Gradients and Nested Sampling

The present state of the art

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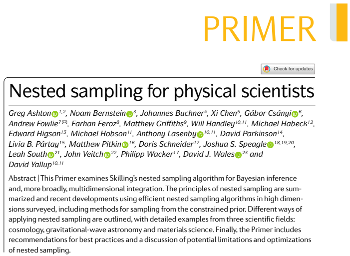
Highlight: state-of-the-art Nature review primer [2205.15570]

- 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?



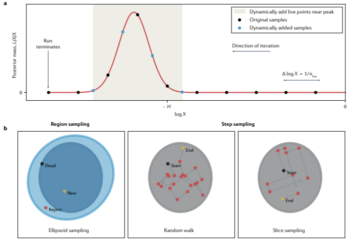
PRIMER

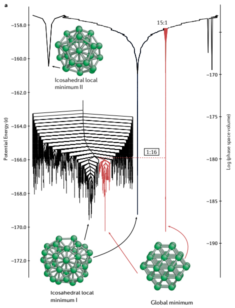
Check for updates

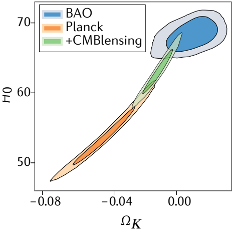
Nested sampling for physical scientists

Greg Ashton[1,2], Noam Bernstein[3], Johannes Buchner[4], Xi Chen[5], Gábor Csányi[6], Andrew Fowlie[7], Farhan Feroz[8], Matthew Griffiths[9], Will Handley[10,11], Michael Habeck[12], Edward Higson[13], Michael Hobson[11], Anthony Lasenby[10,11], David Parkinson[14], Livia B. Pártay[15], Matthew Pitkin[16], Doris Schneider[17], Joshua S. Speagle[18,19,20], Leah South[21], John Veitch[22], Philipp Wacker[17], David J. Wales[23] and David Yallup[10,11]

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.



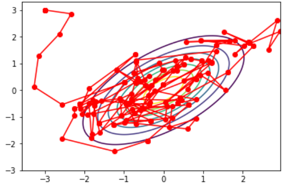


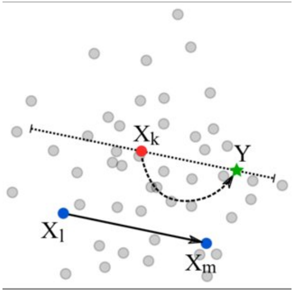


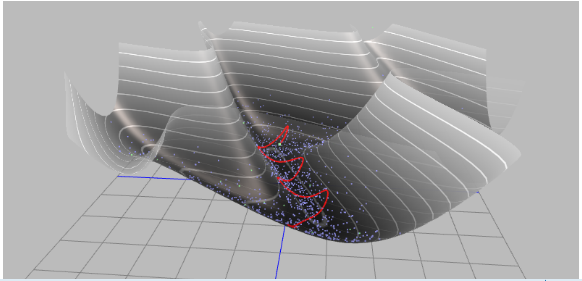
Where is Nested Sampling?

- 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

emcee
the mcmc hammer





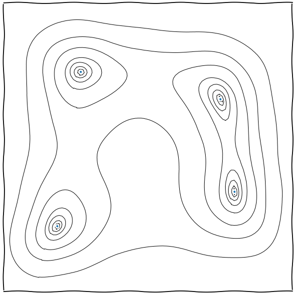


What is Nested Sampling?

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

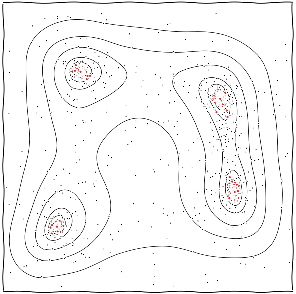
Optimisation

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



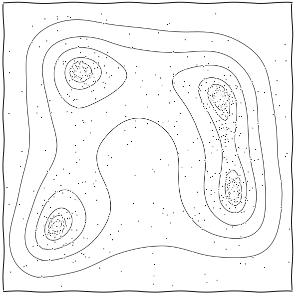
Exploration

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



Integration

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



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

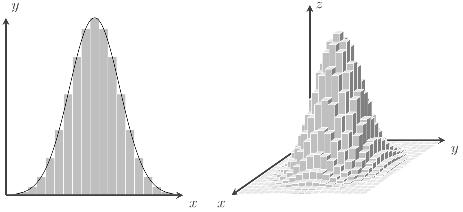
$$\Psi = \int e^{iS} \mathcal{D}x$$

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:

