

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

Will Handley  
[<wh260@cam.ac.uk>](mailto:wh260@cam.ac.uk)

Royal Society University Research Fellow & Turing Fellow  
Astrophysics Group, Cavendish Laboratory, University of Cambridge  
Kavli Institute for Cosmology, Cambridge  
Gonville & Caius College  
[willhandley.co.uk/talks](http://willhandley.co.uk/talks)

18<sup>th</sup> August 2023



The  
**Alan Turing**  
Institute



UNIVERSITY OF  
**CAMBRIDGE**



# Highlight: state-of-the-art Nature review [NatRev]

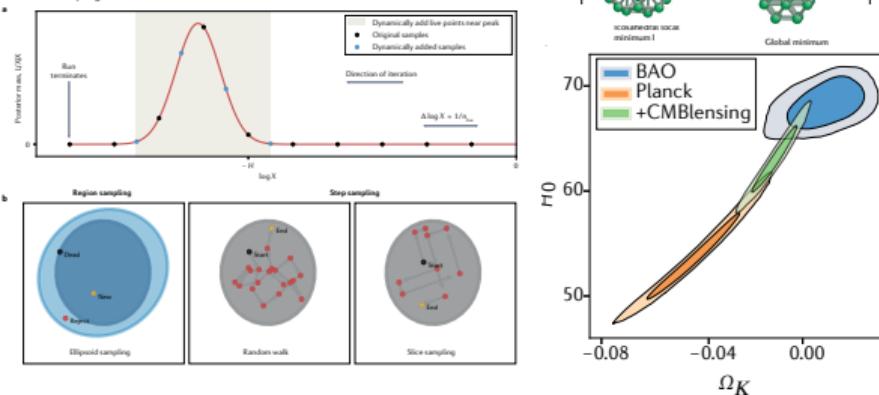
- ▶ Invented by John Skilling in 2004.
- ▶ Recent Nature review primer on nested sampling led by Andrew Fowlie and assembled by the community.
- ▶ Showcases the current set of tools, and applications from chemistry to cosmology.
- ▶ Recent 1.5 day conference in Munich: “Frontiers of Nested Sampling”
- ▶ Planned week-long NSCON 2024
- ▶ In this talk:
  - ▶ User guide to nested sampling
  - ▶ Particle physics applications
  - ▶ Cosmology applications
  - ▶ Machine learning applications

PRIMER

## Nested sampling for physical scientists

Greg Ashton<sup>1,2</sup>, Noam Bernstein<sup>3,4</sup>, Johannes Buchner<sup>5</sup>, Xi Chen<sup>6</sup>, Gábor Csányi<sup>1,6</sup>, Andrew Fowlie<sup>1,2</sup>, Farhan Farooq<sup>6</sup>, Matthew Griffiths<sup>6</sup>, Will Handley<sup>10,11</sup>, Michael Habenek<sup>12</sup>, Edward Higson<sup>13</sup>, Michael Hobson<sup>11</sup>, Anthony Lasenby<sup>14,15,11</sup>, David Parkinson<sup>16</sup>, Liviu B. Pătrășcan<sup>15</sup>, Matthew Pitkin<sup>1,2</sup>, Doris Schneider<sup>17</sup>, Joshua S. Speagle<sup>18,19,20</sup>, Leah South<sup>21</sup>, John Veitch<sup>22</sup>, Philipp Wacker<sup>17</sup>, David J. Wales<sup>1,22</sup> and David Yallup<sup>10,11</sup>

**Abstract** | This Primer examines Skilling’s nested sampling algorithm for Bayesian inference and, more broadly, multidimensional integration. The principles of nested sampling are summarized and recent developments using efficient nested sampling algorithms in high dimensions surveyed, including methods for sampling from the constrained prior. Different ways of applying nested sampling are outlined, with detailed examples from three scientific fields: cosmology, gravitational-wave astronomy and materials science. Finally, the Primer includes recommendations for best practices and a discussion of potential limitations and optimizations of nested sampling.

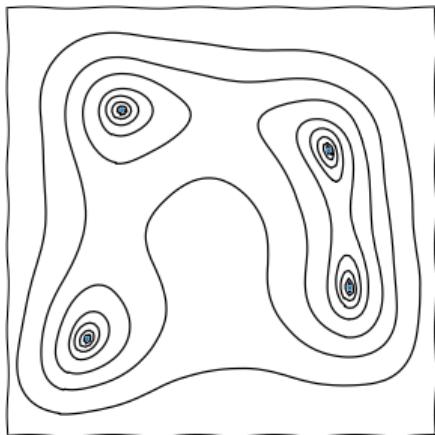


# What is Nested Sampling?

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

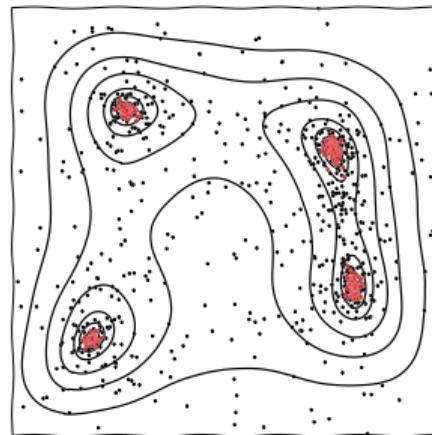
## Optimisation

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



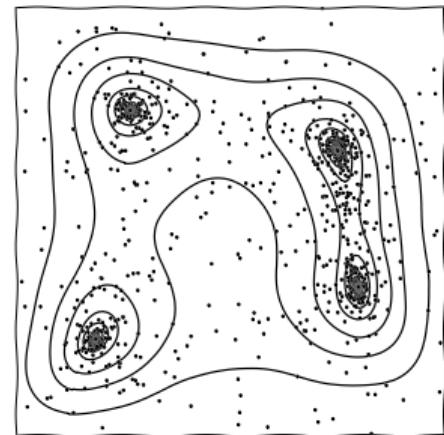
## Exploration

draw/sample  $\theta \sim f$



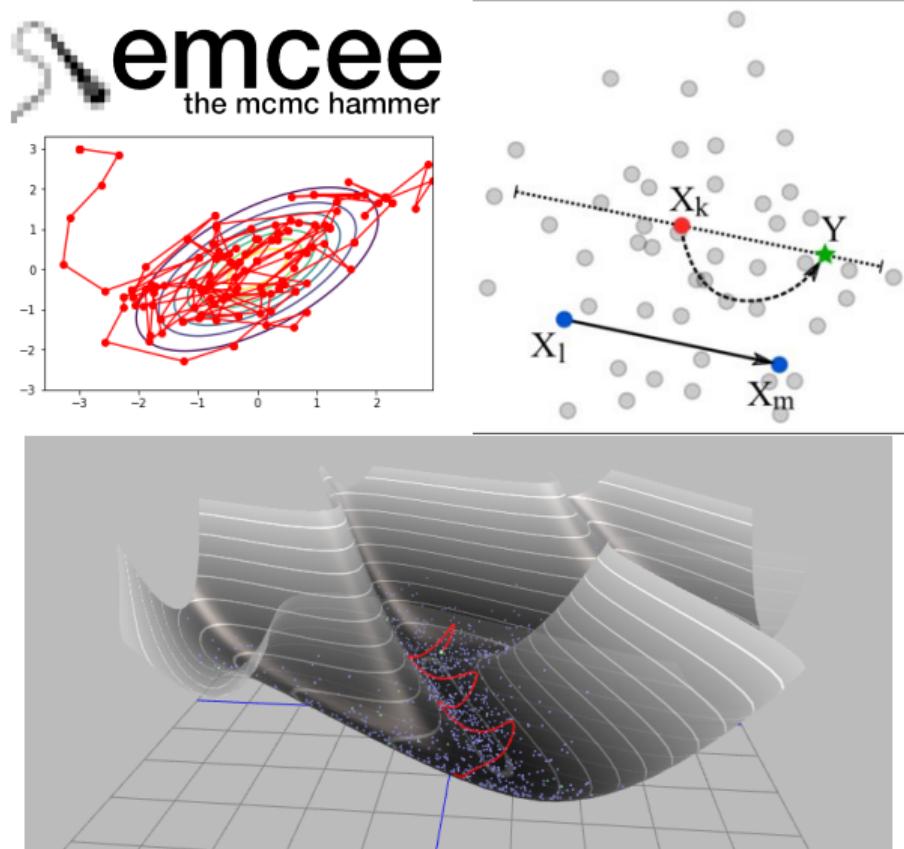
## Integration

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



# 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

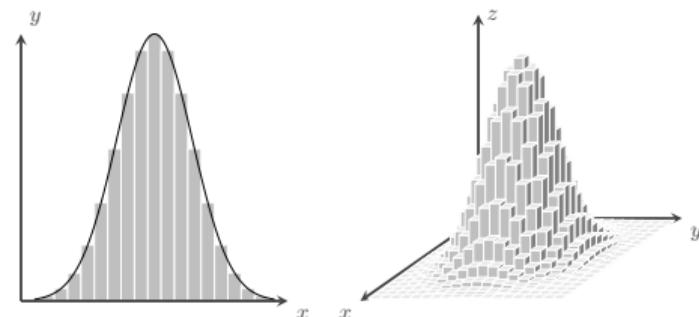
$$\Psi = \int e^{iS} \mathcal{D}x$$

## 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.

# Probabalistic volume estimation

- ▶ Key idea in NS: estimating volumes probabilistically

$$\frac{V_{\text{after}}}{V_{\text{before}}} \approx \frac{n_{\text{in}}}{n_{\text{out}} + n_{\text{in}}}$$

- ▶ This is the **only** way to calculate volume in high dimensions  $d > 3$ .
  - ▶ Geometry is exponentially inefficient.
- ▶ This estimation process does not depend on geometry, topology or dimensionality
- ▶ This really is the unique selling point of nested sampling.

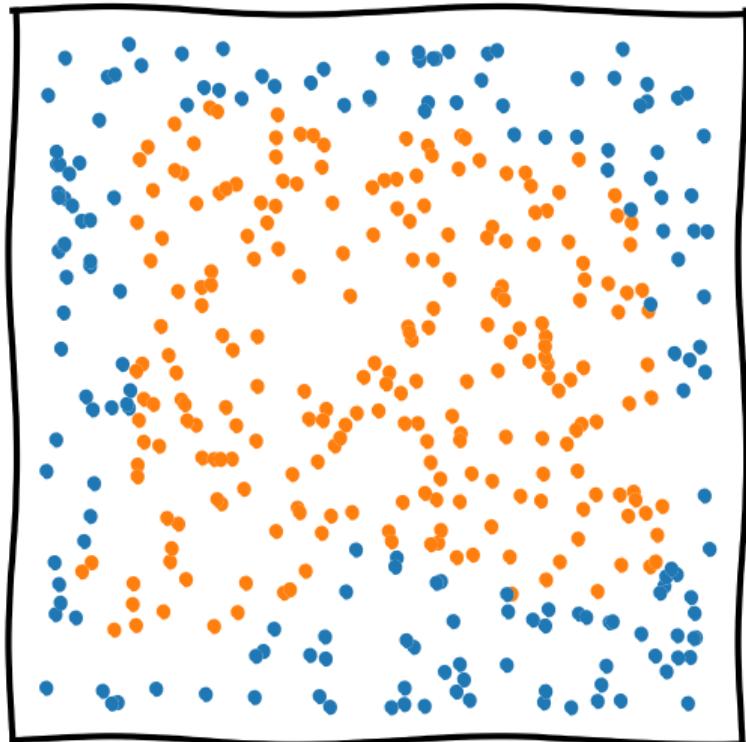


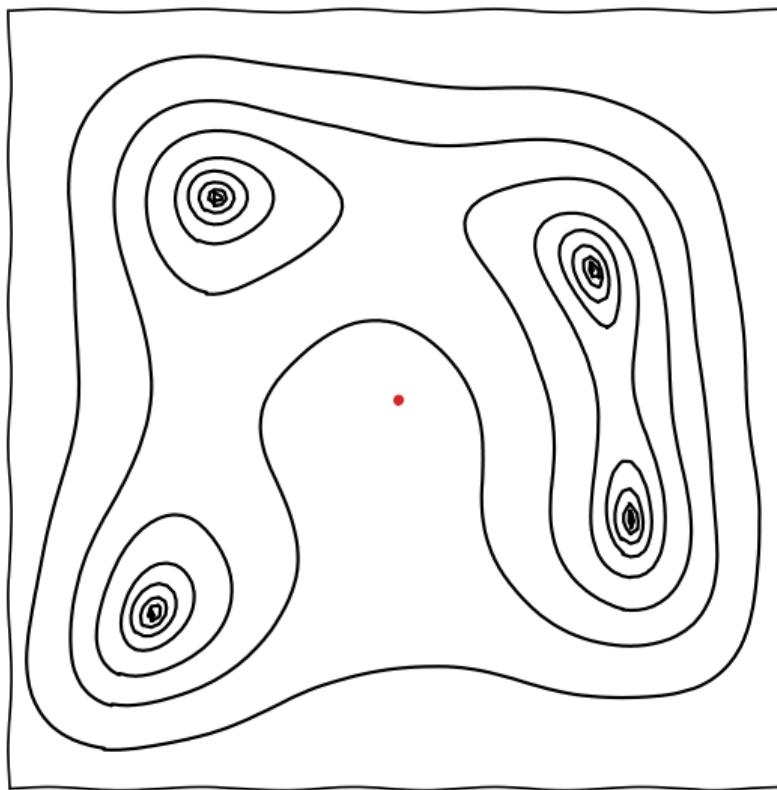
# Probabalistic volume estimation

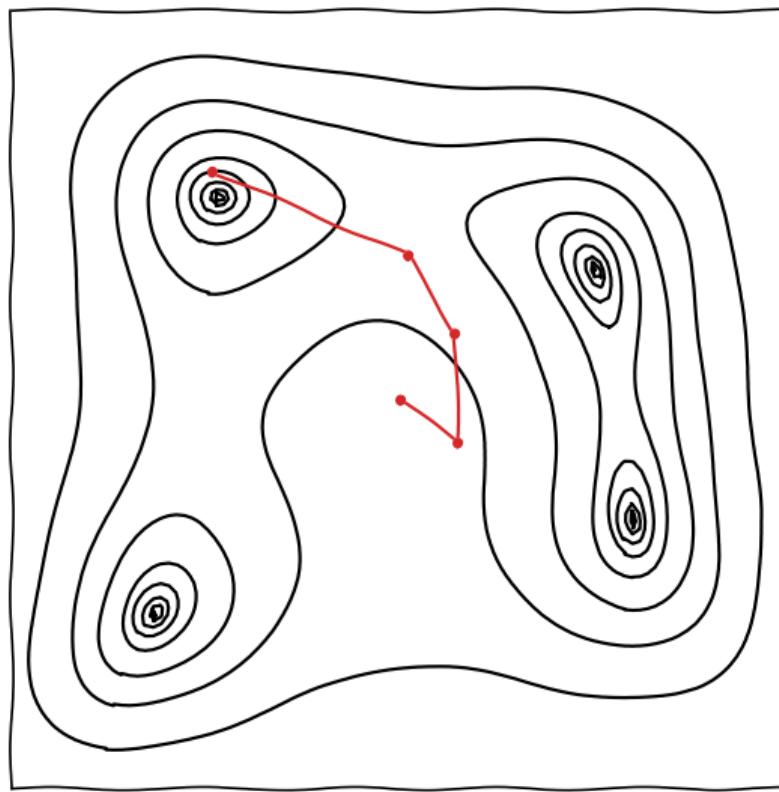
- ▶ Key idea in NS: estimating volumes probabilistically

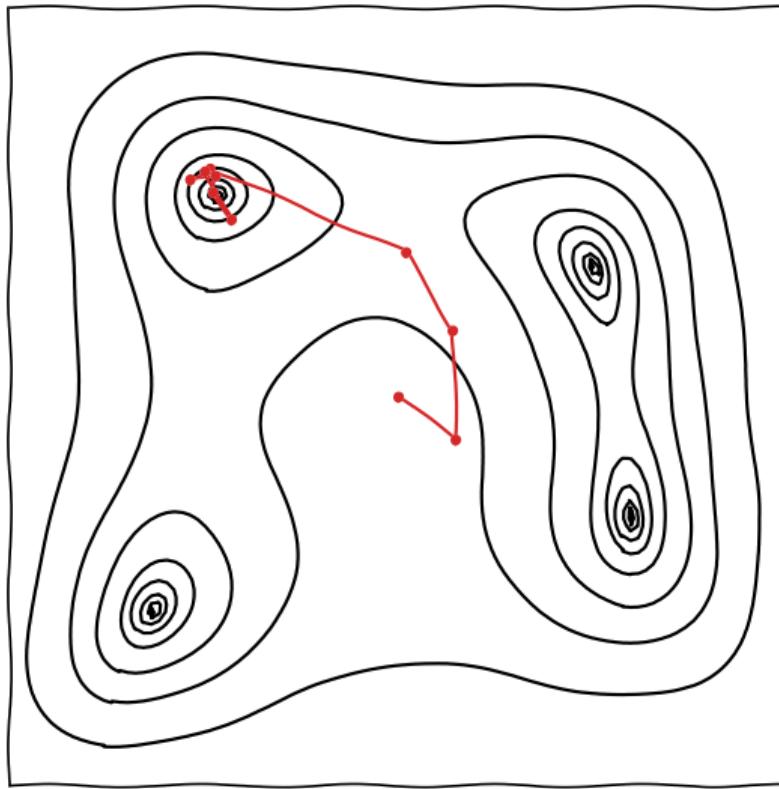
$$\frac{V_{\text{after}}}{V_{\text{before}}} \approx \frac{n_{\text{in}}}{n_{\text{out}} + n_{\text{in}}}$$

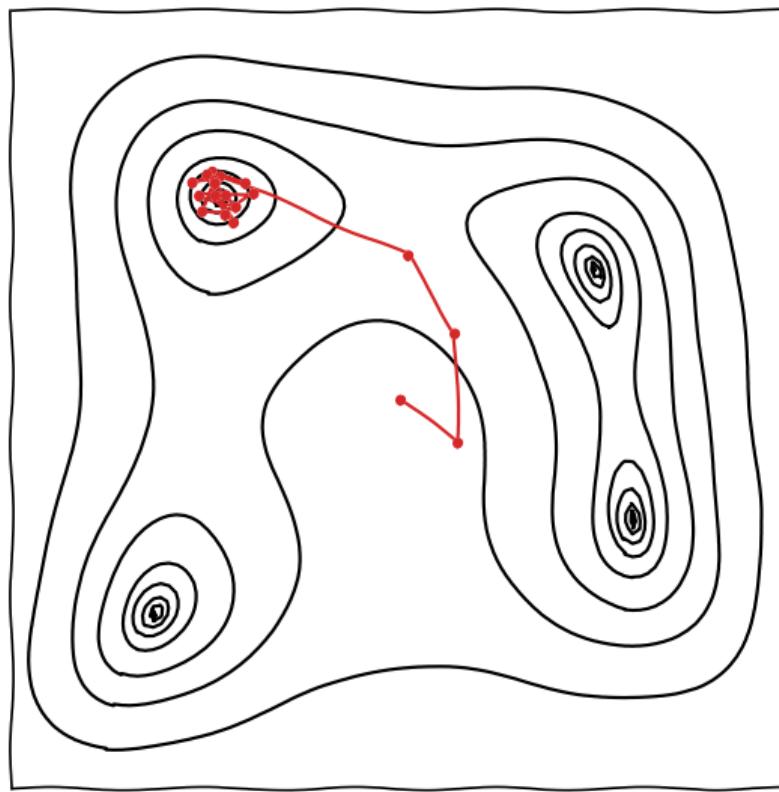
- ▶ This is the **only** way to calculate volume in high dimensions  $d > 3$ .
  - ▶ Geometry is exponentially inefficient.
- ▶ This estimation process does not depend on geometry, topology or dimensionality
- ▶ This really is the unique selling point of nested sampling.

