

Gradients and Nested Sampling

The present state of the art

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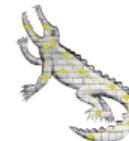
7th July 2023



**The
Alan Turing
Institute**



UNIVERSITY OF
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Highlight: state-of-the-art Nature review primer [2205.15570]

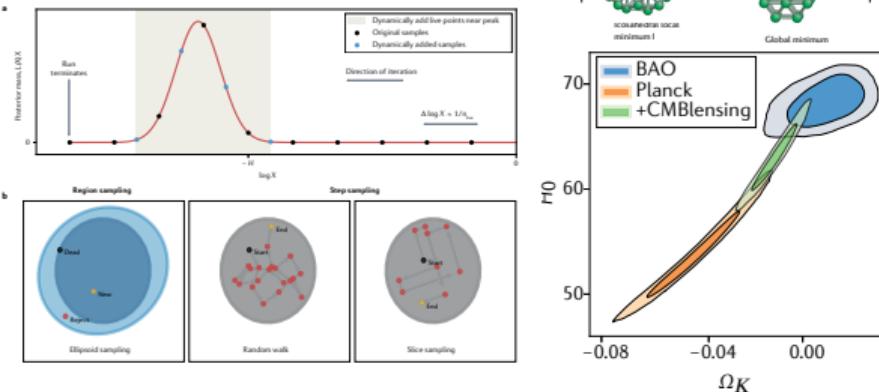
PRIMER

- ▶ 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.
- ▶ Buchner technical review [2101.09675]
- ▶ In this talk
 - ▶ What is nested sampling?
 - ▶ How can it use gradients?

Nested sampling for physical scientists

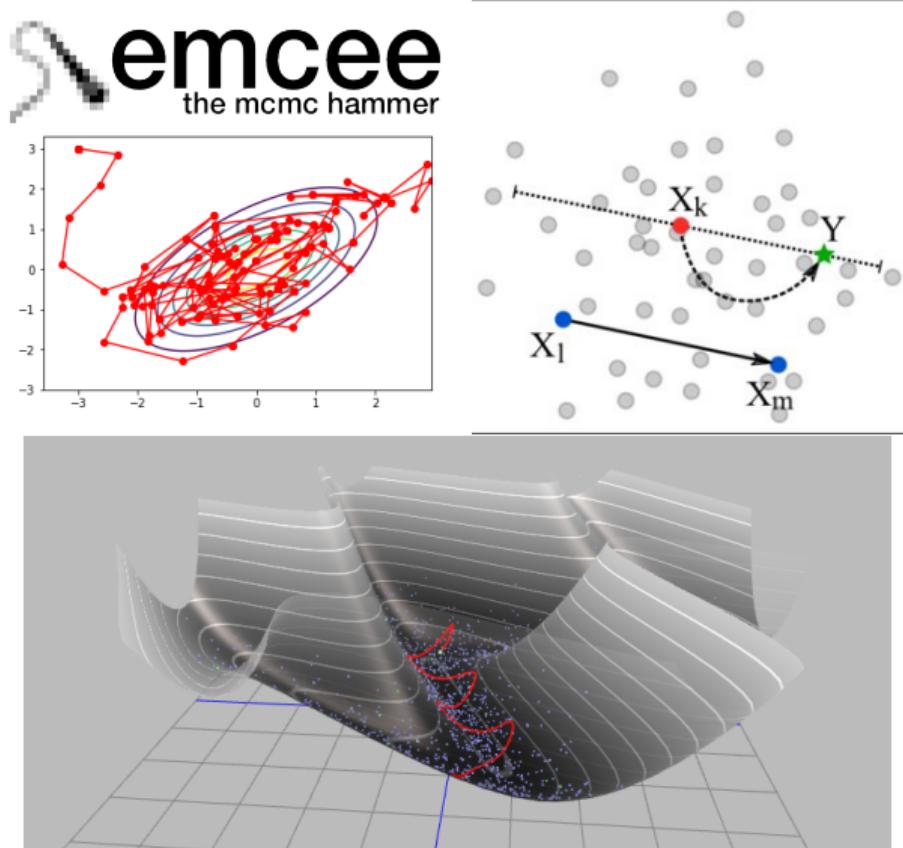
Greg Ashton^{1,2*}, Noam Bernstein^{3,4}, Johannes Buchner⁵, Xi Chen⁶, Gábor Csányi^{1,6}, Andrew Fowlie^{2,7}, Farhan Feraz⁸, Matthew Griffiths⁹, Will Handley^{10,11}, Michael Hobbs¹², Edward Higson¹³, Michael Hobson¹¹, Anthony Lasenby^{10,11}, David Parkinson¹⁴, Liviu B. Părtay¹⁵, Matthew Pritch^{16,17}, Doris Schneider¹¹, Joshua S. Speagle^{18,19,20}, Leah South²¹, John Veitch²², Philipp Wacker¹⁷, David J. Wales^{1,23} and David Yallup^{20,21}

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.



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

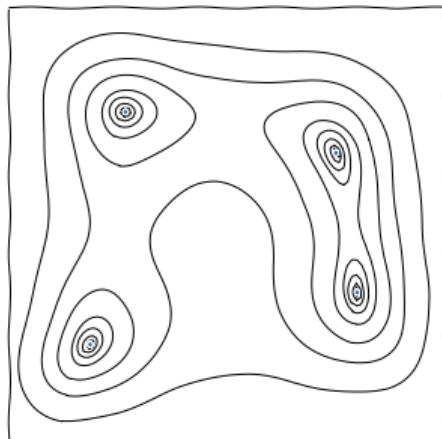


What is Nested Sampling?

- ▶ 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:

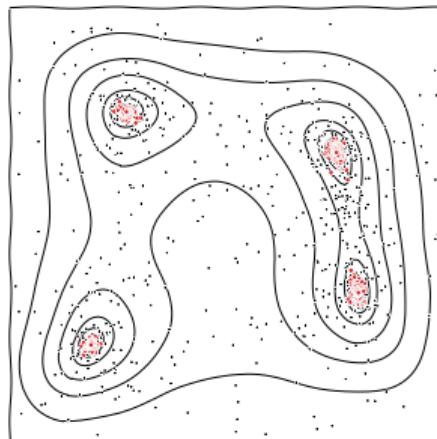
Optimisation

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



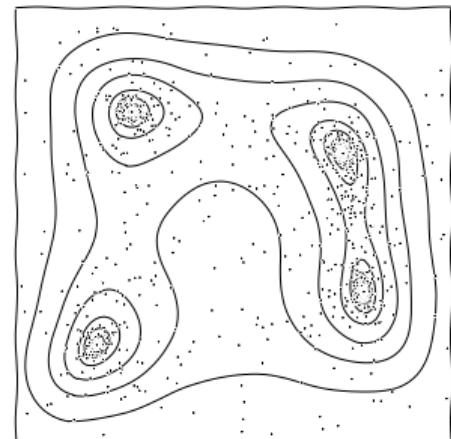
Exploration

draw/sample $\theta \sim f$



Integration

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



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

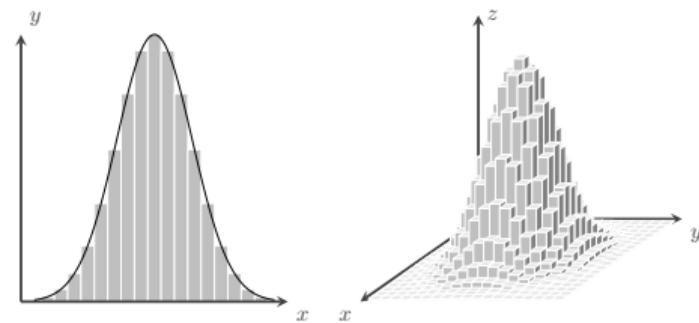
$$\Psi = \int e^{iS} \mathcal{D}x$$

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.
- ▶ Nested sampling integrates **probabilistically**.

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
- ▶ The errors however are not small.

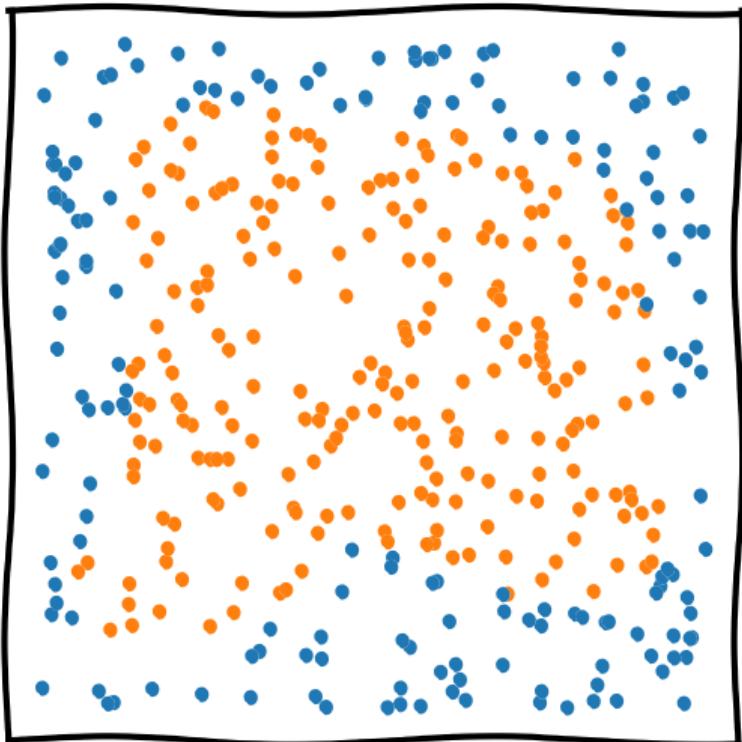


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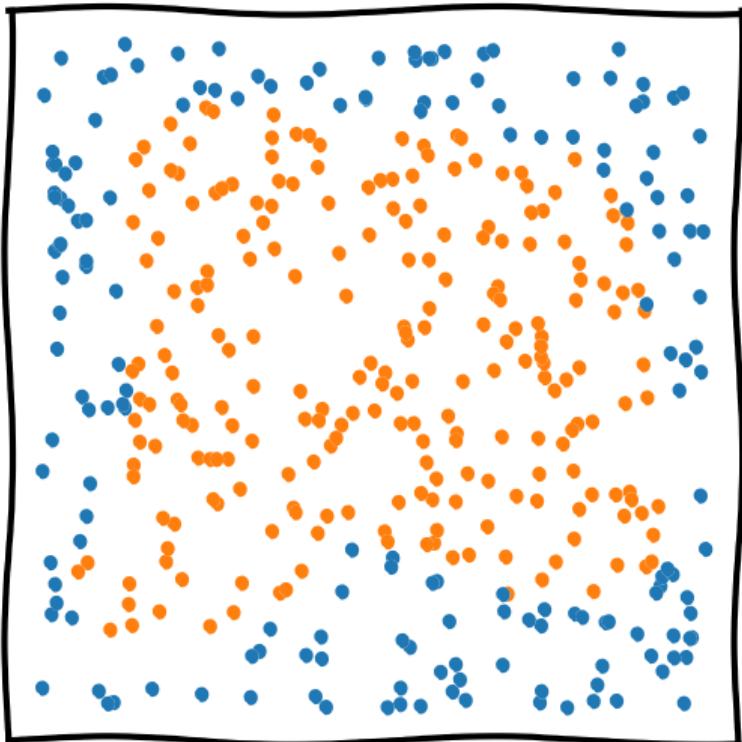


Probabalistic volume estimation

- ▶ Key idea in NS: estimating volumes probabilistically

$$\frac{V_{\text{after}}}{V_{\text{before}}} \approx \frac{n_{\text{in}} + 1}{n_{\text{out}} + n_{\text{in}} + 2}$$

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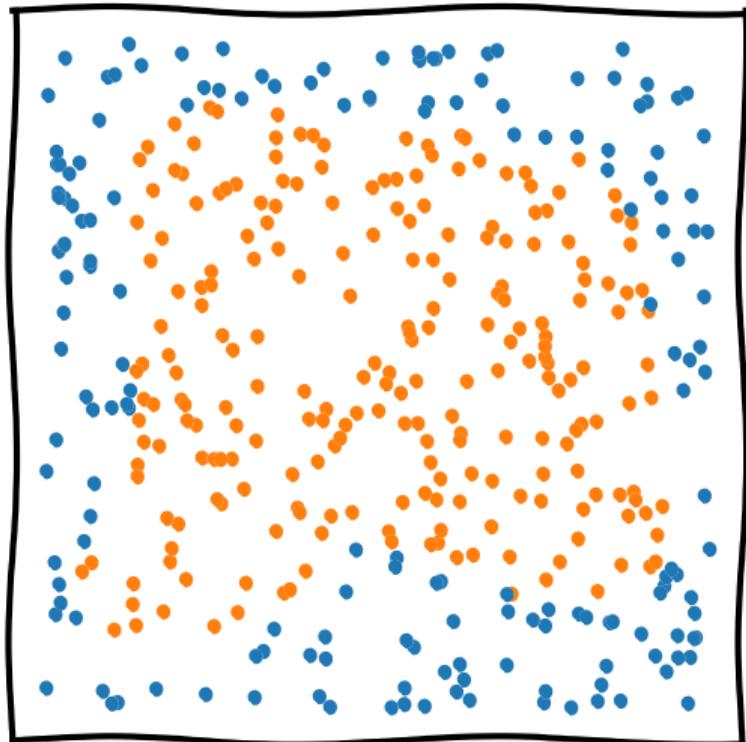


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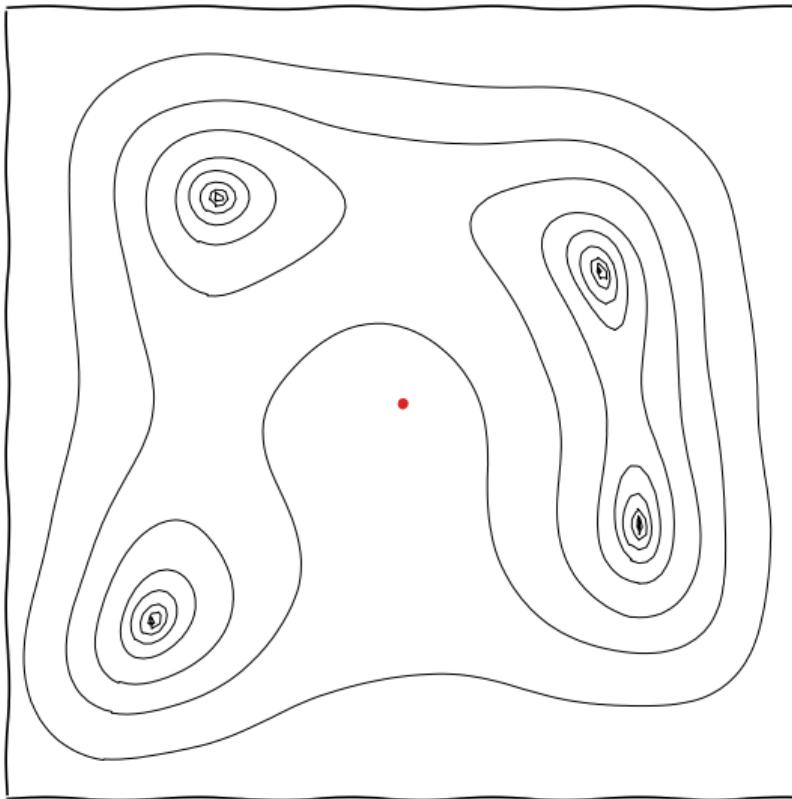
- ▶ Key idea in NS: estimating volumes probabilistically

$$\frac{V_{\text{after}}}{V_{\text{before}}} = \frac{n_{\text{in}} + 1}{n_{\text{out}} + n_{\text{in}} + 2} \pm \sqrt{\frac{(n_{\text{in}}+1)(n_{\text{out}}+1)}{(n_{\text{out}}+n_{\text{in}}+2)^2(n_{\text{out}}+n_{\text{in}}+3)}}$$