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



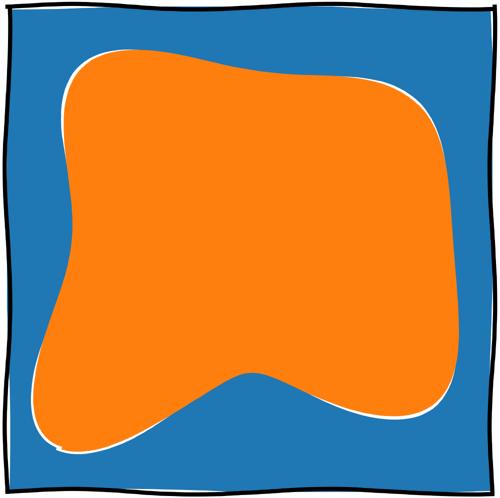
- Curse of dimensionality $\Rightarrow$ exponential scaling.
- Nested sampling integrates **probabilistically**.

Probabalistic volume estimation

- Key idea in NS: estimating volumes probabilistically

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

- 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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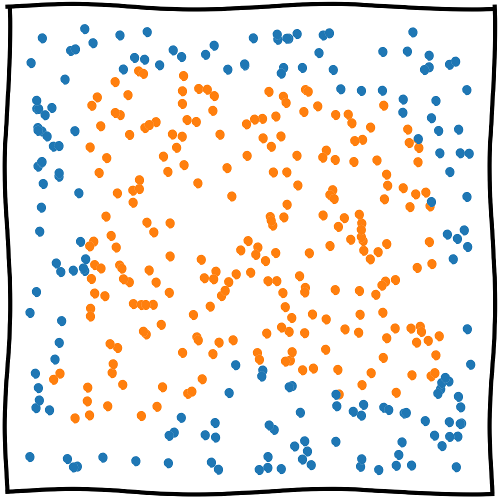

Probabalistic volume estimation

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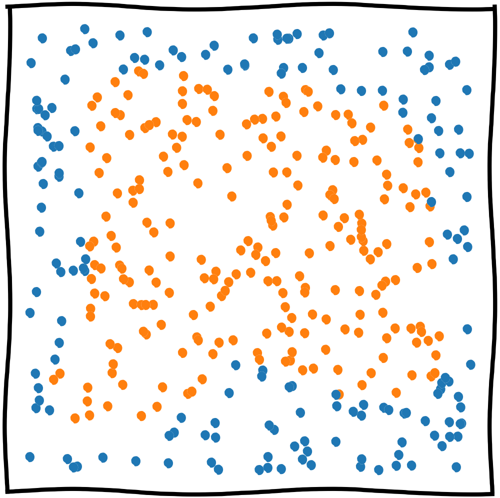

Probabalistic volume estimation

- Key idea in NS: estimating volumes probabilistically

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

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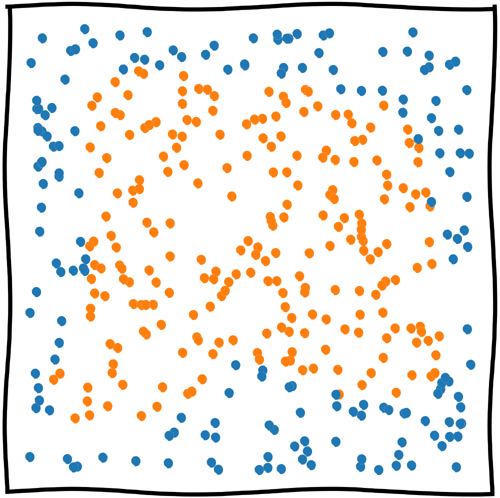
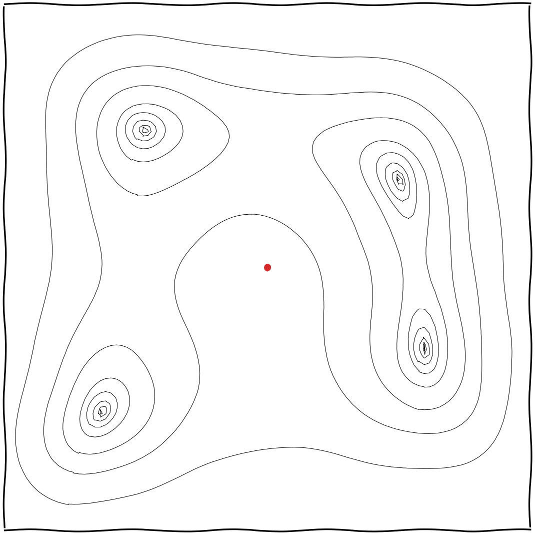