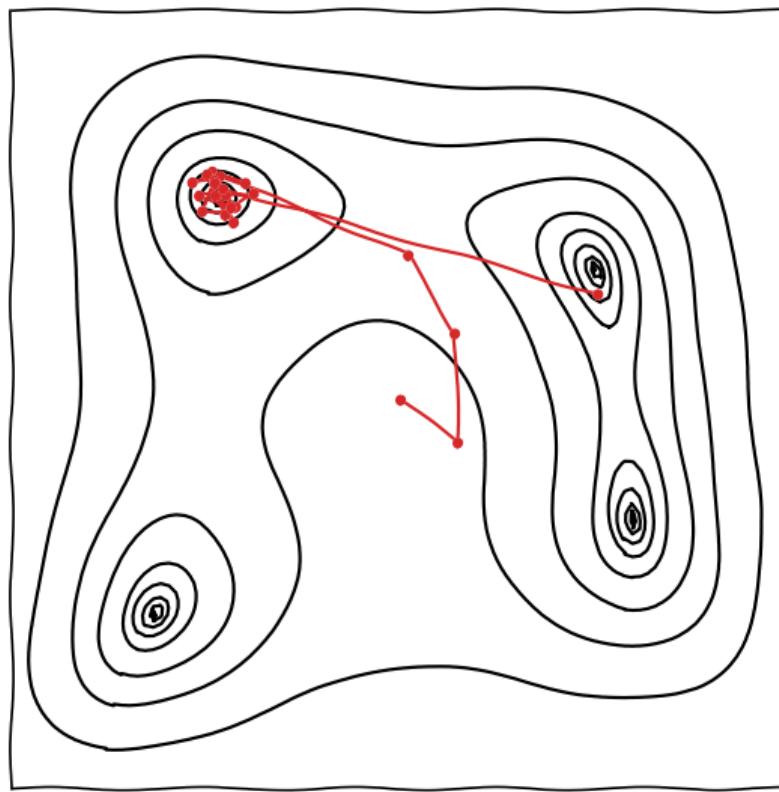


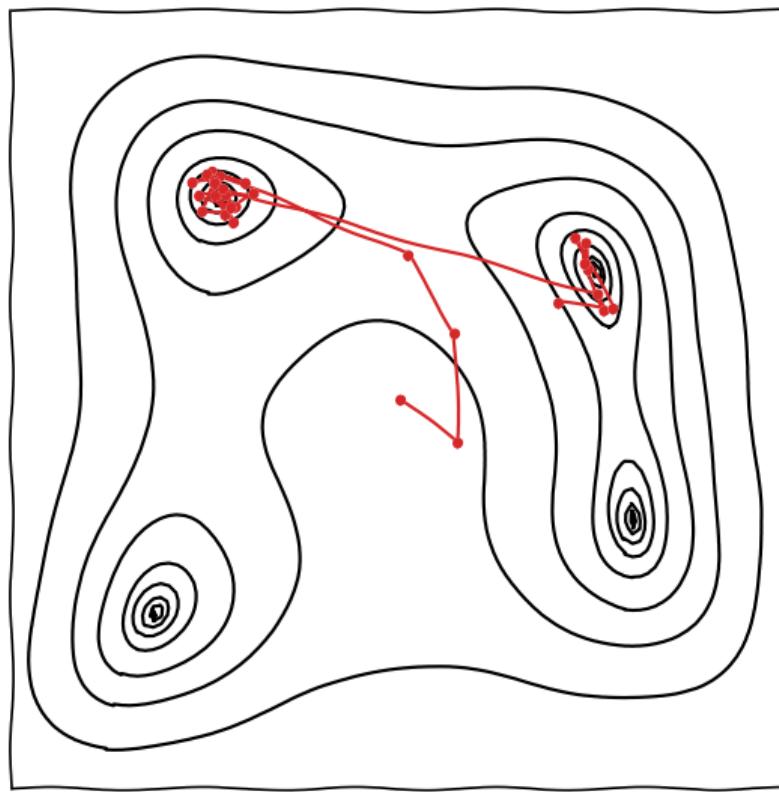




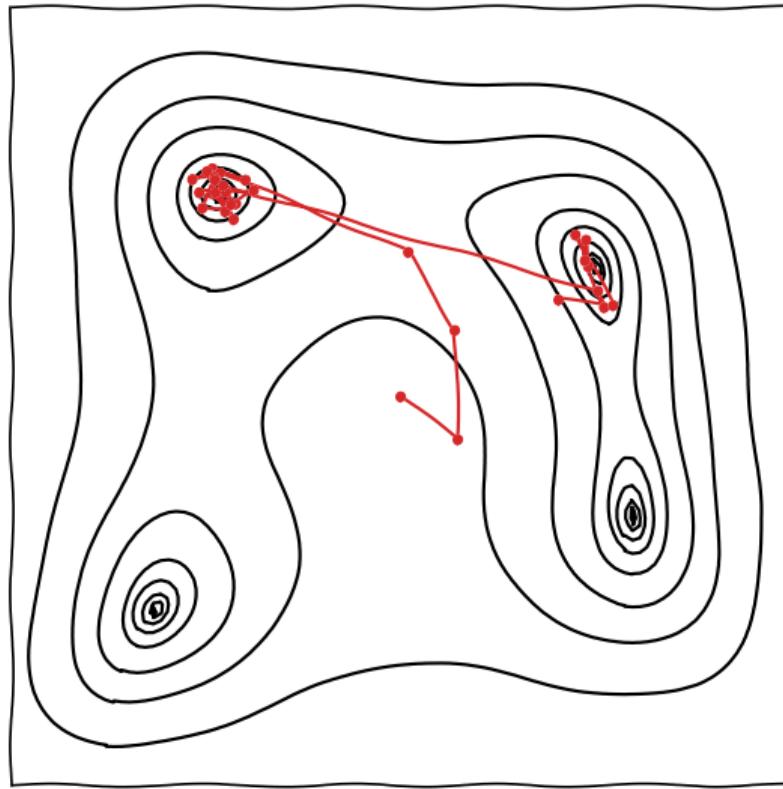




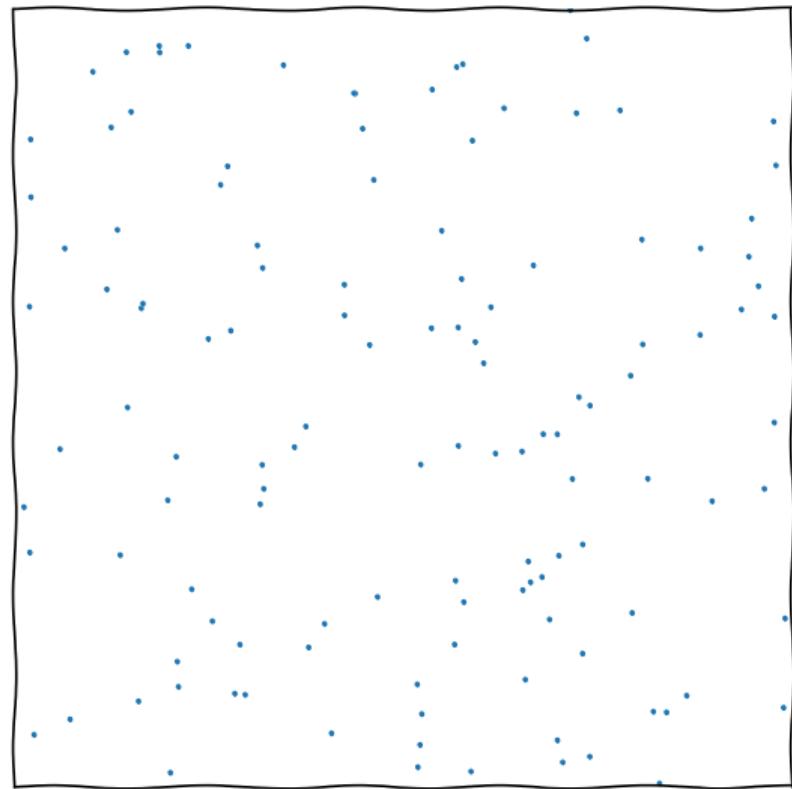




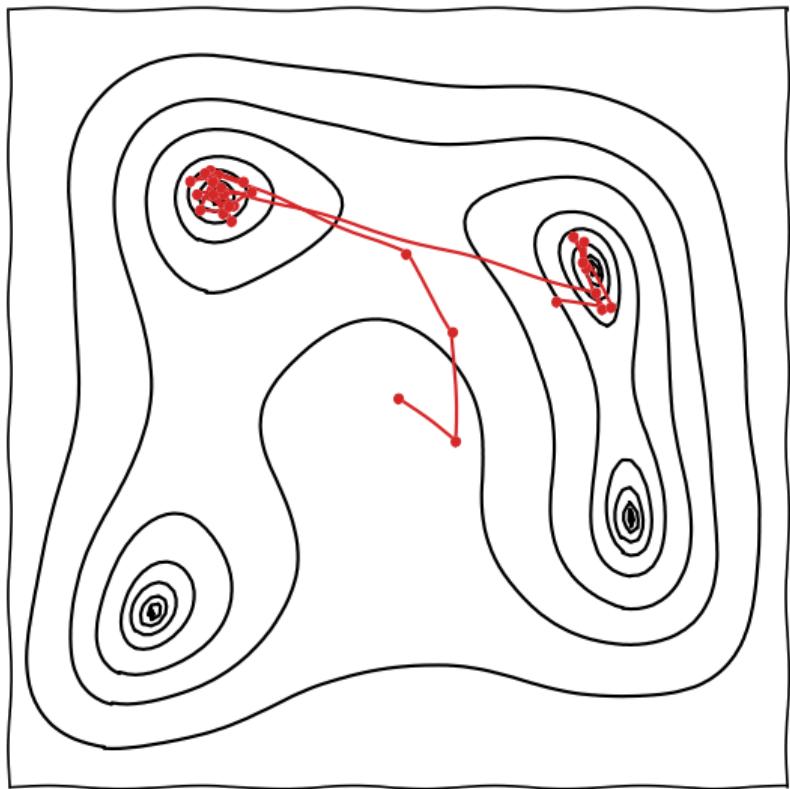
## MCMC



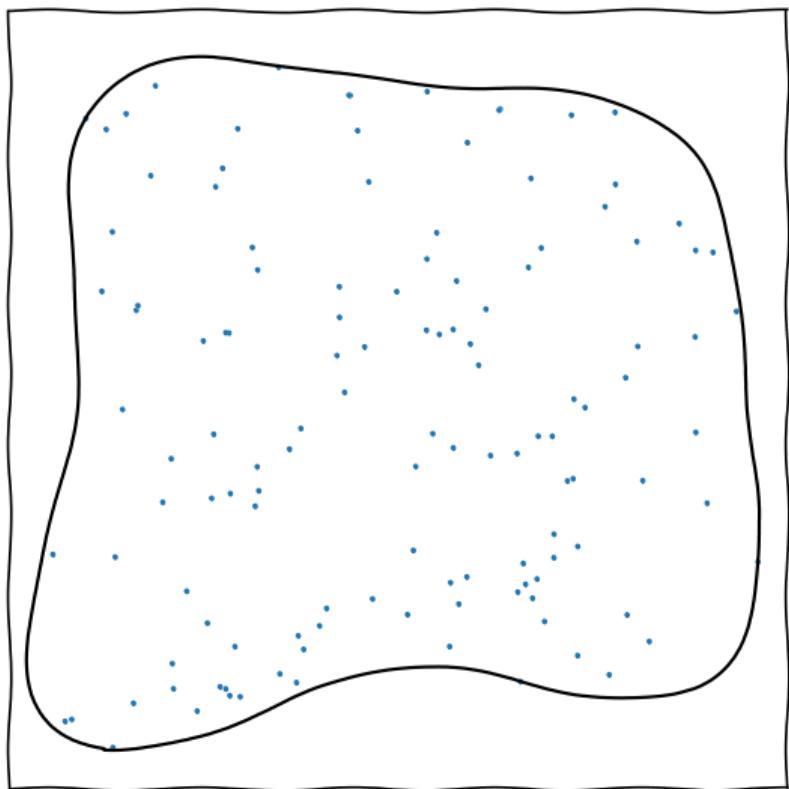
## Nested sampling



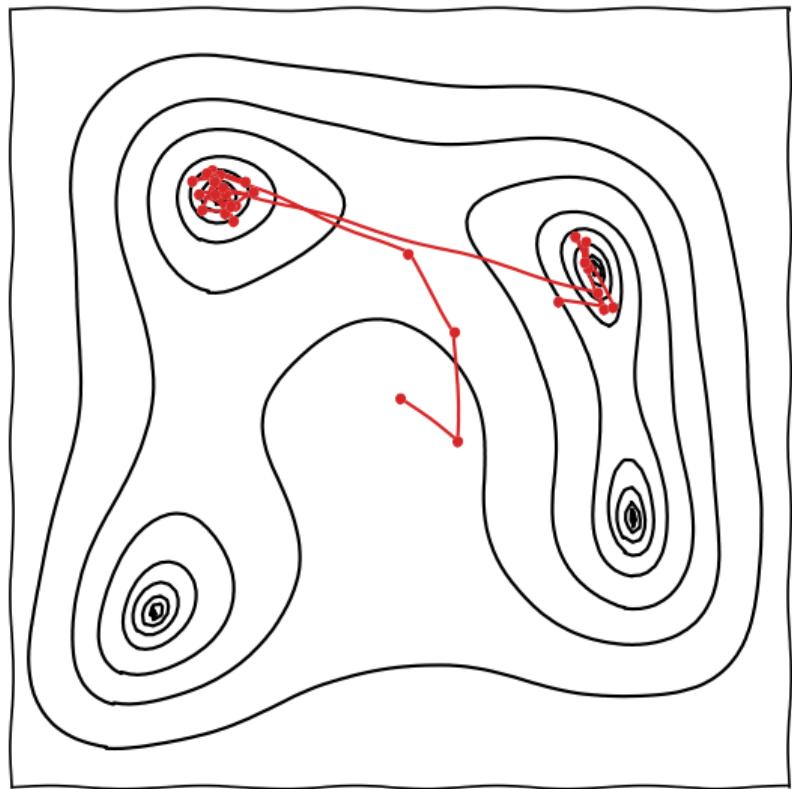
## MCMC



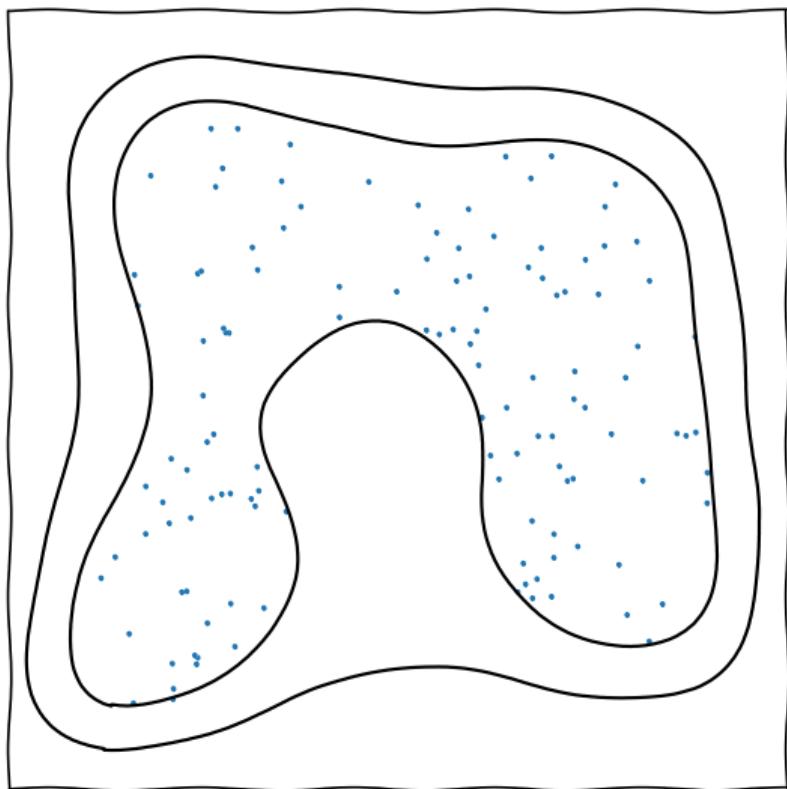
## Nested sampling



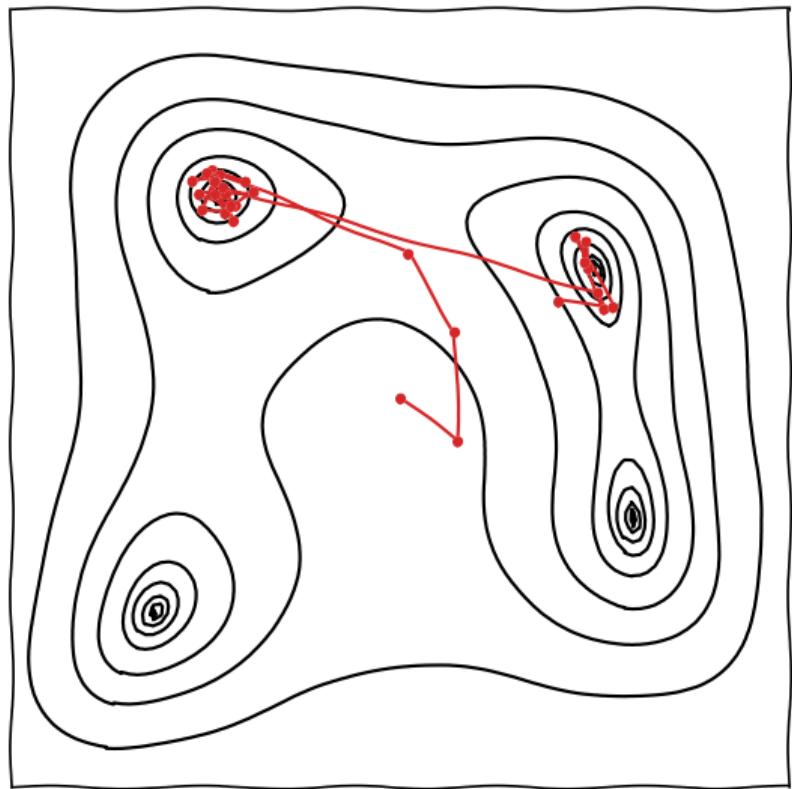
## MCMC



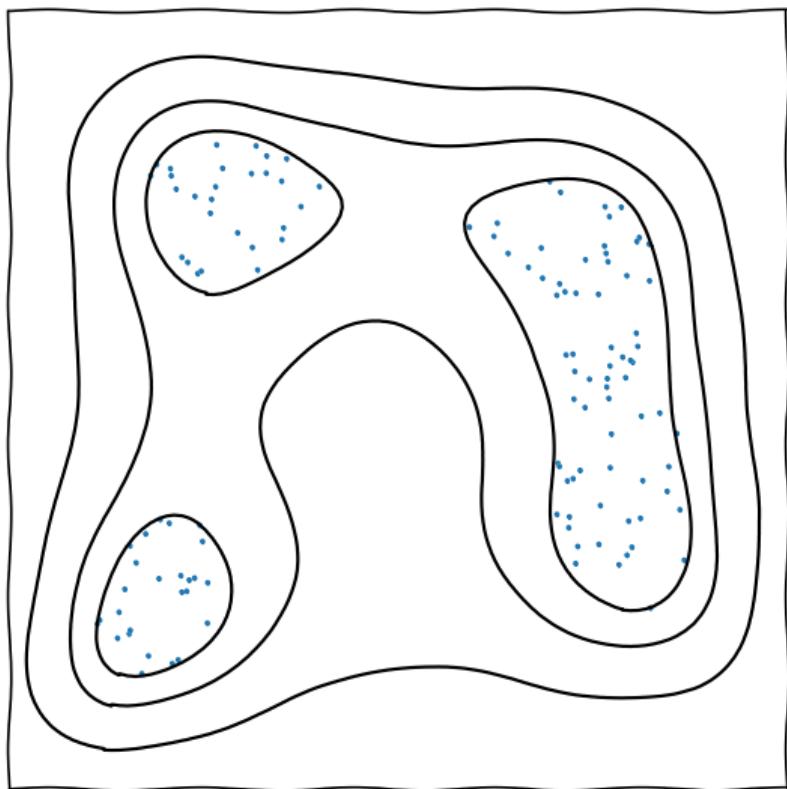
## Nested sampling



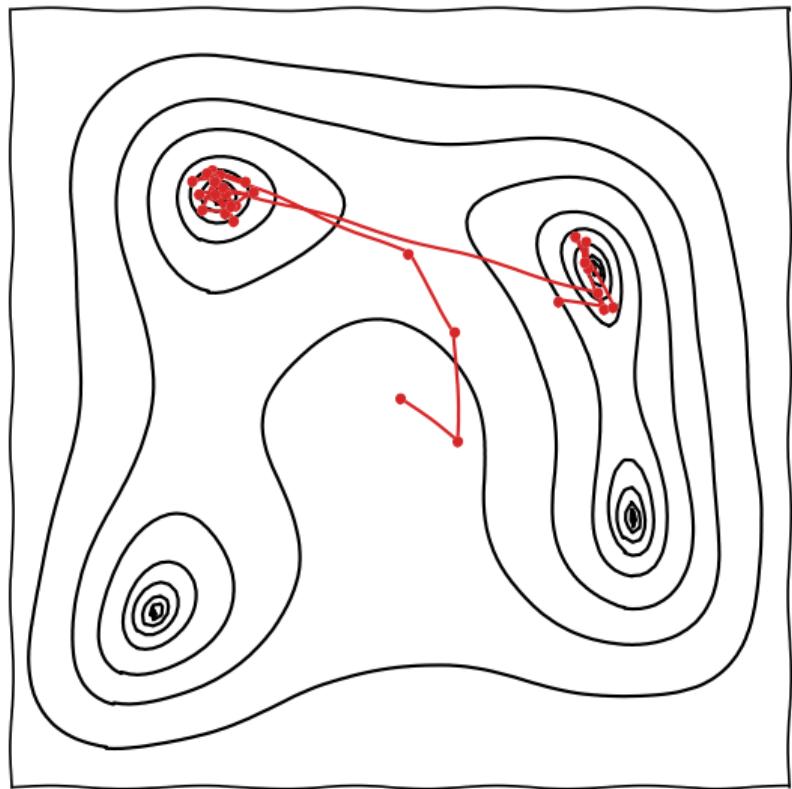
## MCMC



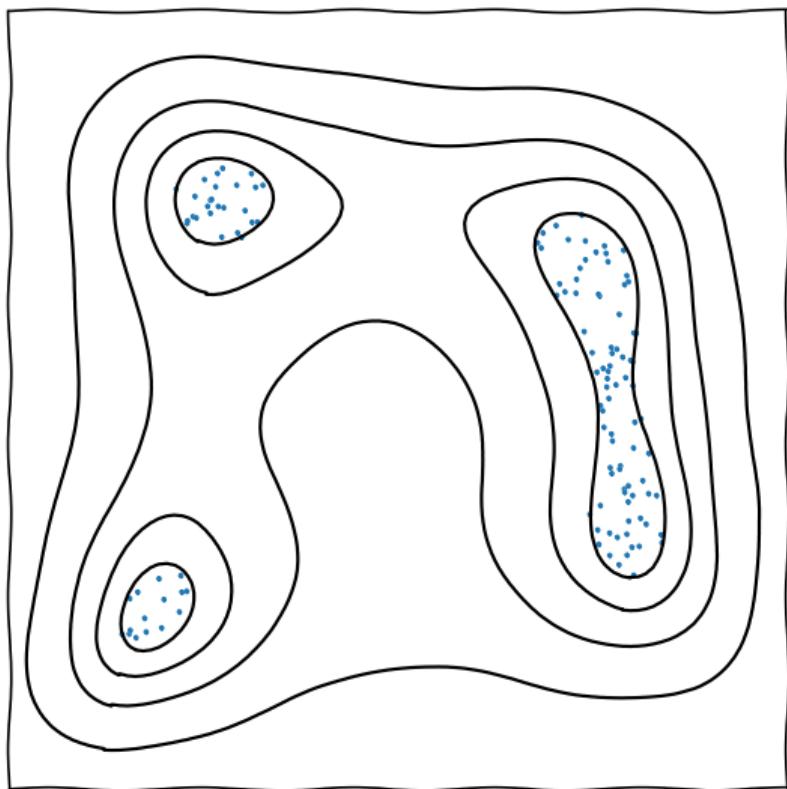
## Nested sampling



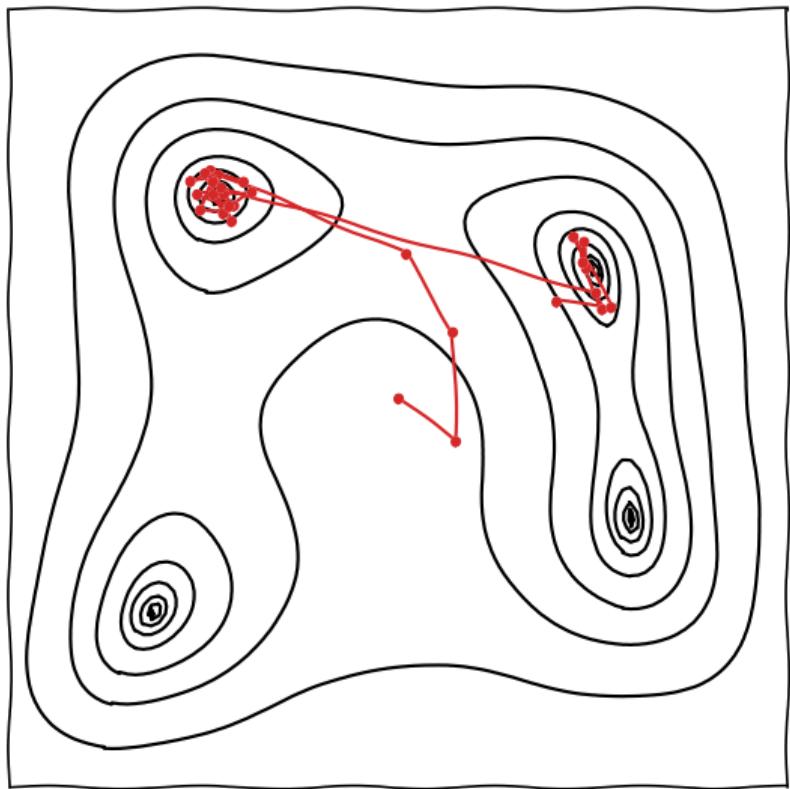
## MCMC



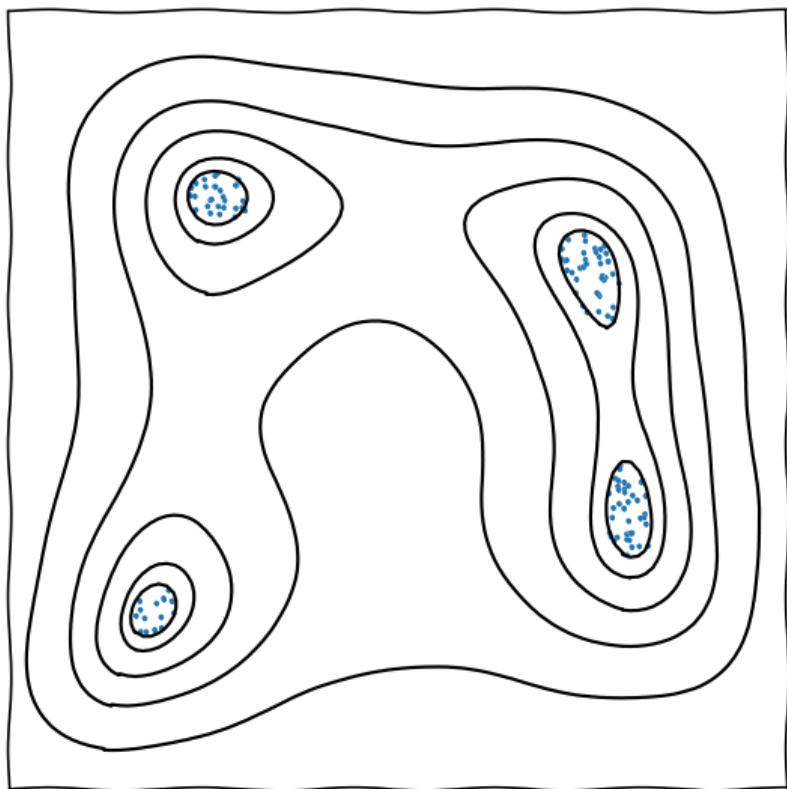
## Nested sampling



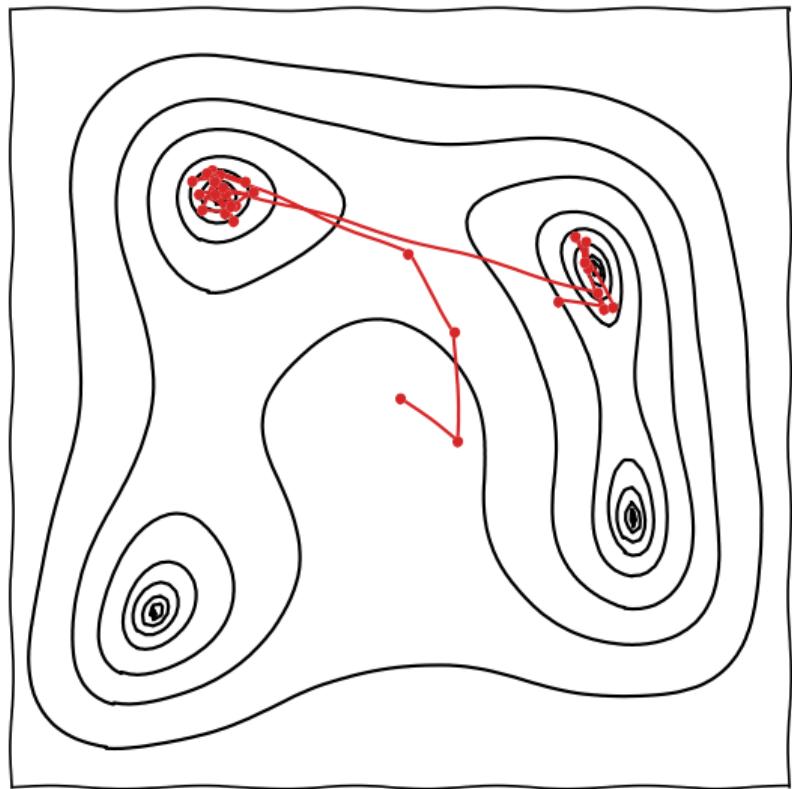