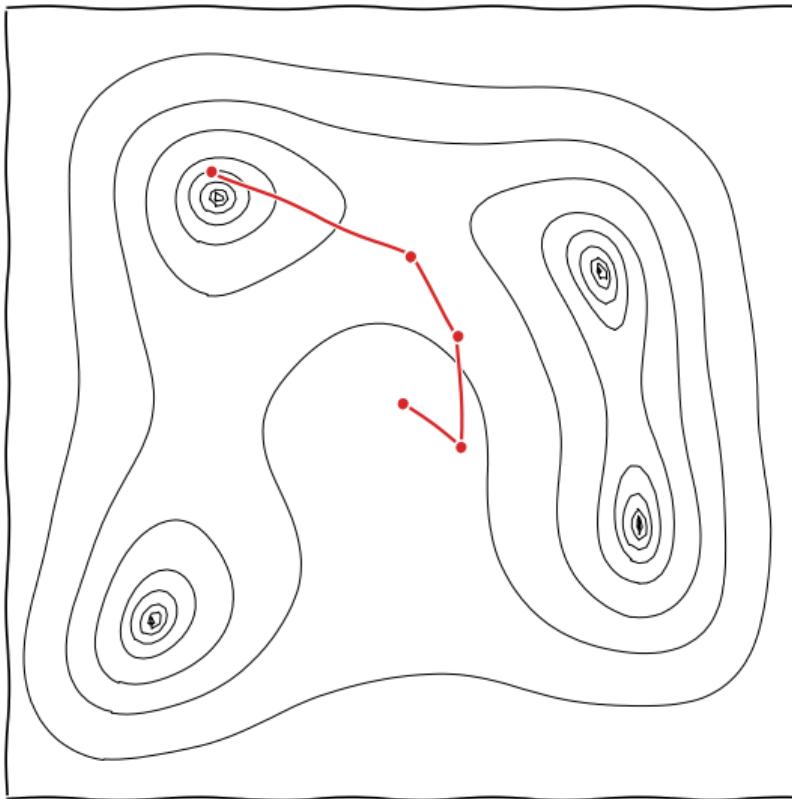
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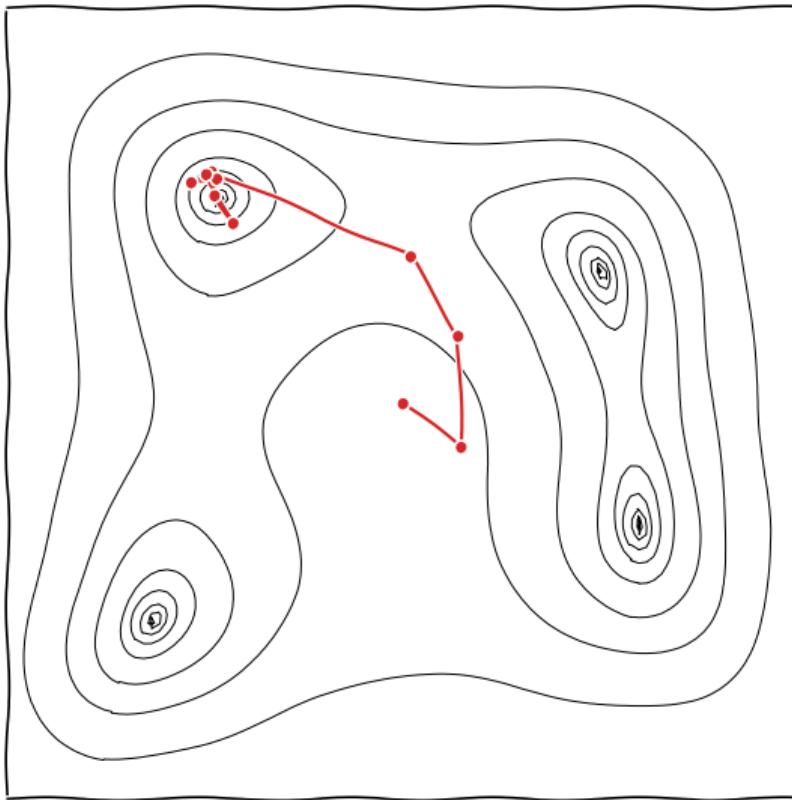
MCMC



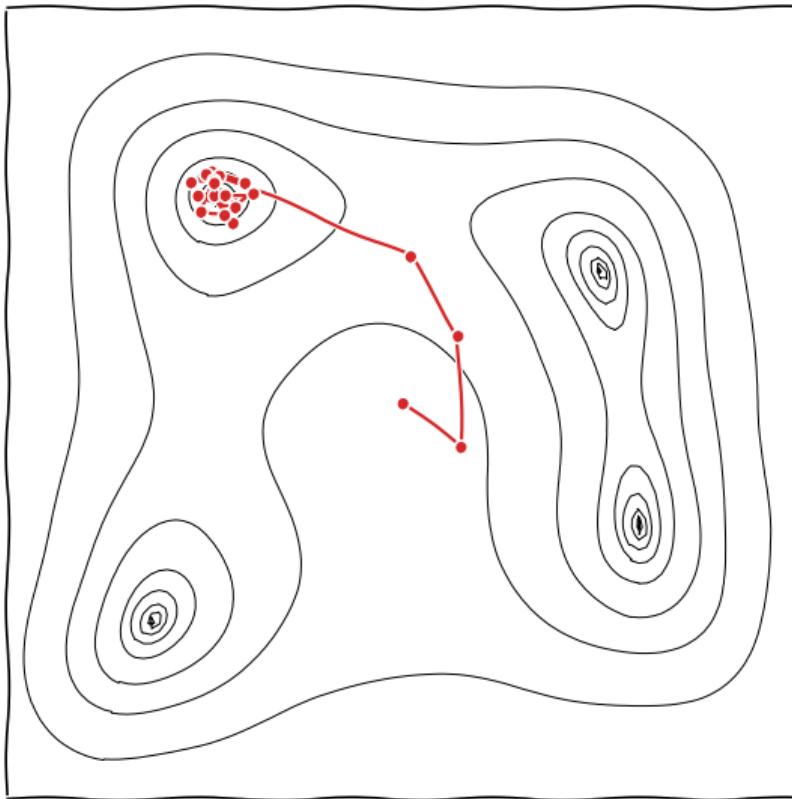
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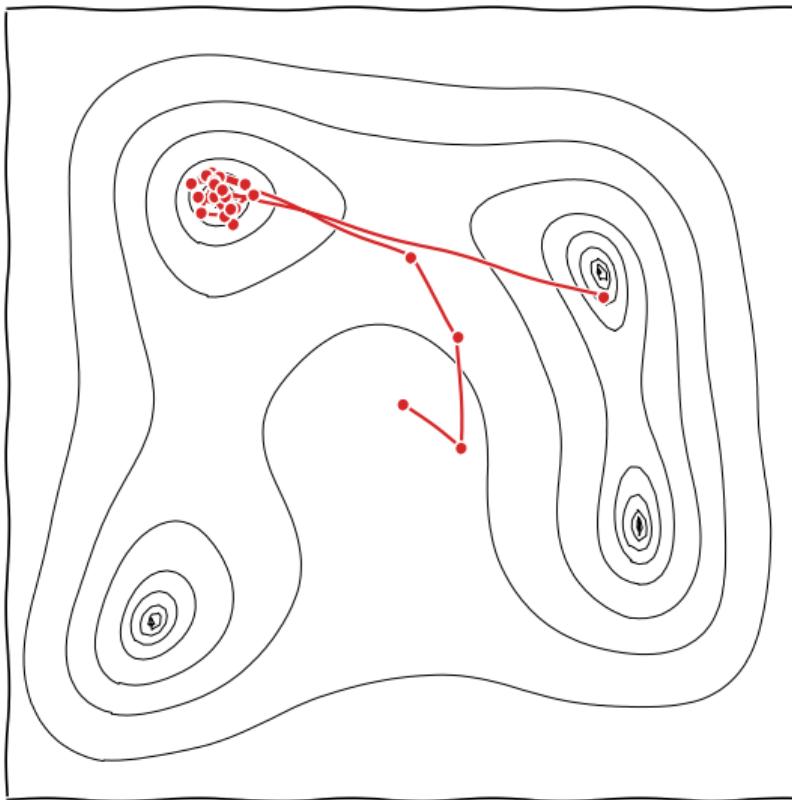
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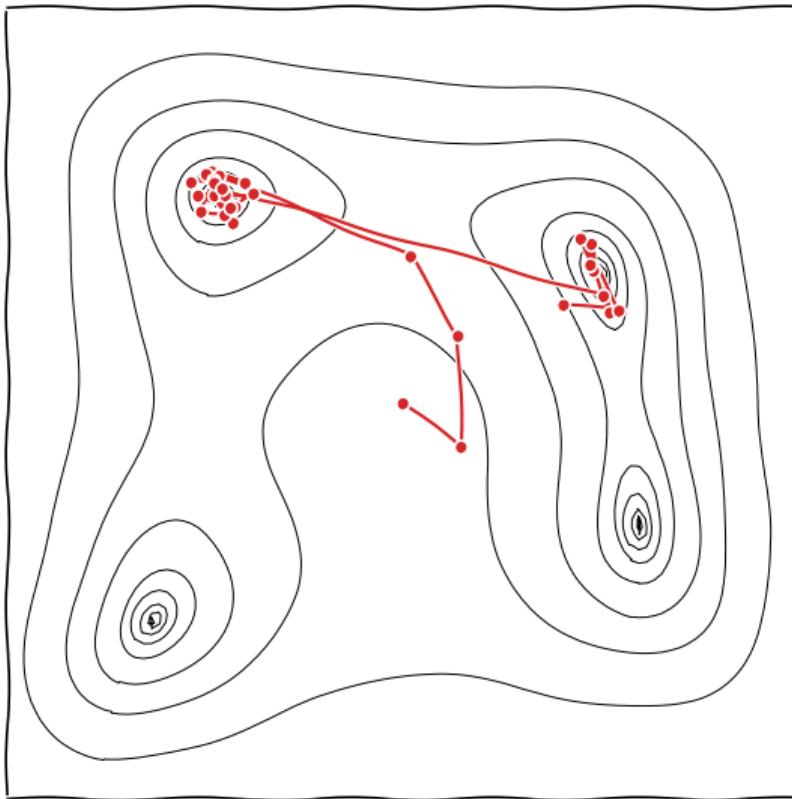
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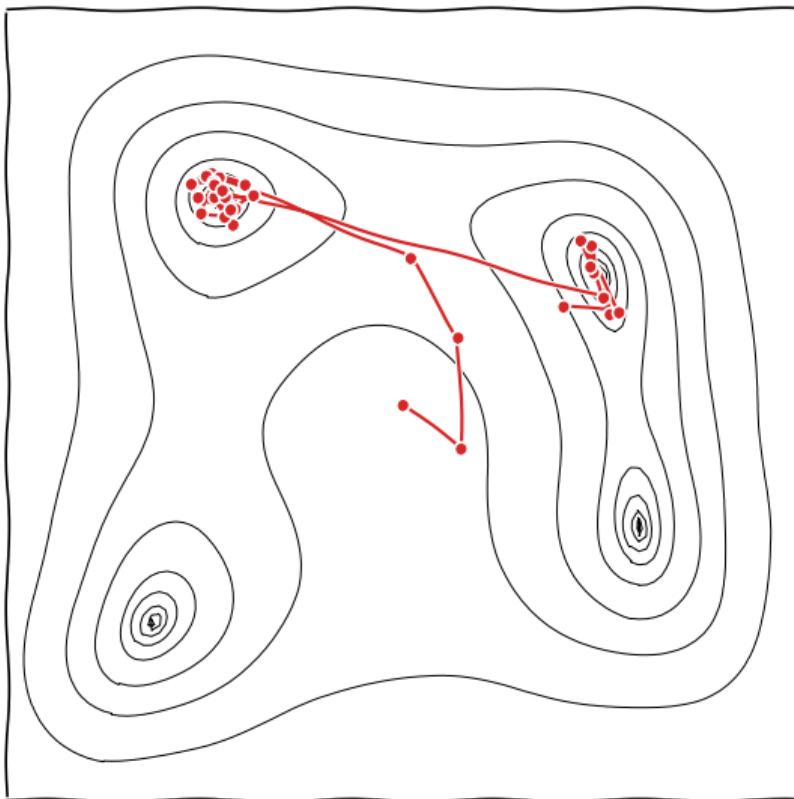
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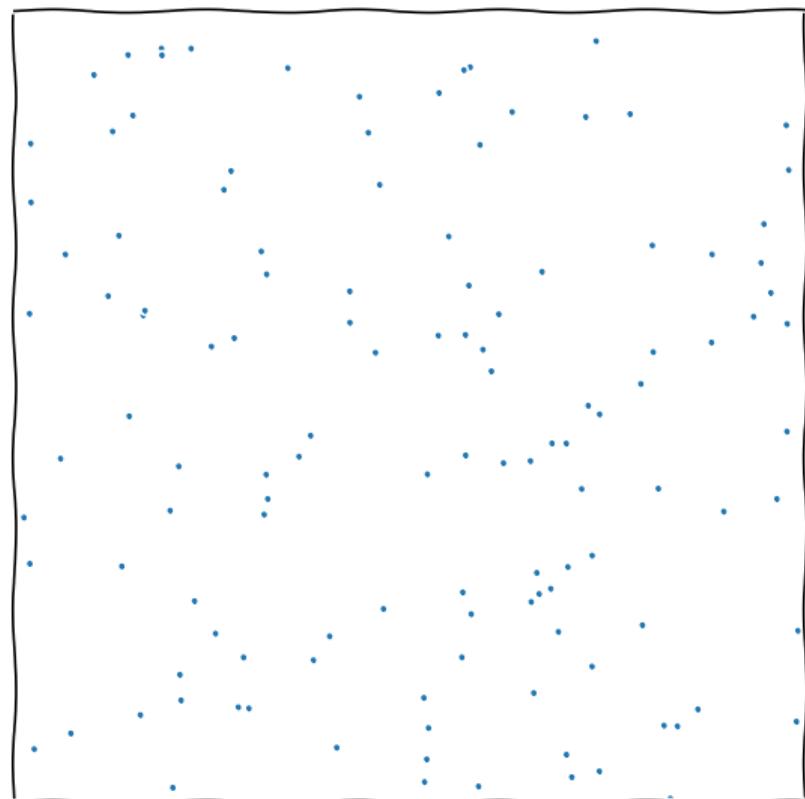
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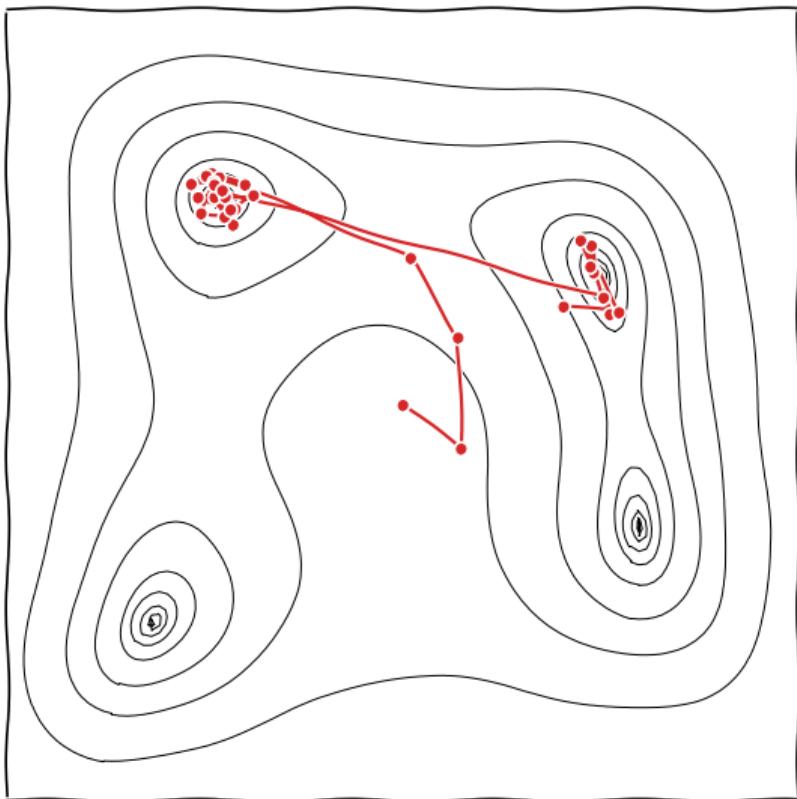
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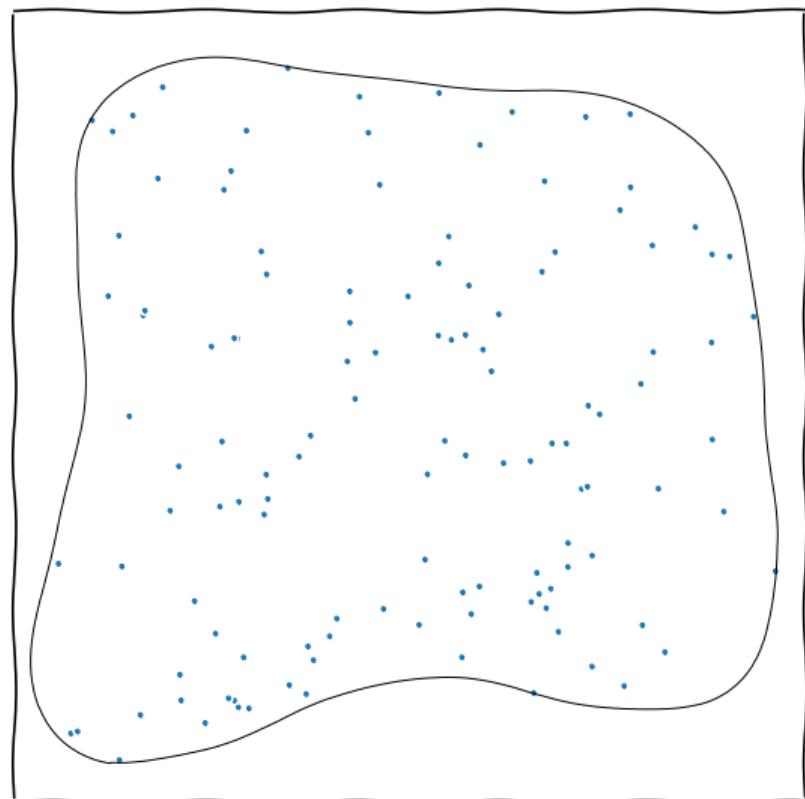
Nested sampling