MCMC



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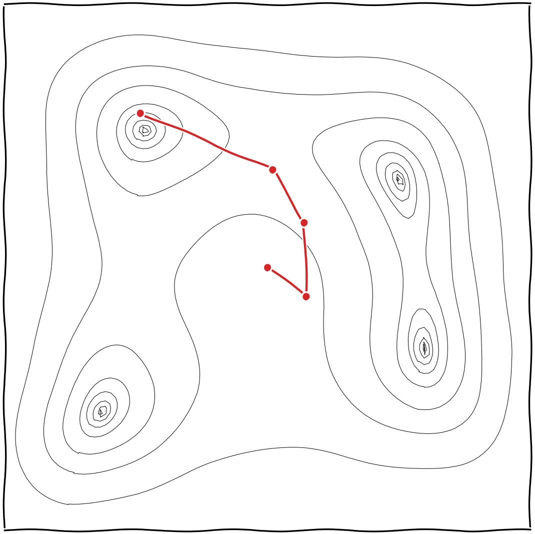

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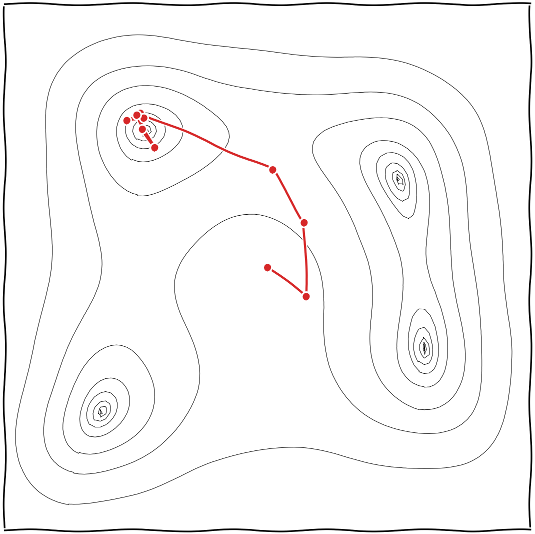

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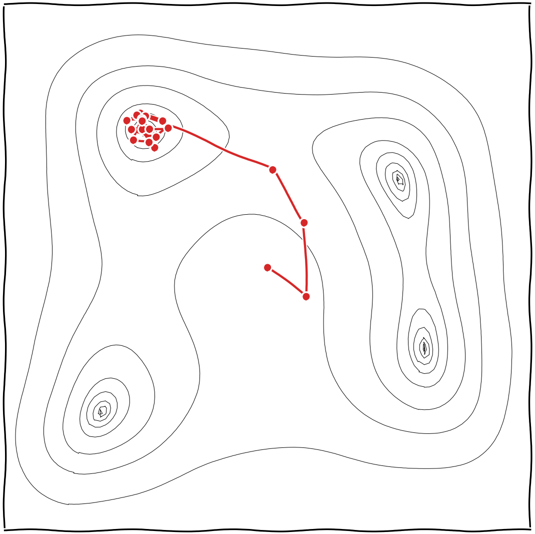

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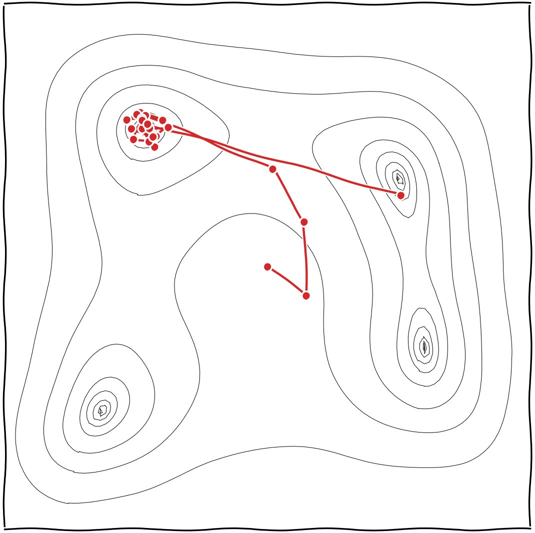

