

Gradients and Nested Sampling

The present state of the art

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7th July 2023



**The
Alan Turing
Institute**



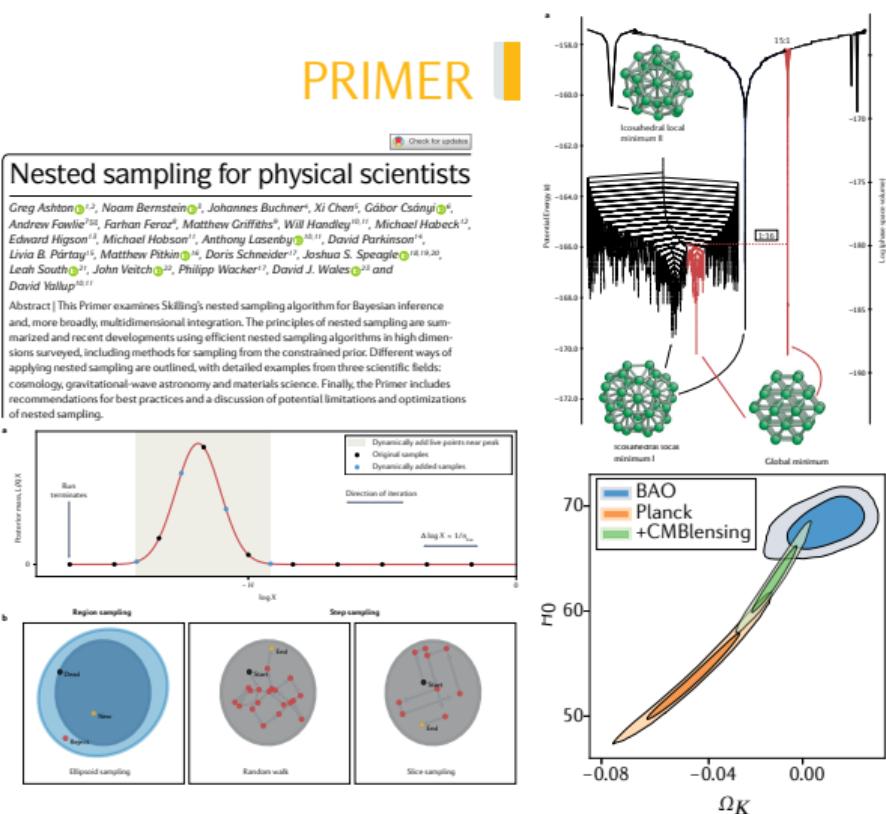
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Highlight: state-of-the-art Nature review primer [2205.15570]

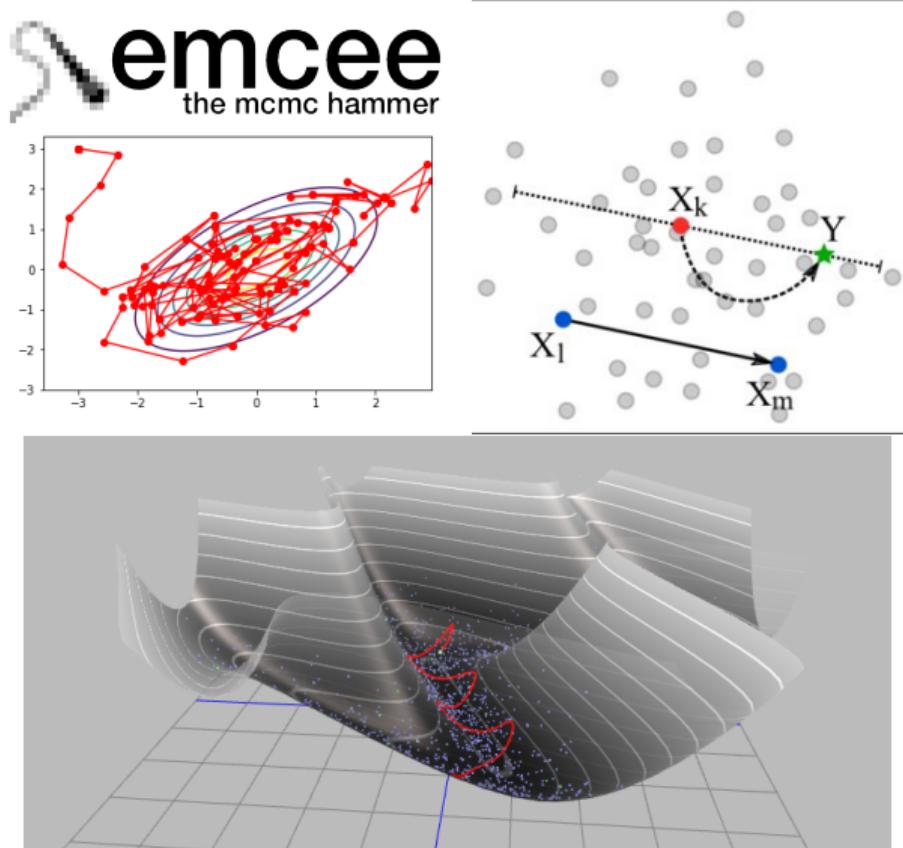
PRIMER

- ▶ 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?



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

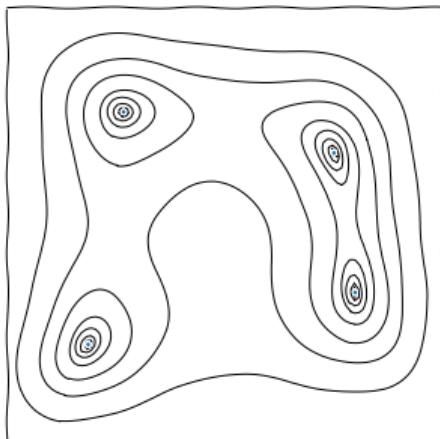


What is Nested Sampling?

- ▶ 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:

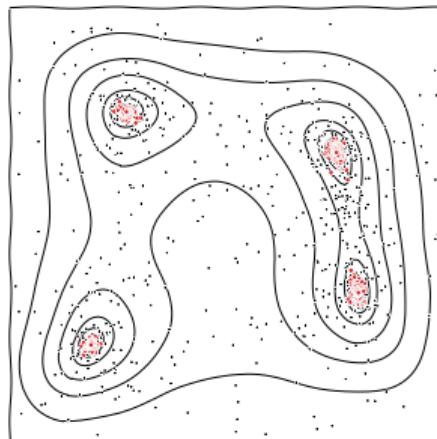
Optimisation

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



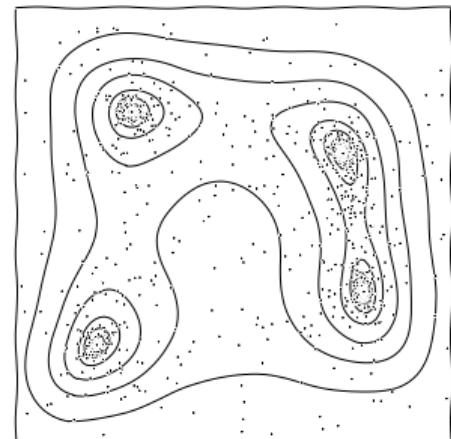
Exploration

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

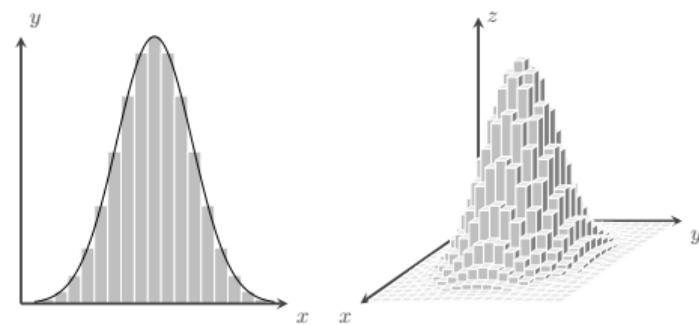
$$\Psi = \int e^{iS} \mathcal{D}x$$

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.

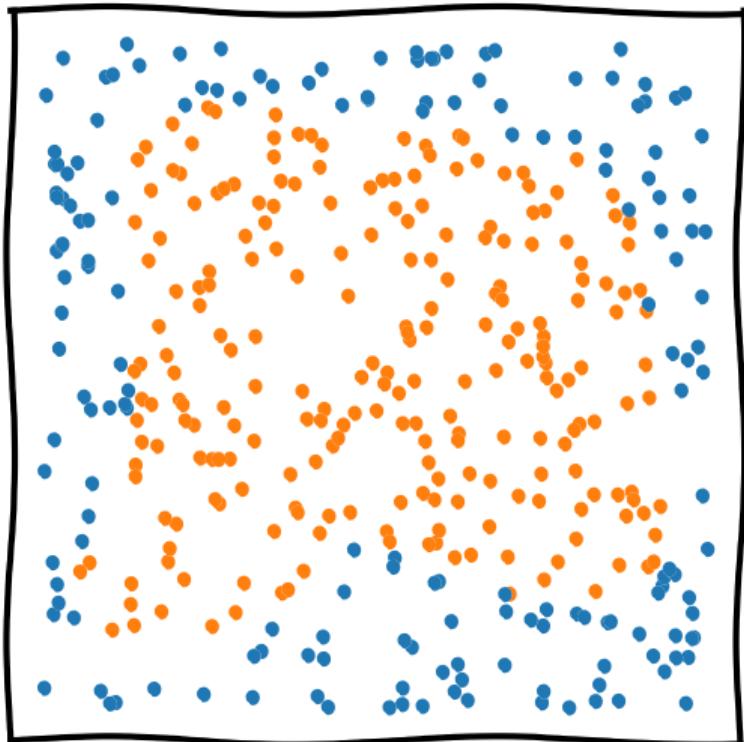


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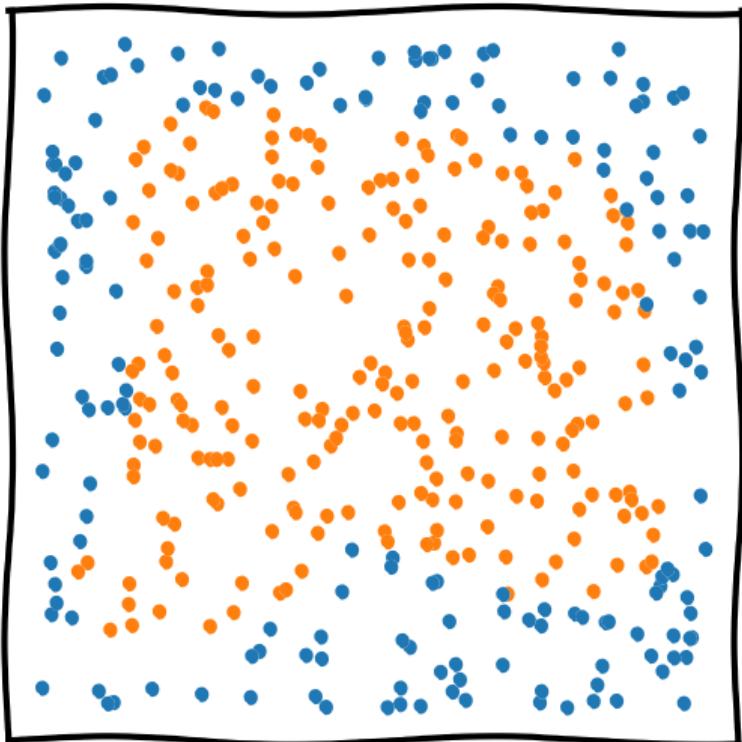


Probabalistic volume estimation

- ▶ 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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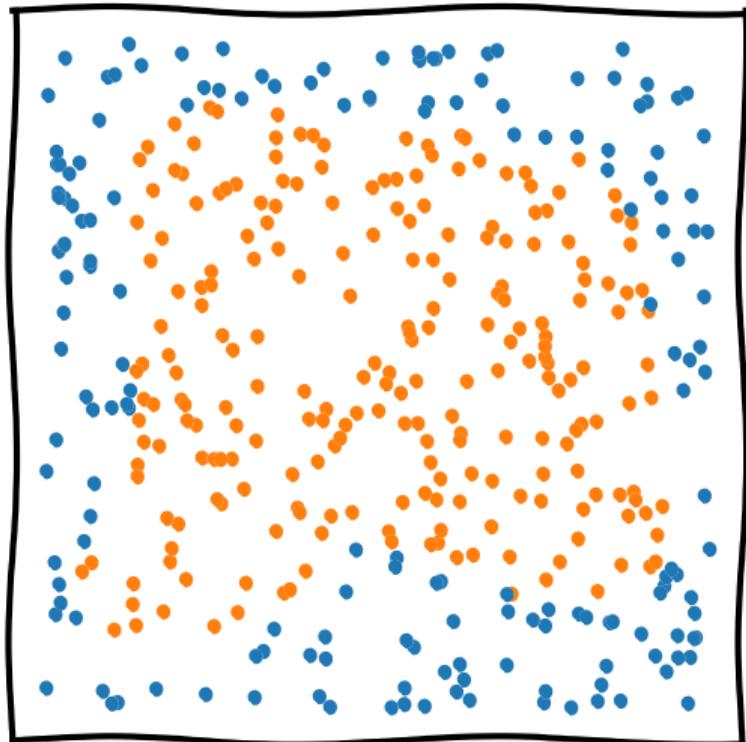


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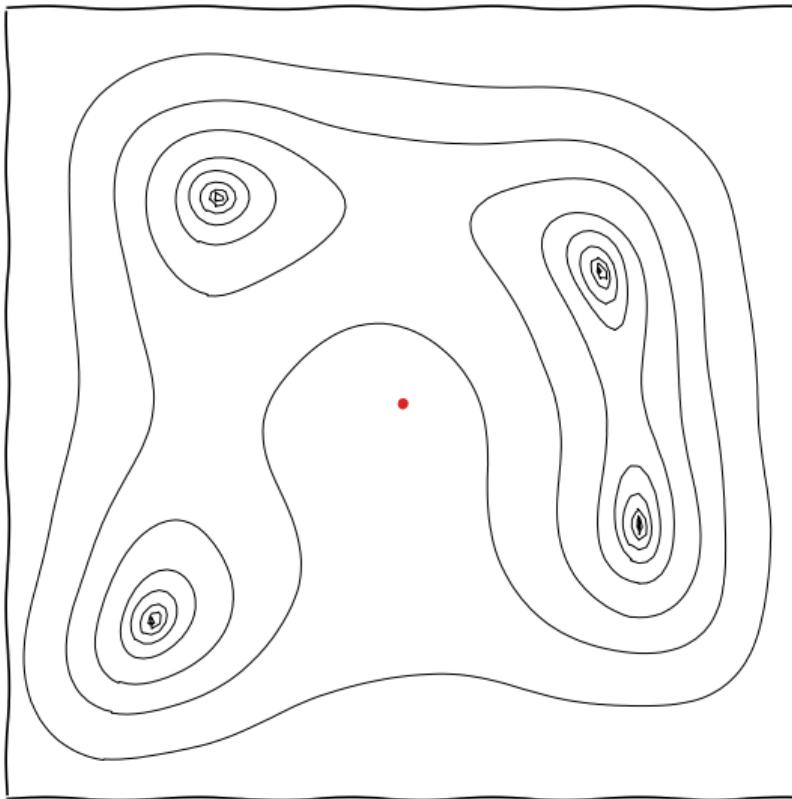
- ▶ Key idea in NS: estimating volumes probabilistically