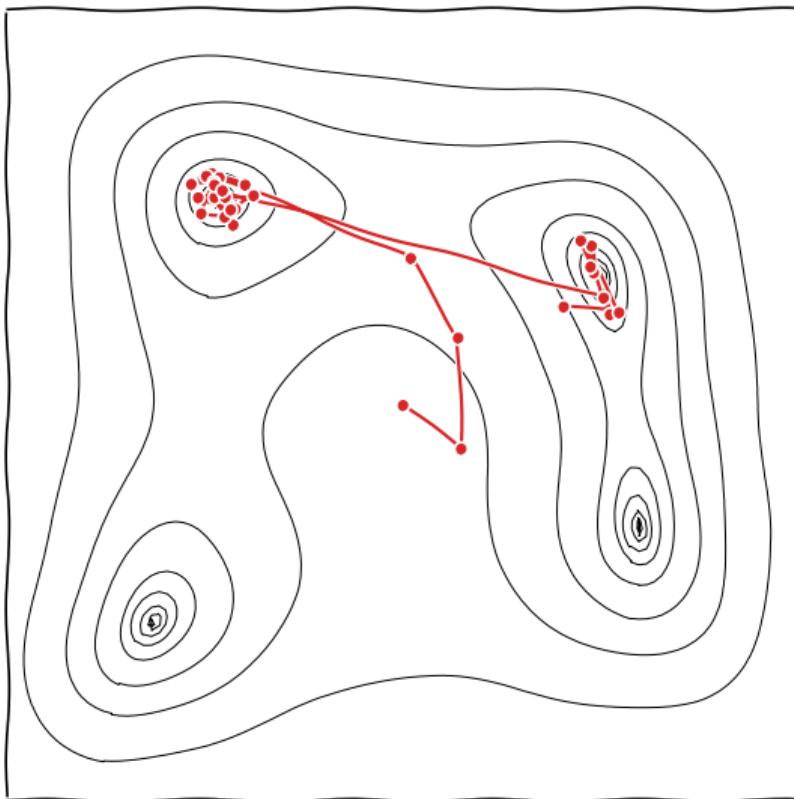
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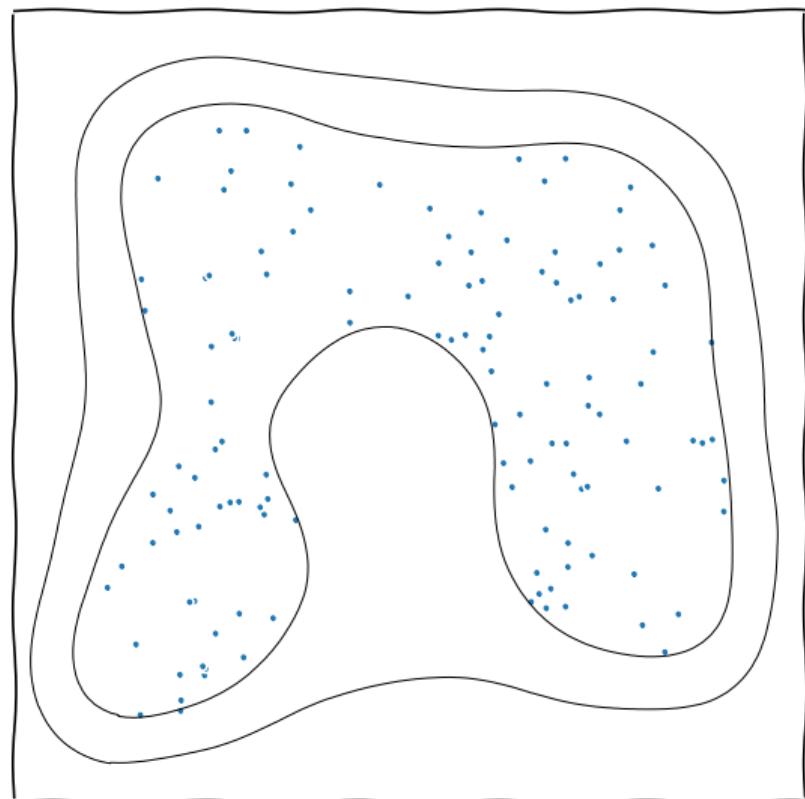
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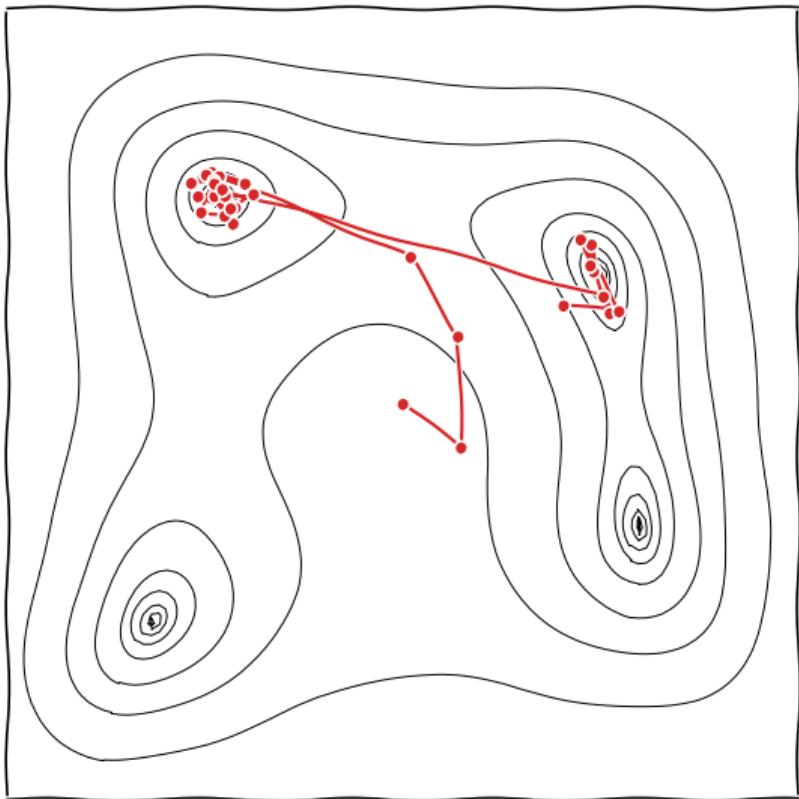
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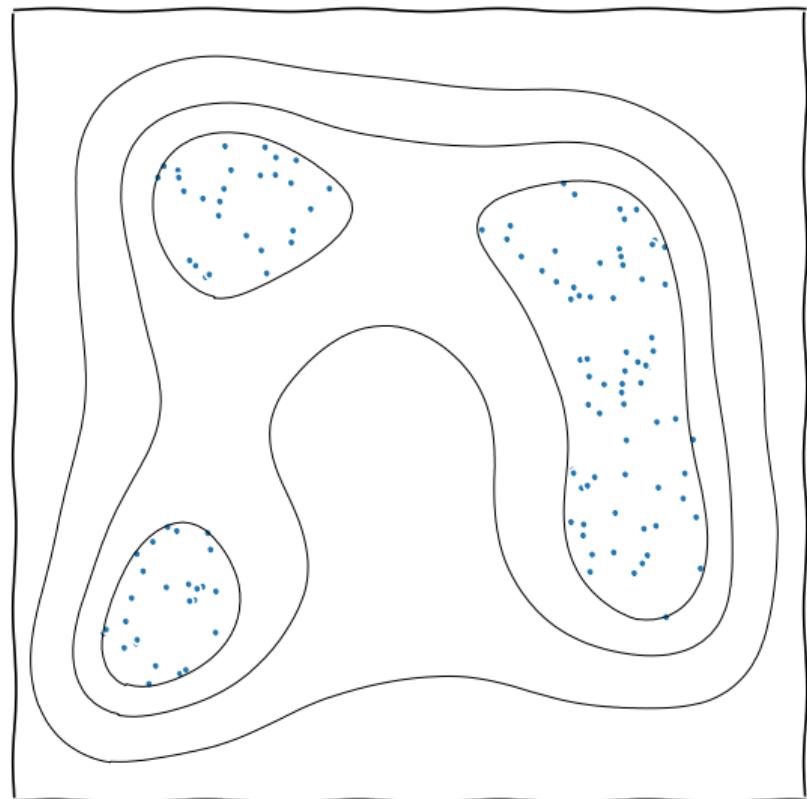
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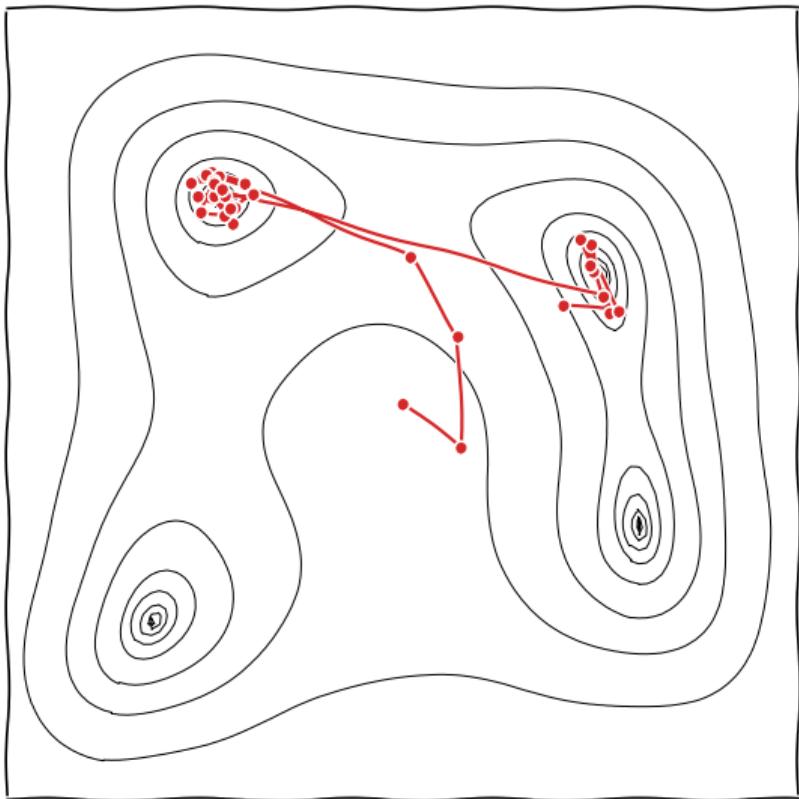
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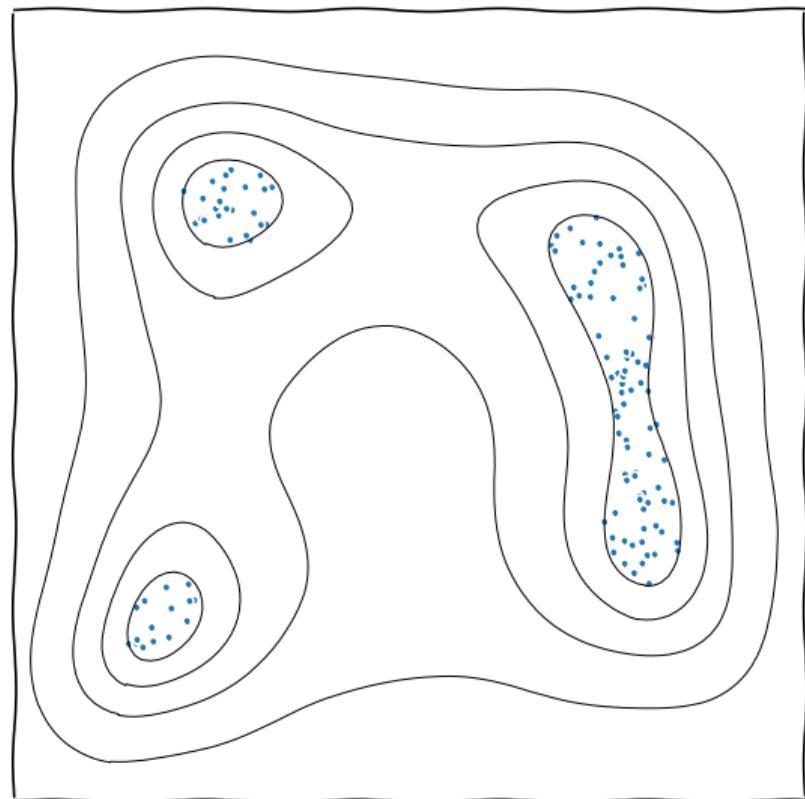
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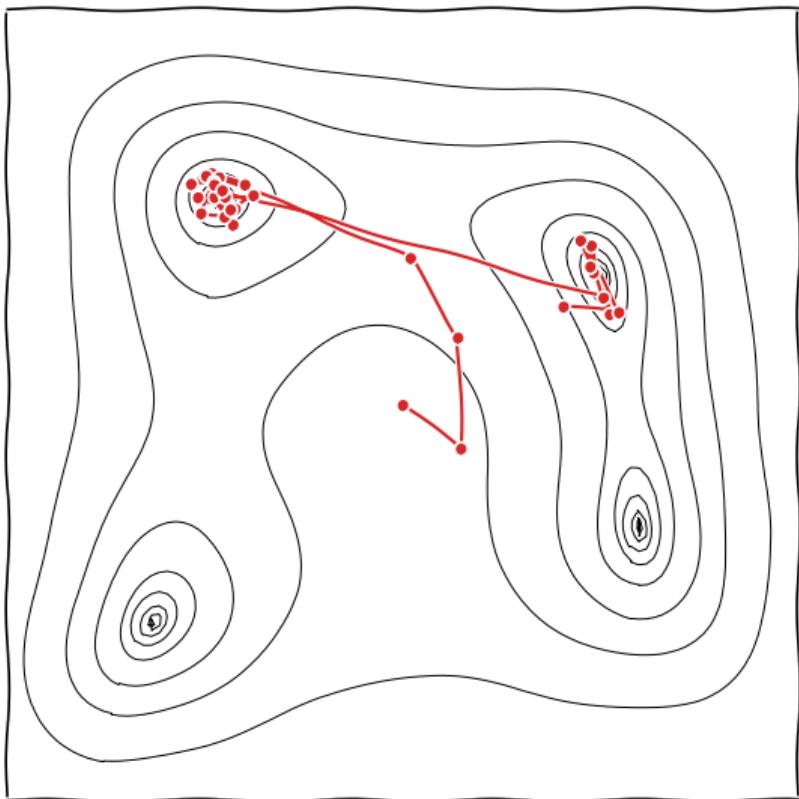
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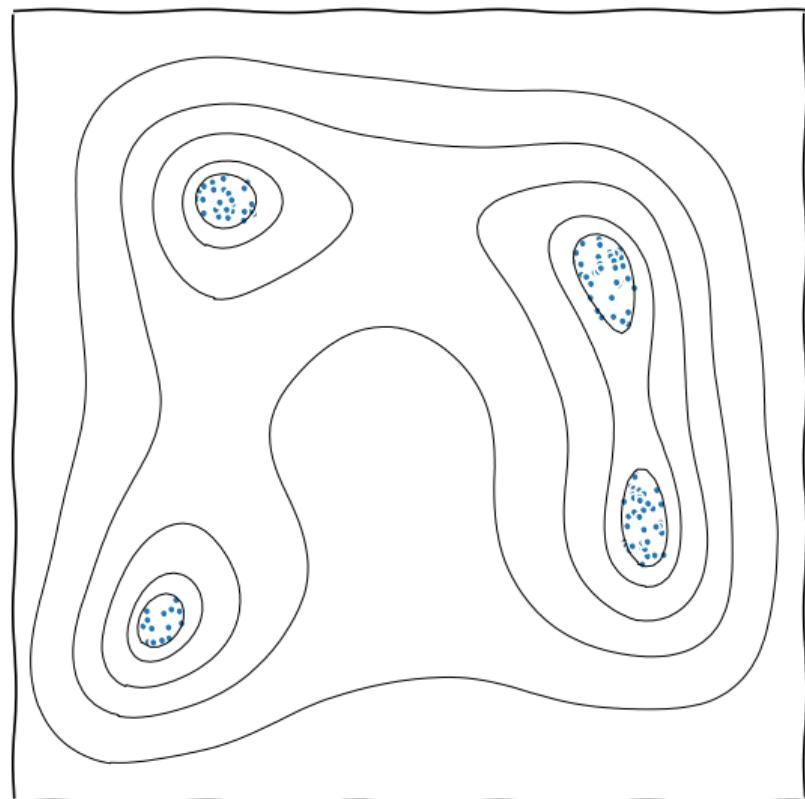