## MCMC



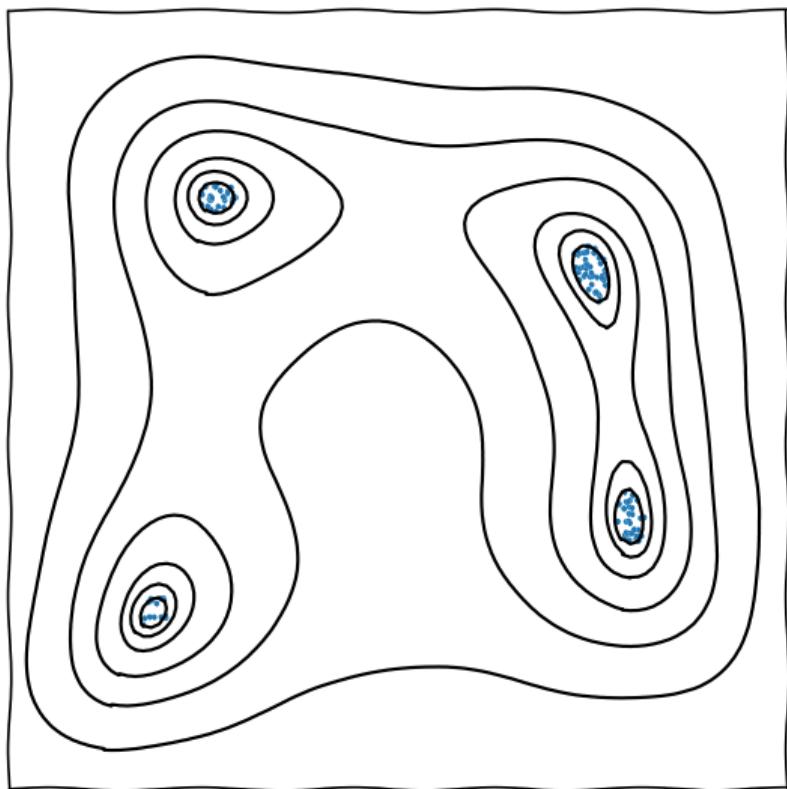
## Nested sampling



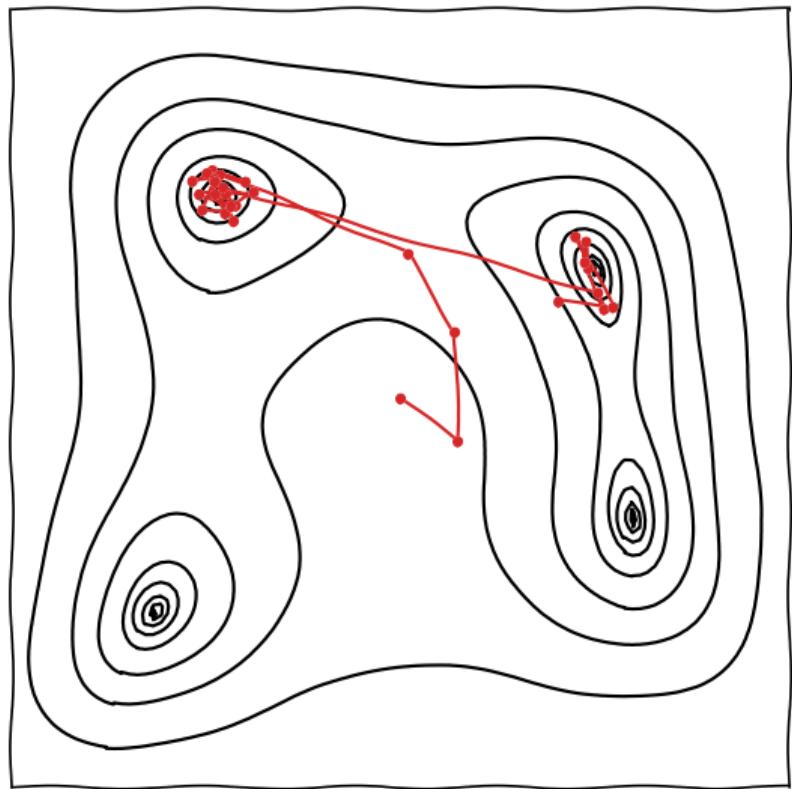
## MCMC



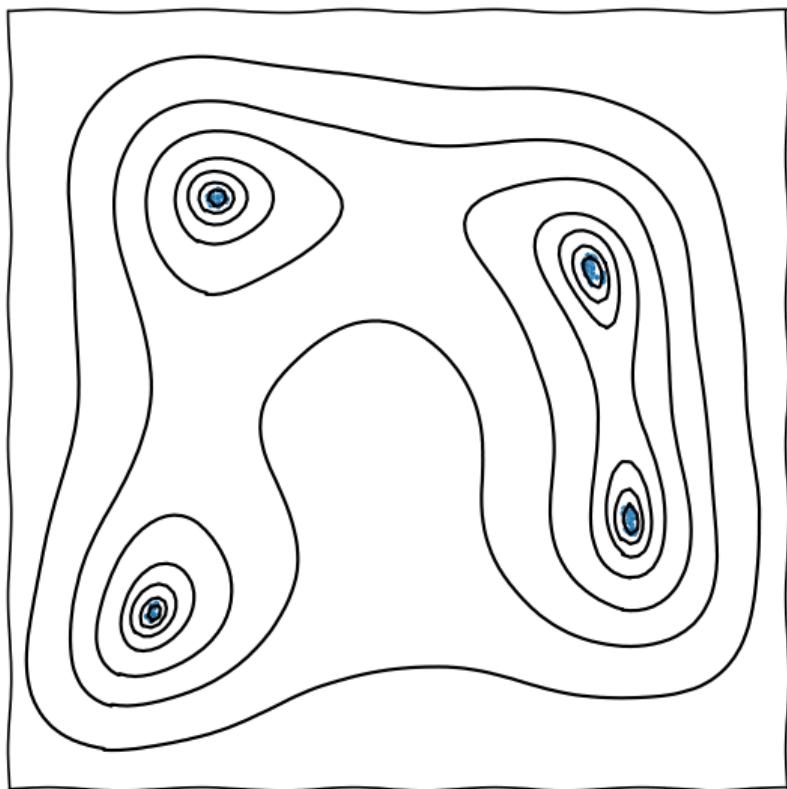
## Nested sampling



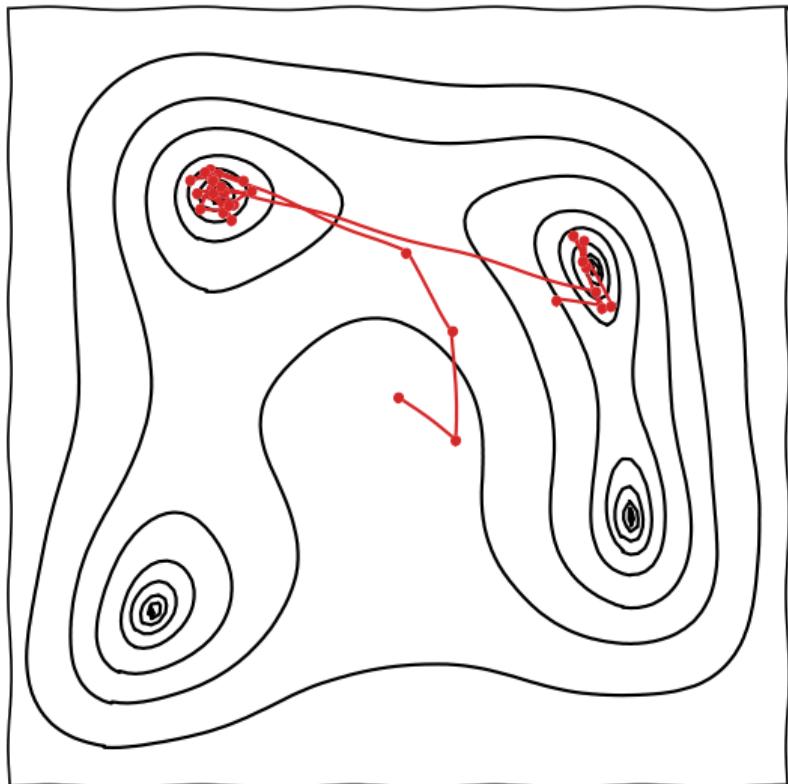
## MCMC



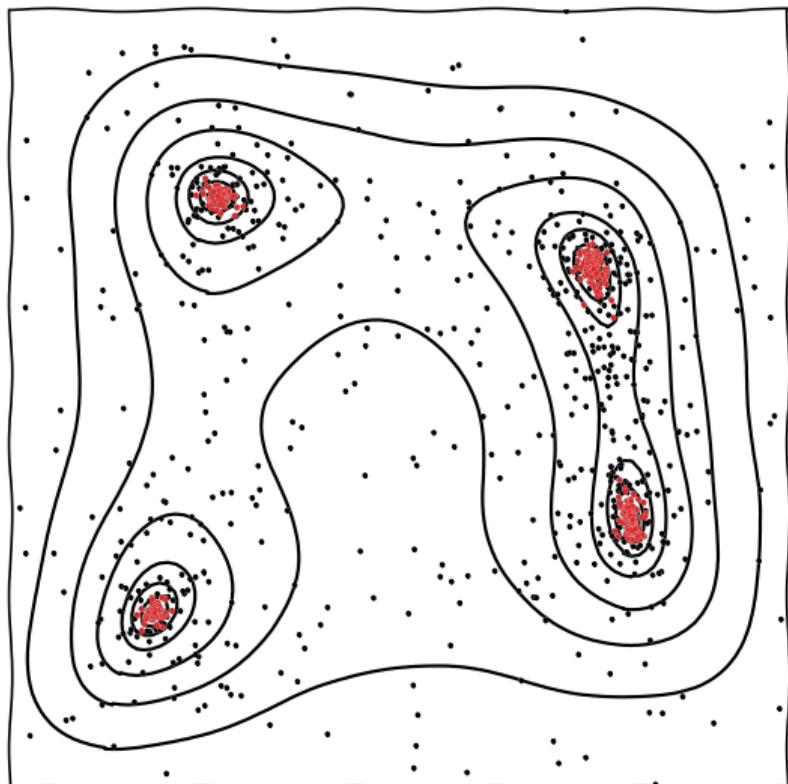
## Nested sampling



## MCMC

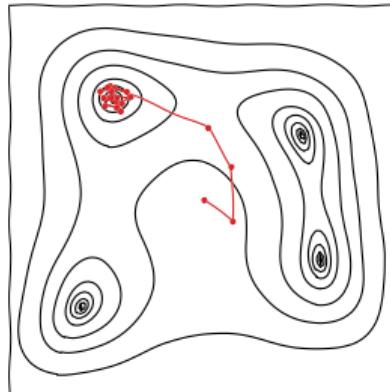


## Nested sampling



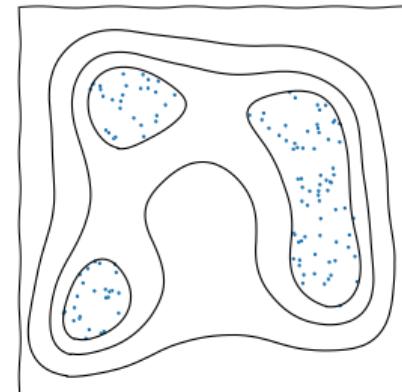
## MCMC

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



## Nested sampling

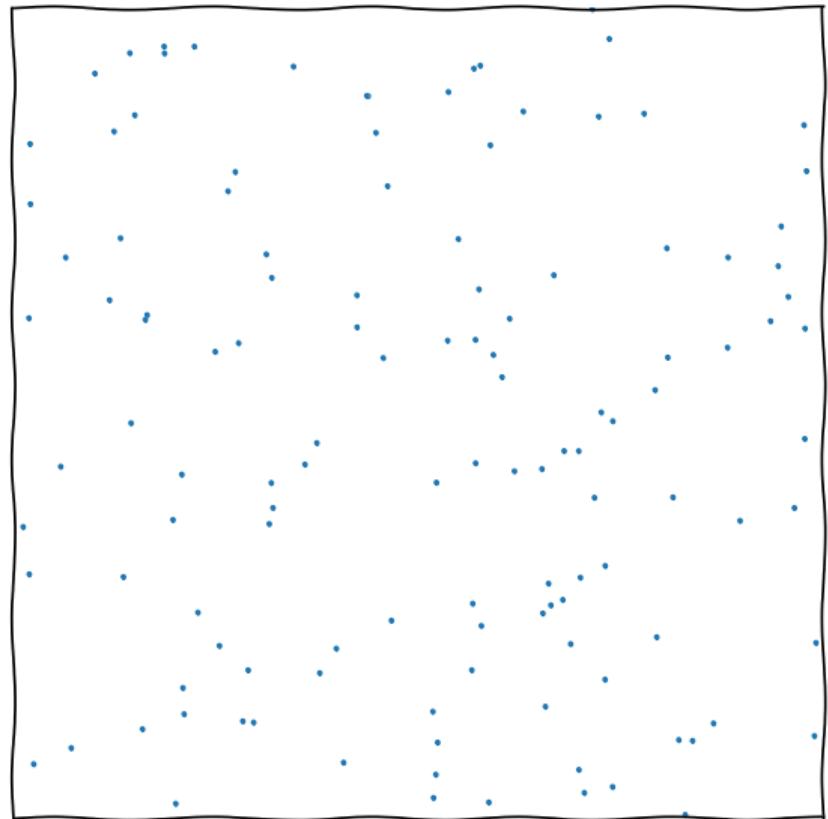
- ▶ Ensemble of “live points”
- ▶ Scans from prior to peak of likelihood
- ▶ Slower, no tuning required
- ▶ Parameter estimation, model comparison, tension quantification
- ▶ Channel capacity optimised for computing partition function