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

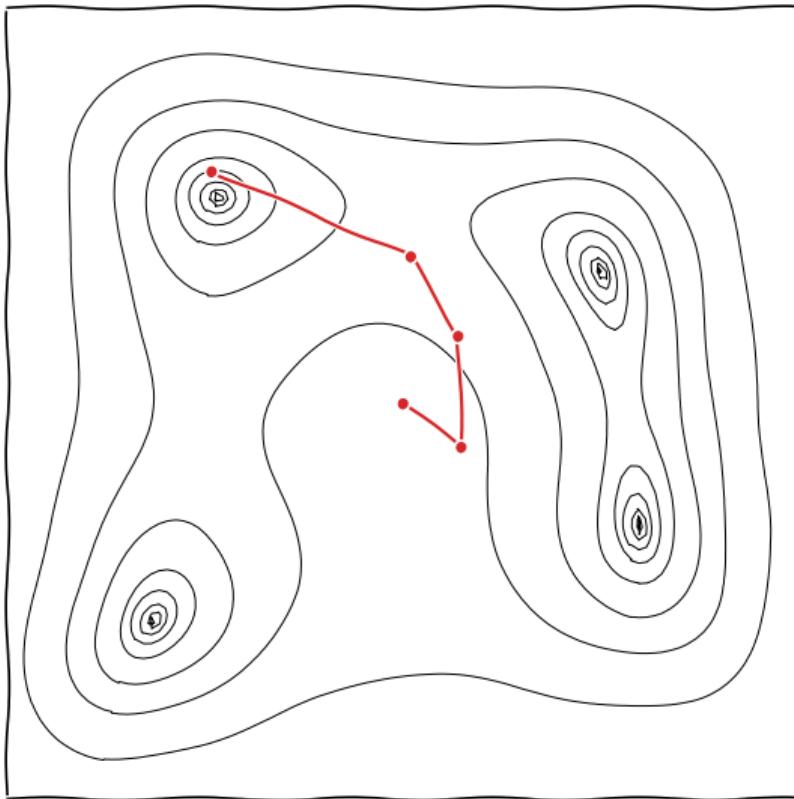
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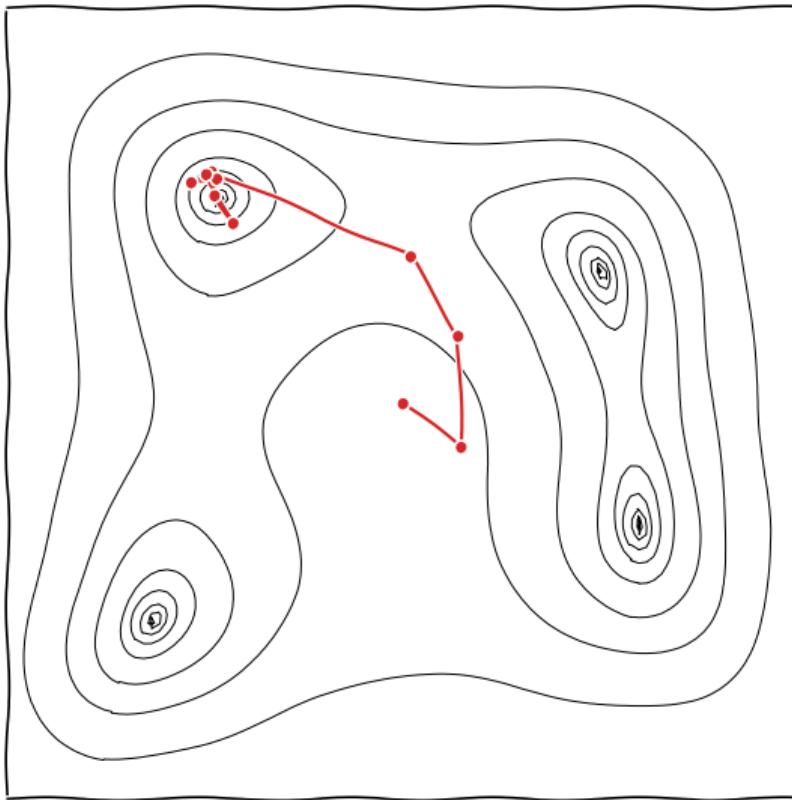
MCMC



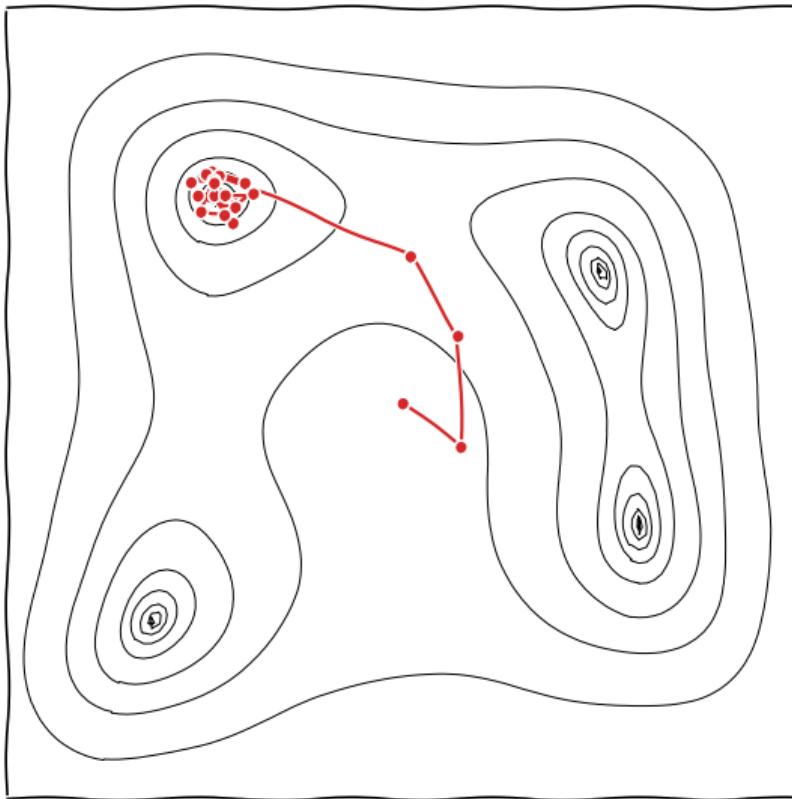
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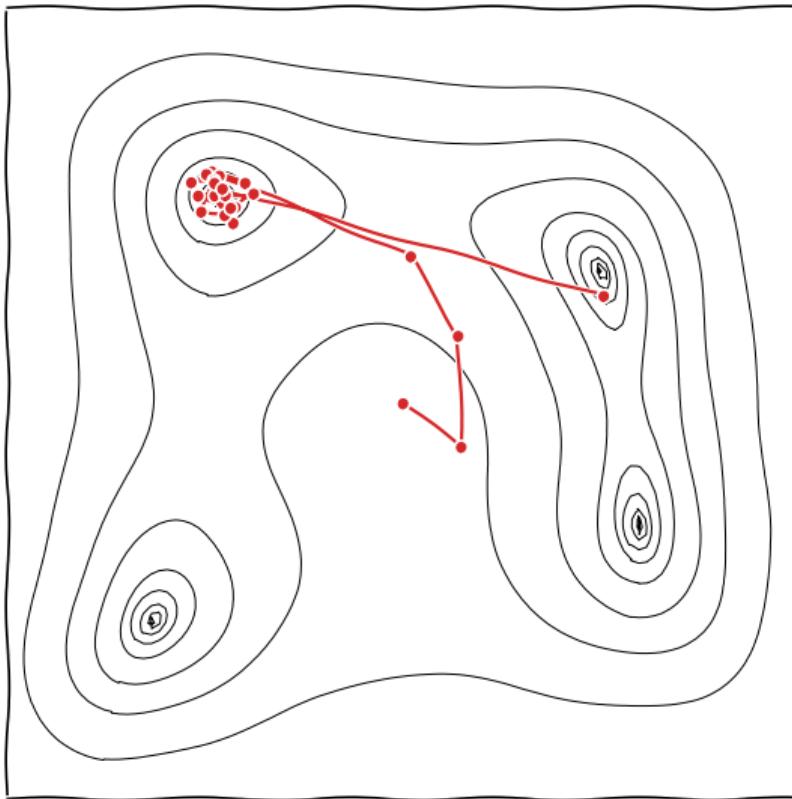
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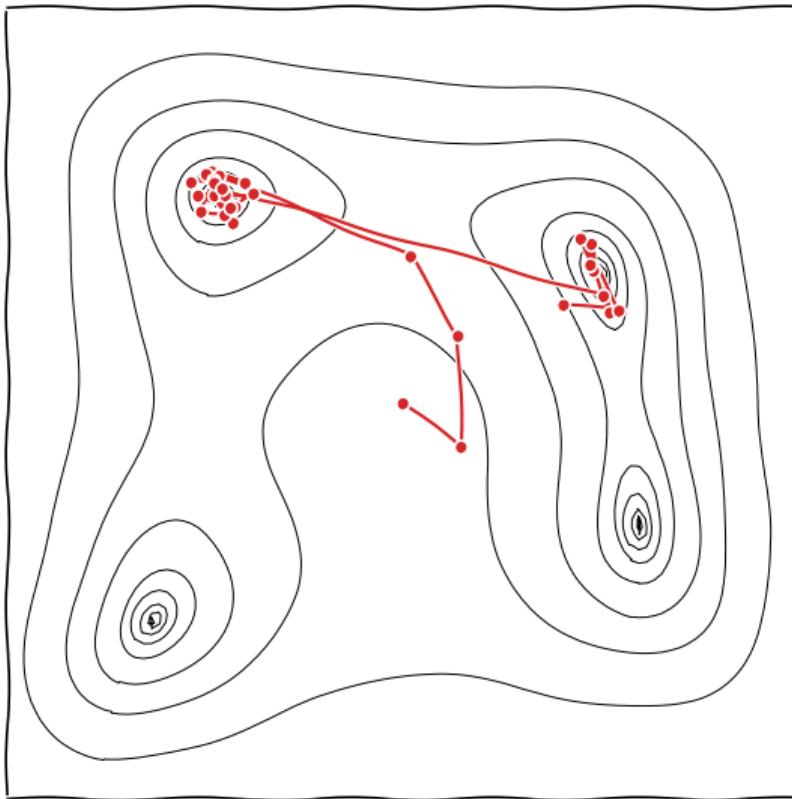
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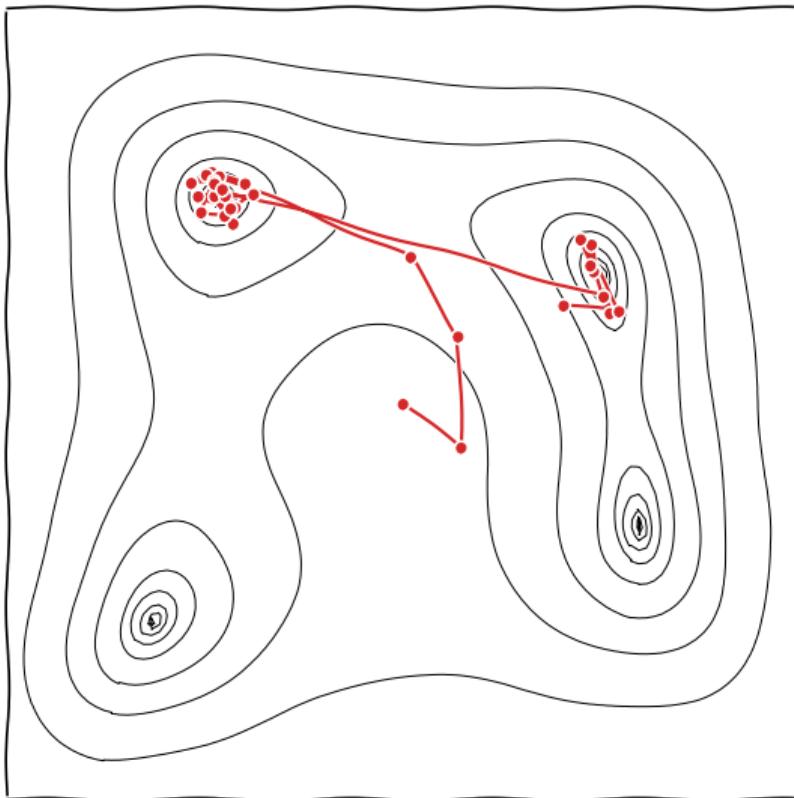
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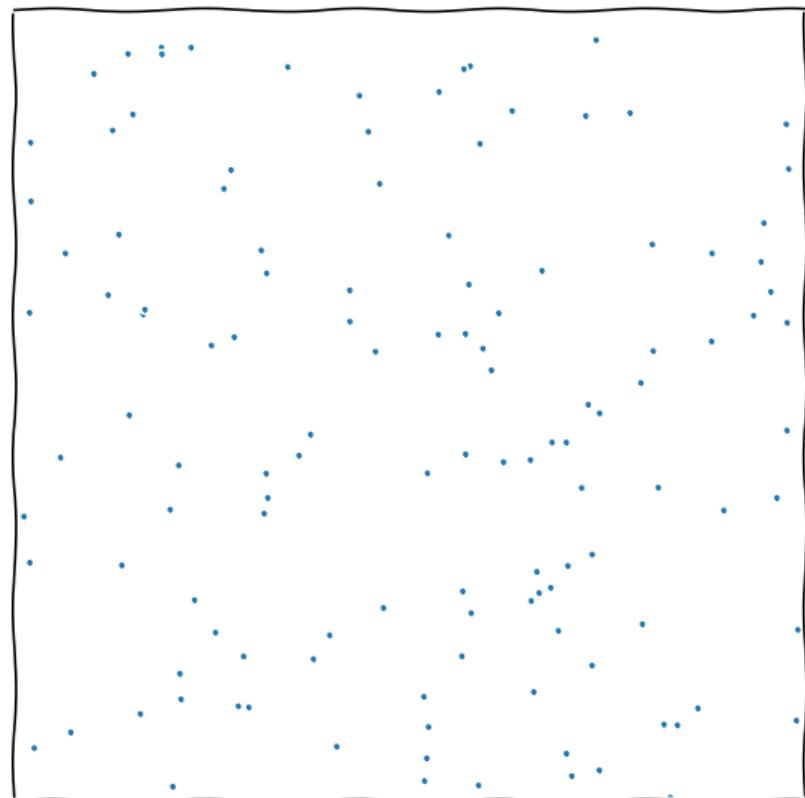
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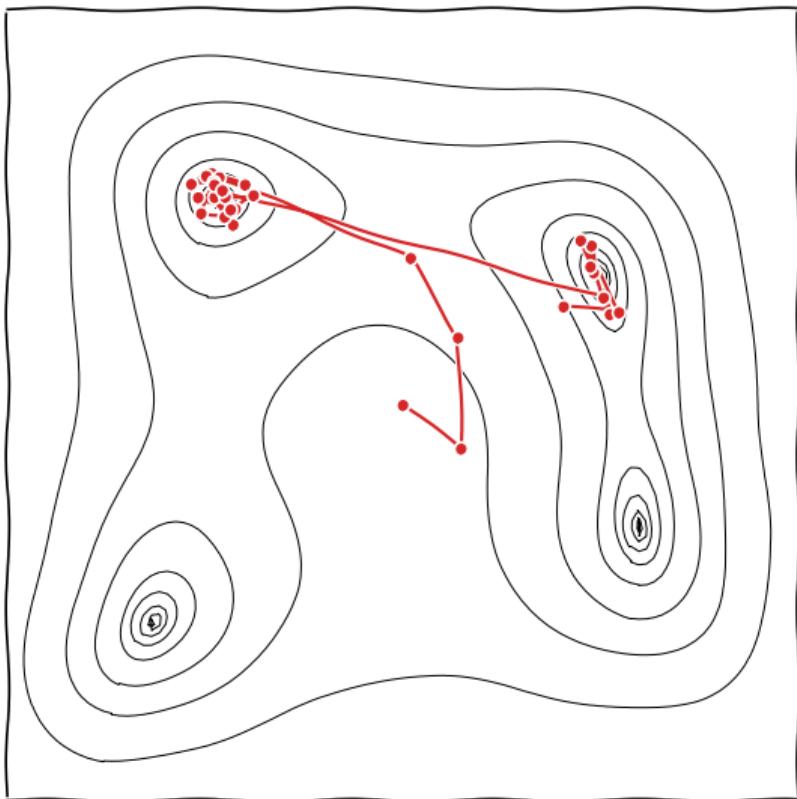
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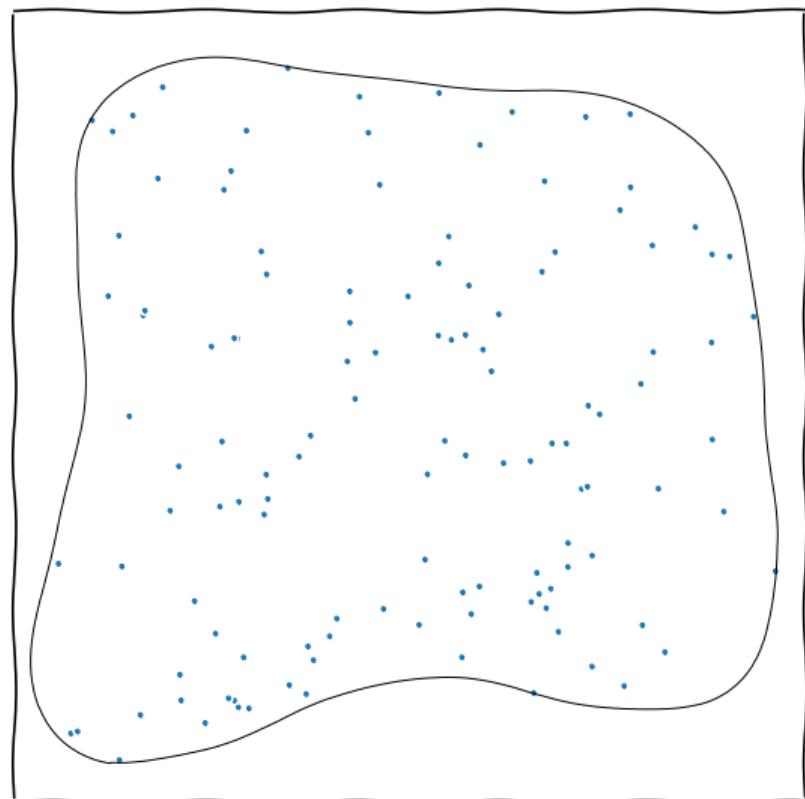
Nested sampling



