## Popper's falsificationism

- ▶ Prefer models that make bold predictions.
- ▶ if proven true, model more likely correct.



- ▶ Falsificationism comes from normalisation

Viewed from parameter-space  $\theta$ :

## Occam's razor

- ▶ Models should be as simple as possible
- ▶ ... but no simpler

- ▶ Occam's razor equation:

$$\log \mathcal{Z} = \langle \log \mathcal{L} \rangle_{\mathcal{P}} - \mathcal{D}_{\text{KL}}$$

- ▶ “Occam penalty”: KL divergence between prior  $\pi$  and posterior  $\mathcal{P}$ .

$$\mathcal{D}_{\text{KL}} \sim \log \frac{\text{Prior volume}}{\text{Posterior volume}}$$

# Conclusions

[github.com/handley-lab](https://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.
- ▶ It's unique traits as the only numerical Lebesgue integrator mean with compute it will continue to grow in importance.