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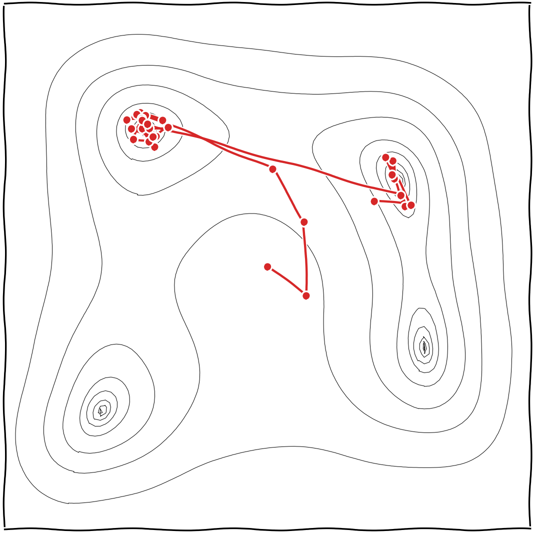

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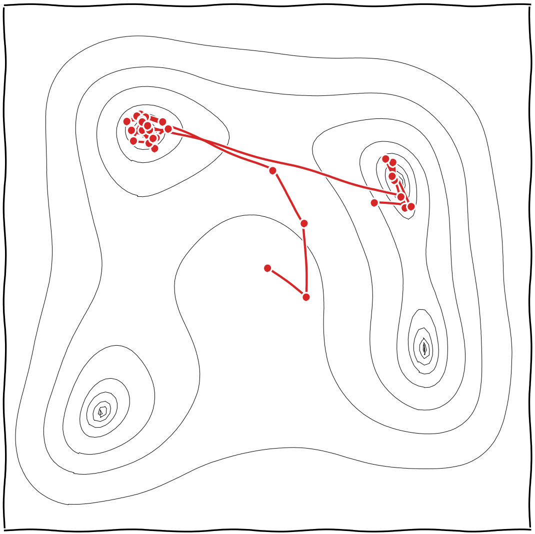
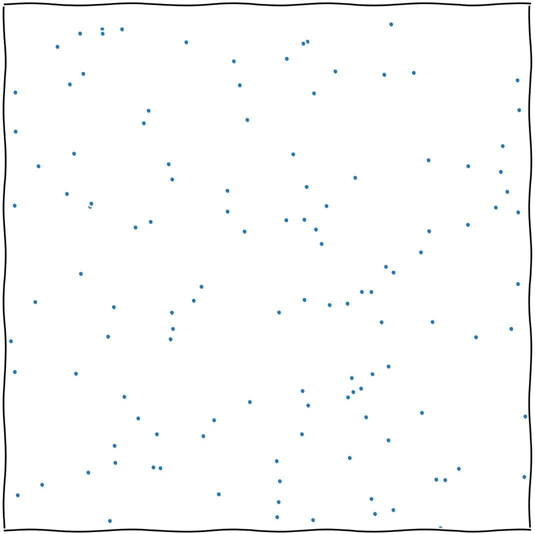


Nested sampling



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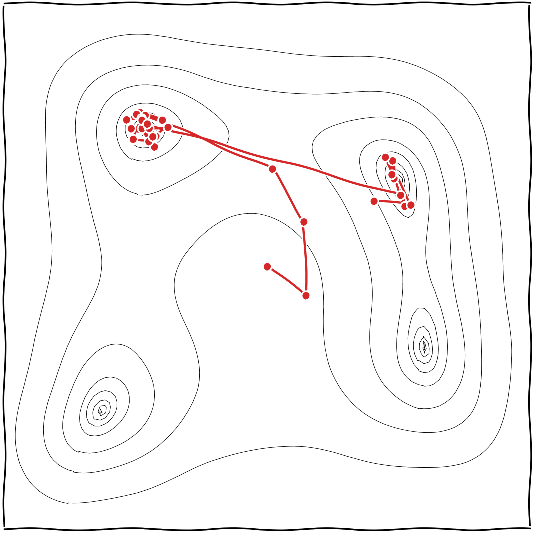

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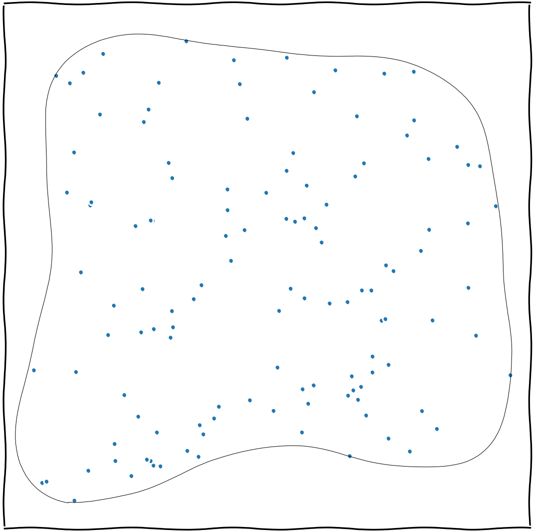