## The nested sampling meta-algorithm

- ▶ 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

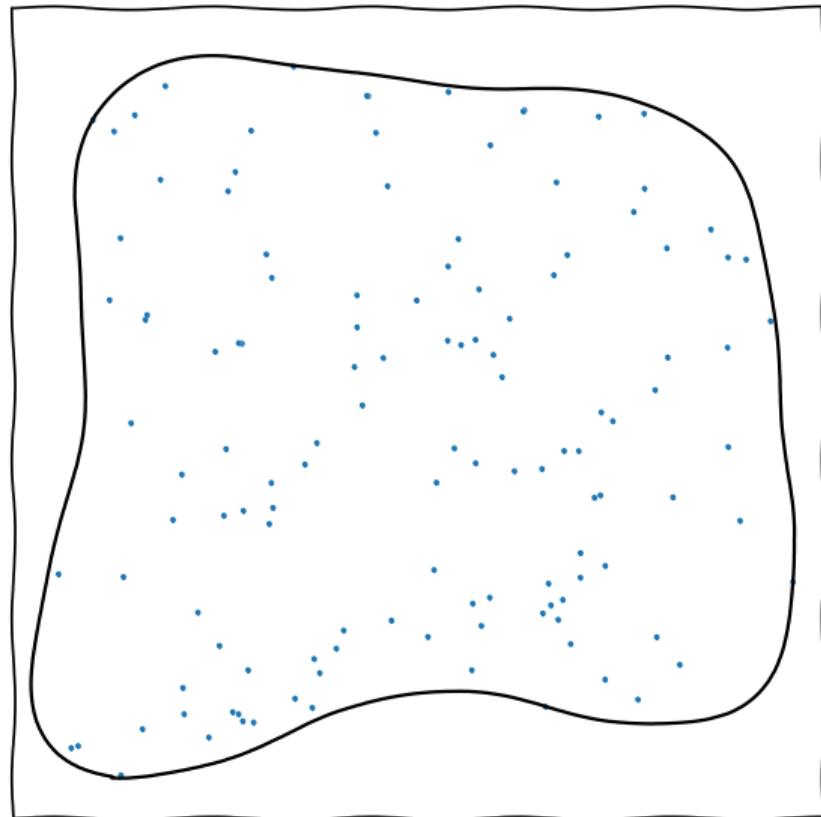
$$\sum_i f(x_i) \Delta V_i, \quad V_i = V_0 e^{-i/n}$$



## The nested sampling meta-algorithm

- ▶ 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

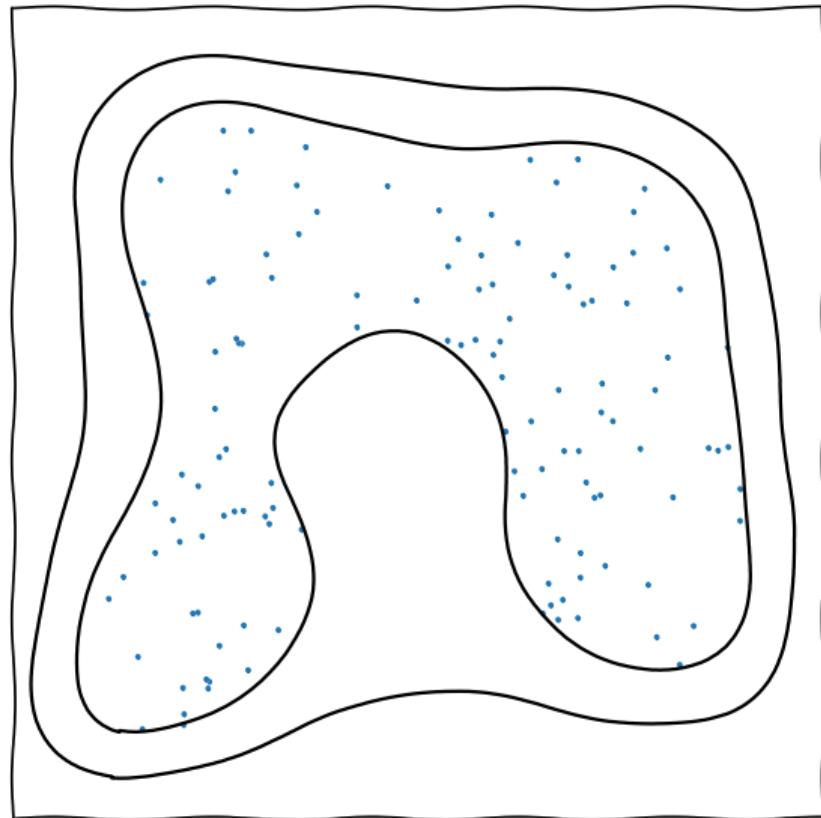
$$\sum_i f(x_i) \Delta V_i, \quad V_i = V_0 e^{-i/n}$$



## The nested sampling meta-algorithm

- ▶ 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

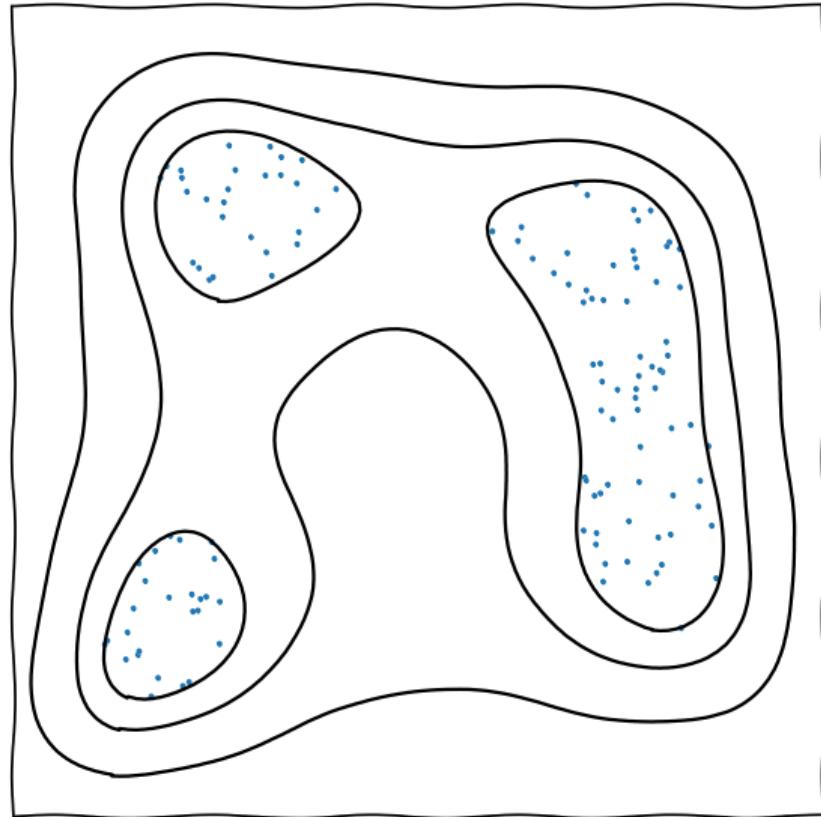
$$\sum_i f(x_i) \Delta V_i, \quad V_i = V_0 e^{-i/n}$$



## The nested sampling meta-algorithm

- ▶ 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

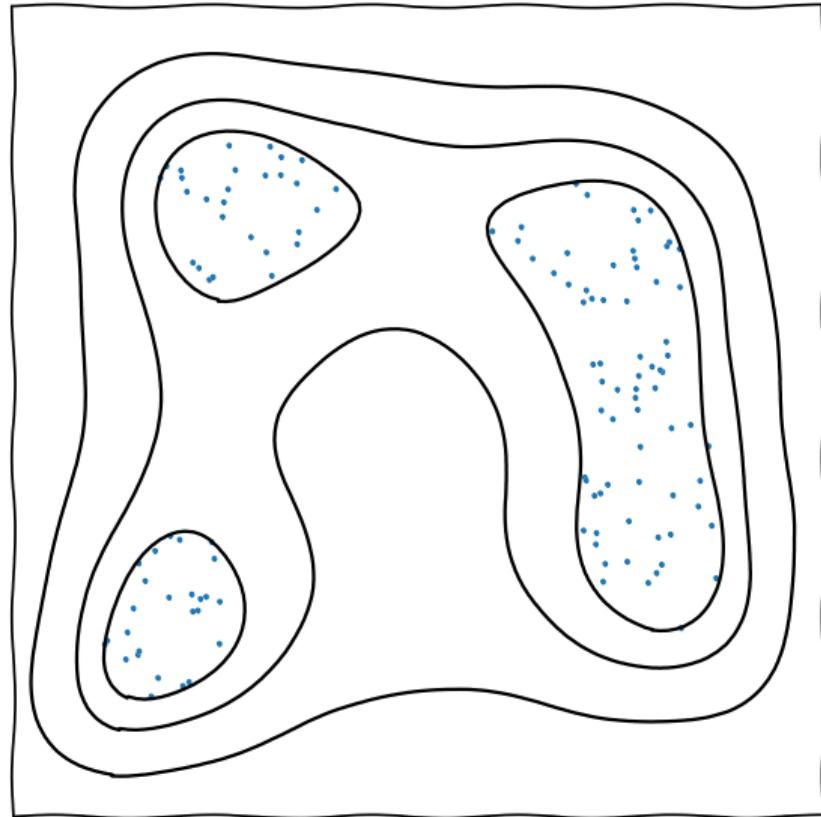
$$\sum_i f(x_i) \Delta V_i, \quad V_i = V_0 e^{-i/n}$$



## The nested sampling meta-algorithm

- ▶ 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  $\sim \frac{1}{n} \pm \frac{1}{n}$  of their volume.
- ▶ This is an exponential contraction, so

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

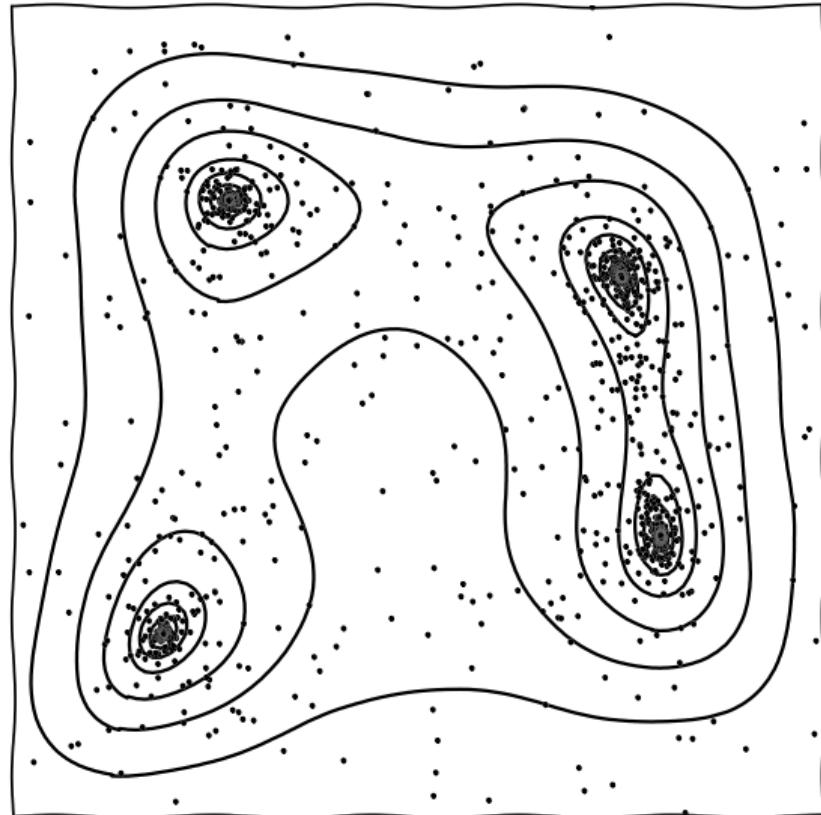


# The nested sampling meta-algorithm: Lebesgue integration

- ▶ At the end, one is left with a set of discarded “dead” points.
- ▶ 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
- ▶ For this kind of numerical, generic, high-dimensional integration, it is the only game in town.



## Sampling from a hard likelihood constraint

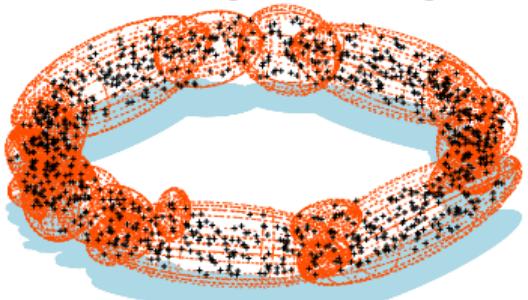
*"It is not the purpose of this introductory paper to develop the technology of navigation within such a volume. We merely note that exploring a hard-edged likelihood-constrained domain should prove to be neither more nor less demanding than exploring a likelihood-weighted space."*

— John Skilling

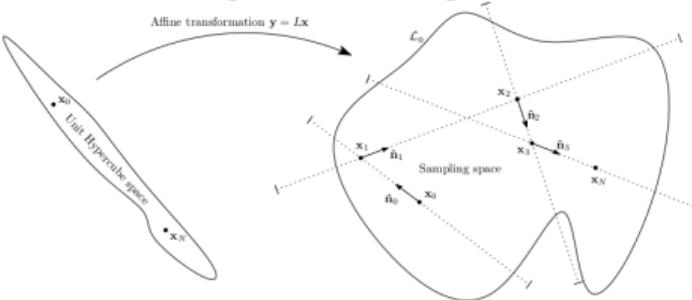
- ▶ A large fraction of the work in NS to date has been in attempting to implement a hard-edged sampler in the NS meta-algorithm  $\{\theta \sim \pi : \mathcal{L}(\theta) > \mathcal{L}_*\}$ .
- ▶ <https://projecteuclid.org/euclid.ba/1340370944>.
- ▶ There has also been much work beyond this (see 'frontiers of nested sampling talk'
  - ▶ See "Frontiers of nested sampling": [willhandley.co.uk/talks](http://willhandley.co.uk/talks)

# Implementations of Nested Sampling [2205.15570](NatReview)

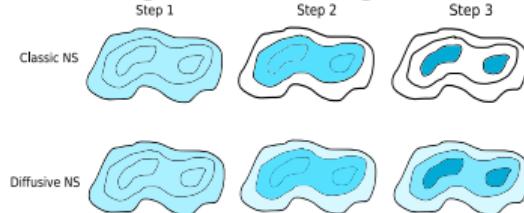
MultiNest [0809.3437]



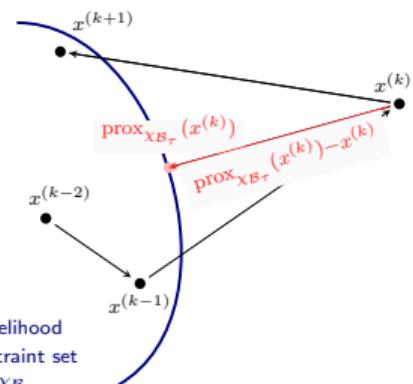
PolyChord [1506.00171]



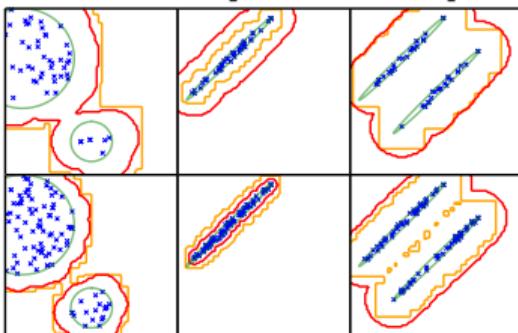
DNest [1606.03757]



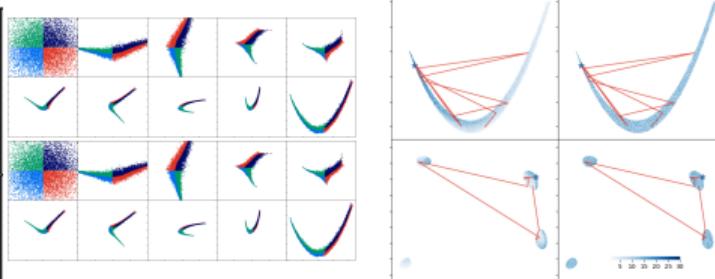
ProxNest [2106.03646]



UltraNest [2101.09604]



NeuralNest [1903.10860]



nessai [2102.11056]

nora [2305.19267]

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  $d > d_0 \sim 10$ .

- ▶ Nested samplers usually come with:

- ▶ *resolution* parameter  $n_{\text{live}}$  (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  $\text{eff}$  or PolyChord chain length  $n_{\text{repeats}}$ .

## 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.

# Applications: 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  $\Lambda$ CDM 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.  $\Lambda$ CDM vs a dynamic dark energy cosmology

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

$$\frac{\mathcal{Z}_M \Pi_M}{\sum_m \mathcal{Z}_m \Pi_m}$$

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

## Tension quantification

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

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

$$\begin{aligned} \log \mathcal{S} &= \langle \log \mathcal{L}_{AB} \rangle_{\mathcal{P}_{AB}} \\ &\quad - \langle \log \mathcal{L}_A \rangle_{\mathcal{P}_A} \\ &\quad - \langle \log \mathcal{L}_B \rangle_{\mathcal{P}_B} \end{aligned}$$

# Applications of nested sampling

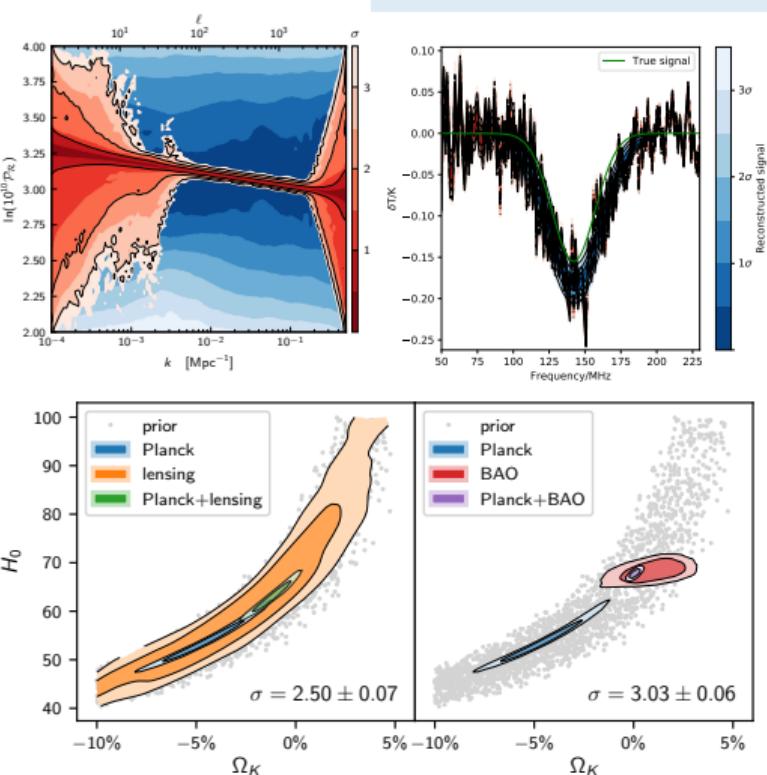
Adam Ormondroyd



PhD

## Cosmology

- ▶ 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  $\Lambda$ CDM 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