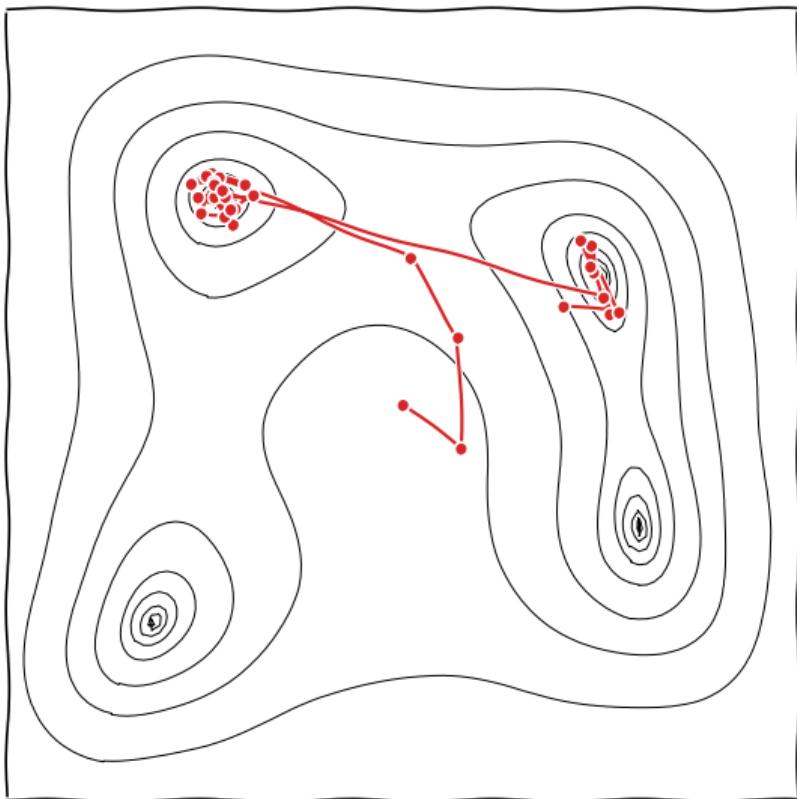
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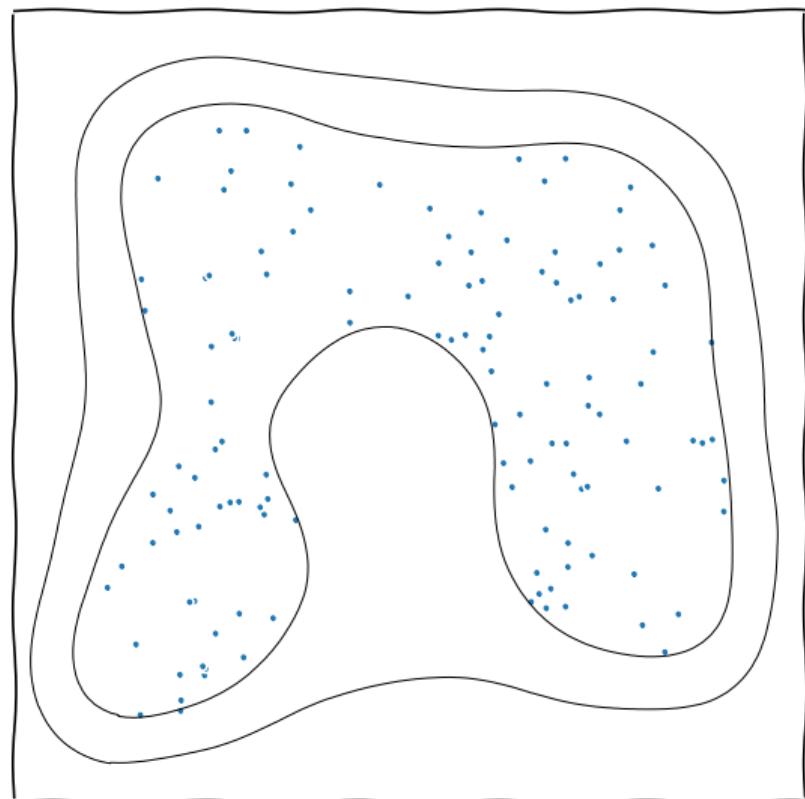
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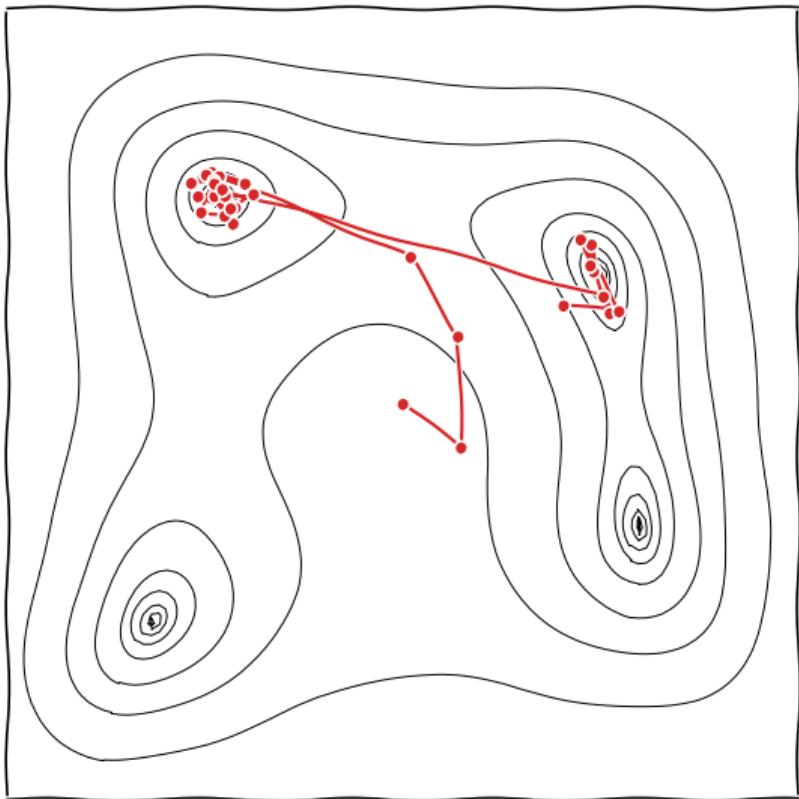
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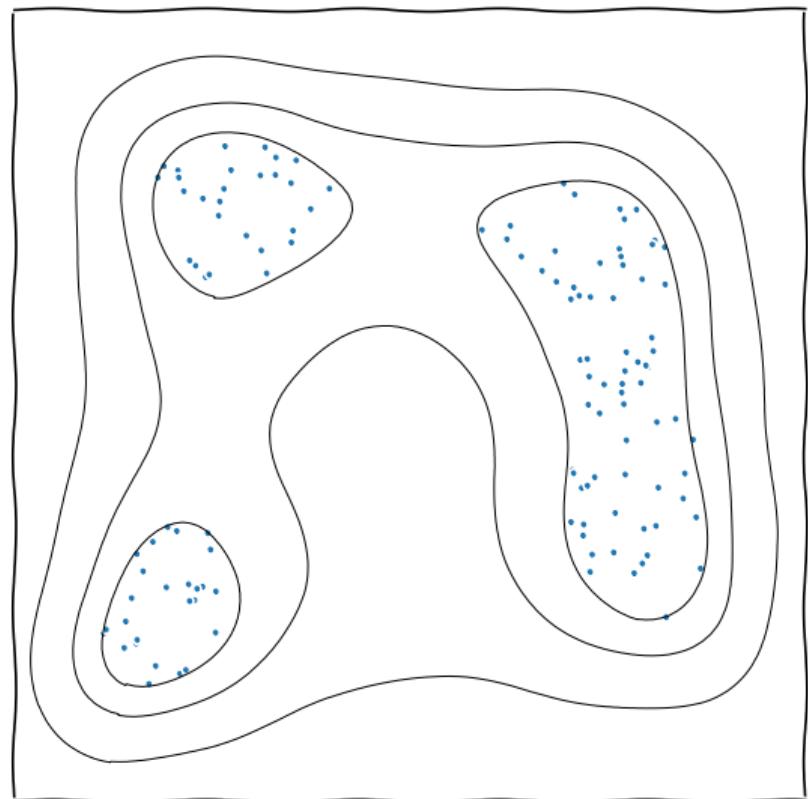
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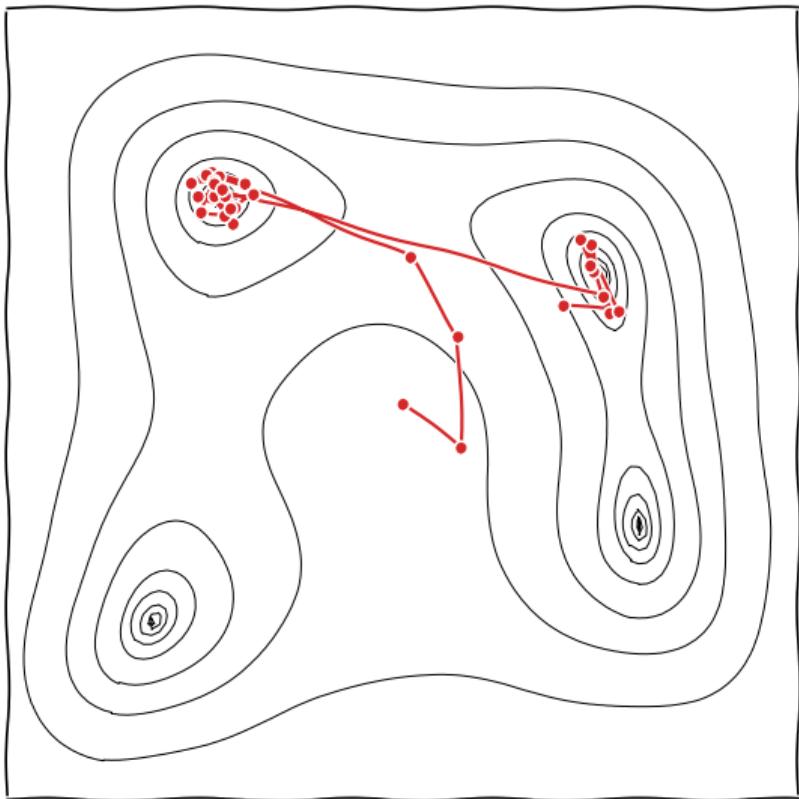
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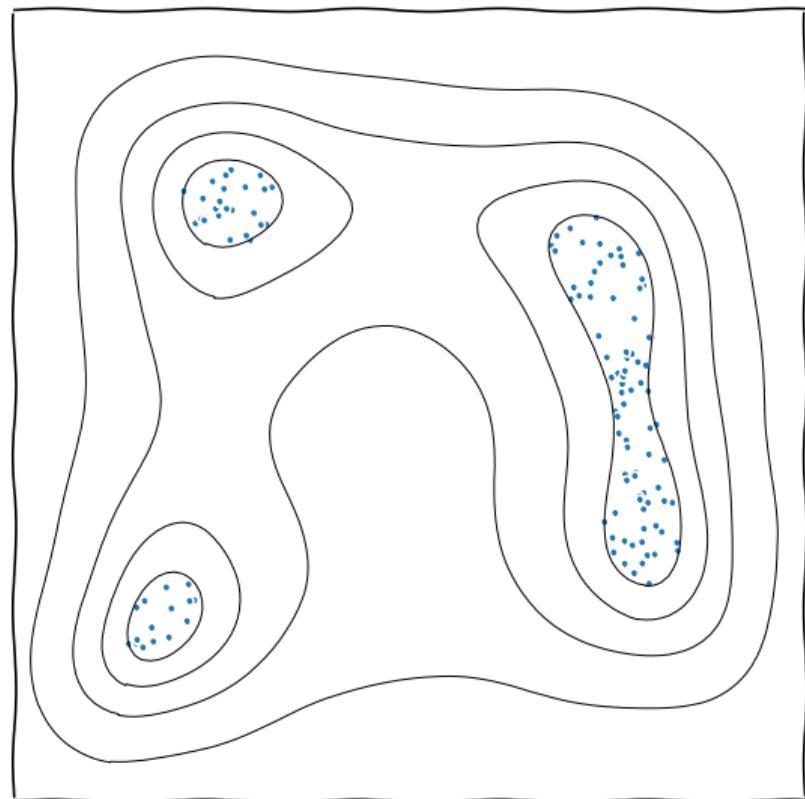
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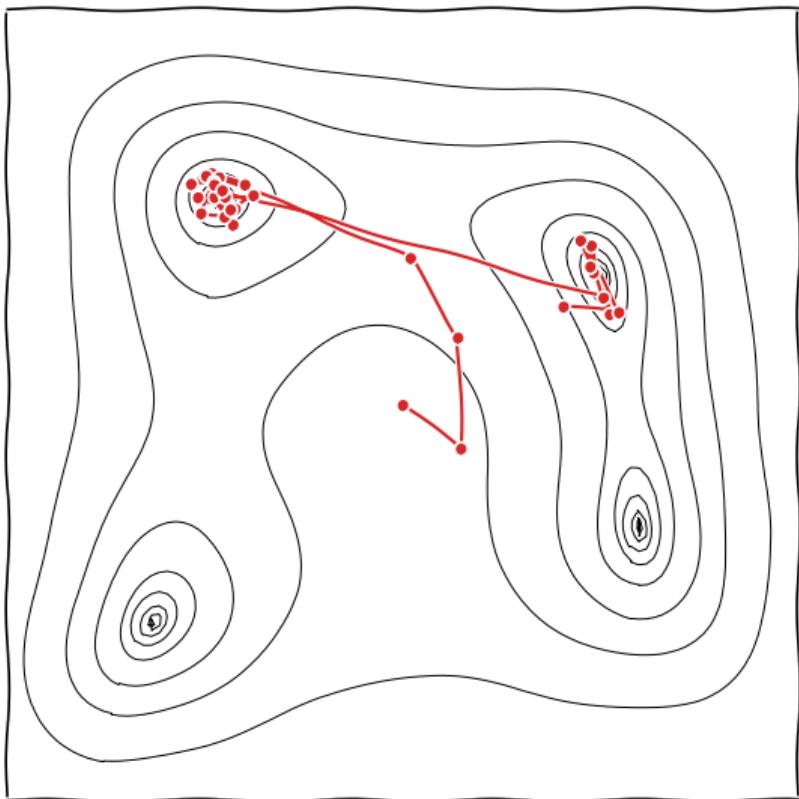
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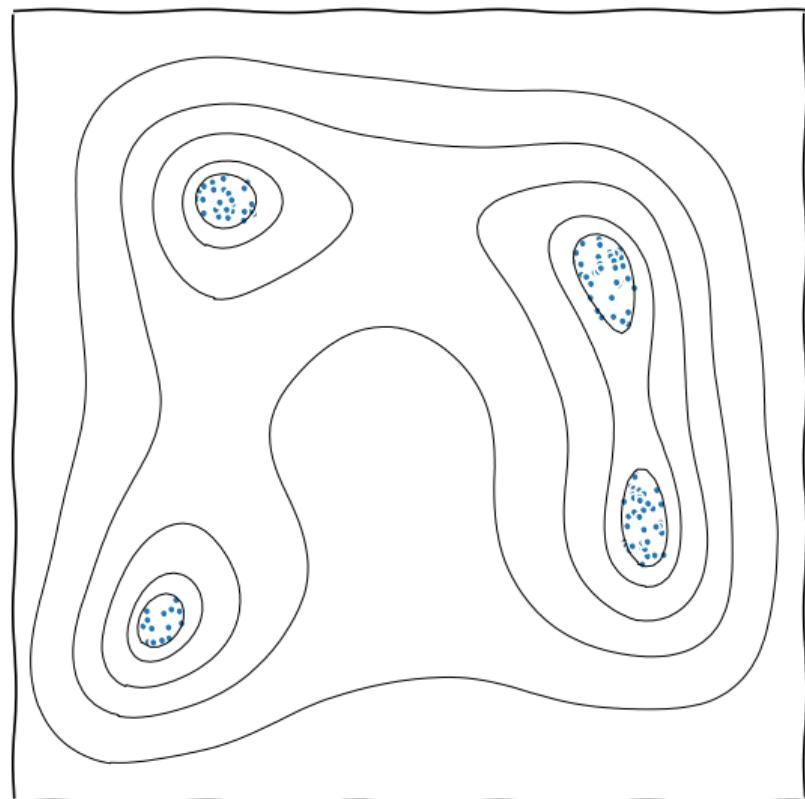