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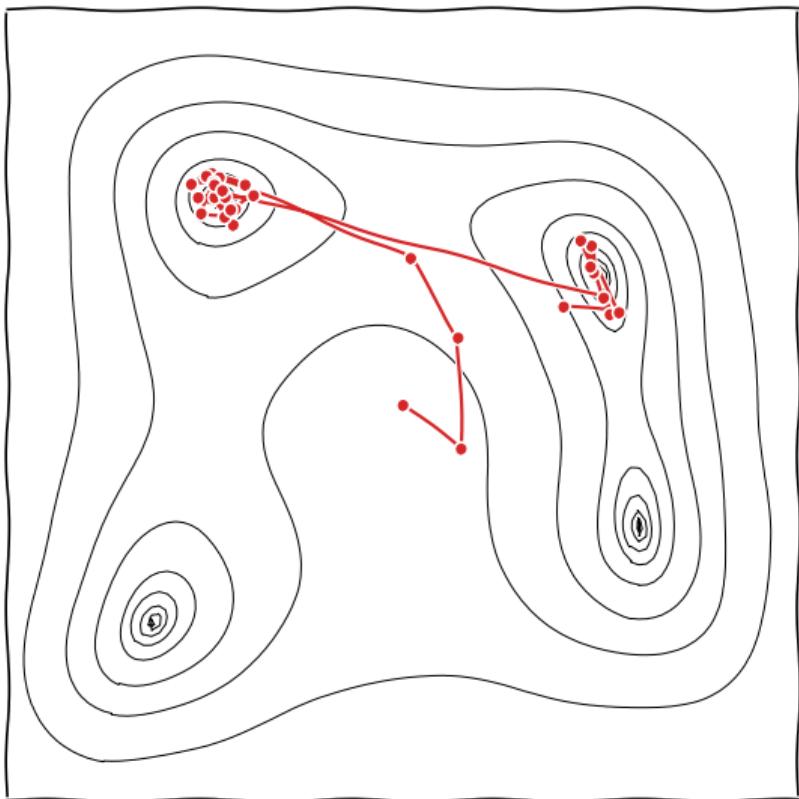
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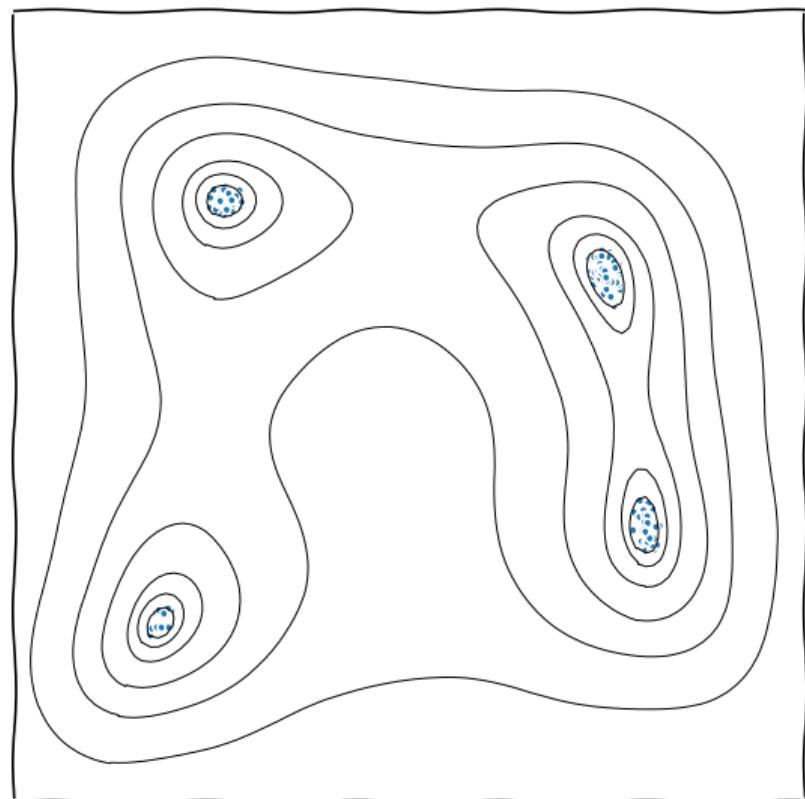
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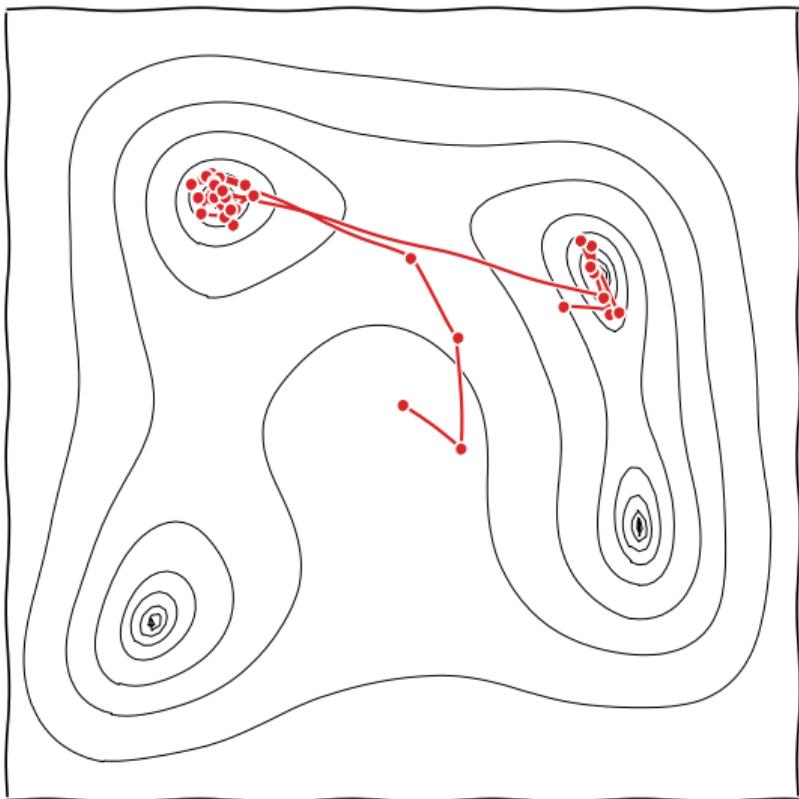
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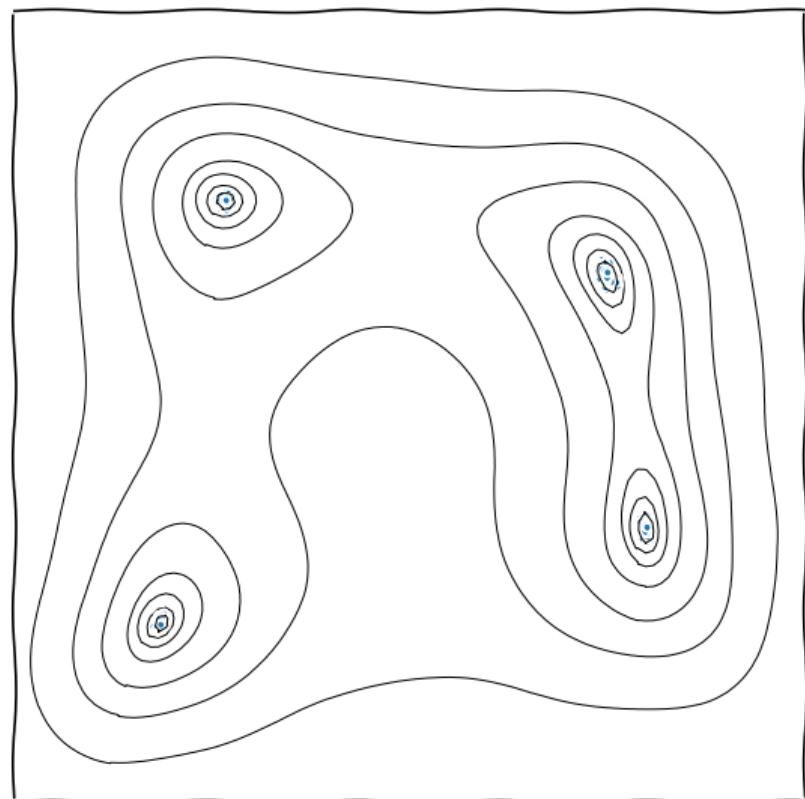
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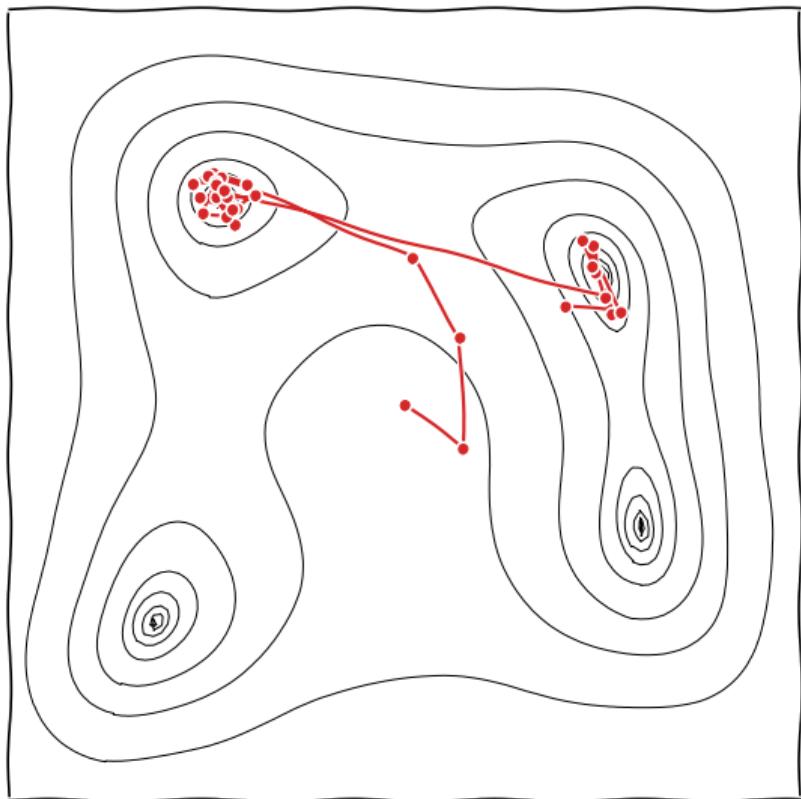
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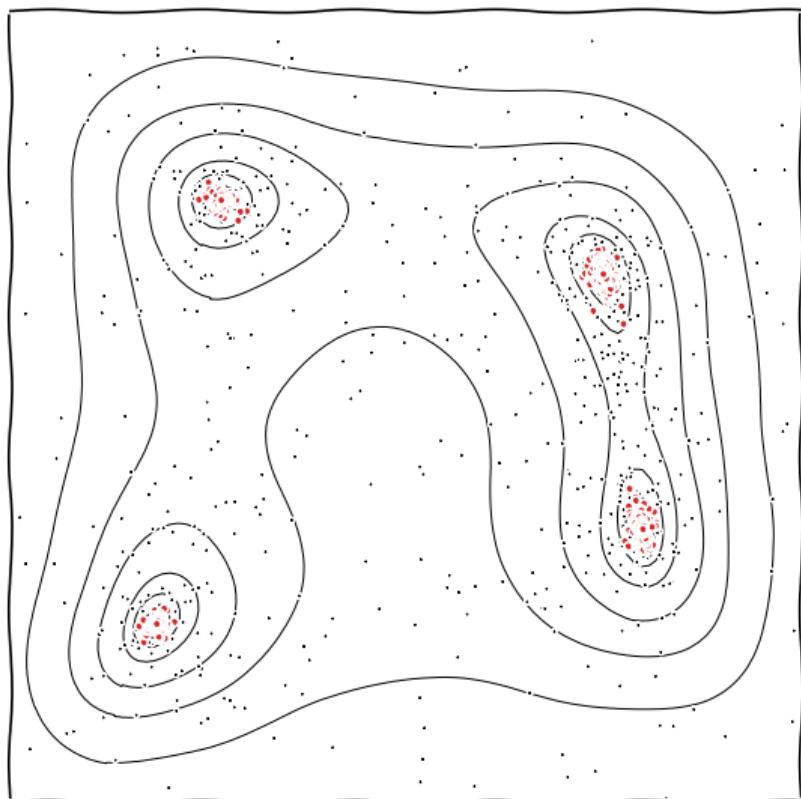
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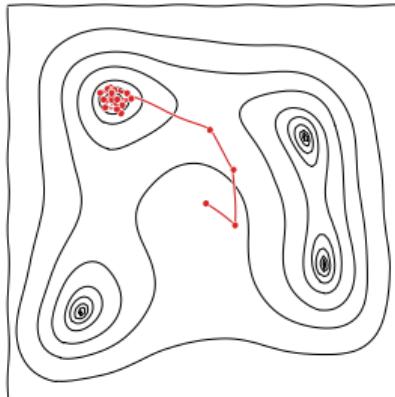