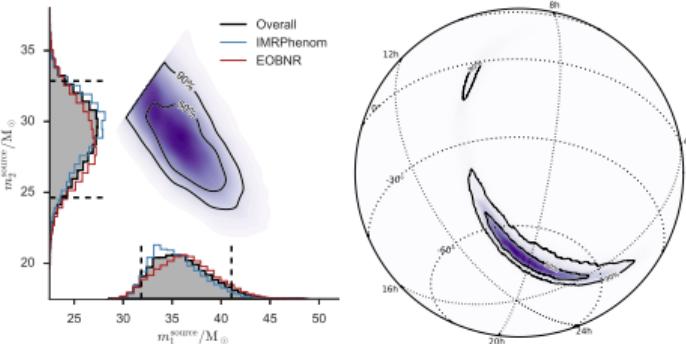
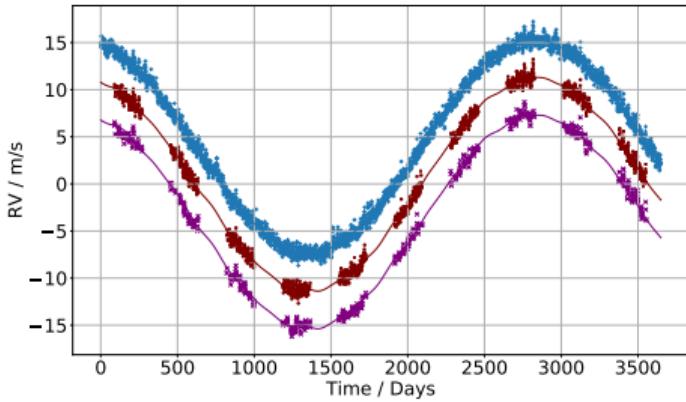
Metha Prathaban

PhD



## Astrophysics

- ▶ 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

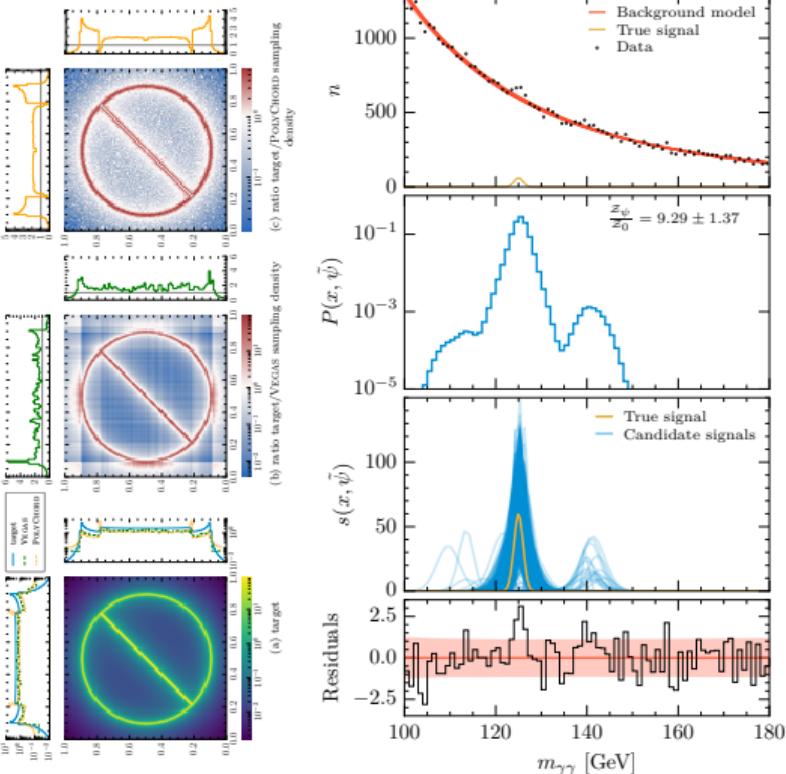
## Particle physics

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  $\Omega$  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



# Applications of nested sampling

## Lattice field theory

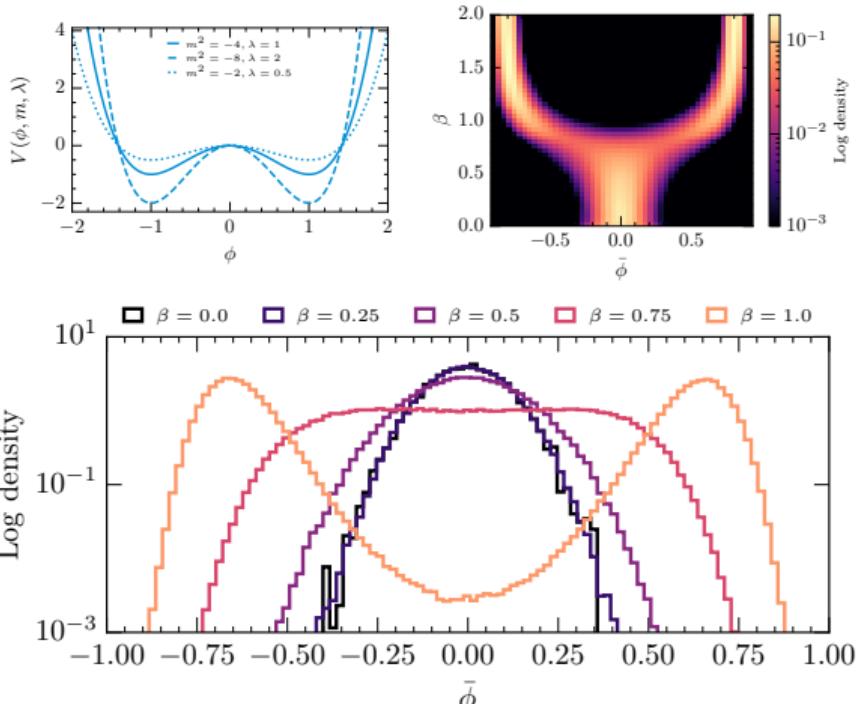
- Consider standard field theory Lagrangian:

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

- 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
- Publication imminent (next week)

David Yallup

PDRA

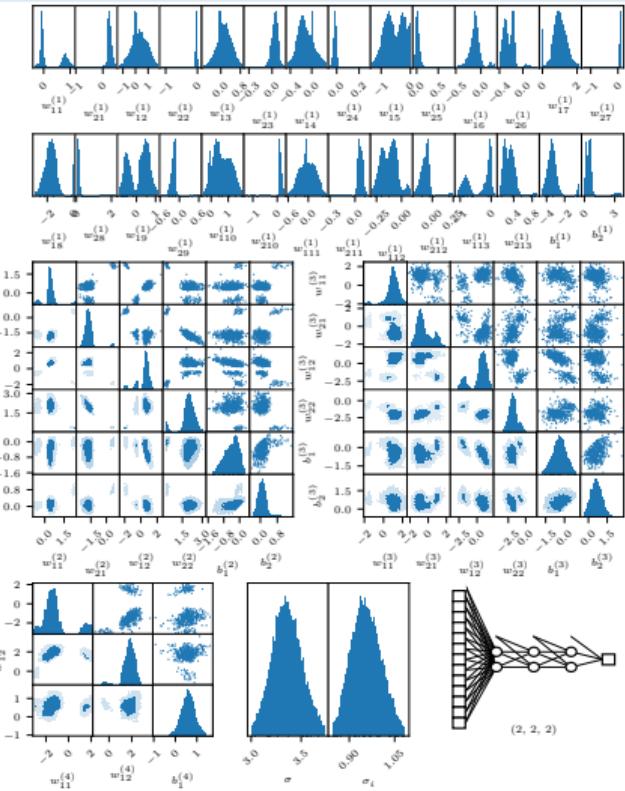




# Applications of nested sampling

## Machine learning

- ▶ 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.



# Applications of nested sampling

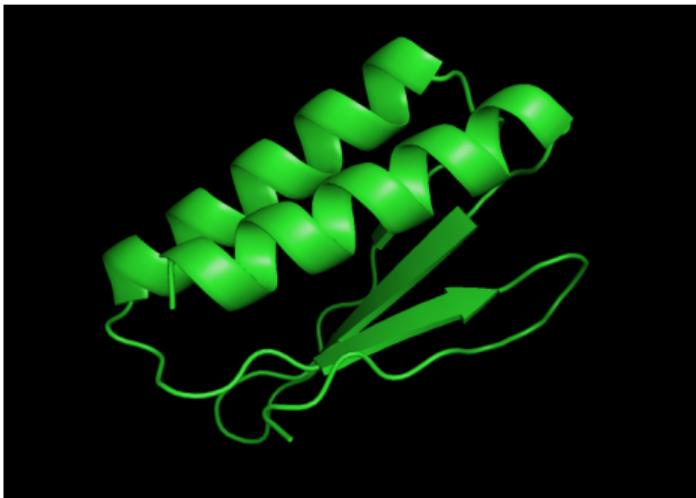
And beyond...

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.



# Applications of nested sampling

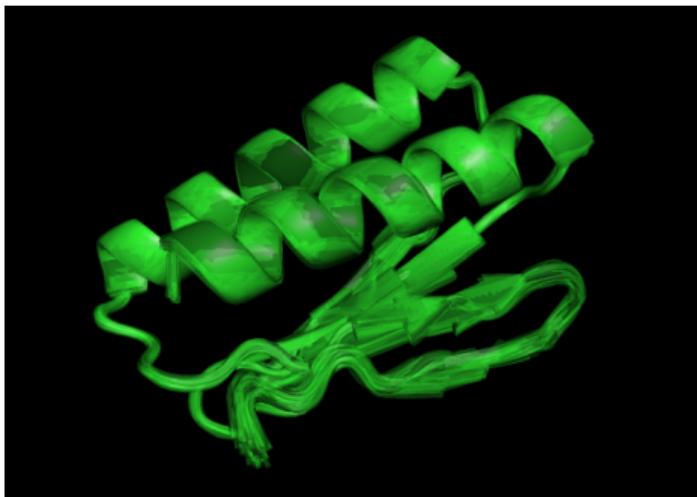
And beyond...

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.



# Applications of nested sampling

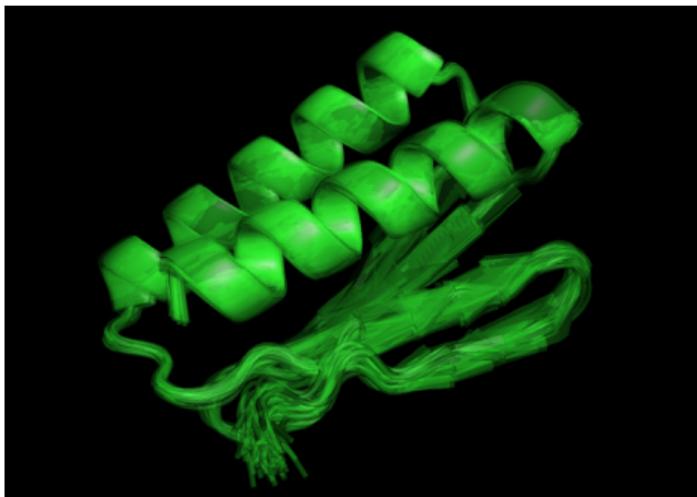
And beyond...

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.



# Applications of nested sampling

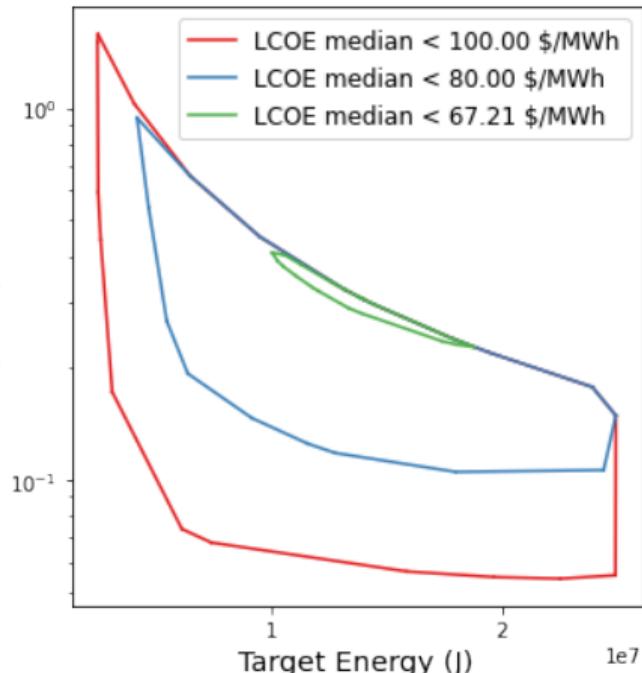
And beyond...

- ▶ 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.



Catherine Watkinson

Senior Data Scientist



# Applications of nested sampling

And beyond...

Thomas Mcaloone

PhD → Data Scientist



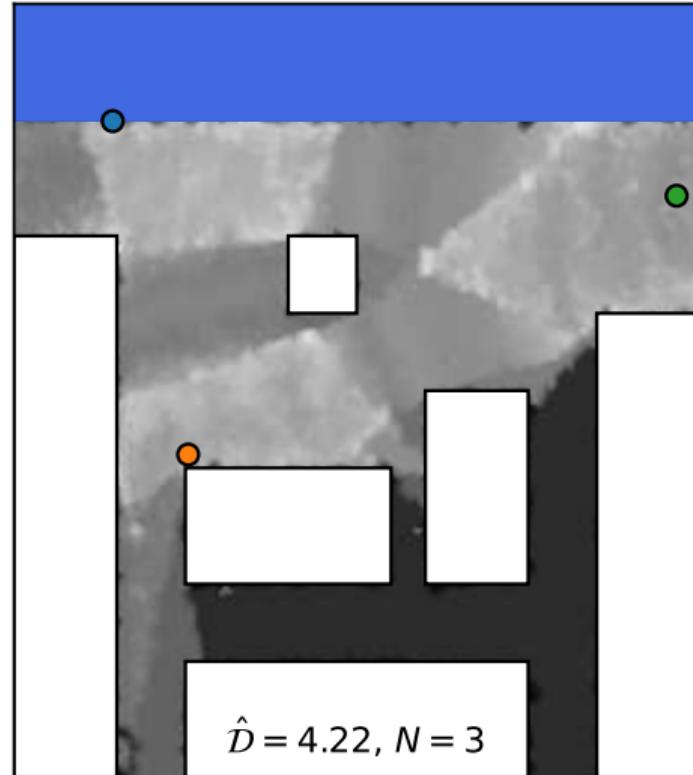
- ▶ Techniques have been spun-out (PolyChord Ltd) to:
- ▶ Protein folding
  - ▶ Navigating free energy surface.
  - ▶ Computing misfolds.
  - ▶ Thermal motion.
- ▶ Nuclear fusion reactor optimisation
  - ▶ multi-objective.
  - ▶ uncertainty propagation.
- ▶ Telecoms & DSTL research (MIDAS)
  - ▶ Optimising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



# Applications of nested sampling

And beyond...

- ▶ 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.



# Applications of nested sampling

And beyond...

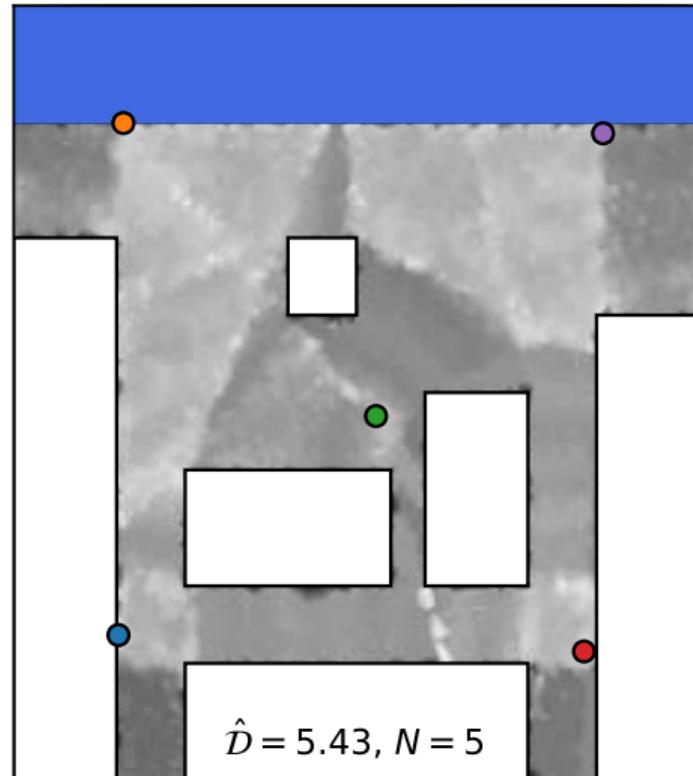
- ▶ Techniques have been spun-out (PolyChord Ltd) to:
- ▶ Protein folding
  - ▶ Navigating free energy surface.
  - ▶ Computing misfolds.
  - ▶ Thermal motion.
- ▶ Nuclear fusion reactor optimisation
  - ▶ multi-objective.
  - ▶ uncertainty propagation.
- ▶ Telecoms & DSTL research (MIDAS)
  - ▶ Optimising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



# Applications of nested sampling

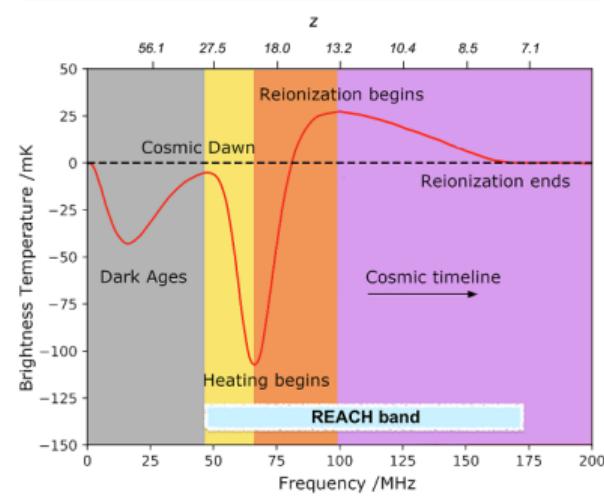
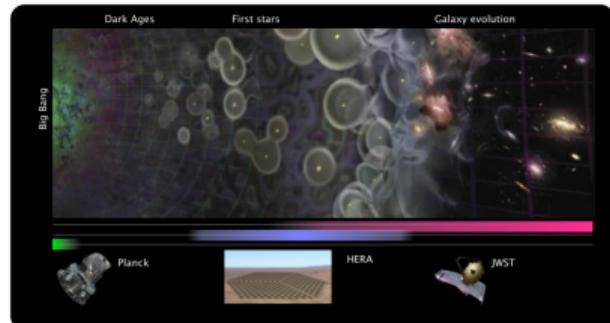
And beyond...

- ▶ 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.



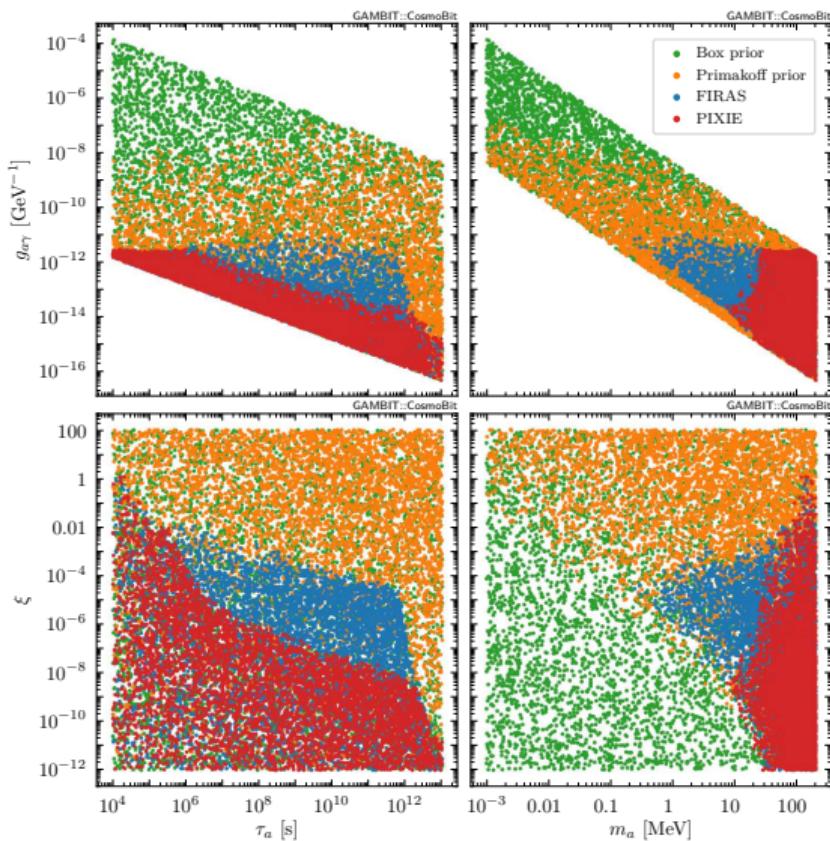
# REACH: Global 21cm cosmology [2210.07409](NatAstro)

- ▶ 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]



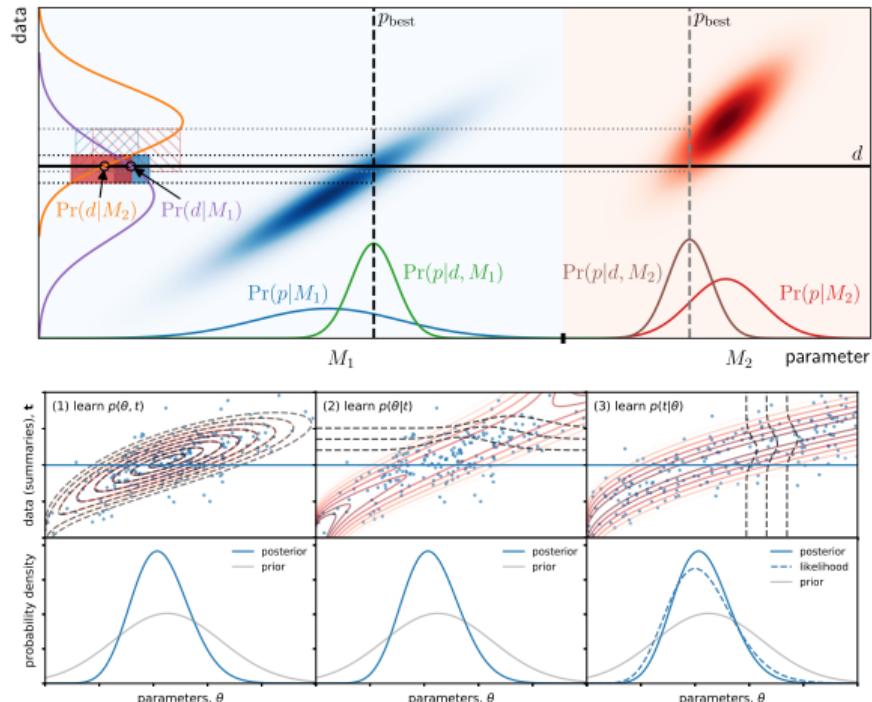
# Likelihood-free inference (aka SBI)

Kilian Scheutwinkel

PhD



- ▶ How do you do inference if you don't know the likelihood  $P(D|\theta)$ ?
  - ▶ e.g. if you can simulate a disease outbreak, how can you infer a posterior on  $R_0$ , or select the most predictive model?
- ▶ If you can forward simulate/model  $\theta \rightarrow D$ , then you have an implicit likelihood.
- ▶ LFI aims to (machine-)learn the likelihood from carefully chosen training data  $\{(\theta, D)\}$ .
- ▶ Nested sampling has much to offer
  - ▶ truncation strategies (PolySwyft)
  - ▶ evidence driven compression
  - ▶ marginalised machine learning
- ▶ In my view, LFI represents the future of inference – in twenty years time this will be as well-used as MCMC techniques are today.