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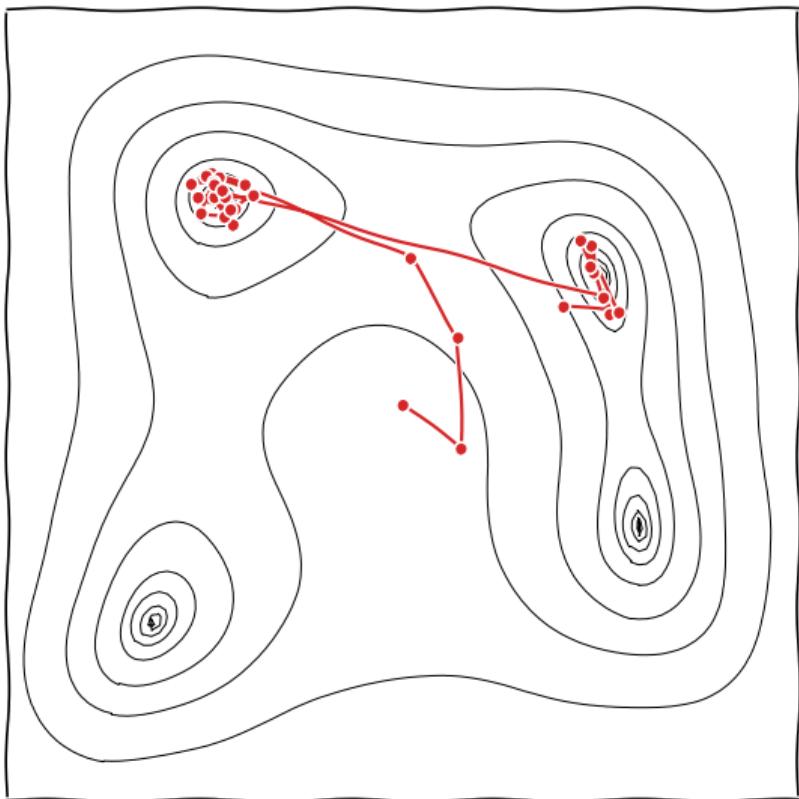
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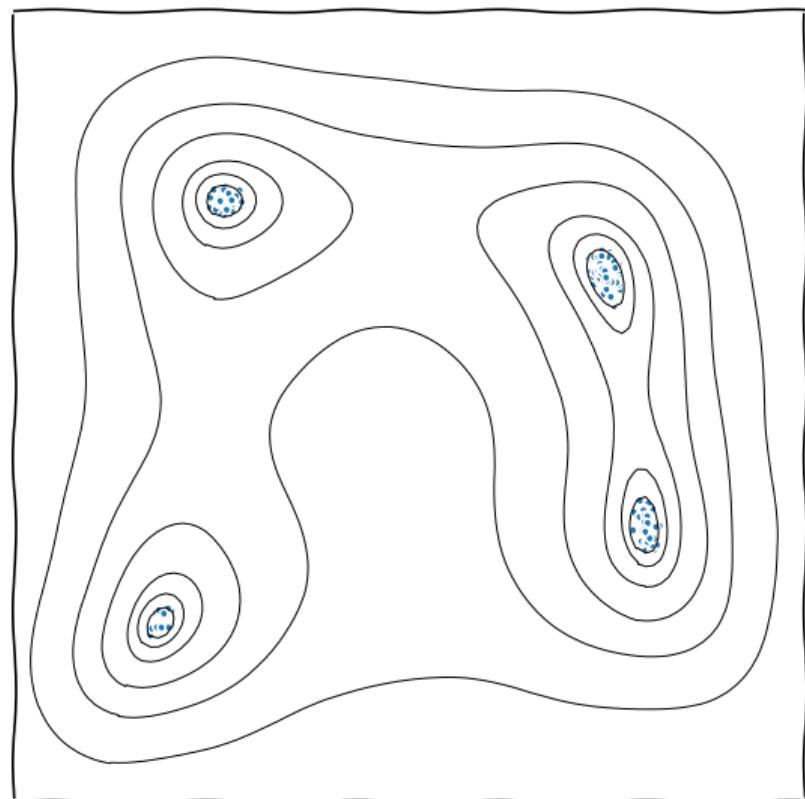
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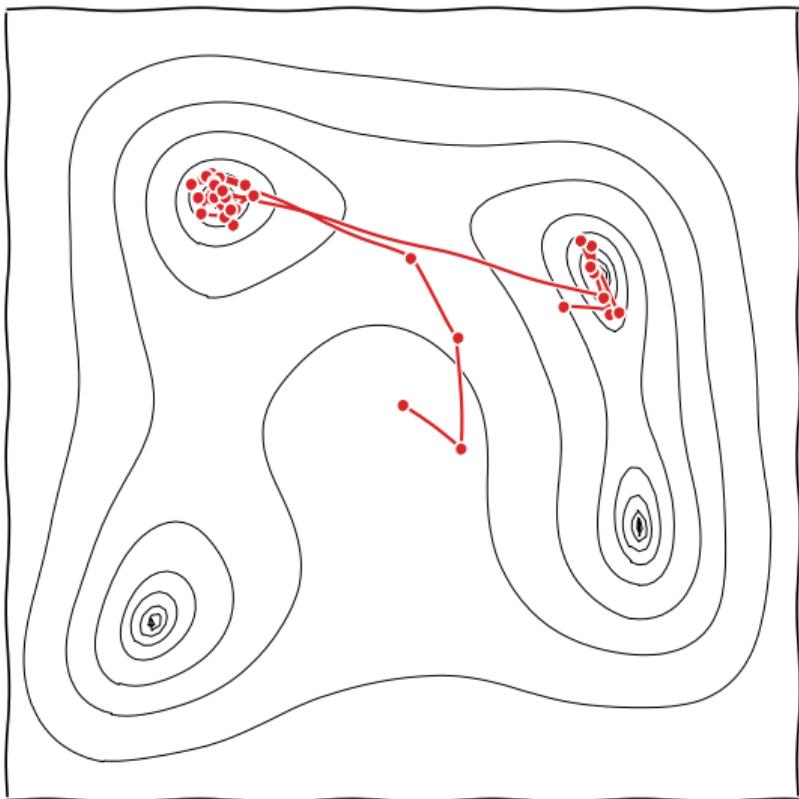
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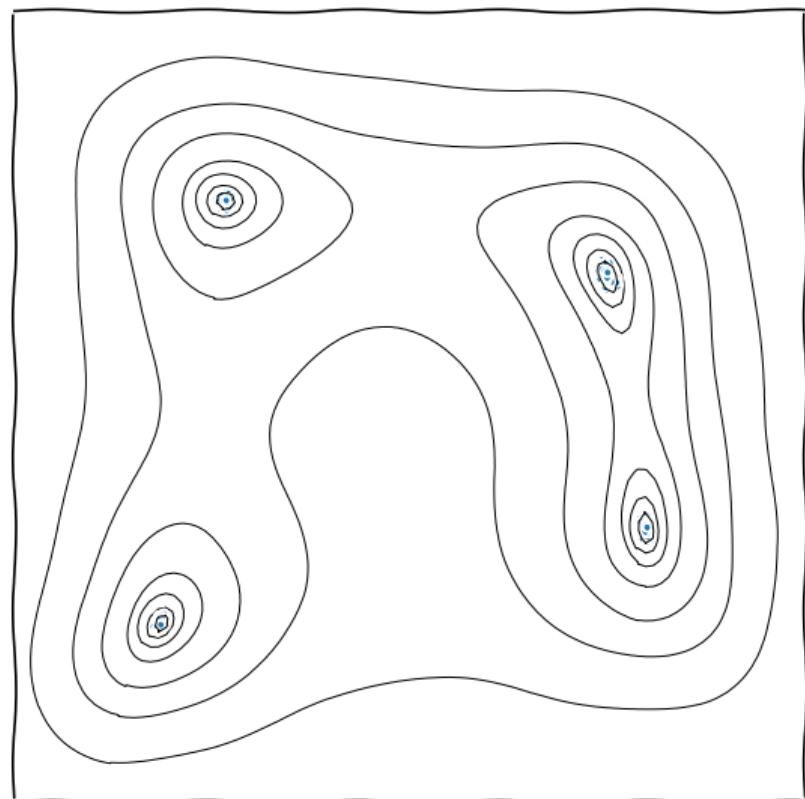
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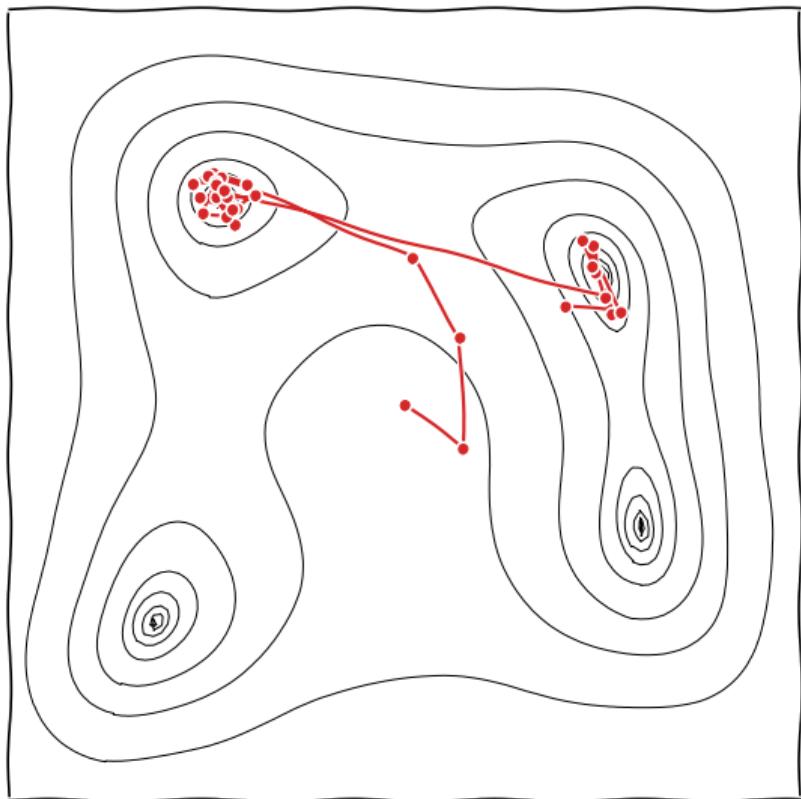
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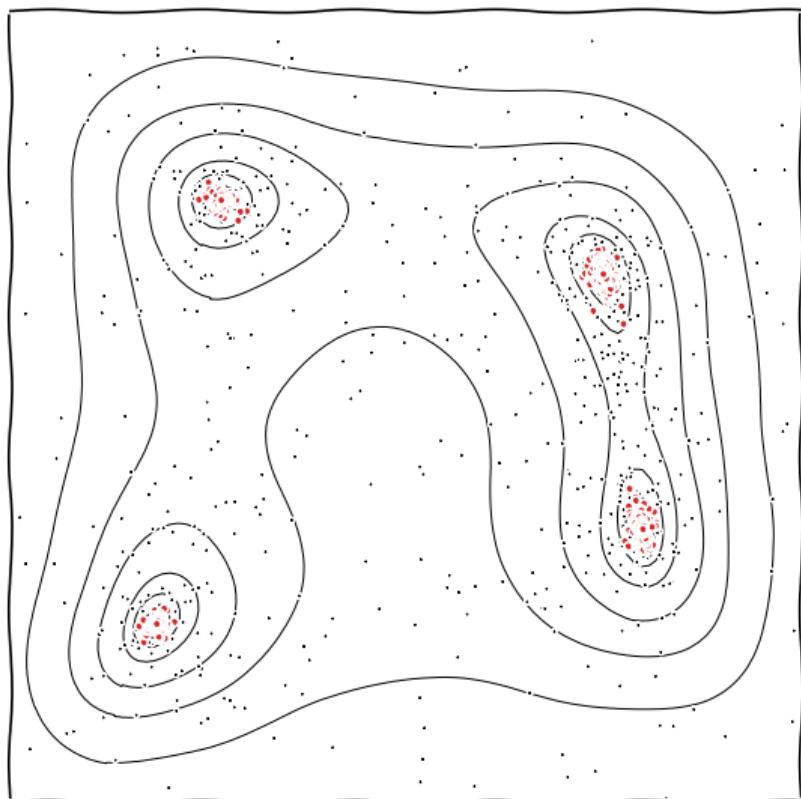
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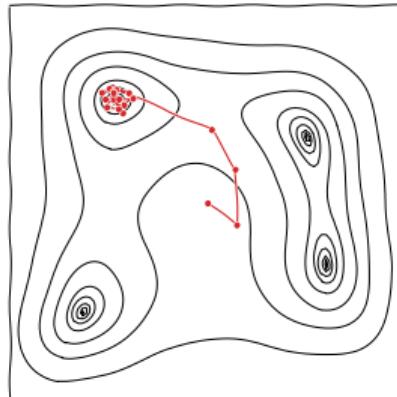