Nested sampling



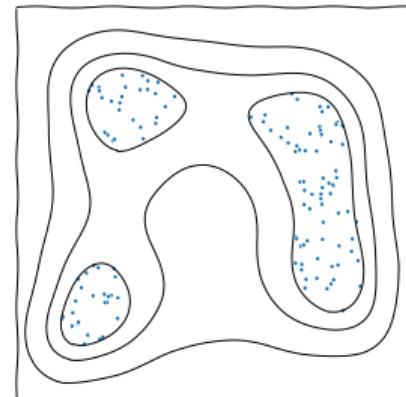
MCMC

- ▶ 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



Nested sampling

- ▶ Sequentially update a set S of n samples:

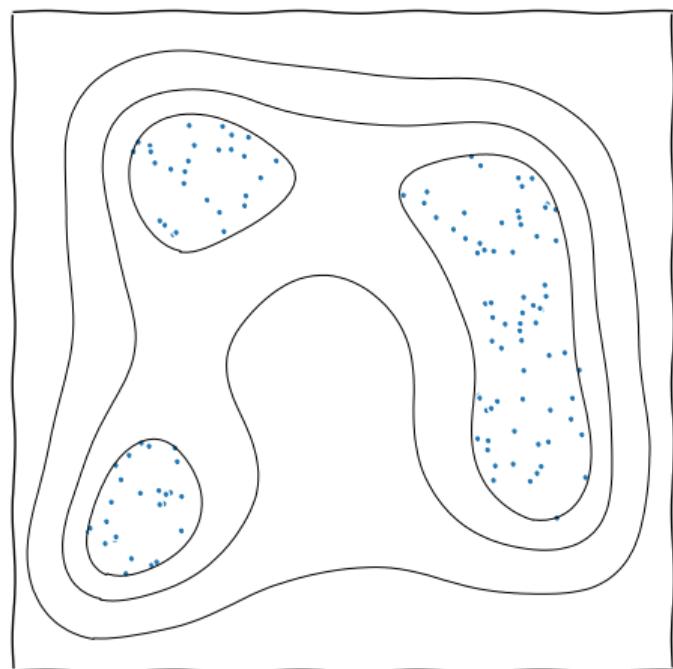
S_0 : Generate n samples uniformly over the space (from the prior π).

S_{i+1} : Delete the lowest likelihood sample in S_i , and replace it with a new uniform sample with higher likelihood.

- ▶ Requires one to be able to sample uniformly within a region, subject to a *hard likelihood constraint*:

$$\{\theta \sim \pi : \mathcal{L}(\theta) > \mathcal{L}_{*.\cdot}\}$$

- ▶ This procedure optimises (multimodally), and can calculate the **evidence** & **posterior** weights.
- ▶ The evolving ensemble of live points allows algorithms to perform self-tuning and mode clustering.

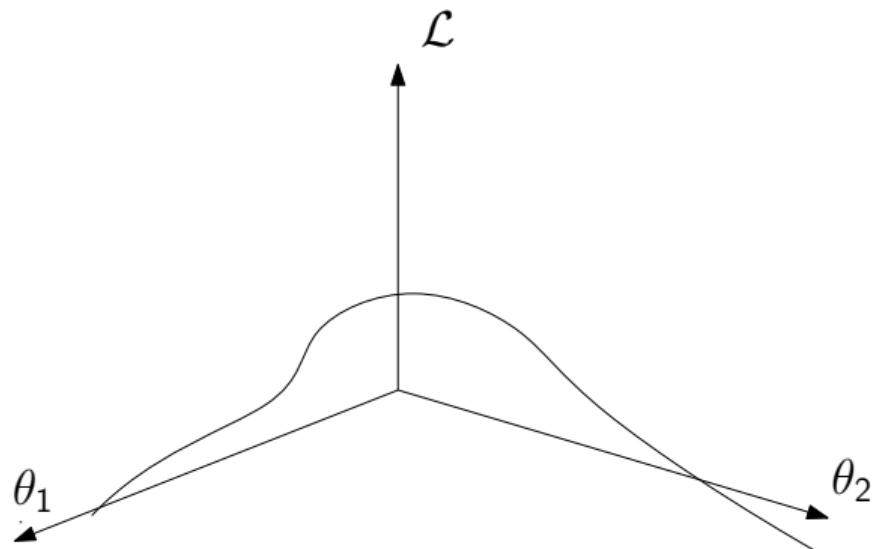


(Lesbesgue) Integrating with nested sampling

- ▶ At each iteration, the likelihood contour shrinks in volume X by $\approx 1/n$.
- ▶ Nested sampling zooms in to the peak of the function \mathcal{L} exponentially.

$$\mathcal{Z} \approx \sum_i \Delta \mathcal{L}_i X_i, \quad X_{i+1} \approx \frac{n}{n+1} X_i, \quad X_0 = 1.$$

- ▶ At the end, one is left with a set of discarded points.
- ▶ These may be weighted to form weighted posterior samples using $w_i = \mathcal{L}_i \Delta X_i$.
- ▶ Estimates the density of states, and is therefore a partition function calculator
 $Z(\beta) = \sum_i \mathcal{L}_i^\beta \Delta X_i$.

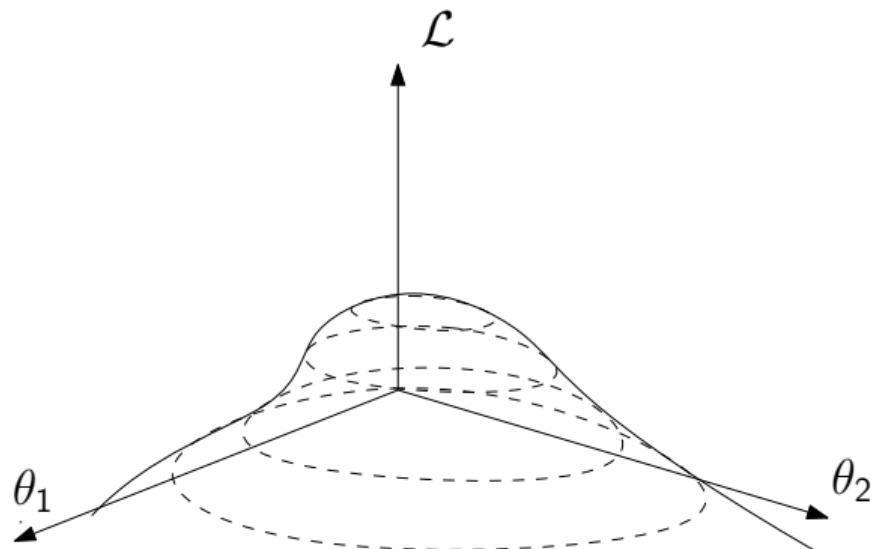


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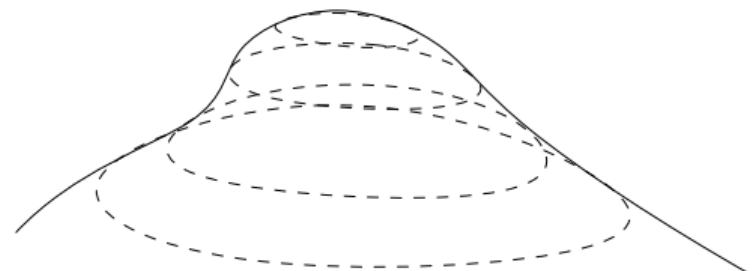


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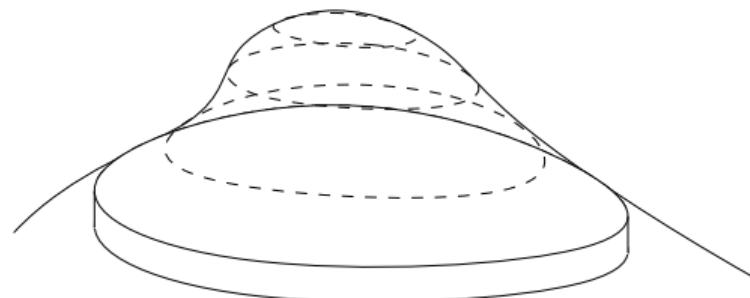


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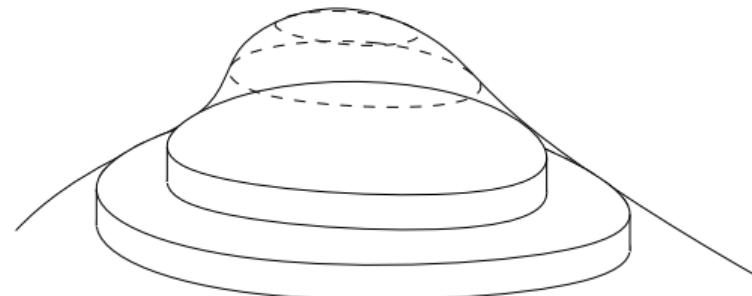


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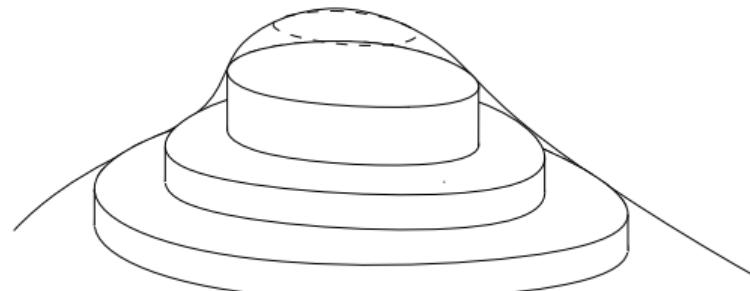


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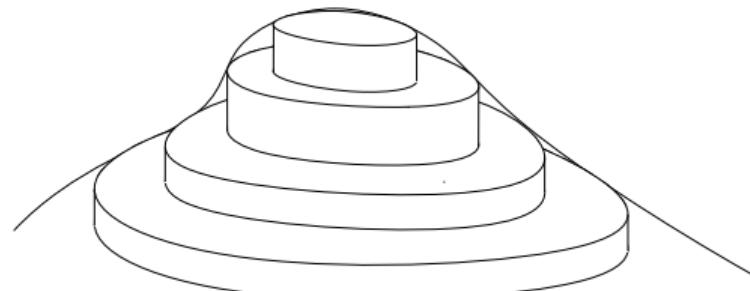


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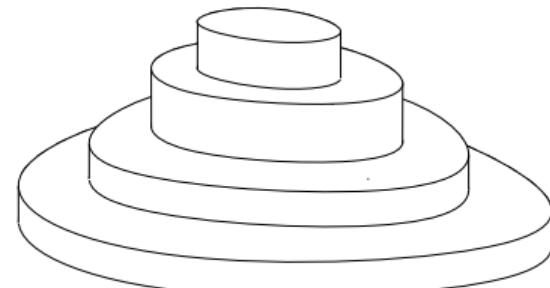


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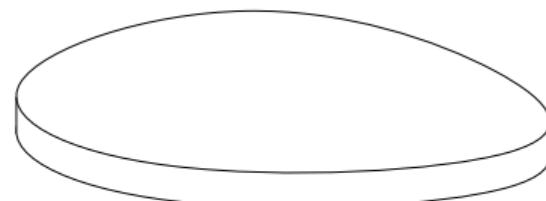


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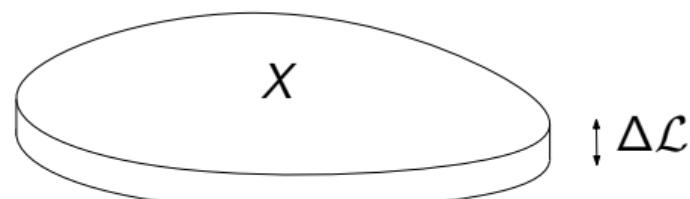


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$$\mathcal{Z} \approx \sum_i \Delta \mathcal{L}_i X_i, \quad X_{i+1} \approx \frac{n}{n+1} X_i, \quad X_0 = 1.$$

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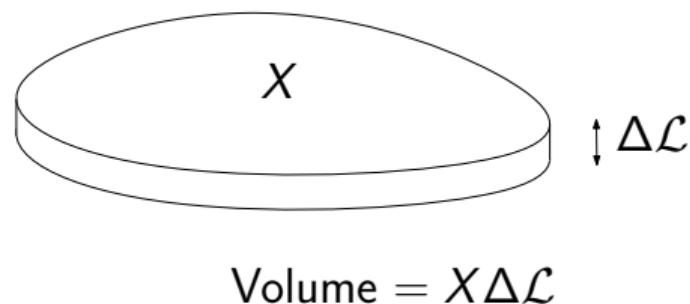


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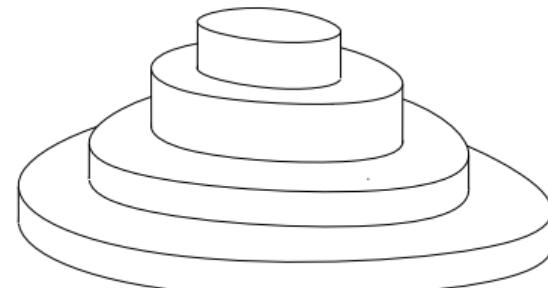