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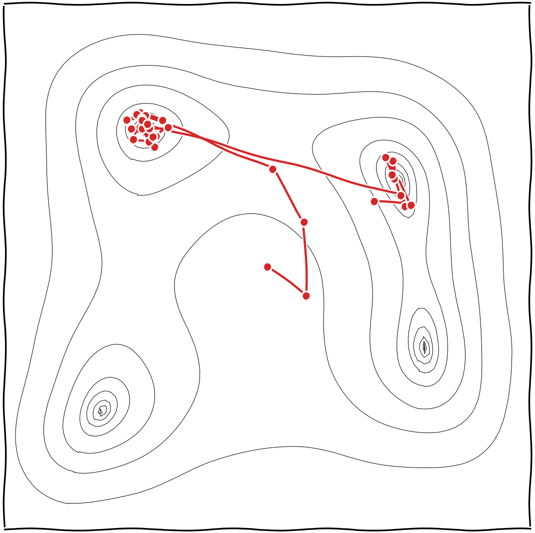

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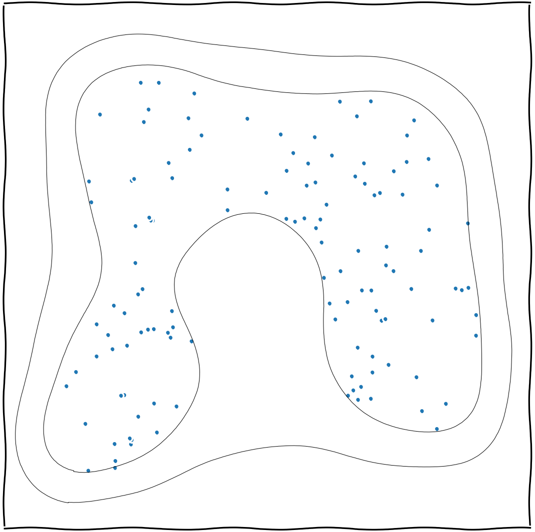

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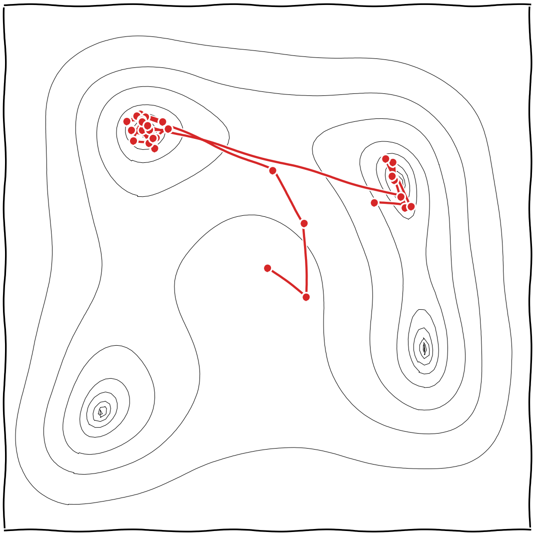

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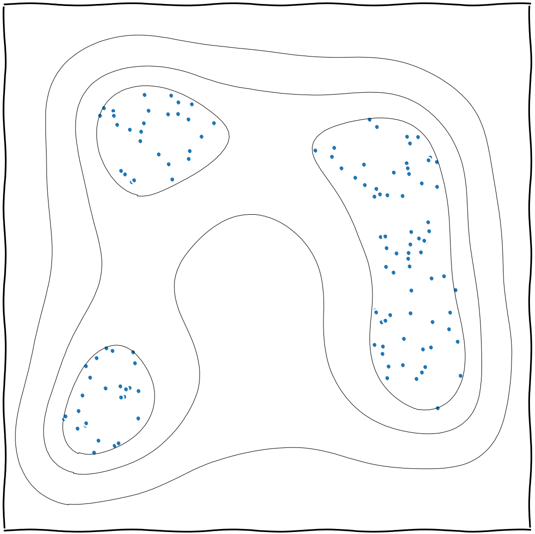