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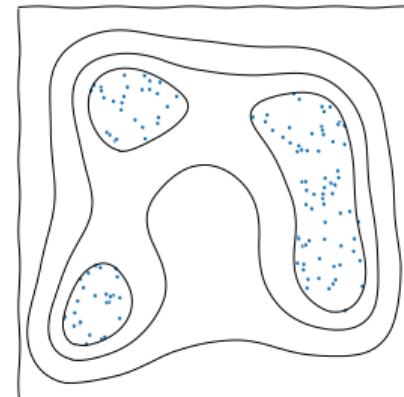
MCMC

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



Nested sampling

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



Nested sampling

- ▶ Sequentially update a set S of n samples:

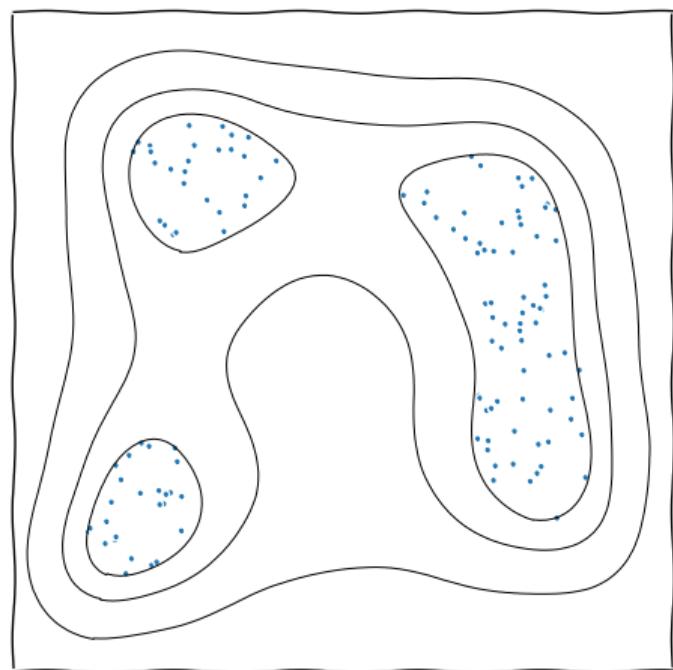
S_0 : Generate n samples uniformly over the space (from the prior π).

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.

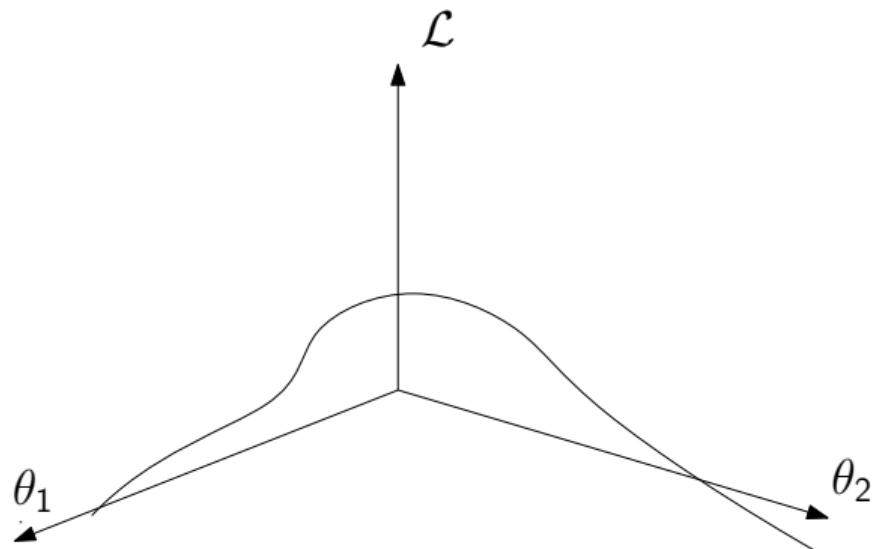


(Lesbesgue) Integrating with nested sampling

- ▶ 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
 $Z(\beta) = \sum_i \mathcal{L}_i^\beta \Delta X_i$.

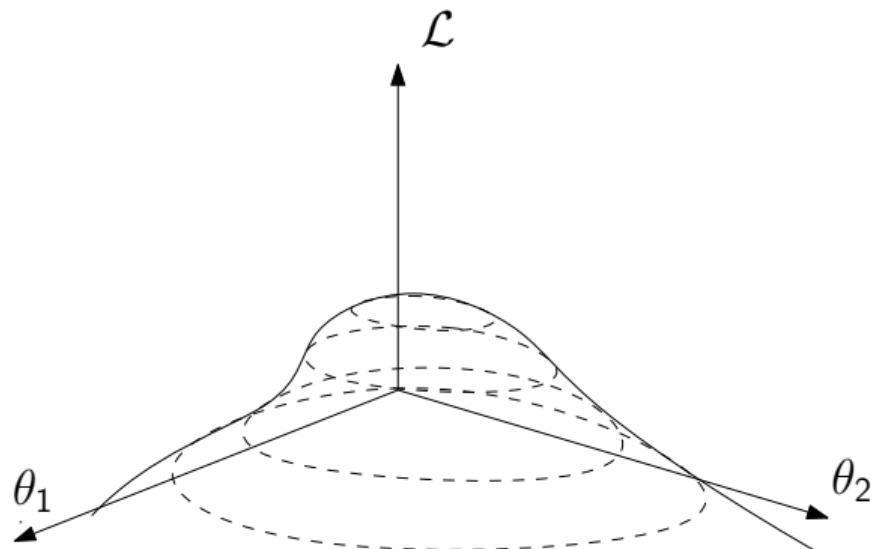


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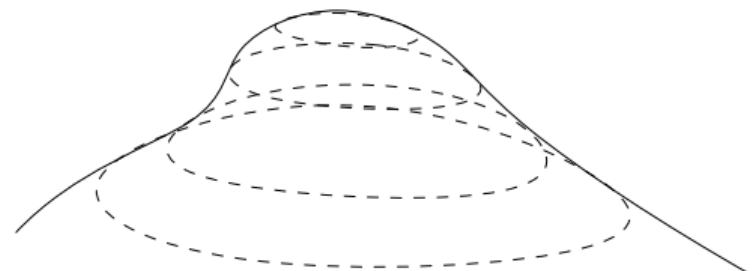


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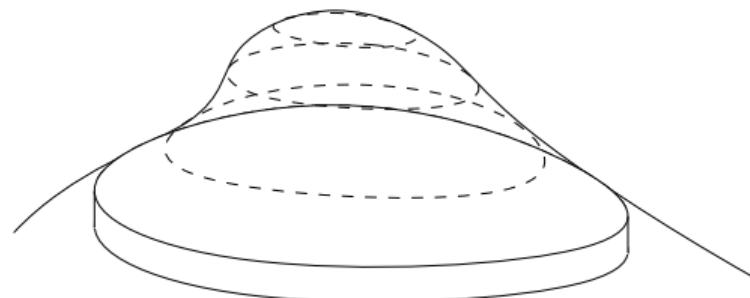


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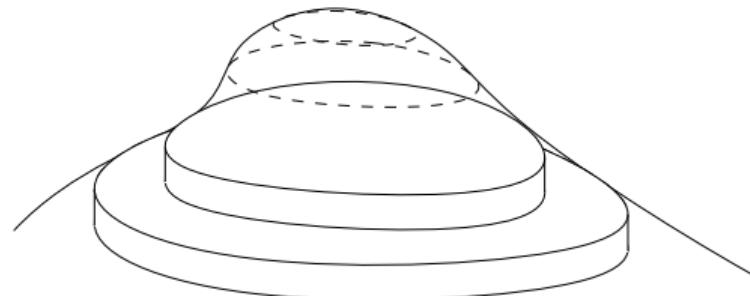


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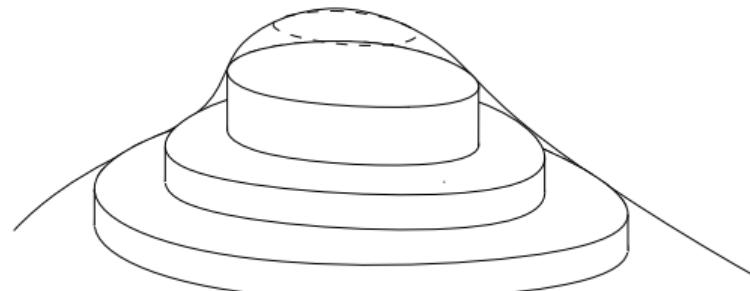


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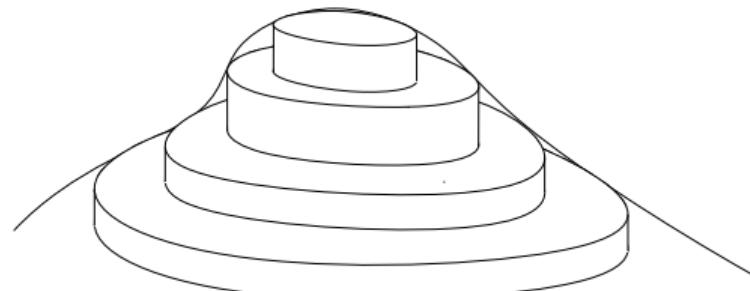


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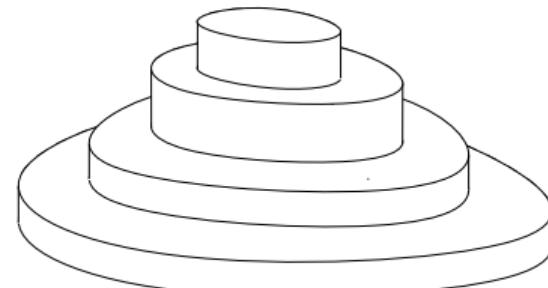


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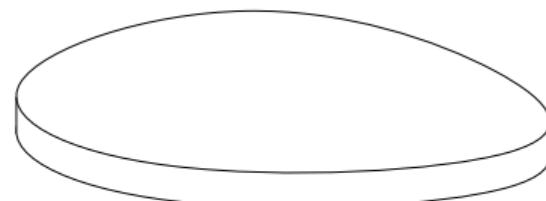


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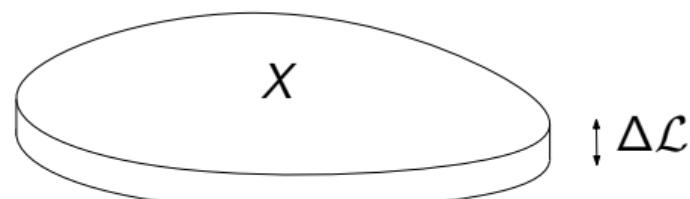


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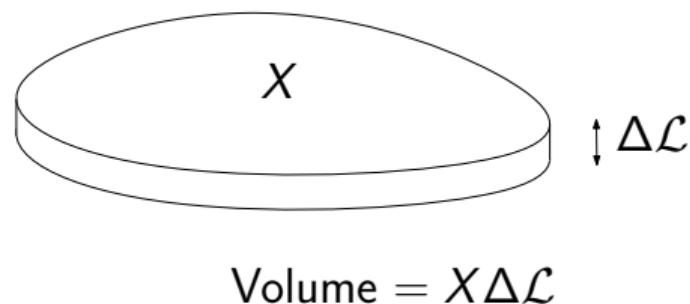


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- ▶ Estimates the density of states, and is therefore a partition function calculator
 $Z(\beta) = \sum_i \mathcal{L}_i^\beta \Delta X_i$.