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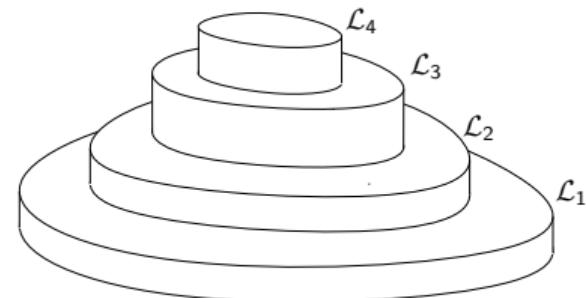


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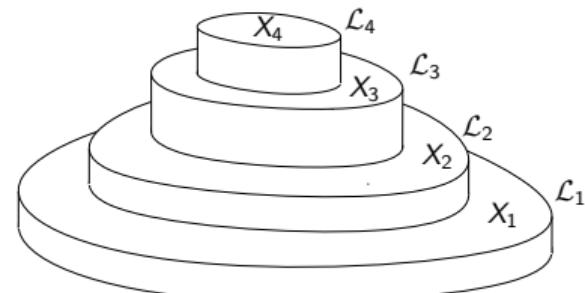


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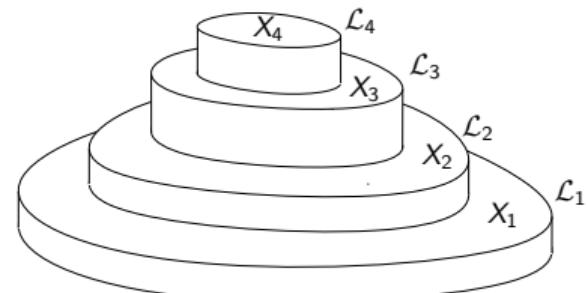
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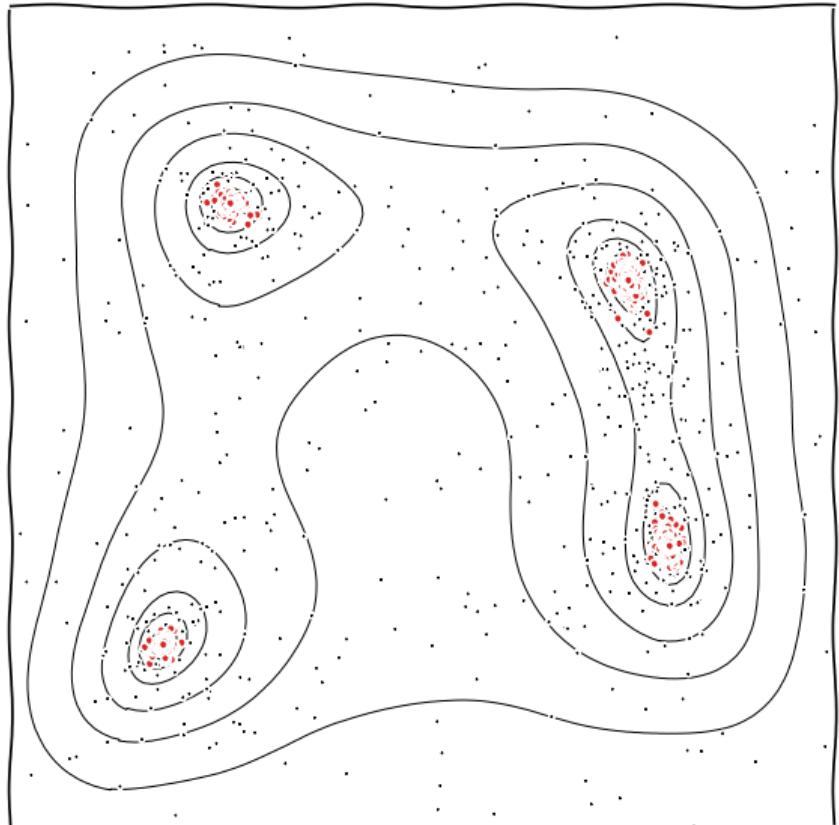


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Sampling from a hard likelihood constraint

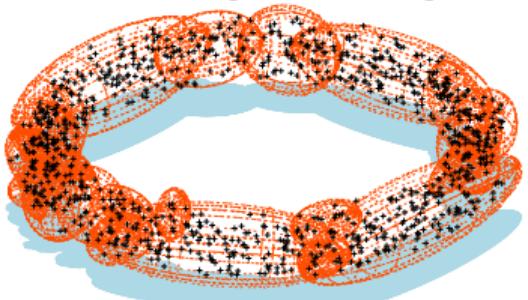
"It is not the purpose of this introductory paper to develop the technology of navigation within such a volume. We merely note that exploring a hard-edged likelihood-constrained domain should prove to be neither more nor less demanding than exploring a likelihood-weighted space."

— John Skilling

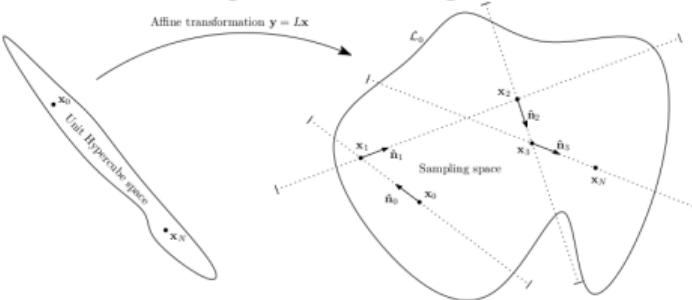
- ▶ A large fraction of the work in NS to date has been in attempting to implement a hard-edged sampler in the NS meta-algorithm $\{\theta \sim \pi : \mathcal{L}(\theta) > \mathcal{L}_*\}$.
- ▶ <https://projecteuclid.org/euclid.ba/1340370944>.
- ▶ There has also been much work beyond this (see "Frontiers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

Implementations of Nested Sampling [2205.15570](NatReview)

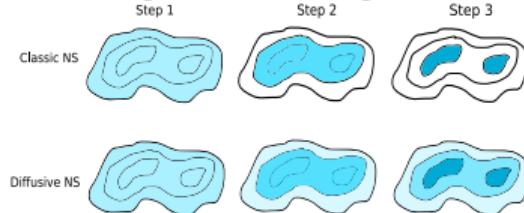
MultiNest [0809.3437]



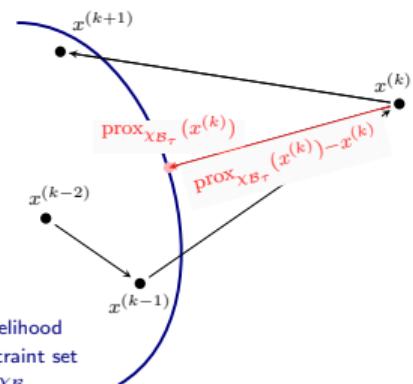
PolyChord [1506.00171]



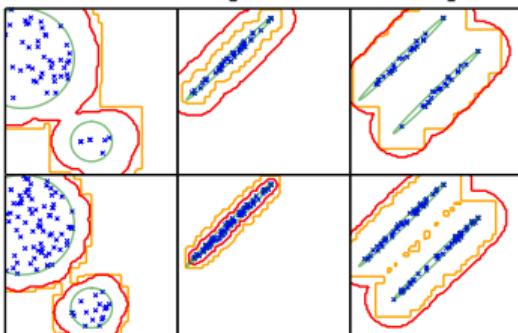
DNest [1606.03757]



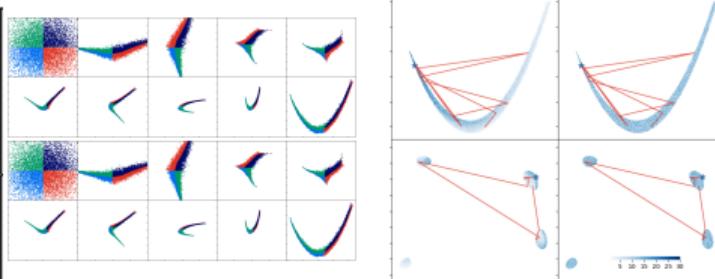
ProxNest [2106.03646]



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_{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} .

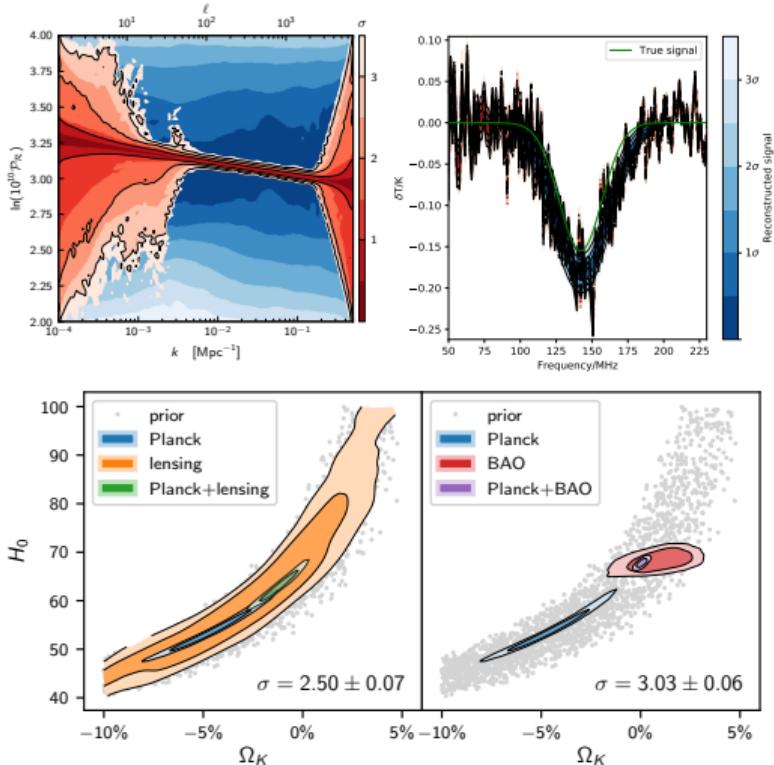
Chain-based samplers

- ▶ 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 of nested sampling

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 Λ 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.

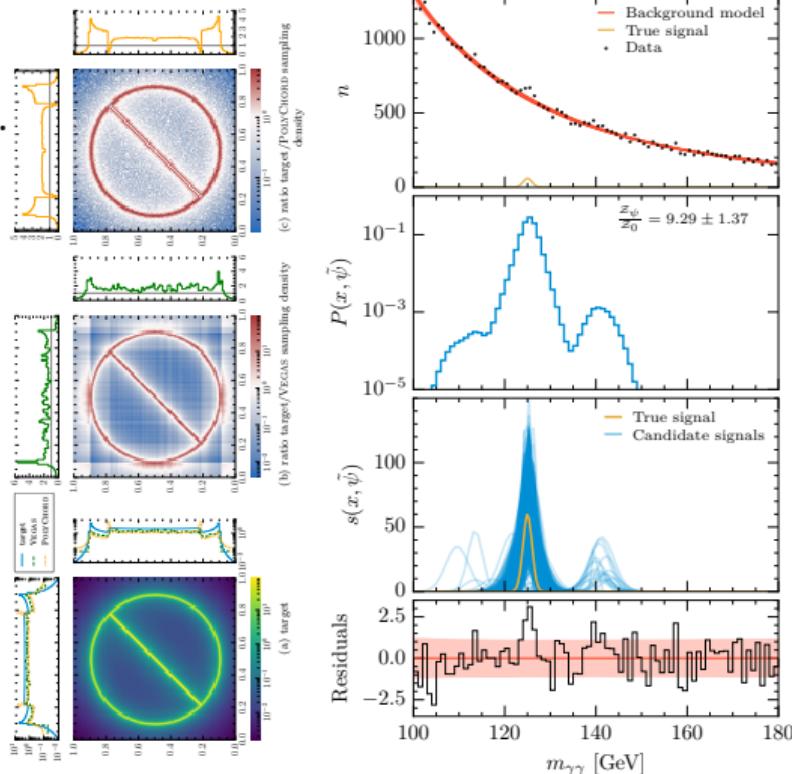


▪

Applications of nested sampling

Particle physics

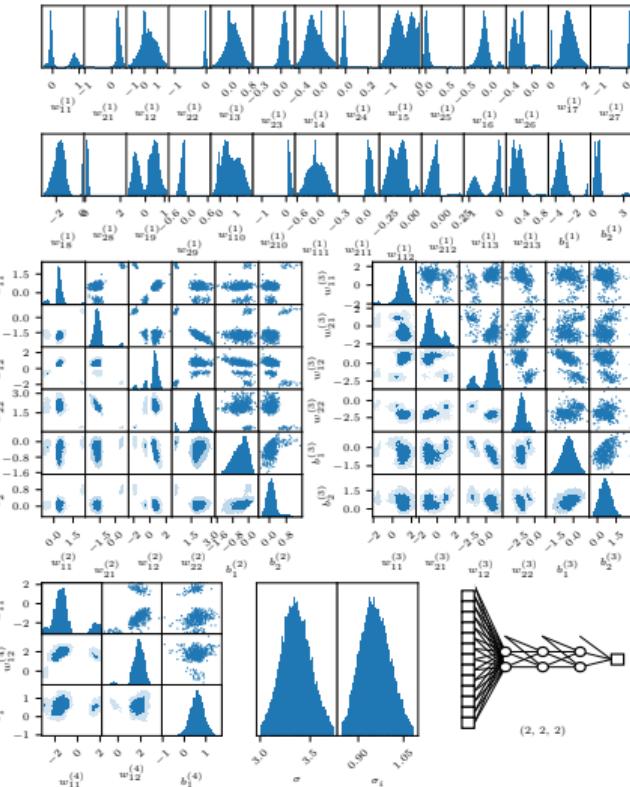
- ▶ Nested sampling for cross section computation/event generation $\sigma = \int_{\Omega} d\Phi |\mathcal{M}|^2$.
- ▶ Nested sampling can explore the phase space Ω and compute integral blind with comparable efficiency to HAAG/RAMBO [2205.02030].
- ▶ Bayesian sparse reconstruction [1809.04598] applied to bump hunting allows evidence-based detection of signals in phenomenological backgrounds [2211.10391].
- ▶ Now applying to lattice field theory, and lattice gravity Lagrangians.
- ▶ Fine tuning quantification



Applications of nested sampling

Machine learning

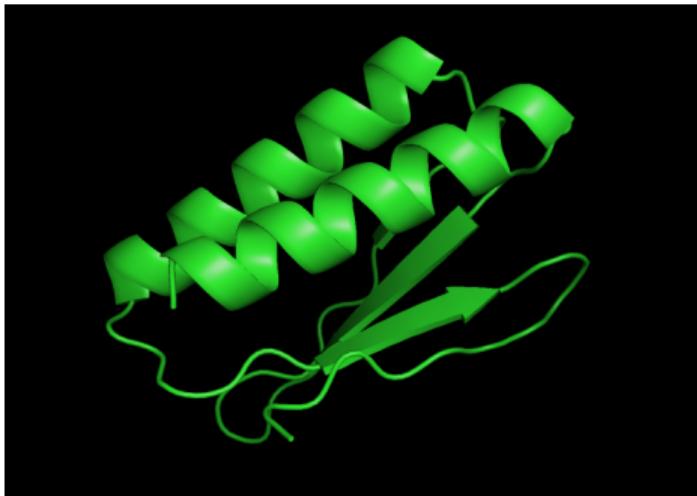
- ▶ Machine learning requires:
 - ▶ Training to find weights
 - ▶ Choice of architecture/topology/hyperparameters
- ▶ Bayesian NNs treat training as a model fitting problem
- ▶ Compute posterior of weights (parameter estimation), rather than optimisation (gradient descent)
- ▶ Use evidence to determine 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.



Applications of nested sampling

and beyond...