# unimpeded: PLA for the next generation

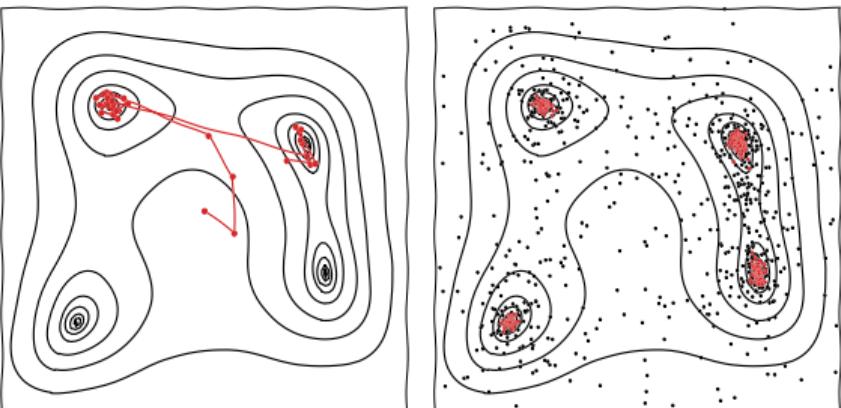
Harry Bevins



PhD→JRF

- ▶ DiRAC 2020 RAC allocation of 30MCPUh
- ▶ Main goal: Planck Legacy Archive equivalent
- ▶ Parameter estimation → Model comparison
- ▶ MCMC → Nested sampling
- ▶ Planck → {Planck, DESY1, BAO, ...}
- ▶ Pairwise combinations
- ▶ Suite of tools for processing these
  - ▶ anesthetic 2.0
  - ▶ unimpeded 1.0
  - ▶ zenodo archive
  - ▶ margarine
- ▶ MCMC chains also available.
- ▶ Library of bijectors emulators for fast re-use

# DiRAC



# CosmoTension

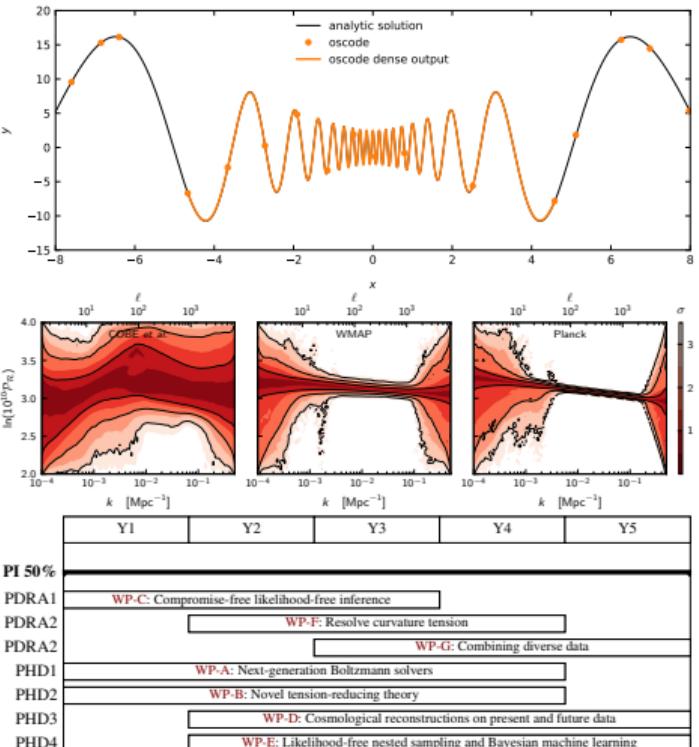
Resolving cosmological tensions with diverse data, novel theories and Bayesian machine learning

Will Barker

PhD→JRF



- ▶ ERC grant ⇒ UKRI Frontier, commencing 2023.
- ▶ Funds 3 PDRAs and 4 PhDs over 5 years.
- ▶ Research programme centered around combining novel theories of gravity, Boltzmann solvers [1906.01421], reconstruction [1908.00906], nested sampling & likelihood free inference.
- ▶ Aims to disentangle cosmological tensions  $H_0$ ,  $\sigma_8$ ,  $\Omega_K$  with next-generation data analysis techniques.

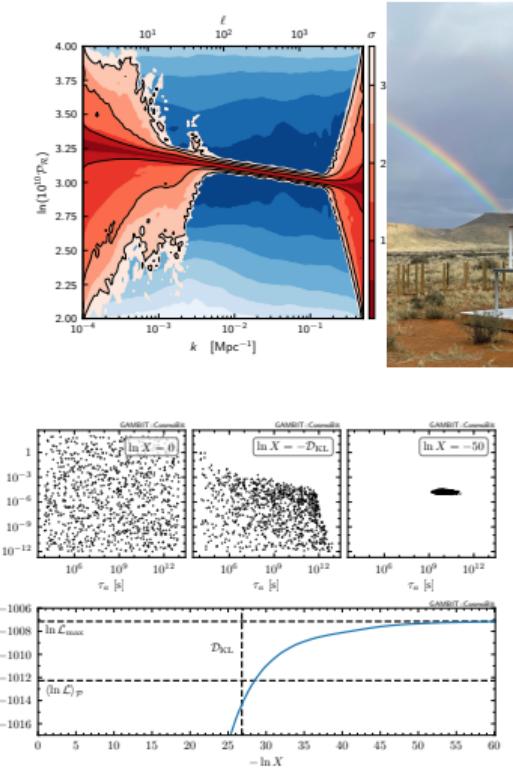
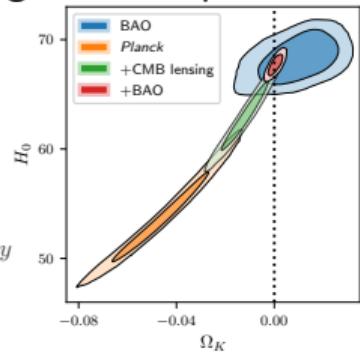
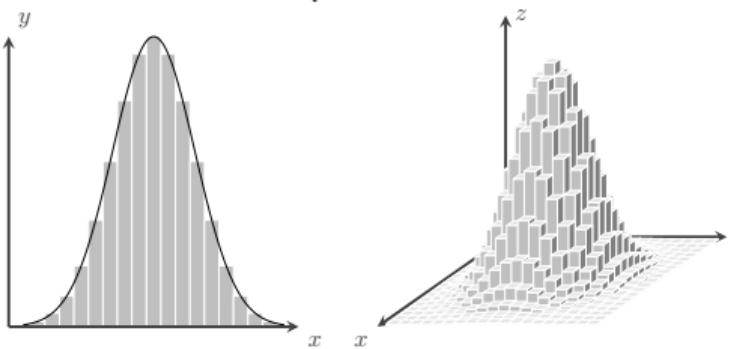


# Conclusions

[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 & machine learning.
- ▶ It's unique traits as the only numerical Lebesgue integrator mean with compute it will continue to grow in importance.



# How does Nested Sampling compare to other approaches?

- ▶ In all cases:
    - + NS can handle multimodal functions
    - + NS computes evidences, partition functions and integrals
    - + NS is self-tuning/black-box
- Modern Nested Sampling algorithms can do this in  $\sim \mathcal{O}(100s)$  dimensions

## Optimisation

- ▶ Gradient descent
  - NS cannot use gradients
  - + NS does not require gradients
- ▶ Genetic algorithms
  - + NS discarded points have statistical meaning

## Sampling

- ▶ Metropolis-Hastings?
  - Nothing beats well-tuned customised MH
  - + NS is self tuning
- ▶ Hamiltonian Monte Carlo?
  - In millions of dimensions, HMC is king
  - + NS does not require gradients

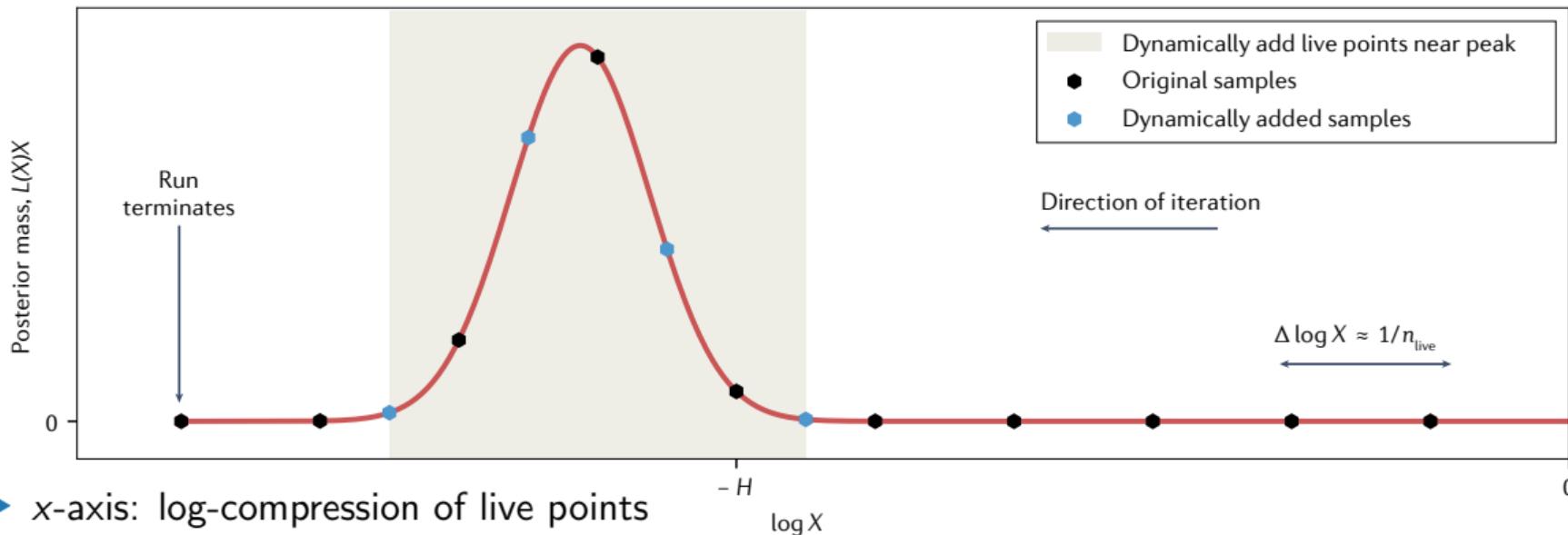
## Integration

- ▶ Thermodynamic integration
  - protective against phase transitions
  - + No annealing schedule tuning
- ▶ Sequential Monte Carlo
  - SMC experts classify NS as a kind of SMC
  - + NS is athermal

# Nested Sampling: a user's guide

1. Nested sampling is a likelihood scanner, rather than posterior explorer.
  - ▶ This means typically most of its time is spent on burn-in rather than posterior sampling.
  - ▶ Changing the stopping criterion from  $10^{-3}$  to 0.5 does little to speed up the run, but can make results very unreliable.
2. The number of live points  $n_{\text{live}}$  is a resolution parameter.
  - ▶ Run time is linear in  $n_{\text{live}}$ , posterior and evidence accuracy goes as  $\frac{1}{\sqrt{n_{\text{live}}}}$ .
  - ▶ Set low for exploratory runs  $\sim \mathcal{O}(10)$  and increased to  $\sim \mathcal{O}(1000)$  for production standard.
3. Most algorithms come with additional reliability parameter(s).
  - ▶ e.g. MultiNest:  $\text{eff}$ , PolyChord:  $n_{\text{repeats}}$ .
  - ▶ These are parameters which have no gain if set too conservatively, but increase the reliability.
  - ▶ Check that results do not degrade if you reduce them from defaults, otherwise increase.

# Time complexity of nested sampling



► Time complexity

$$T = n_{\text{live}} \times T_{\mathcal{L}} \times T_{\text{sampler}} \times D_{\text{KL}}(\mathcal{P} \parallel \pi)$$

► Error complexity  $\sigma \propto \sqrt{D_{\text{KL}}(\mathcal{P} \parallel \pi) / n_{\text{live}}}$

# Occam's Razor [2102.11511]

- ▶ Bayesian inference quantifies Occam's Razor:
  - ▶ “Entities are not to be multiplied without necessity” — William of Occam
  - ▶ “Everything should be kept as simple as possible, but not simpler” — Albert Einstein”
- ▶ Properties of the evidence: rearrange Bayes' theorem for parameter estimation

$$\mathcal{P}(\theta) = \frac{\mathcal{L}(\theta)\pi(\theta)}{\mathcal{Z}} \quad \Rightarrow \quad \log \mathcal{Z} = \log \mathcal{L}(\theta) - \log \frac{\mathcal{P}(\theta)}{\pi(\theta)}.$$

- ▶ Evidence is composed of a “goodness of fit” term and “Occam Penalty”.
- ▶ RHS true for all  $\theta$ . Take max likelihood value  $\theta_*$ :
- ▶ Be more Bayesian and take posterior average to get the “Occam's razor equation”

$$\log \mathcal{Z} = -\chi^2_{\min} - \text{Mackay penalty.}$$

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

- ▶ Natural regularisation which penalises models with too many parameters.

# Kullback Liebler divergence

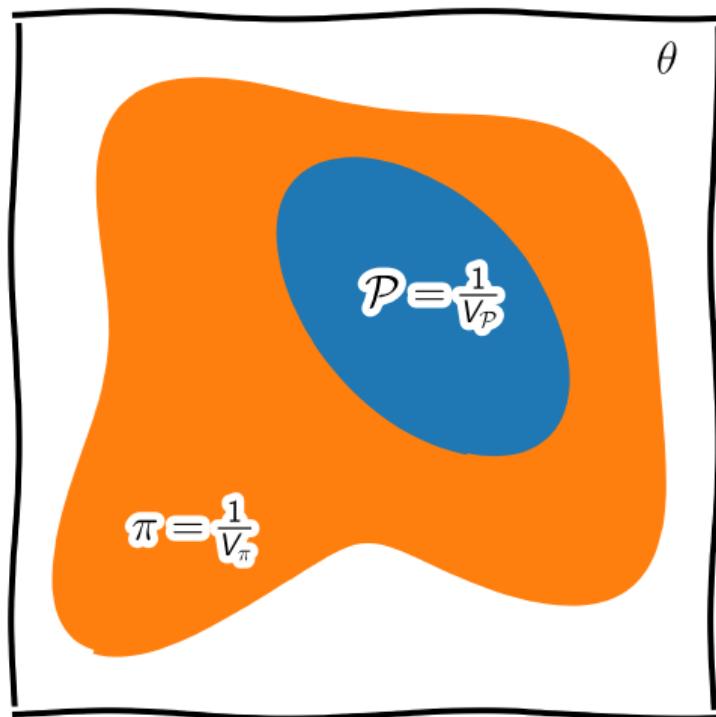
- The KL divergence between prior  $\pi$  and posterior  $\mathcal{P}$  is defined as:

$$\mathcal{D}_{\text{KL}} = \left\langle \log \frac{\mathcal{P}}{\pi} \right\rangle_{\mathcal{P}} = \int \mathcal{P}(\theta) \log \frac{\mathcal{P}(\theta)}{\pi(\theta)} d\theta.$$

- Whilst not a distance,  $\mathcal{D} = 0$  when  $\mathcal{P} = \pi$ .
- Occurs in the context of machine learning as an objective function for training functions.
- In Bayesian inference it can be understood as a log-ratio of “volumes”:

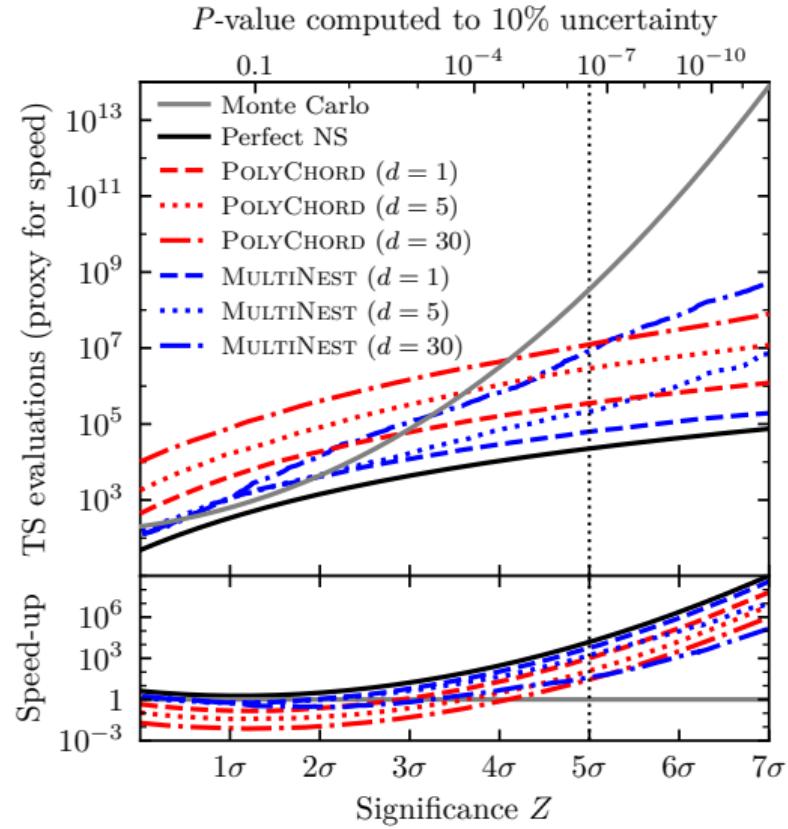
$$\mathcal{D}_{\text{KL}} \approx \log \frac{V_\pi}{V_{\mathcal{P}}}.$$

(this is exact for top-hat distributions).



# Statistics: fast estimation of small $p$ -values [2106.02056](PRL)

- ▶ 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.