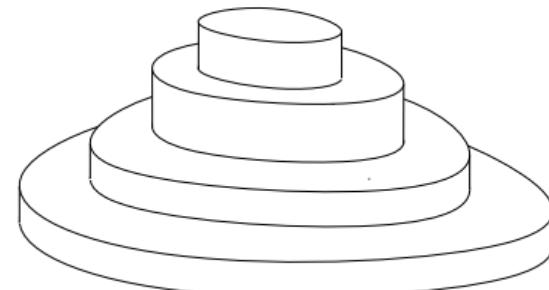


(Lesbesgue) Integrating with nested sampling

- ▶ 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.

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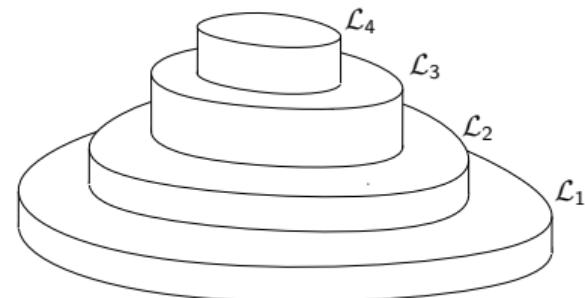


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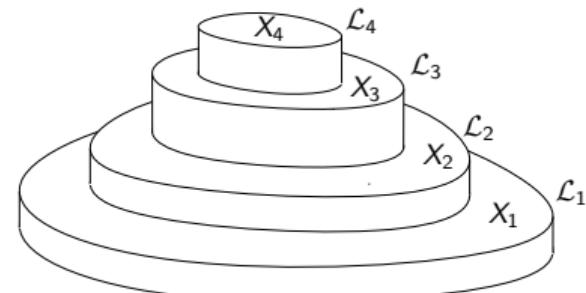


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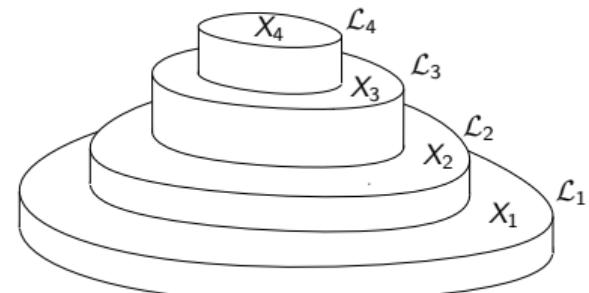
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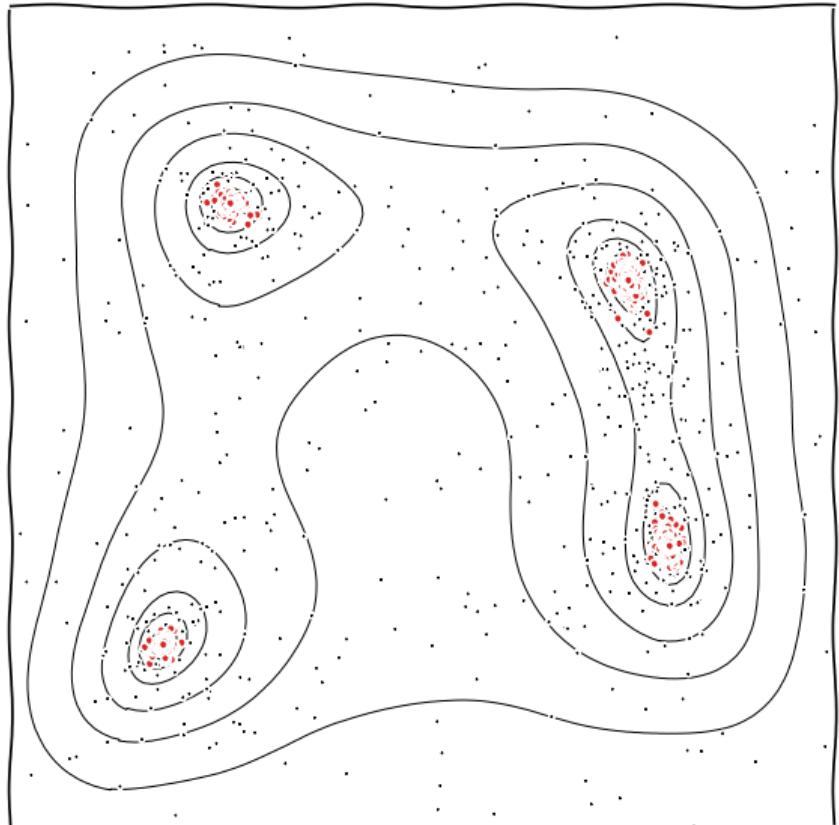


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Sampling from a hard likelihood constraint

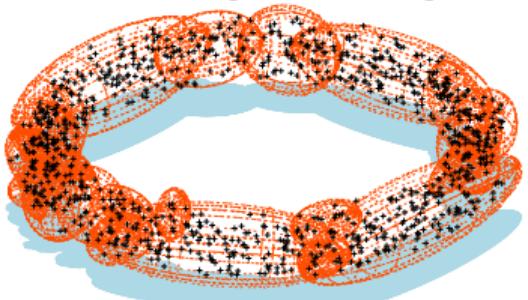
"It is not the purpose of this introductory paper to develop the technology of navigation within such a volume. We merely note that exploring a hard-edged likelihood-constrained domain should prove to be neither more nor less demanding than exploring a likelihood-weighted space."

— John Skilling

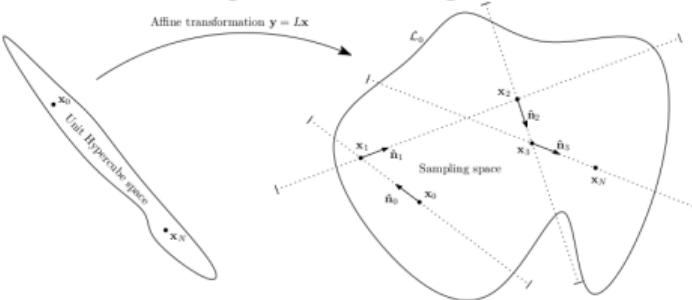
- ▶ A large fraction of the work in NS to date has been in attempting to implement a hard-edged sampler in the NS meta-algorithm $\{\theta \sim \pi : \mathcal{L}(\theta) > \mathcal{L}_*\}$.
- ▶ <https://projecteuclid.org/euclid.ba/1340370944>.
- ▶ There has also been much work beyond this (see "Frontiers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

Implementations of Nested Sampling [2205.15570](NatReview)

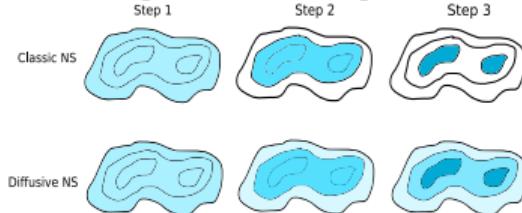
MultiNest [0809.3437]



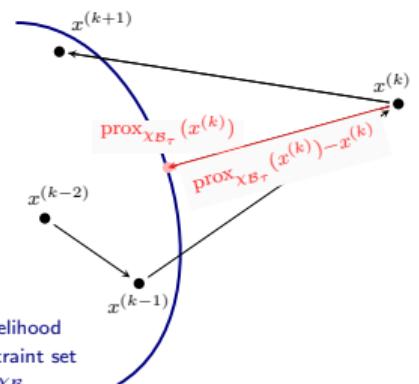
PolyChord [1506.00171]



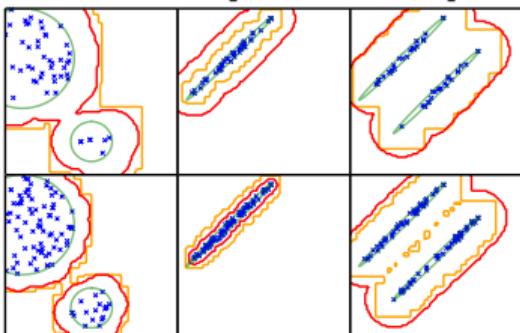
DNest [1606.03757]



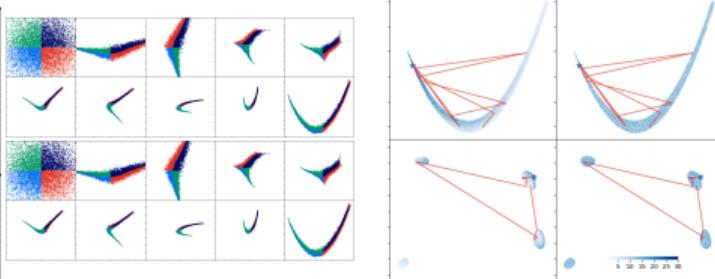
ProxNest [2106.03646]



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} .

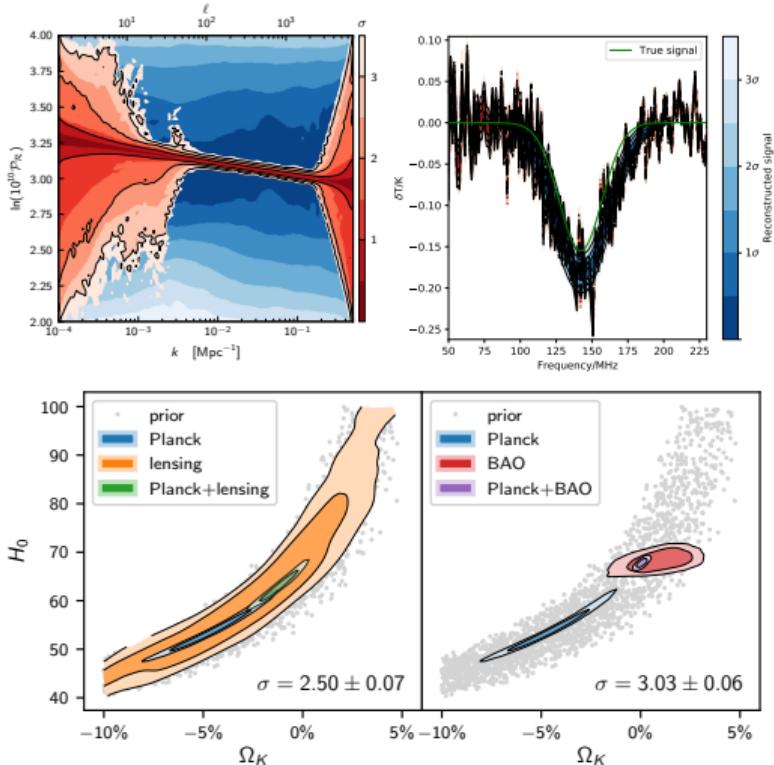
Chain-based samplers

- ▶ 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.

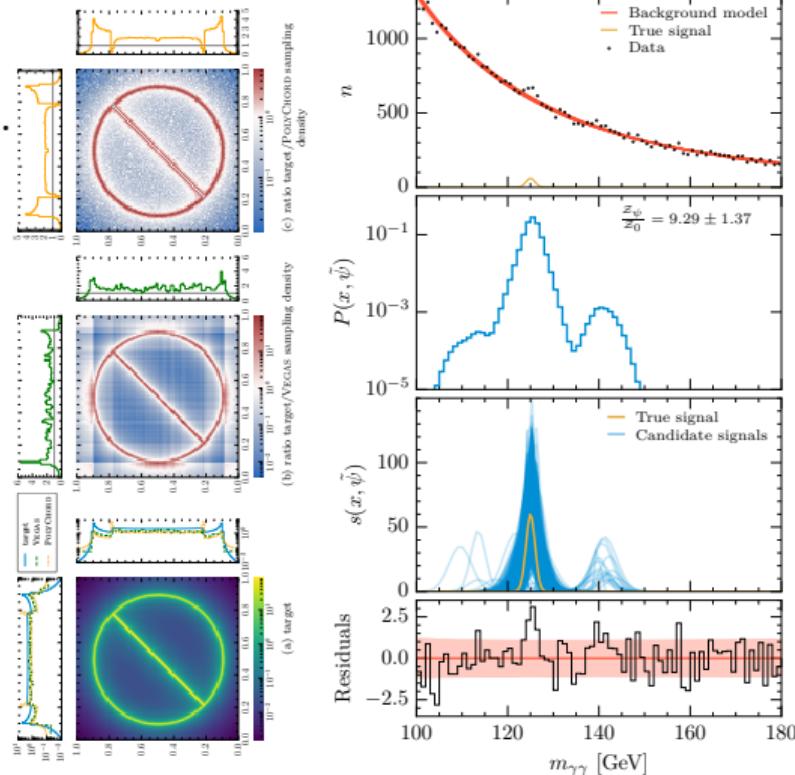


▪

Applications of nested sampling

Particle physics

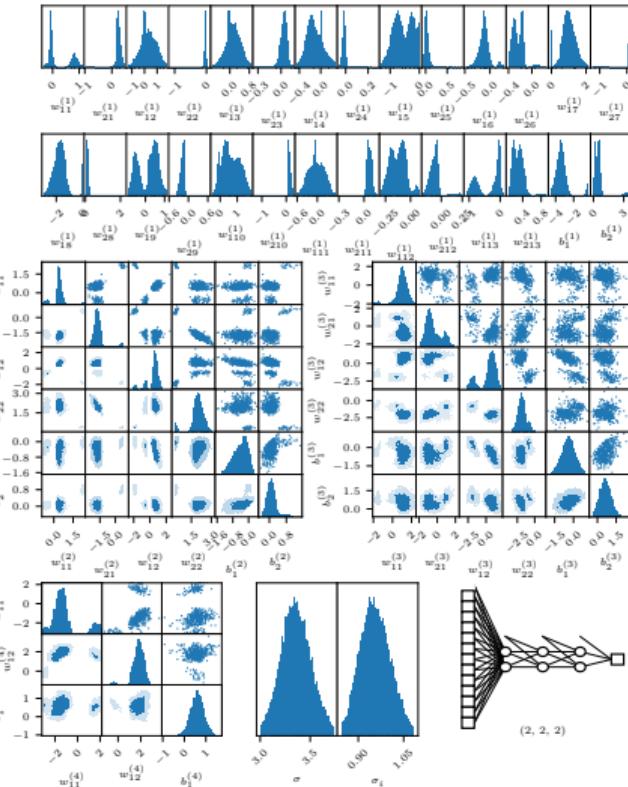
- ▶ Nested sampling for cross section computation/event generation $\sigma = \int_{\Omega} d\Phi |\mathcal{M}|^2$.
- ▶ Nested sampling can explore the phase space Ω and compute integral blind with comparable efficiency to HAAG/RAMBO [2205.02030].
- ▶ Bayesian sparse reconstruction [1809.04598] applied 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