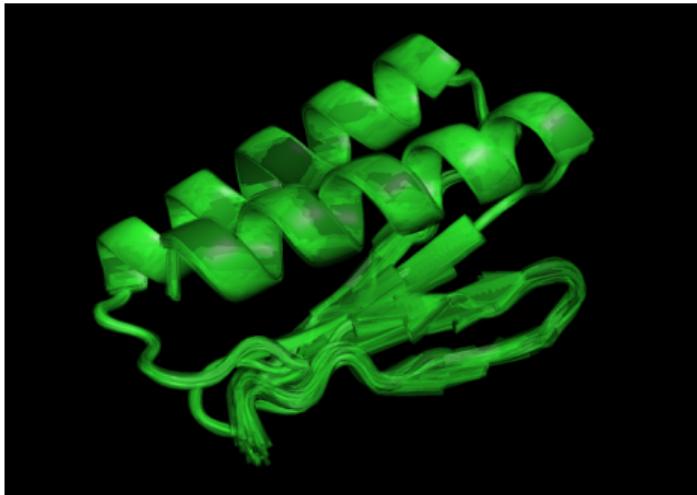
- ▶ Techniques have been spun-out (PolyChord Ltd) to:
- ▶ Protein folding
 - ▶ Navigating free energy surface.
 - ▶ Computing misfolds.
 - ▶ Thermal motion.
- ▶ Nuclear fusion reactor optimisation
 - ▶ multi-objective.
 - ▶ uncertainty propagation.
- ▶ Telecoms & DSTL research (MIDAS)
 - ▶ Optimising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



Applications of nested sampling

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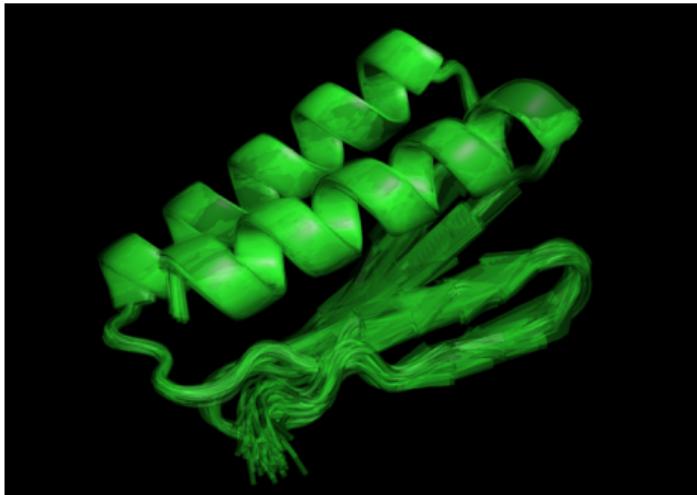
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How does Nested Sampling compare to other approaches?

- ▶ 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

Advantages and disadvantages of nested sampling

Advantages

- ▶ Doesn't need gradients
- ▶ Ensemble sampler
- ▶ Multimodal exploration
- ▶ Very Parallelisable

Disadvantages

- ▶ Doesn't use gradients
- ▶ Slow (but steady)
- ▶ Struggles with stochastic likelihoods (nondeterminism)
- ▶ Limited to $\sim \mathcal{O}(10^3)$ dimensions

Unique elements

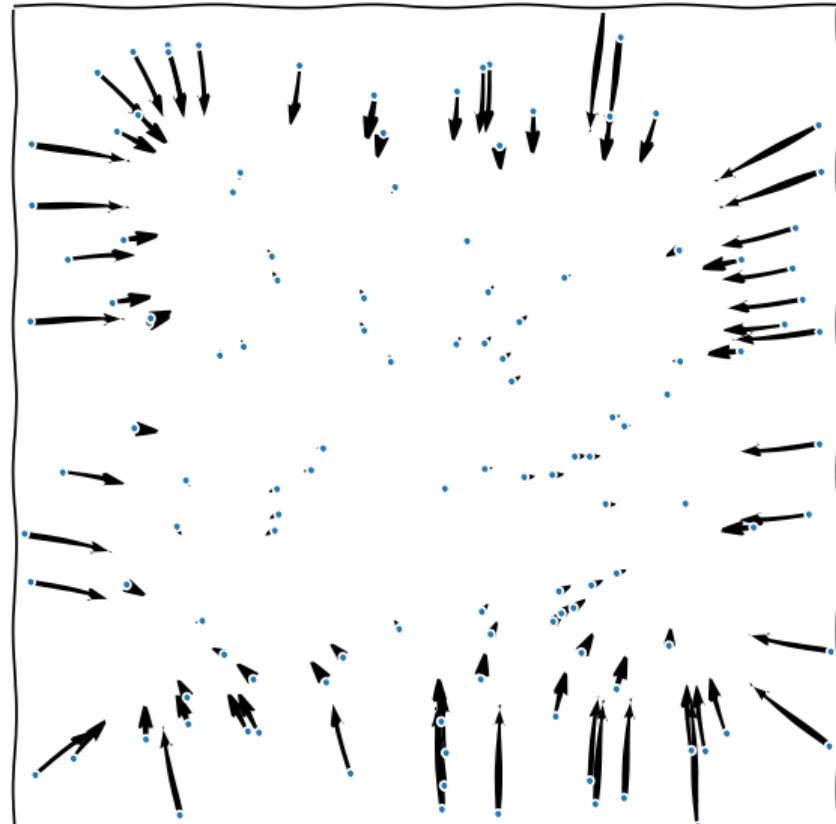
- ▶ Ensemble sampler
- ▶ Estimates volumes, entropies and evidences
- ▶ Athermal evolution
- ▶ Order statistics

Gradients in nested sampling

- The challenge: Sample uniformly within likelihood contour:

$$\{\theta \sim \pi : \mathcal{L}(\theta) > \mathcal{L}_{*}\}$$

making use of $\nabla_{\theta} \log \mathcal{L}$

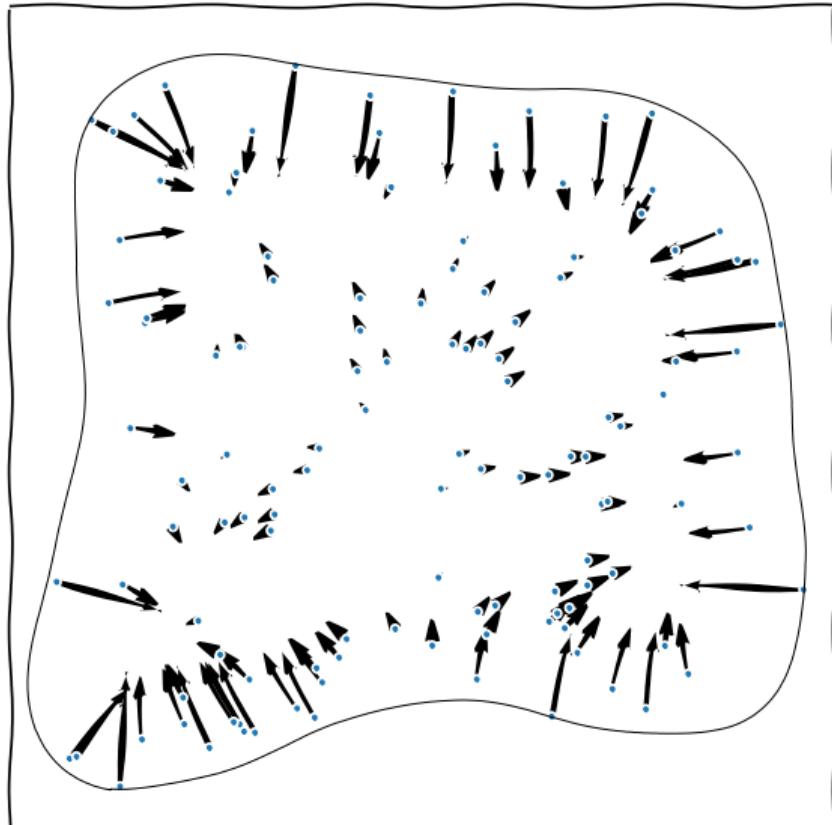


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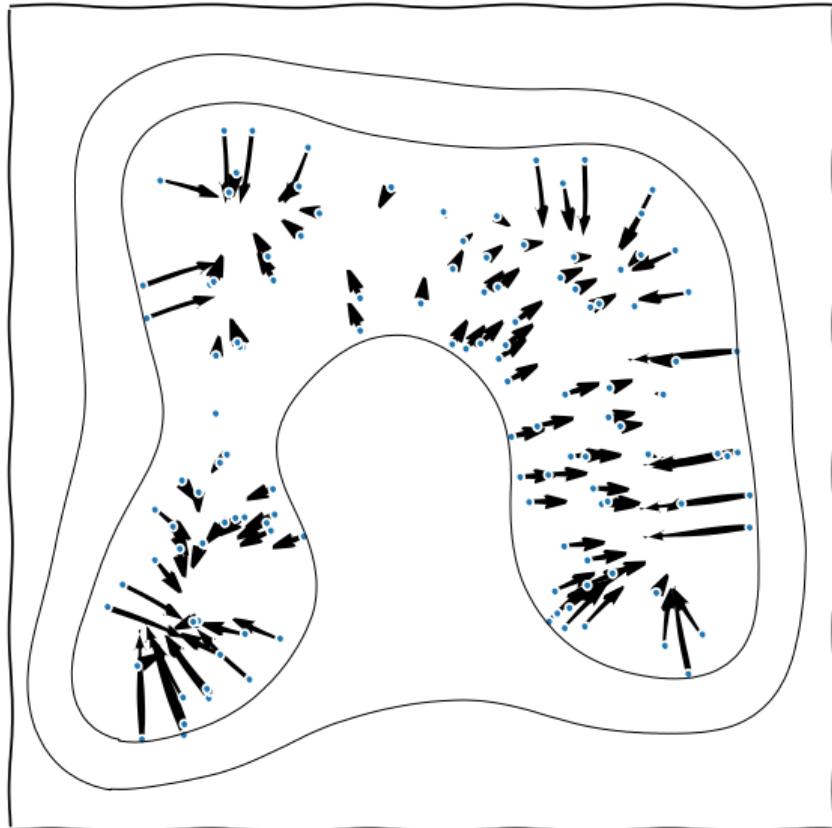


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Why doesn't HMC work?

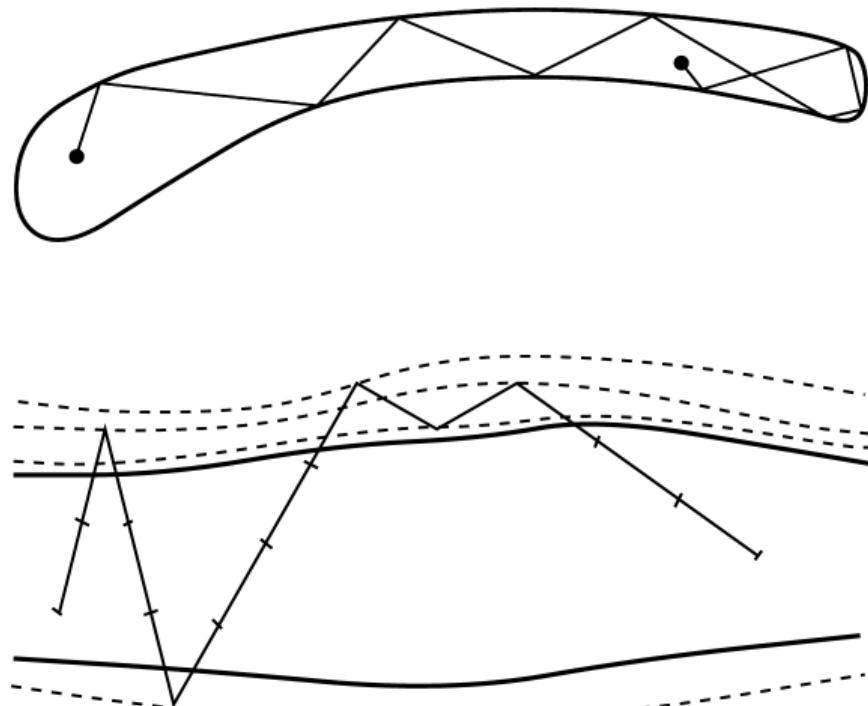
“Tabletop” distributions are difficult to sample!

- ▶ Nested sampling requires you to sample from the truncated *prior*, not the likelihood
- ▶ Other than at the boundaries, it is not obvious how to use a likelihood gradient to navigate the prior.
- ▶ In addition, since nested sampling begins in the tails, proceeding through the typical set and onto the peak, the normalisation of the gradient is typically wildly misnormalised

Constrained Hamiltonian Monte Carlo [1005.0157]

aka: Gailean nested sampling [1312.5638]; Reflective slice sampling [physics/0009028]

- ▶ The primary way to sample from “Tabletop” distributions is with reflection:
 - ▶ Define start x_0 , velocity v ,
 - ▶ Update $x_{i+1} = x_i + v\Delta t$
 - ▶ When you reach the edge, reflect using \hat{n} :
 $v \rightarrow v - 2(v \cdot \hat{n})\hat{n}$
 - ▶ n can be taken to be $\nabla \log P$
- ▶ In practice since don’t know the exact boundary, care needs to be taken to generate unbiased samples
 - ▶ e.g. by reflecting whenever one is outside, not just once to get us back in.
- ▶ Radford Neal [physics/0009028] section 7 is best reference for this.



Historical attempts

[Betancourt](#) Hamiltonian constrained nested sampling [1005.0157].

[Feroz](#) Galilean Nested Sampling [1312.5638].

[Speagle](#) Incorporated into dynesty [1904.02180].

[Habeck](#) Habeck Demonic nested sampling – uses thermodynamic analogy to soften the hard boundary with a Maxwell daemon [doi:10.1063/1.4905971].

[Baldock](#) Total Enthalpy HMC, incorporating momenta in a more HMC like way, but specialised to materials science [1710.11085].

[Cai](#) ProxNest for high-dimensional convex imaging problems [2106.03646].

Things we have tried/are trying

Pablo Lemos Updated existing HMC/Galilean nested sampling to use differentiable programming (jax/torch) – code release imminent

Boris Deletic Masters project with C++ implementation for lattice field theory calculations

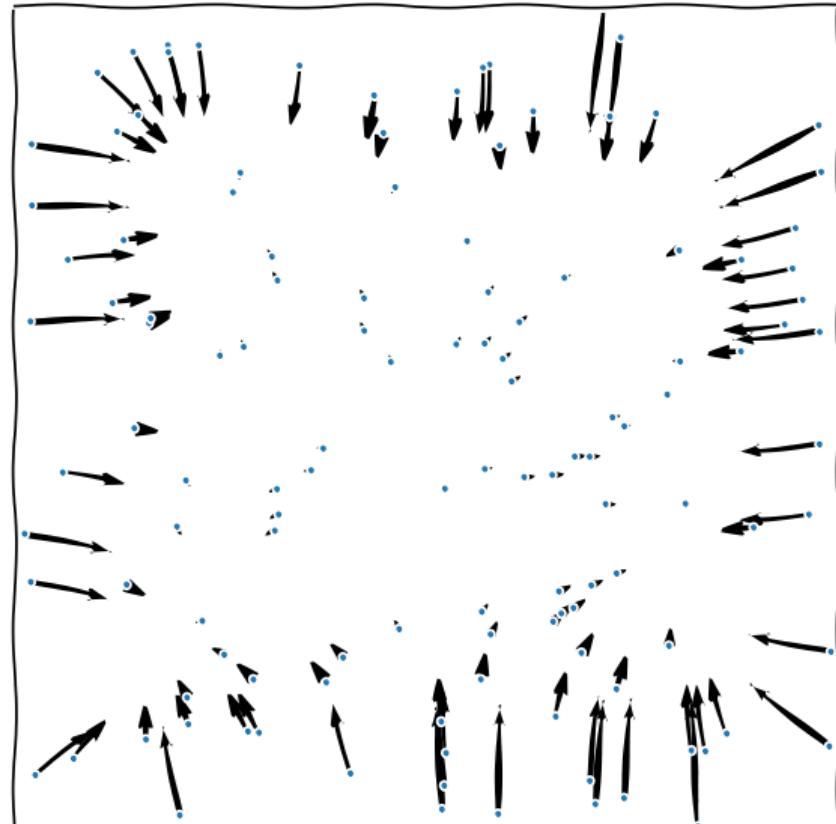
Stephen Thorpe Curved slice sampling.