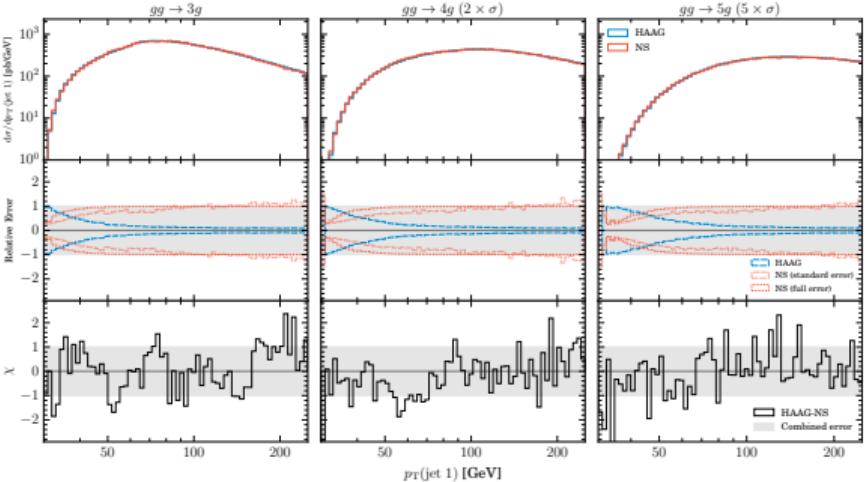
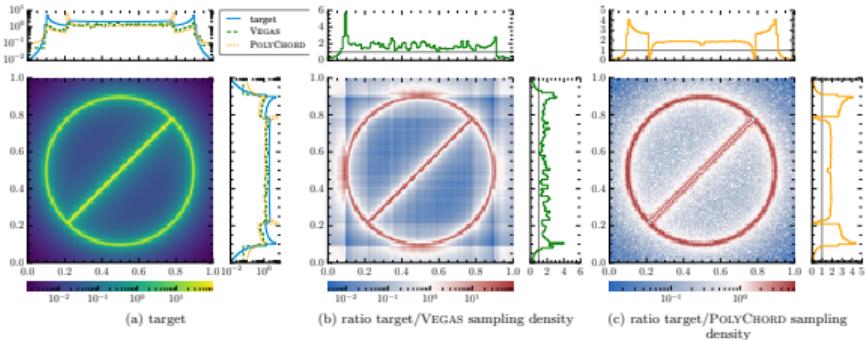
# Exploration of phase space [2106.02056]

- ▶ Nested sampling for cross section computation/event generation.
- ▶ Numerically compute collisional cross section

$$\sigma = \int_{\Omega} d\Phi |\mathcal{M}|^2,$$

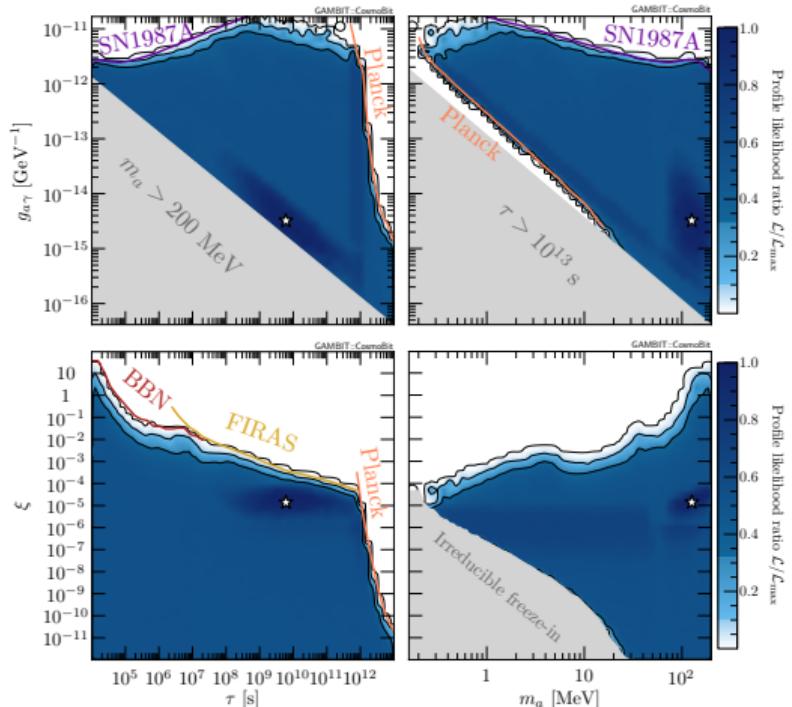
$\Omega$  phase space of kinematic configurations  $\Phi$ , each with matrix element  $\mathcal{M}(\Phi)$ .

- ▶ Current state of the art e.g. HAAG (improvement on RAMBO) requires knowledge of  $\mathcal{M}(\Phi)$ .
- ▶ Nested sampling can explore the phase space and compute integral blind with comparable efficiency.



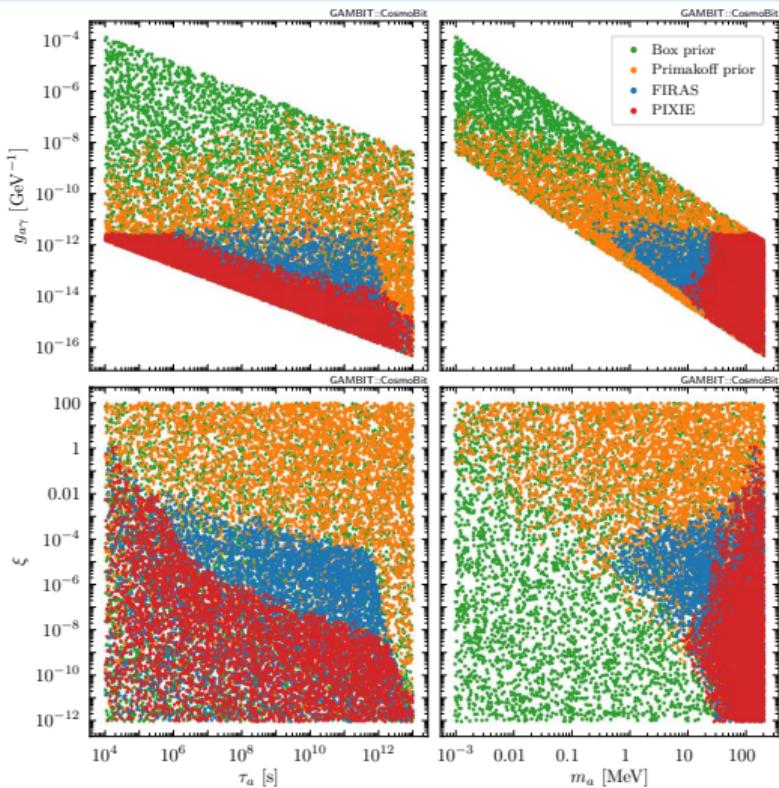
# Quantification of fine tuning [2101.00428] [2205.13549]

- ▶ Example: Cosmological constraints on decaying axion-like particles [2205.13549].
- ▶ Subset of parameters  $\xi, m_a, \tau, g_{a\gamma}$ : ALP fraction, mass, lifetime and photon coupling. (Also vary cosmology,  $\tau_n$  and nuisance params)
- ▶ Data: CMB, BBN, FIRAS, SMM, BAO.
- ▶ Standard profile likelihood fit shows ruled out regions and best-fit point.



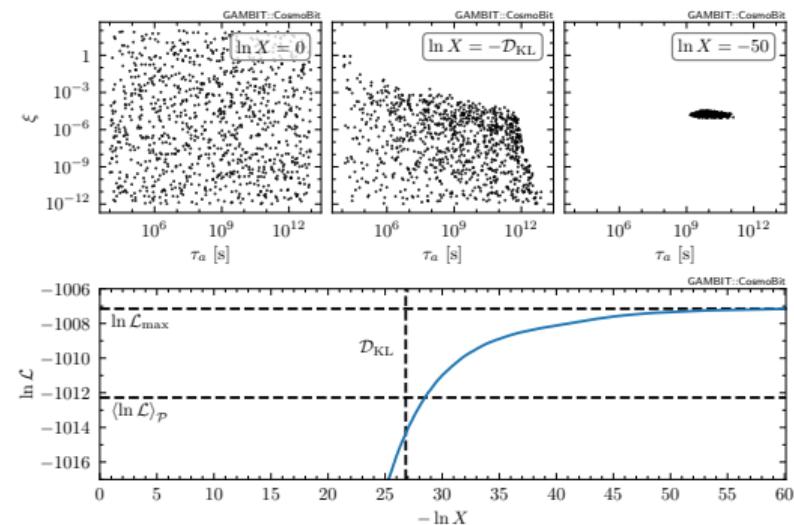
# Quantification of fine tuning [2101.00428] [2205.13549]

- ▶ Example: Cosmological constraints on decaying axion-like particles [2205.13549].
- ▶ Subset of parameters  $\xi, m_a, \tau, g_{a\gamma}$ : ALP fraction, mass, lifetime and photon coupling. (Also vary cosmology,  $\tau_n$  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  $\mathcal{D}_{KL}$ .
  - ▶ 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.



# Quantification of fine tuning [2101.00428] [2205.13549]

- ▶ Example: Cosmological constraints on decaying axion-like particles [2205.13549].
- ▶ Subset of parameters  $\xi, m_a, \tau, g_{a\gamma}$ : ALP fraction, mass, lifetime and photon coupling. (Also vary cosmology,  $\tau_n$  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  $\mathcal{D}_{KL}$ .
  - ▶ 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.

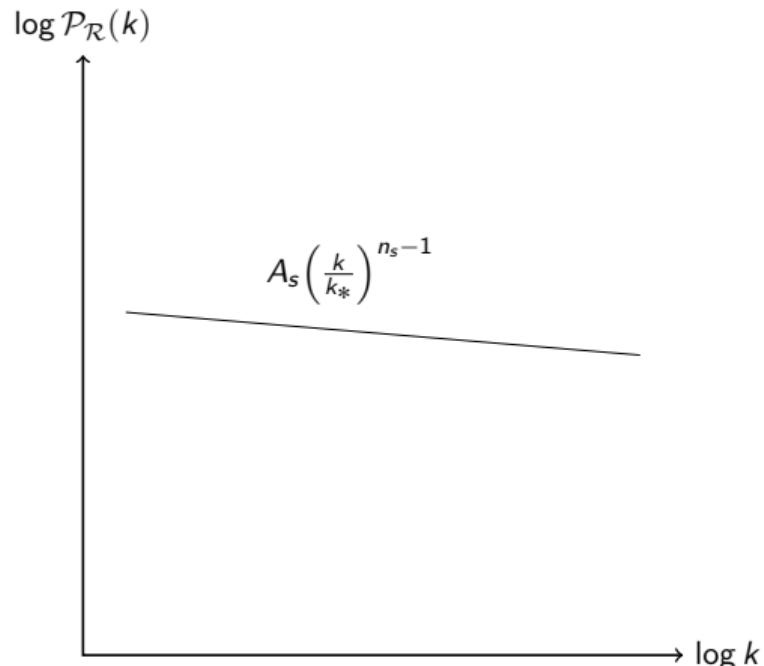


# Primordial power spectrum $\mathcal{P}_{\mathcal{R}}(k)$ reconstruction [1908.00906]

- ▶ Traditionally parameterise the primordial power spectrum with  $(A_s, n_s)$

$$\mathcal{P}_{\mathcal{R}}(k) = A_s \left( \frac{k}{k_*} \right)^{n_s - 1}$$

- ▶ To add more degrees of freedom, can add “running” parameters  $n_{\text{run}}$  (higher order polynomial in index)
- ▶ Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: “FlexKnots”
- ▶ Let the Bayesian evidence decide when you’ve introduced too many parameters

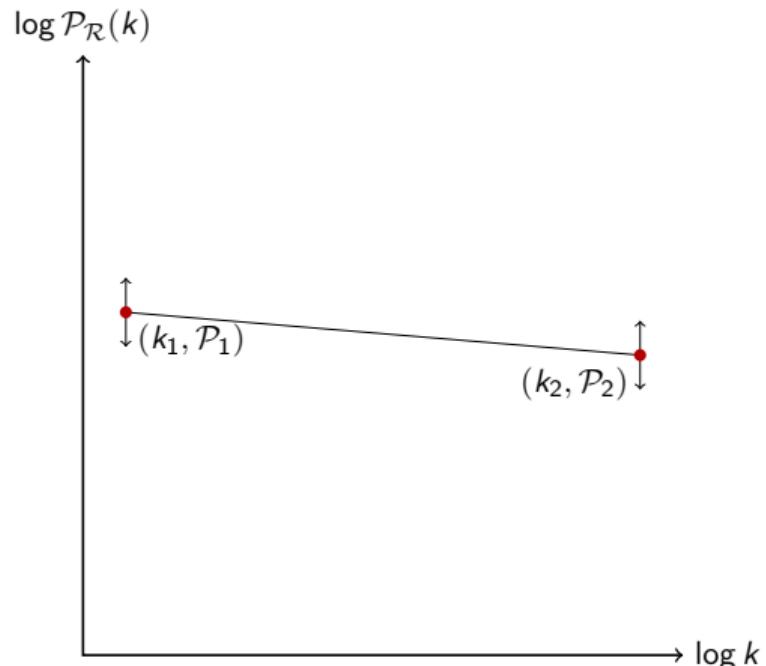


# Primordial power spectrum $\mathcal{P}_{\mathcal{R}}(k)$ reconstruction [1908.00906]

- Traditionally parameterise the primordial power spectrum with  $(A_s, n_s)$

$$\mathcal{P}_{\mathcal{R}}(k) = A_s \left( \frac{k}{k_*} \right)^{n_s - 1}$$

- To add more degrees of freedom, can add “running” parameters  $n_{\text{run}}$  (higher order polynomial in index)
- Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: “FlexKnots”
- Let the Bayesian evidence decide when you’ve introduced too many parameters

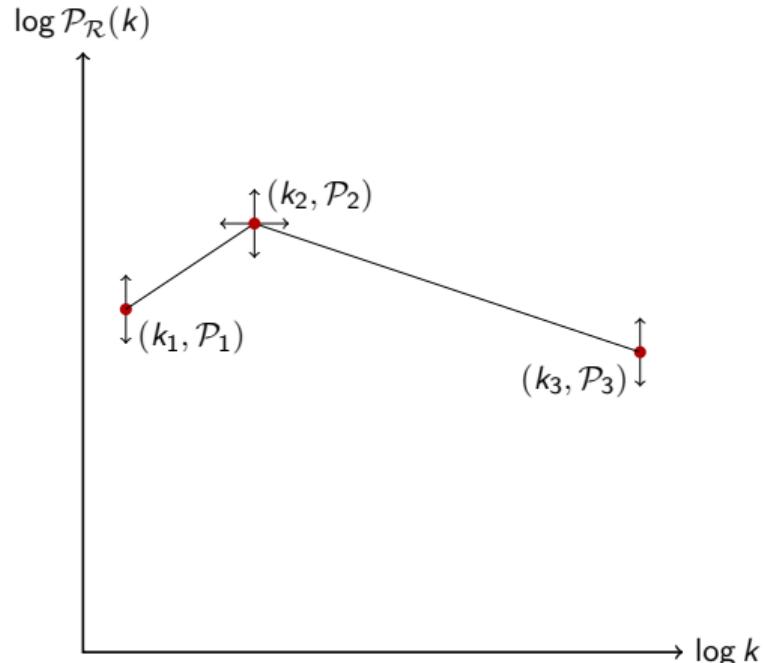


# Primordial power spectrum $\mathcal{P}_{\mathcal{R}}(k)$ reconstruction [1908.00906]

- Traditionally parameterise the primordial power spectrum with  $(A_s, n_s)$

$$\mathcal{P}_{\mathcal{R}}(k) = A_s \left( \frac{k}{k_*} \right)^{n_s - 1}$$

- To add more degrees of freedom, can add “running” parameters  $n_{\text{run}}$  (higher order polynomial in index)
- Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: “FlexKnots”
- Let the Bayesian evidence decide when you’ve introduced too many parameters

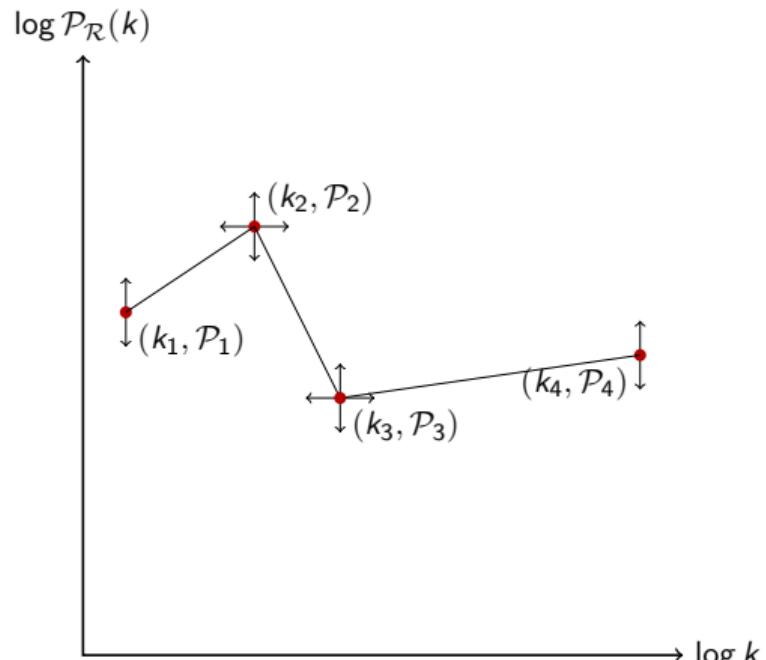


# Primordial power spectrum $\mathcal{P}_{\mathcal{R}}(k)$ reconstruction [1908.00906]

- Traditionally parameterise the primordial power spectrum with  $(A_s, n_s)$

$$\mathcal{P}_{\mathcal{R}}(k) = A_s \left( \frac{k}{k_*} \right)^{n_s - 1}$$

- To add more degrees of freedom, can add “running” parameters  $n_{\text{run}}$  (higher order polynomial in index)
- Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: “FlexKnots”
- Let the Bayesian evidence decide when you’ve introduced too many parameters

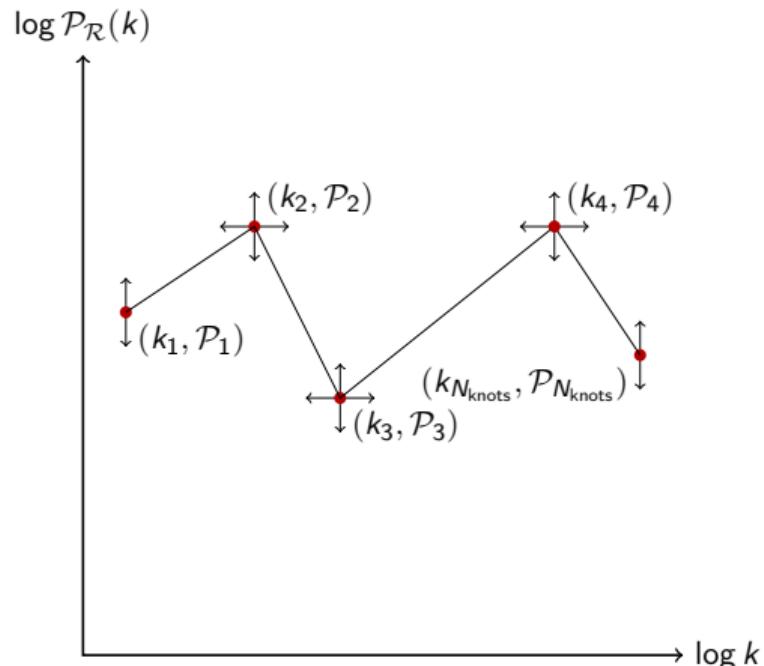


# Primordial power spectrum $\mathcal{P}_{\mathcal{R}}(k)$ reconstruction [1908.00906]

- Traditionally parameterise the primordial power spectrum with  $(A_s, n_s)$

$$\mathcal{P}_{\mathcal{R}}(k) = A_s \left( \frac{k}{k_*} \right)^{n_s - 1}$$

- To add more degrees of freedom, can add “running” parameters  $n_{\text{run}}$  (higher order polynomial in index)
- Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: “FlexKnots”
- Let the Bayesian evidence decide when you’ve introduced too many parameters

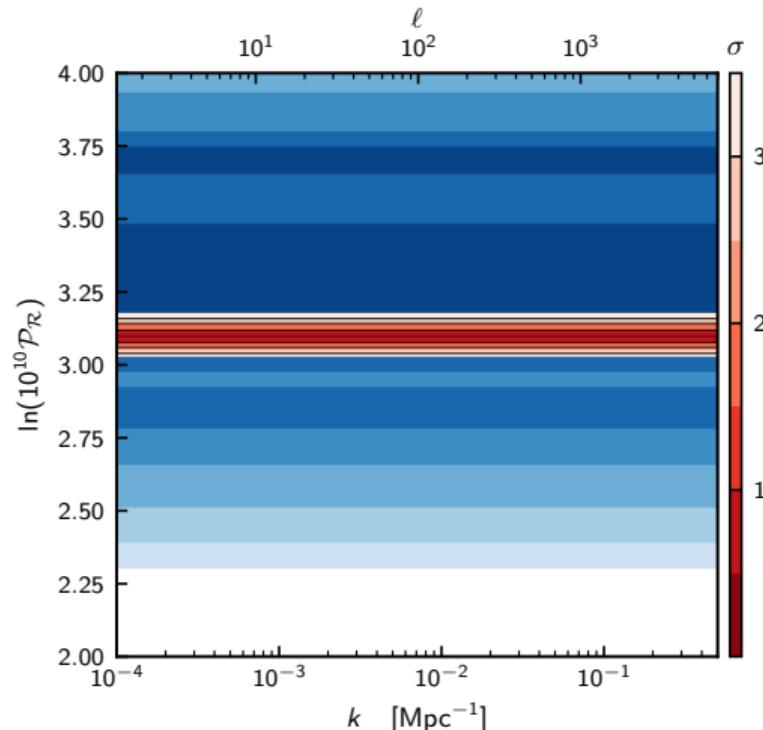


## 0 internal knots

- Traditionally parameterise the primordial power spectrum with  $(A_s, n_s)$

$$\mathcal{P}_{\mathcal{R}}(k) = A_s \left( \frac{k}{k_*} \right)^{n_s - 1}$$

- To add more degrees of freedom, can add “running” parameters  $n_{\text{run}}$  (higher order polynomial in index)
- Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: “FlexKnots”
- Let the Bayesian evidence decide when you’ve introduced too many parameters