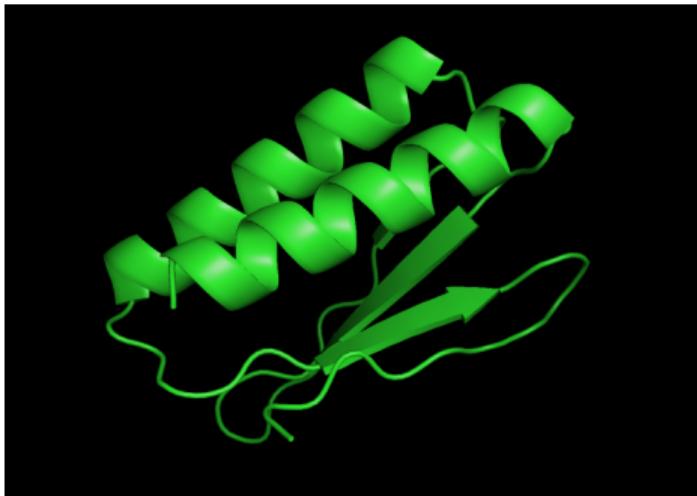
- ▶ Machine learning requires:
 - ▶ Training to find weights
 - ▶ Choice of architecture/topology/hyperparameters
- ▶ Bayesian NNs treat training as a model fitting problem
- ▶ Compute posterior of weights (parameter estimation), rather than optimisation (gradient descent)
- ▶ Use evidence to determine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

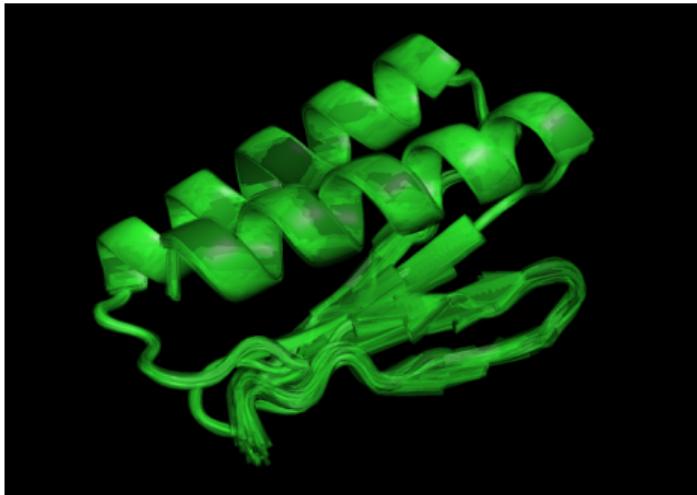
- ▶ Techniques have been spun-out (PolyChord Ltd) to:
- ▶ Protein folding
 - ▶ Navigating free energy surface.
 - ▶ Computing misfolds.
 - ▶ Thermal motion.
- ▶ Nuclear fusion reactor optimisation
 - ▶ multi-objective.
 - ▶ uncertainty propagation.
- ▶ Telecoms & DSTL research (MIDAS)
 - ▶ Optimising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



Applications of nested sampling

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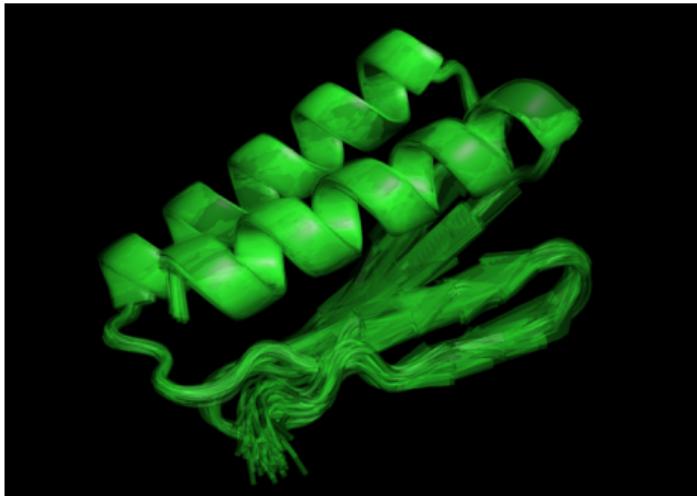
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How does Nested Sampling compare to other approaches?

- ▶ 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

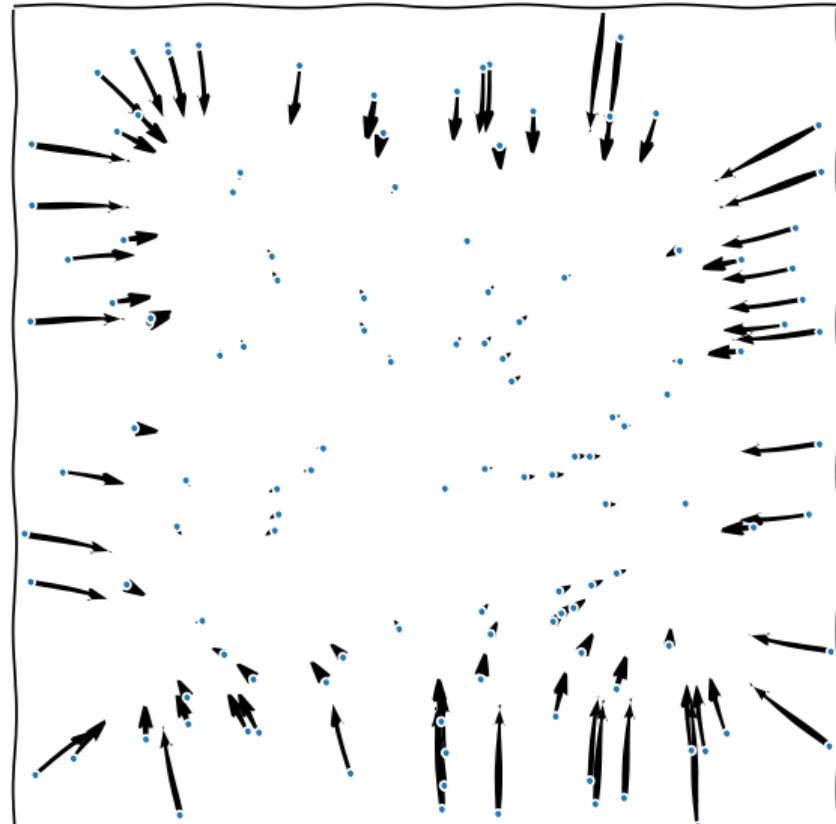
- ▶ Ensemble sampler
- ▶ Estimates volumes, entropies and evidences
- ▶ Athermal evolution
- ▶ Order statistics

Gradients in nested sampling

- The challenge: Sample uniformly within likelihood contour:

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

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

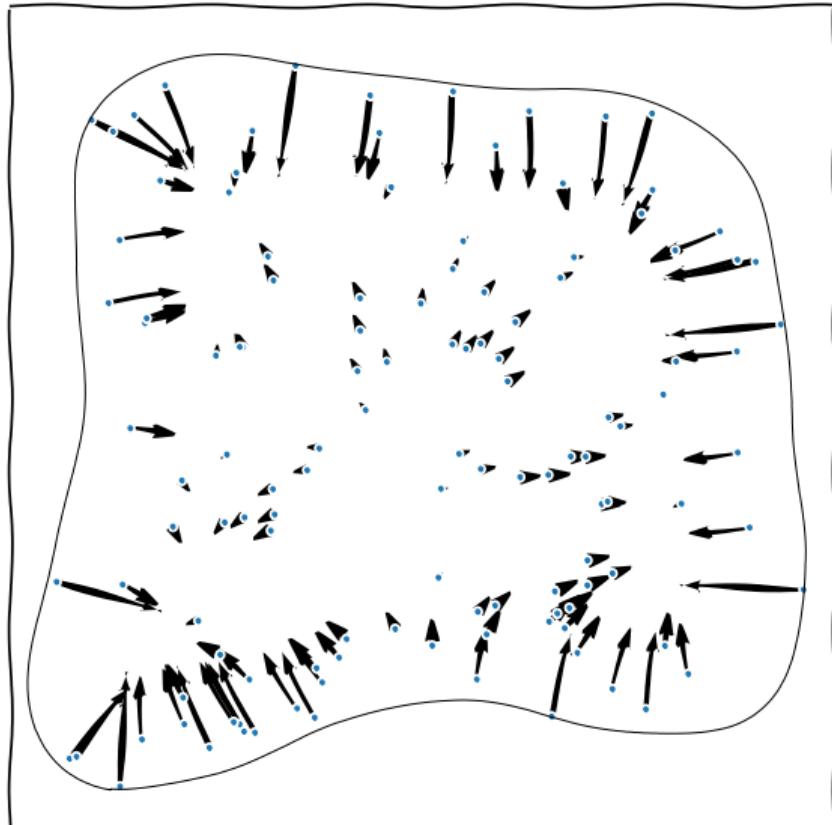


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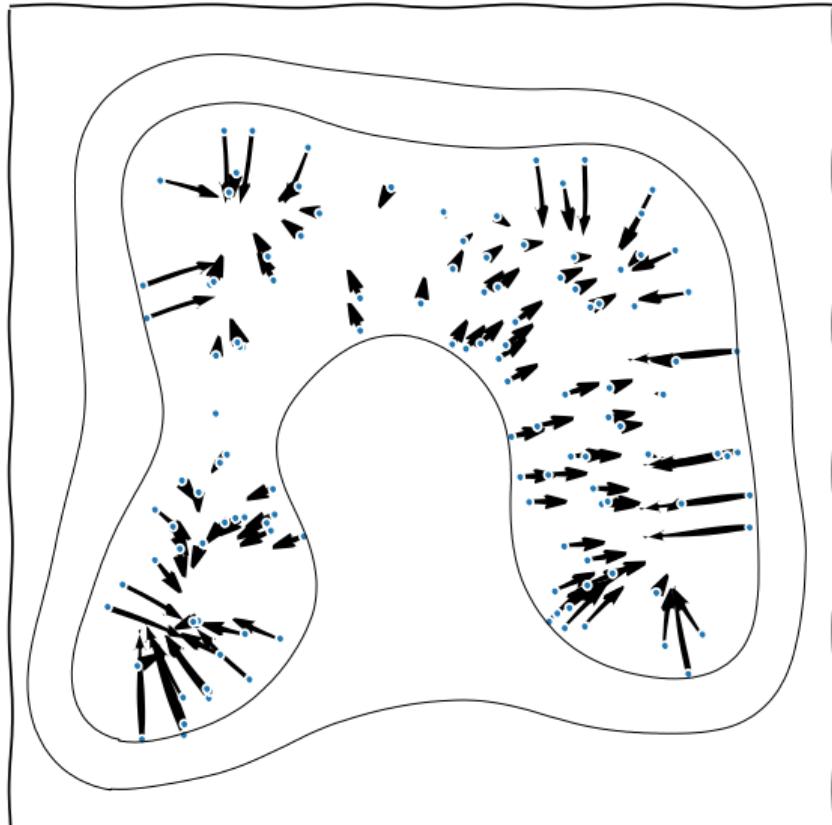


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Why doesn't HMC work?

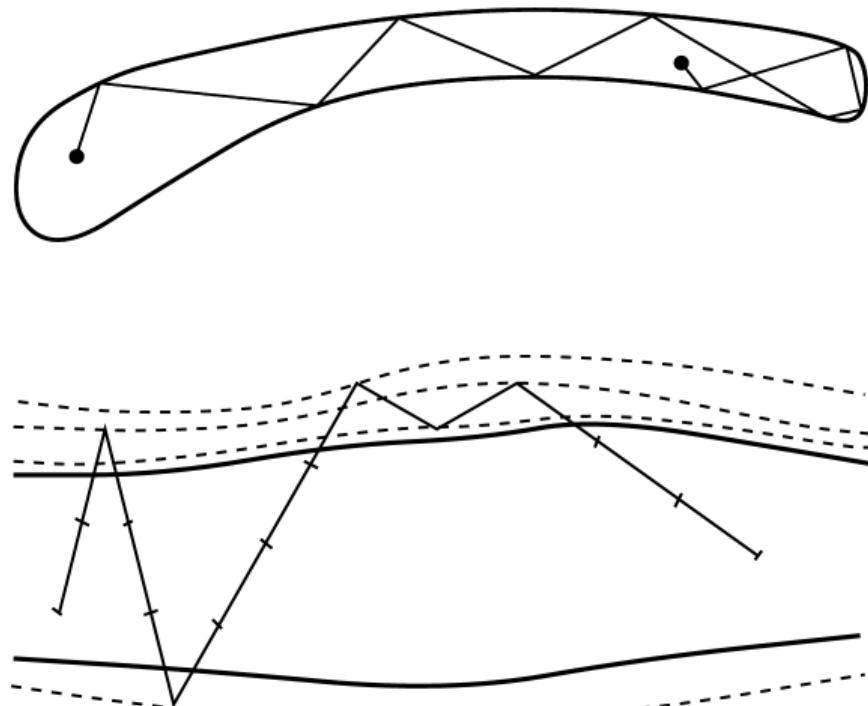
“Tabletop” distributions are difficult to sample!

- ▶ 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

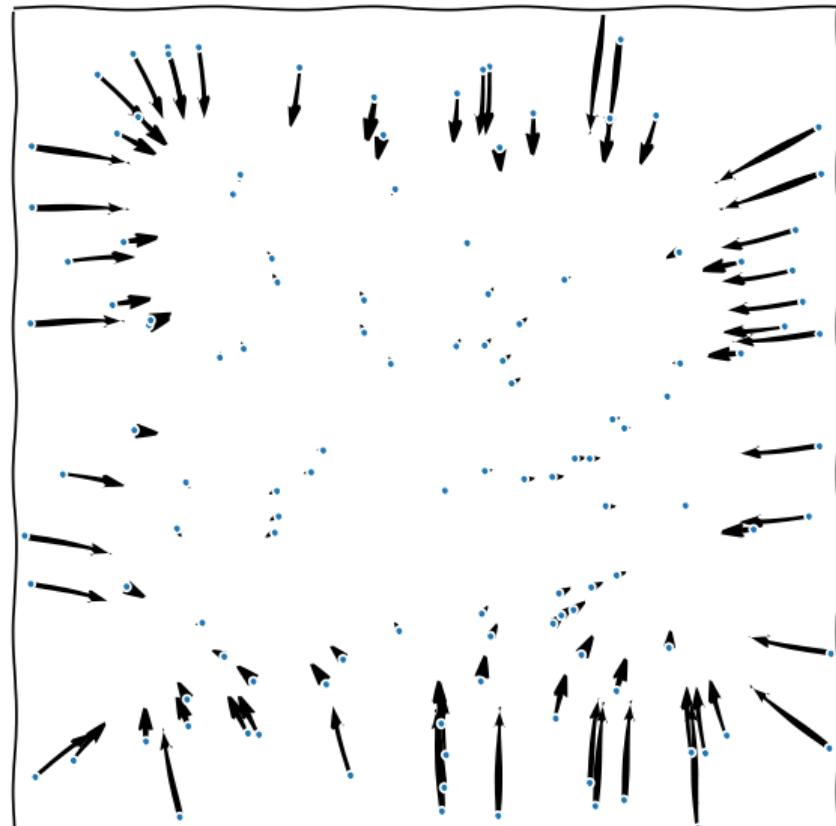
Stephen Thorpe Curved slice sampling.