Sam Leeney Variety of options under exploration:

- ▶ Tuning the HMC mass matrix with iteration number
- ▶ Posterior repartitioning [1908.04655] to “borrow” some of the likelihood
- ▶ Sampling with X rather than \mathcal{L} .

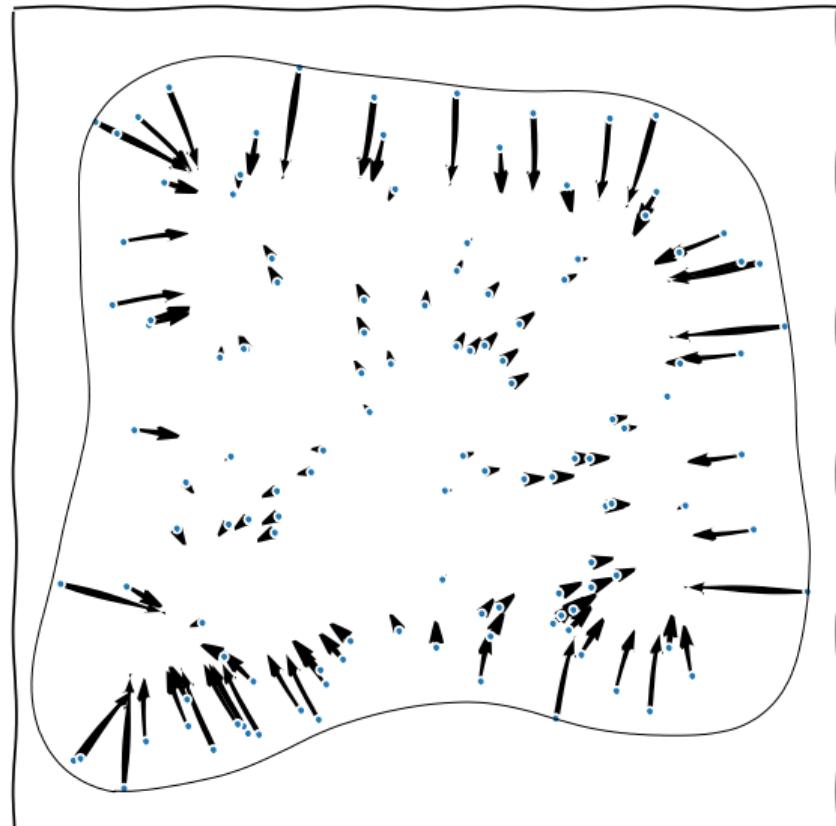
Nested sampling with gradients

- ▶ Current techniques don't make use of:
- ▶ We have "cloud" of gradients at every point
- ▶ We have an estimate of the prior volume X
- ▶ $\nabla \log X \propto \nabla \log L$



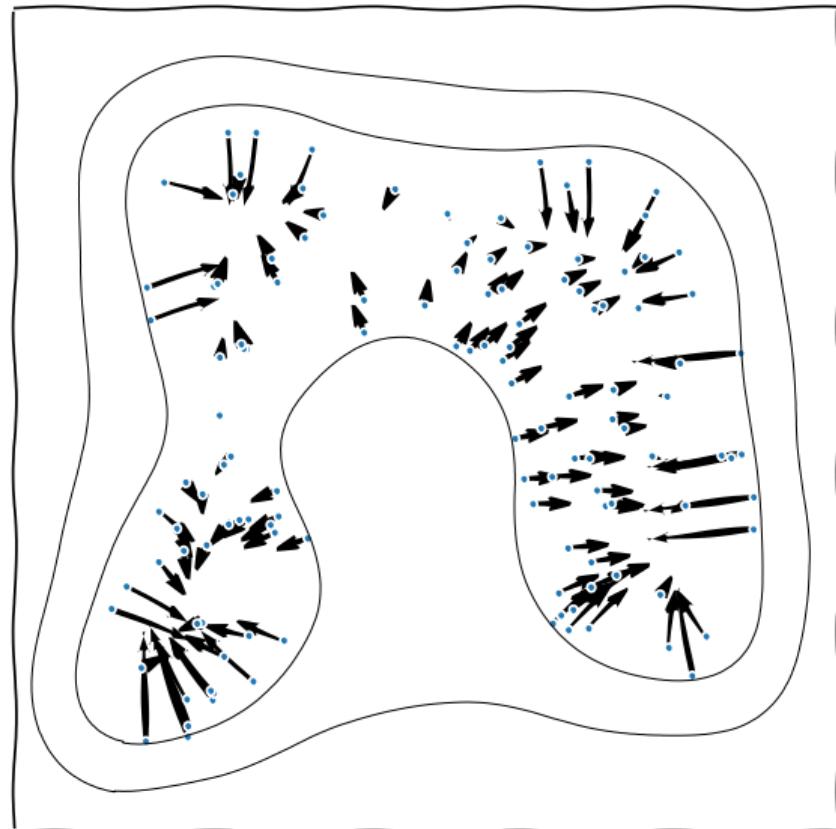
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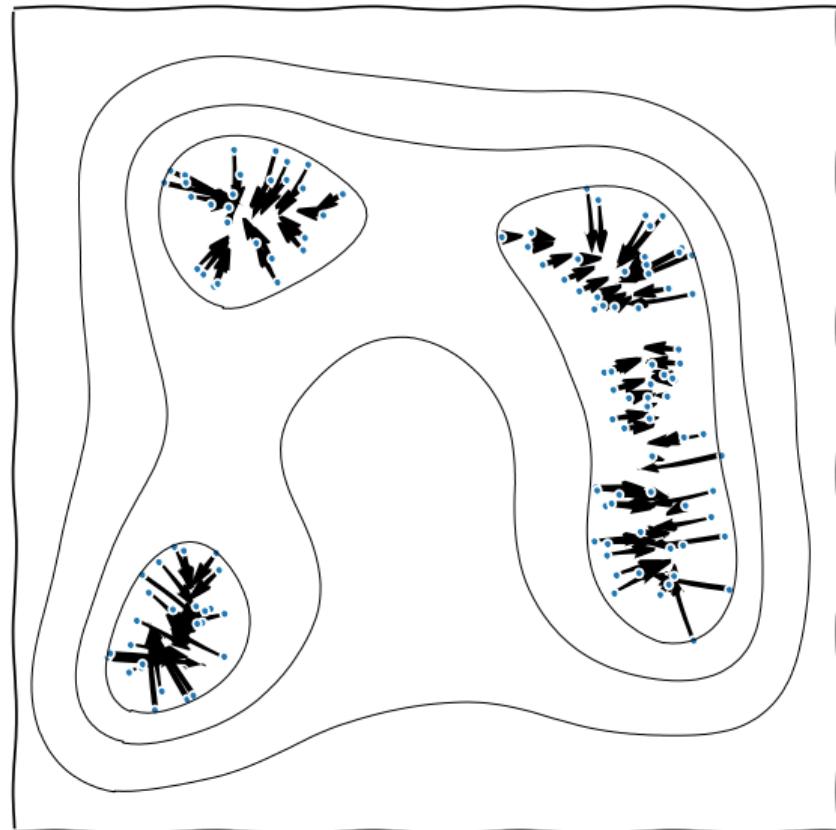
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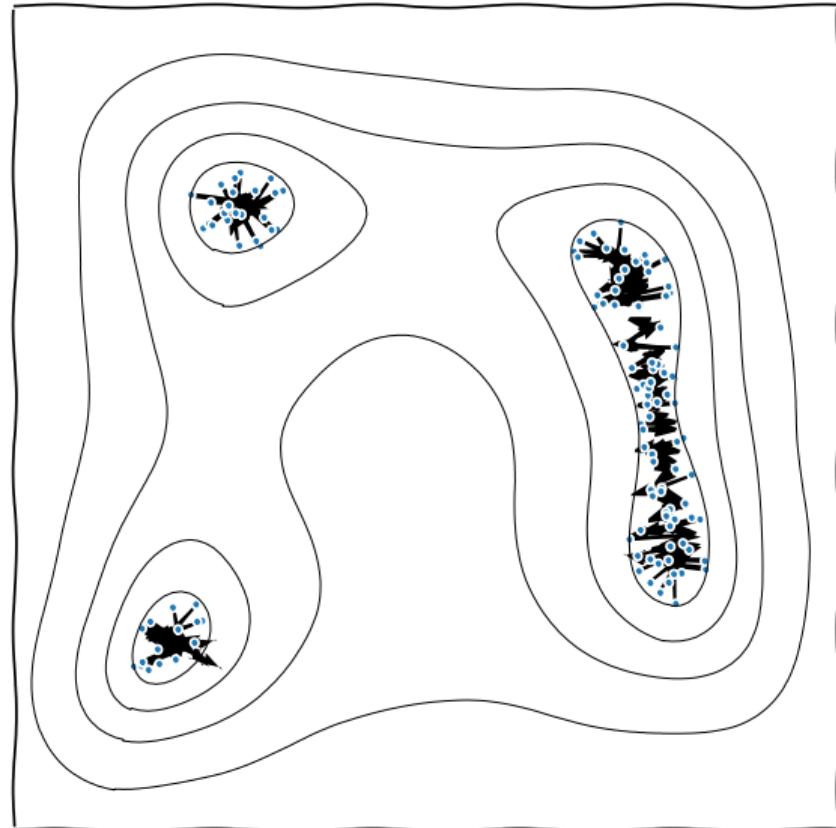
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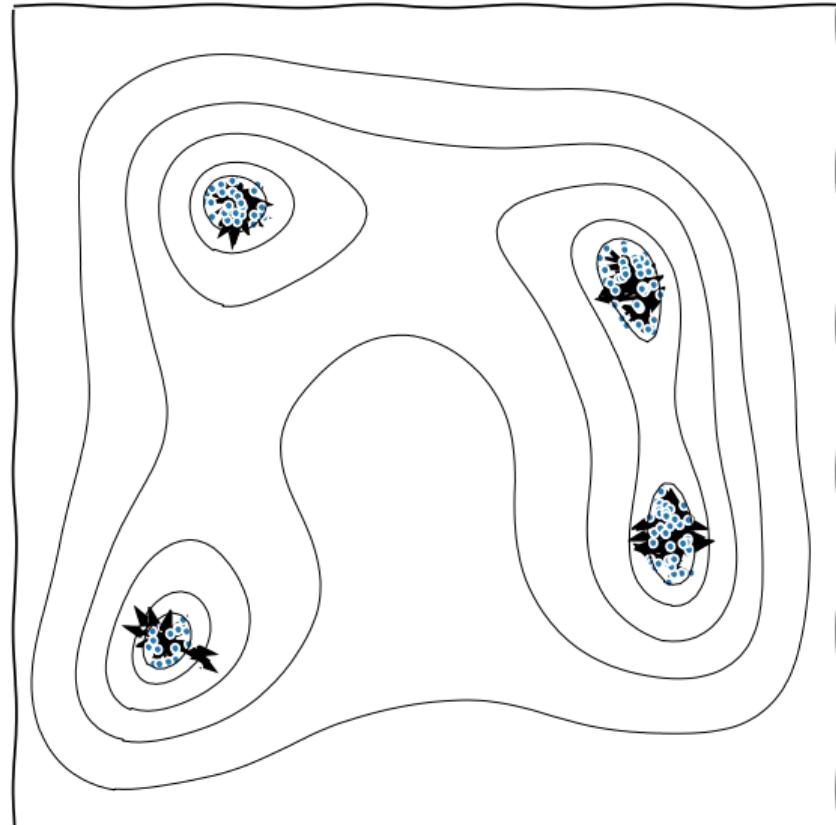
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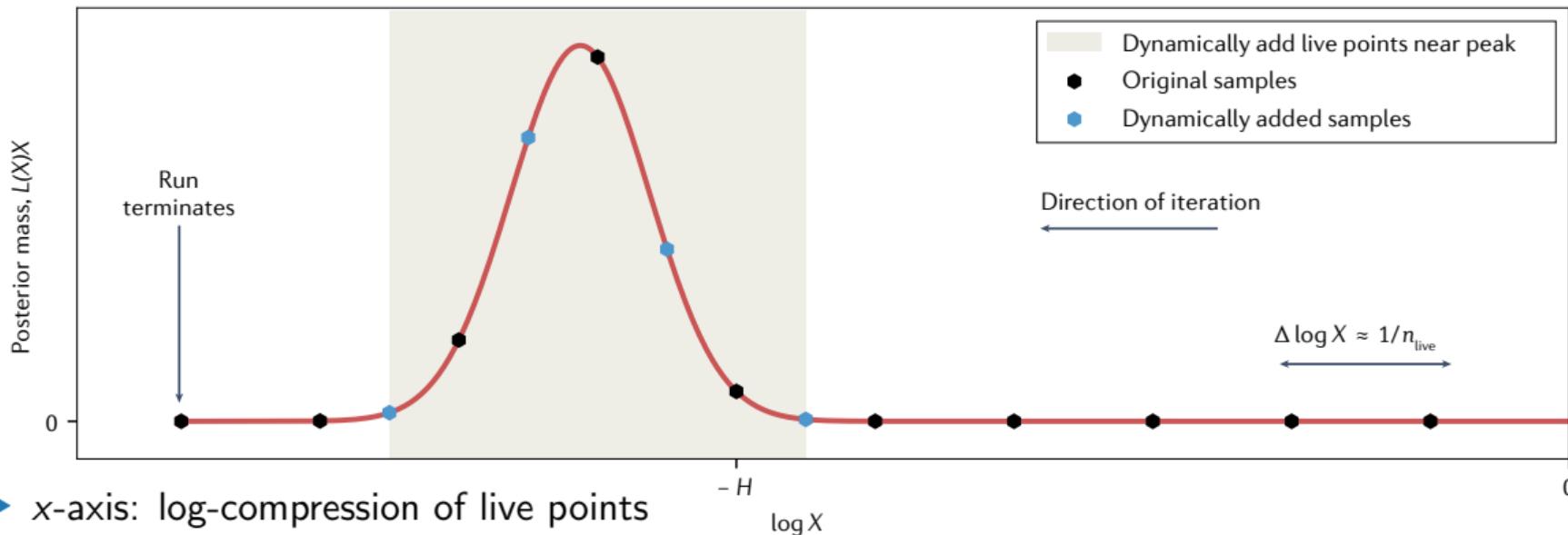
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Conclusions

- ▶ Nested sampling is a robust, 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 a variety of fields
- ▶ It can't currently use gradients very effectively.
- ▶ If it could, probabilistic programming means there are a lot of analyses which would benefit.
- ▶ One of my main aims this week is to see if there are any options from other fields

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