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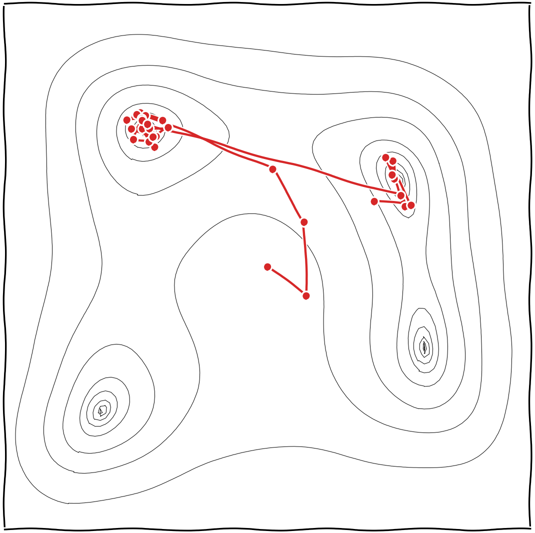

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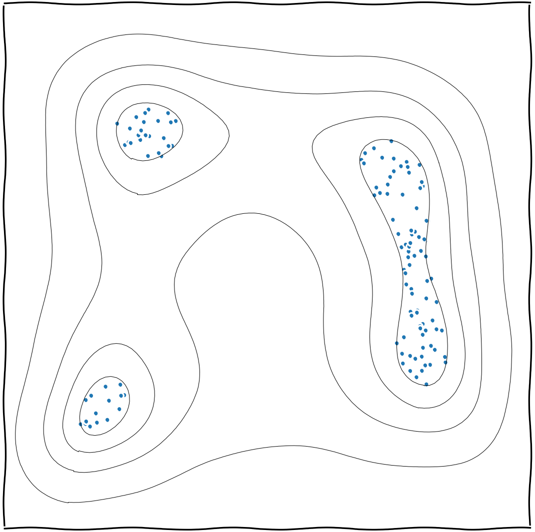

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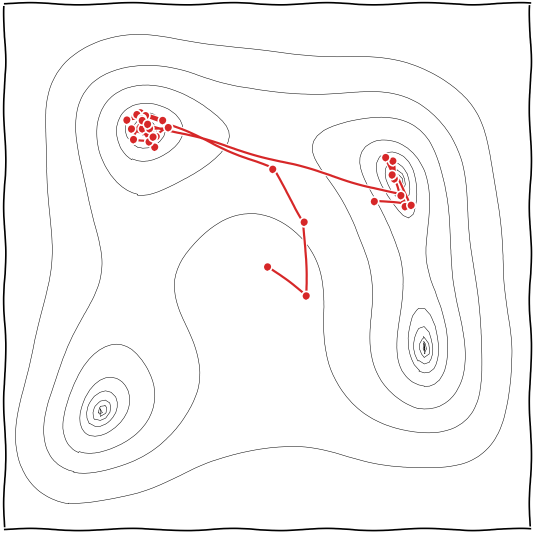

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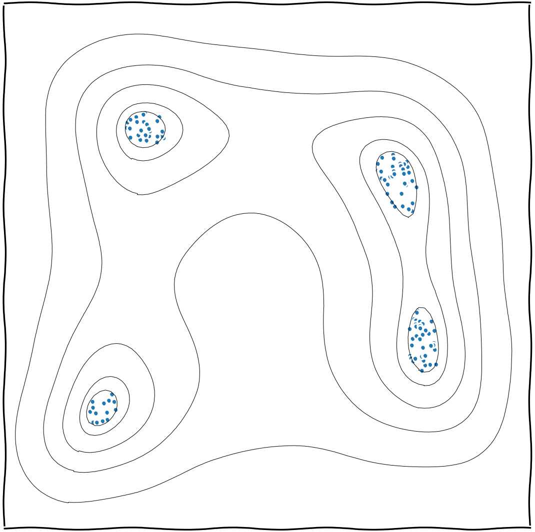

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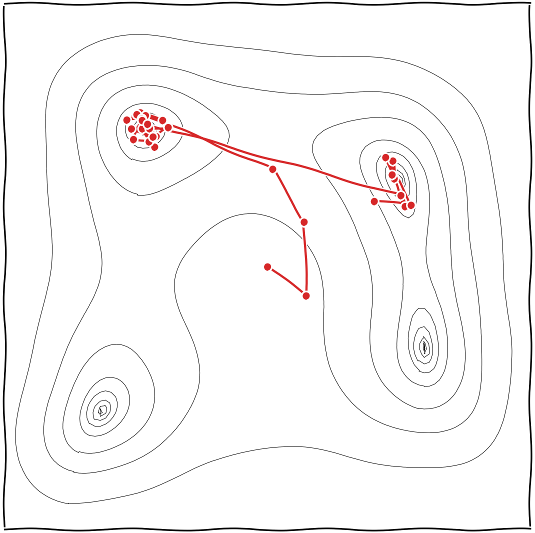