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} .

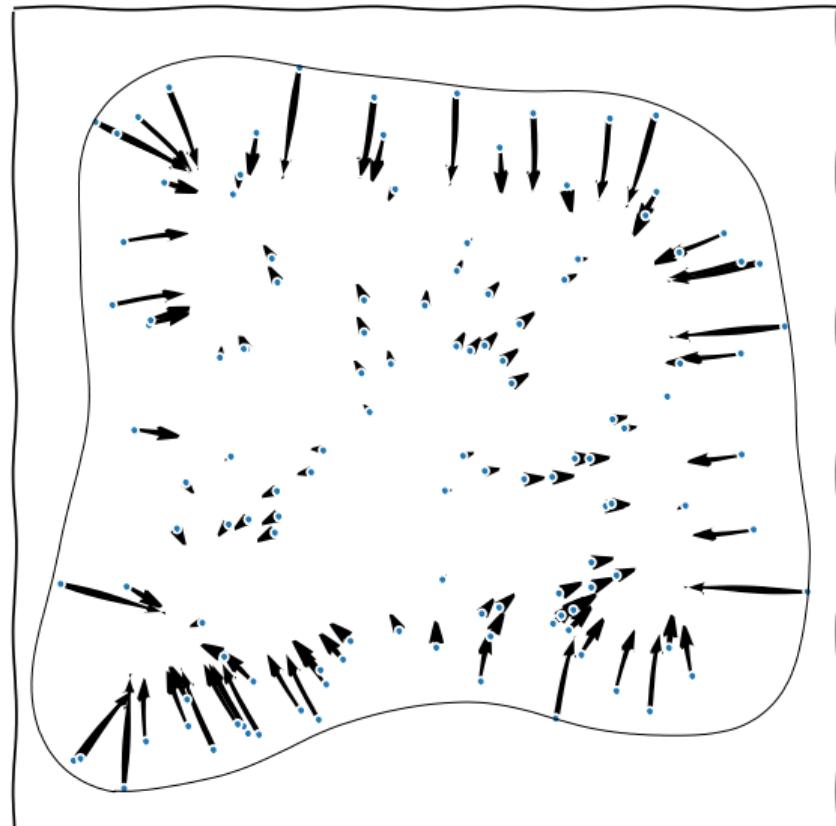
Nested sampling with gradients

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



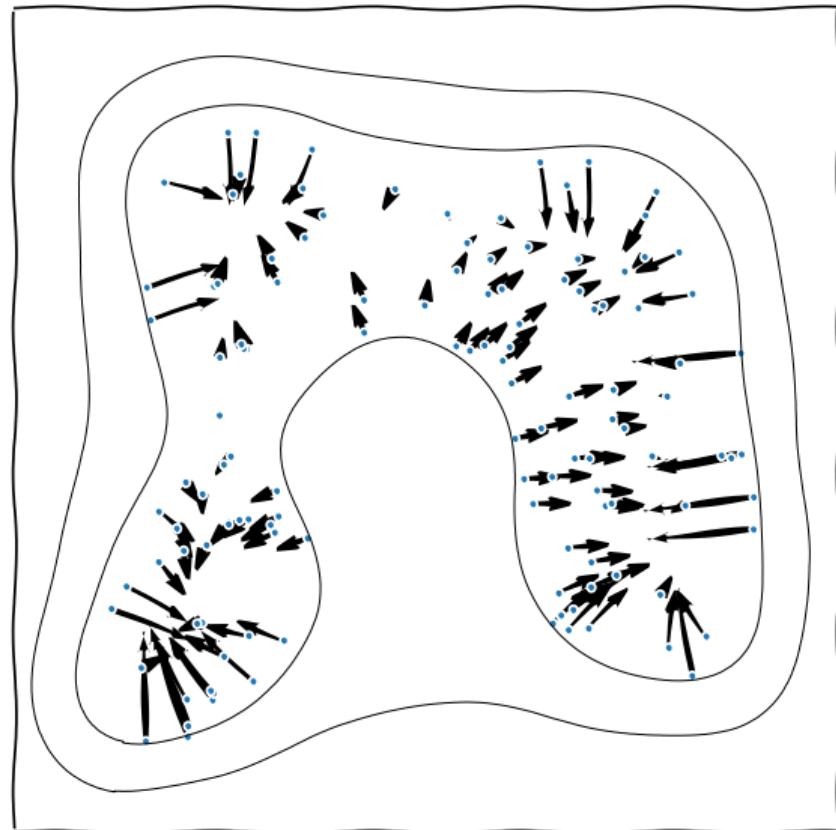
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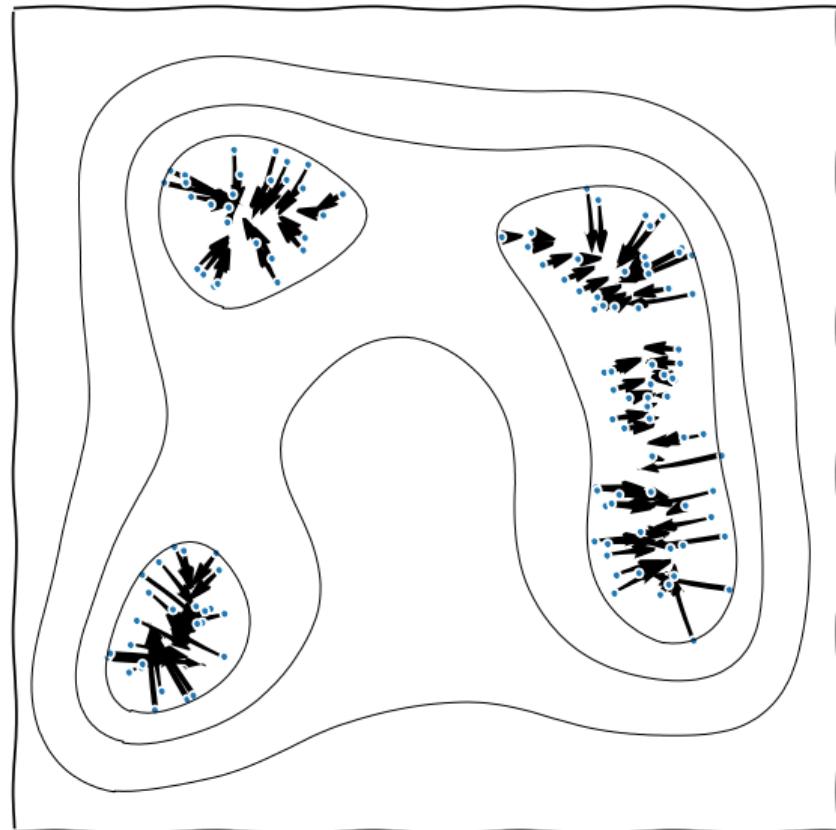
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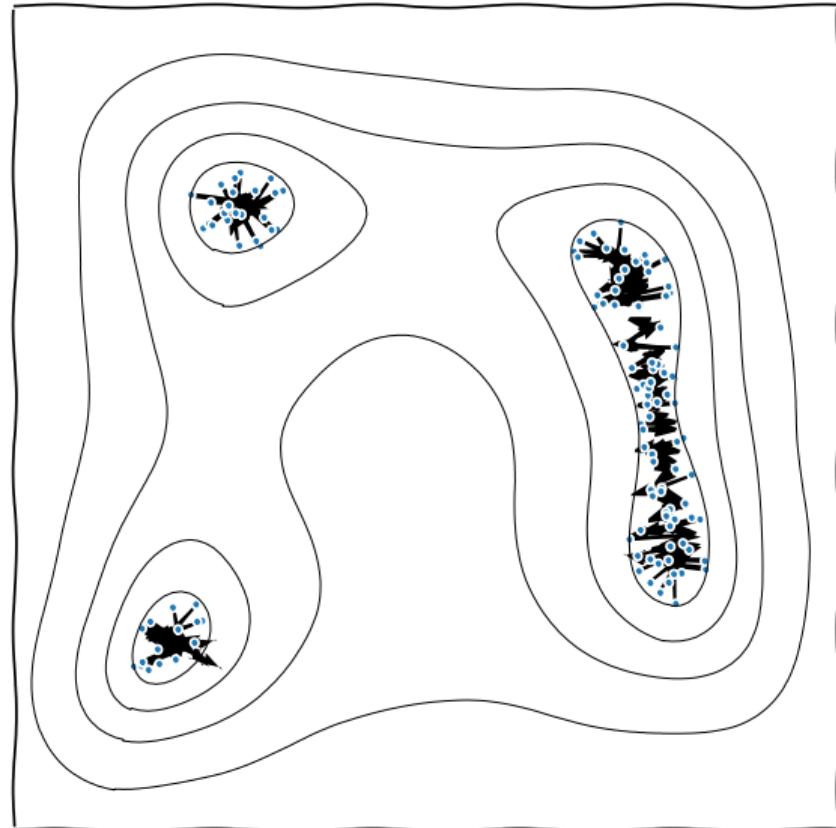
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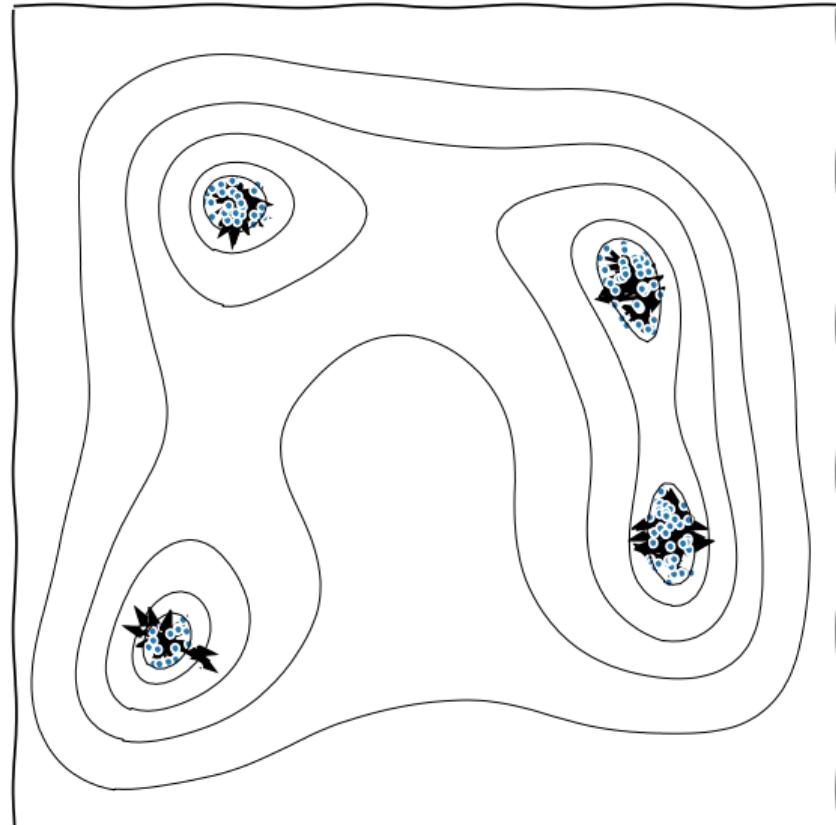
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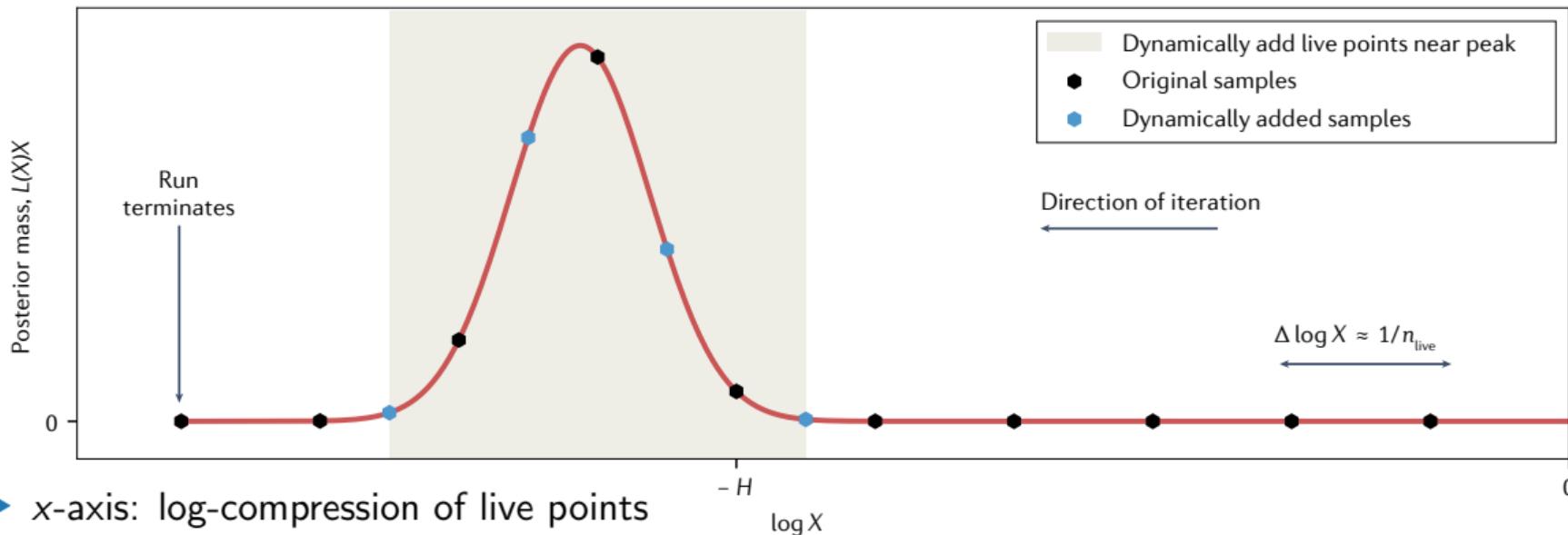
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Conclusions

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