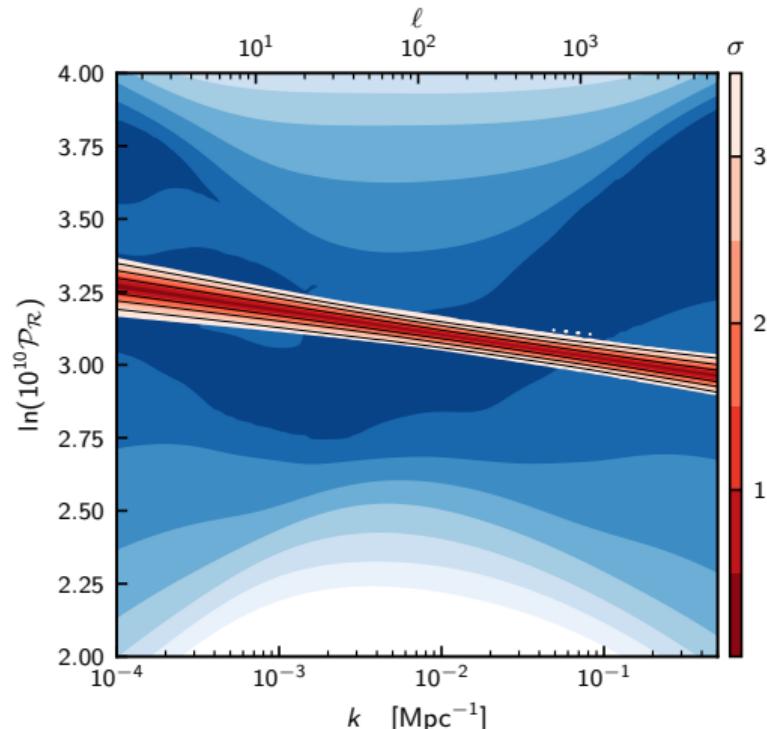


# 1 internal knot

- Traditionally parameterise the primordial power spectrum with  $(A_s, n_s)$

$$\mathcal{P}_R(k) = A_s \left( \frac{k}{k_*} \right)^{n_s - 1}$$

- To add more degrees of freedom, can add “running” parameters  $n_{\text{run}}$  (higher order polynomial in index)
- Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: “FlexKnots”
- Let the Bayesian evidence decide when you’ve introduced too many parameters

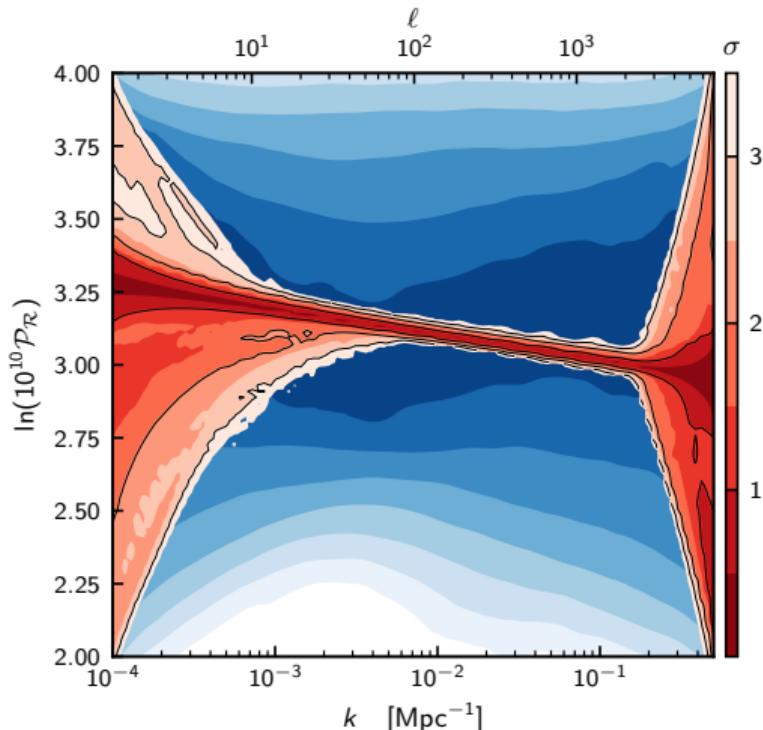


## 2 internal knots

- Traditionally parameterise the primordial power spectrum with  $(A_s, n_s)$

$$\mathcal{P}_R(k) = A_s \left( \frac{k}{k_*} \right)^{n_s - 1}$$

- To add more degrees of freedom, can add “running” parameters  $n_{\text{run}}$  (higher order polynomial in index)
- Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: “FlexKnots”
- Let the Bayesian evidence decide when you’ve introduced too many parameters

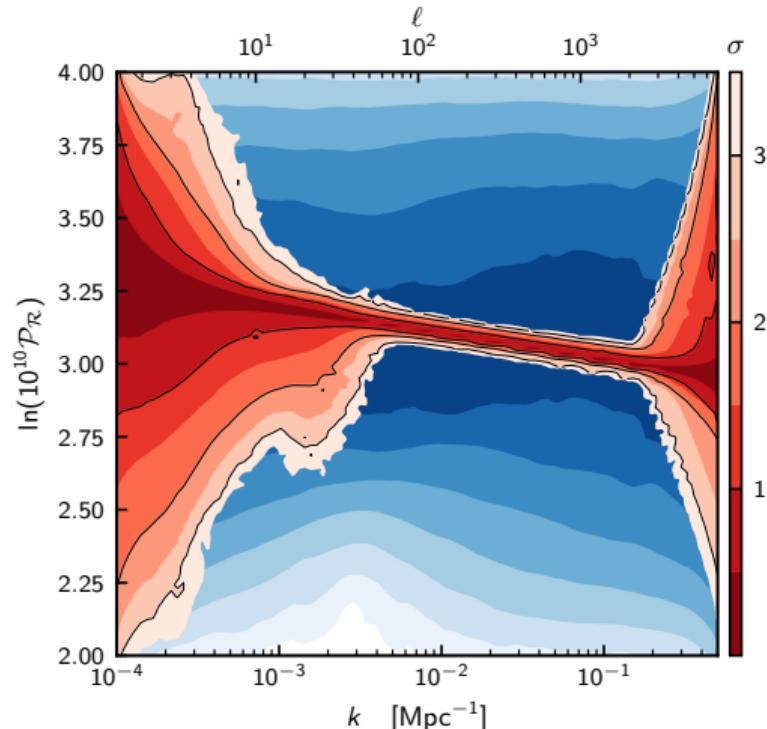


### 3 internal knots

- Traditionally parameterise the primordial power spectrum with  $(A_s, n_s)$

$$\mathcal{P}_{\mathcal{R}}(k) = A_s \left( \frac{k}{k_*} \right)^{n_s - 1}$$

- To add more degrees of freedom, can add “running” parameters  $n_{\text{run}}$  (higher order polynomial in index)
- Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: “FlexKnots”
- Let the Bayesian evidence decide when you’ve introduced too many parameters

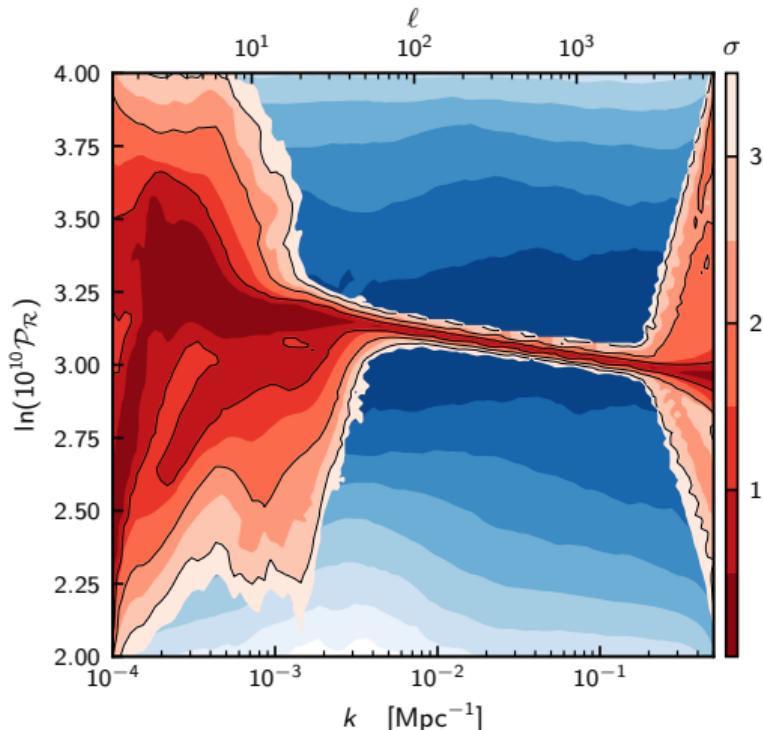


## 4 internal knots

- Traditionally parameterise the primordial power spectrum with  $(A_s, n_s)$

$$\mathcal{P}_R(k) = A_s \left( \frac{k}{k_*} \right)^{n_s - 1}$$

- To add more degrees of freedom, can add “running” parameters  $n_{\text{run}}$  (higher order polynomial in index)
- Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: “FlexKnots”
- Let the Bayesian evidence decide when you’ve introduced too many parameters

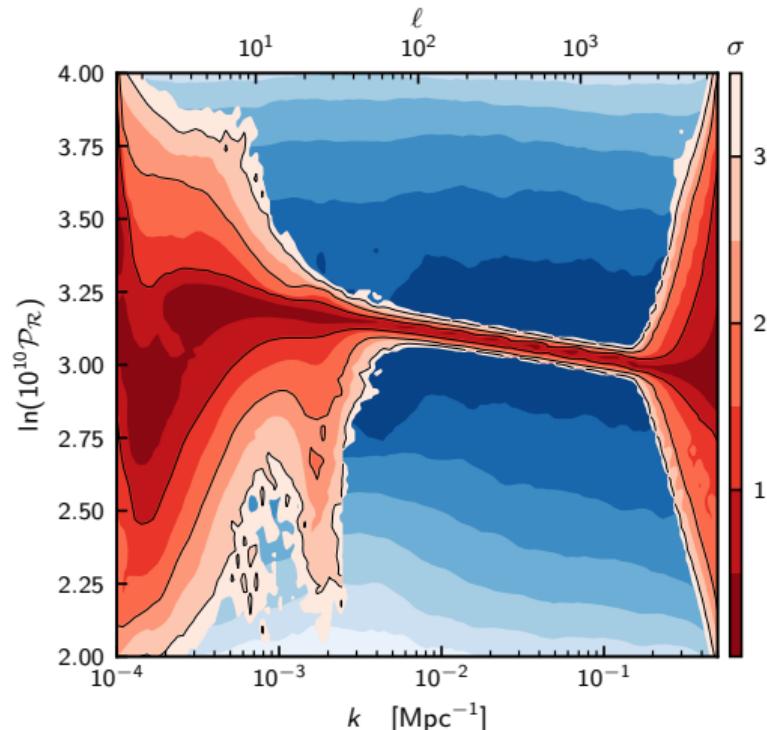


## 5 internal knots

- Traditionally parameterise the primordial power spectrum with  $(A_s, n_s)$

$$\mathcal{P}_R(k) = A_s \left( \frac{k}{k_*} \right)^{n_s - 1}$$

- To add more degrees of freedom, can add “running” parameters  $n_{\text{run}}$  (higher order polynomial in index)
- Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: “FlexKnots”
- Let the Bayesian evidence decide when you’ve introduced too many parameters

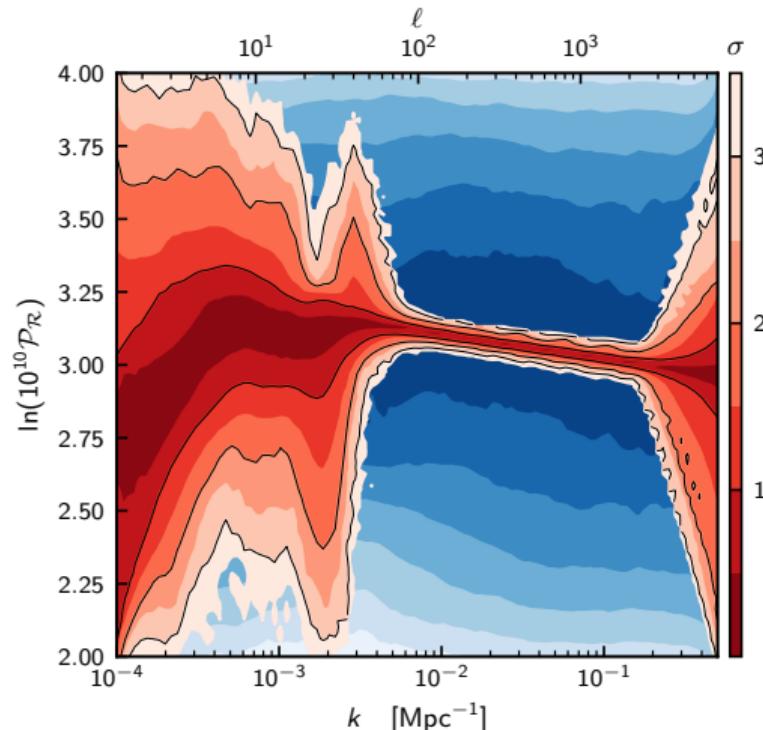


## 6 internal knots

- Traditionally parameterise the primordial power spectrum with  $(A_s, n_s)$

$$\mathcal{P}_R(k) = A_s \left( \frac{k}{k_*} \right)^{n_s - 1}$$

- To add more degrees of freedom, can add “running” parameters  $n_{\text{run}}$  (higher order polynomial in index)
- Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: “FlexKnots”
- Let the Bayesian evidence decide when you’ve introduced too many parameters

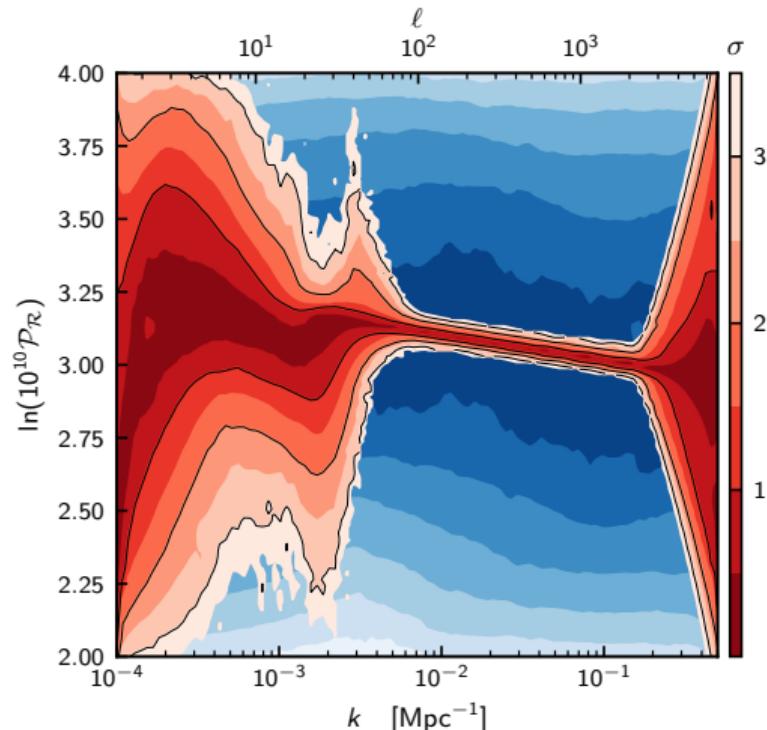


## 7 internal knots

- Traditionally parameterise the primordial power spectrum with  $(A_s, n_s)$

$$\mathcal{P}_R(k) = A_s \left( \frac{k}{k_*} \right)^{n_s - 1}$$

- To add more degrees of freedom, can add “running” parameters  $n_{\text{run}}$  (higher order polynomial in index)
- Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: “FlexKnots”
- Let the Bayesian evidence decide when you’ve introduced too many parameters

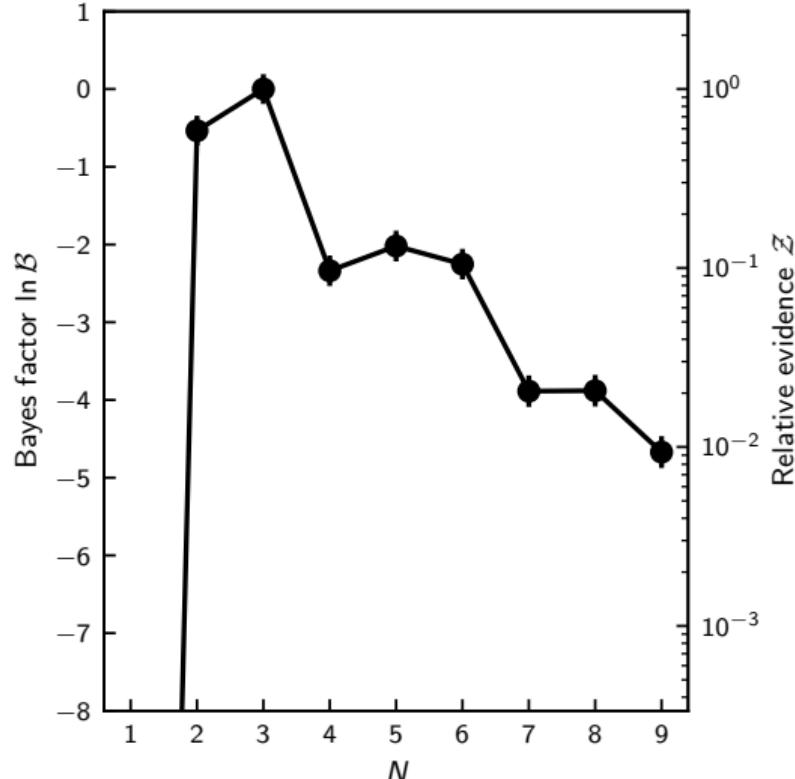


# Bayes Factors

- ▶ Traditionally parameterise the primordial power spectrum with  $(A_s, n_s)$

$$\mathcal{P}_R(k) = A_s \left( \frac{k}{k_*} \right)^{n_s - 1}$$

- ▶ To add more degrees of freedom, can add “running” parameters  $n_{\text{run}}$  (higher order polynomial in index)
- ▶ Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: “FlexKnots”
- ▶ Let the Bayesian evidence decide when you’ve introduced too many parameters

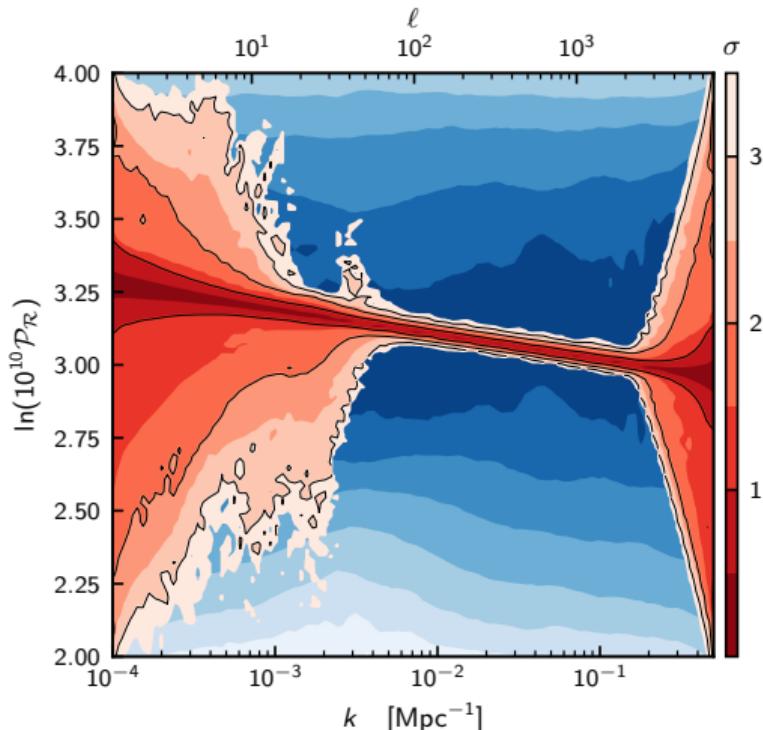


# Marginalised plot

- Traditionally parameterise the primordial power spectrum with  $(A_s, n_s)$

$$\mathcal{P}_R(k) = A_s \left( \frac{k}{k_*} \right)^{n_s - 1}$$

- To add more degrees of freedom, can add “running” parameters  $n_{\text{run}}$  (higher order polynomial in index)
- Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: “FlexKnots”
- Let the Bayesian evidence decide when you’ve introduced too many parameters



# Kullback-Liebler divergences

- Traditionally parameterise the primordial power spectrum with  $(A_s, n_s)$

$$\mathcal{P}_R(k) = A_s \left( \frac{k}{k_*} \right)^{n_s - 1}$$

- To add more degrees of freedom, can add “running” parameters  $n_{\text{run}}$  (higher order polynomial in index)
- Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: “FlexKnots”
- Let the Bayesian evidence decide when you’ve introduced too many parameters