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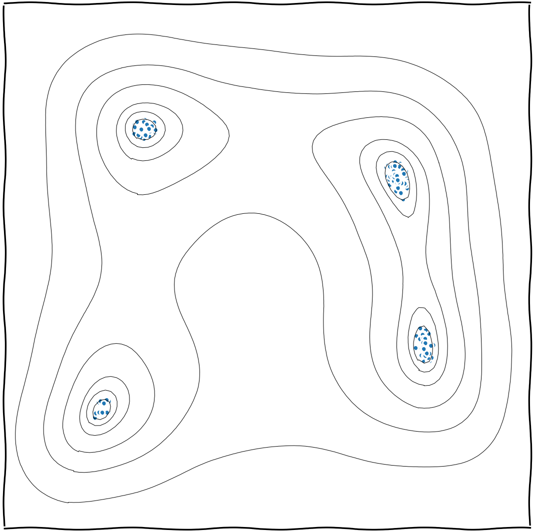

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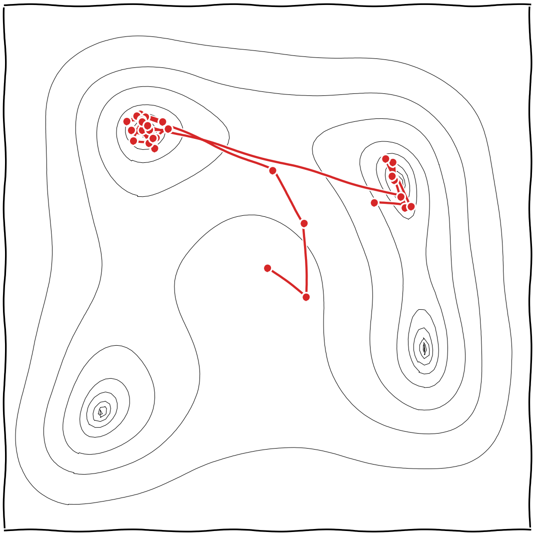

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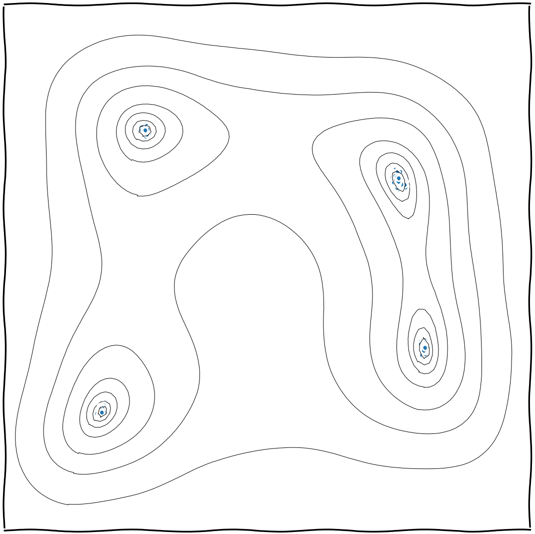

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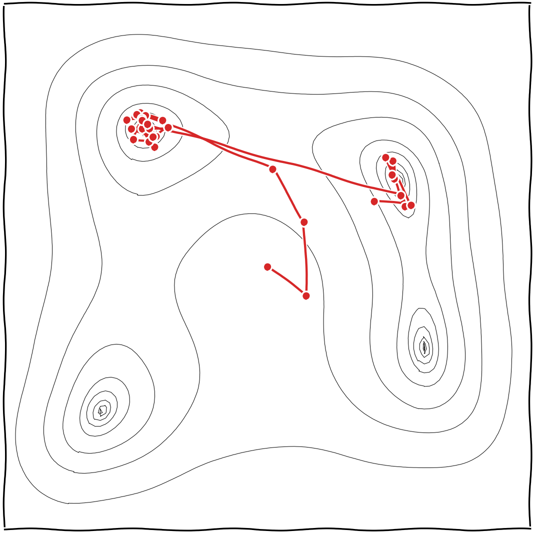

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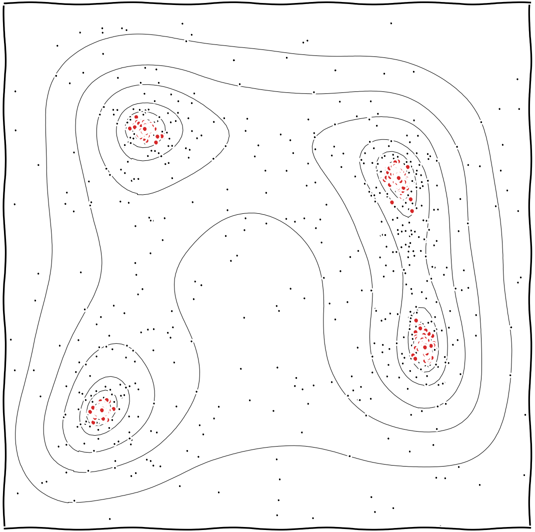
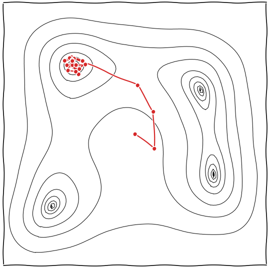


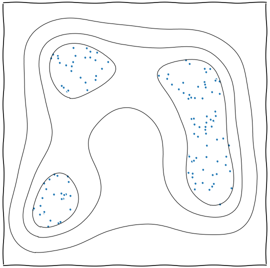
MCMC

- 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:

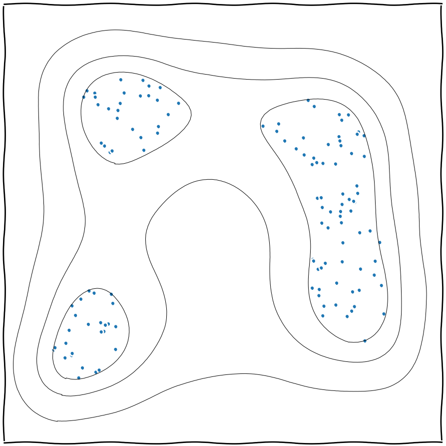
  S_0: Generate n samples uniformly over the space (from the prior π).

  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*:

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

- 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.



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

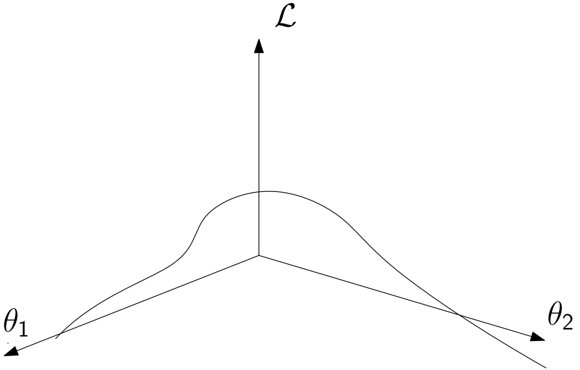
$$\mathcal{Z} \approx \sum_i \Delta\mathcal{L}_i X_i, \quad X_{i+1} \approx \frac{n}{n+1} X_i, \quad X_0 = 1.$$

- Although this is only approximate, we can quantify the error

$$P(X_i|X_{i-1}) = \frac{X_i^{n-1}}{nX_{i-1}^n} \times [0 < X_i < X_{i-1}].$$

- Integral can be discretised in several ways

$$\mathcal{Z} \approx \sum_i \Delta\mathcal{L}_i X_i = \sum_i \mathcal{L}_i \Delta X_i = \sum_i \tfrac{\mathcal{L}_i + \mathcal{L}_{i-1}}{2}(X_{i-1} - X_i).$$



(Lesbesgue) Integrating with nested sampling

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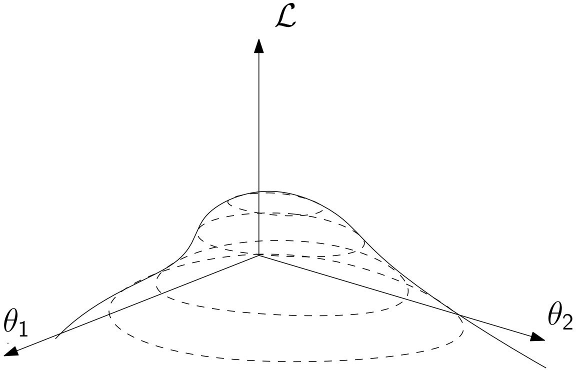

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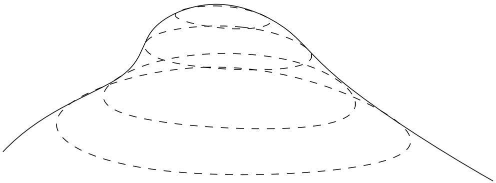

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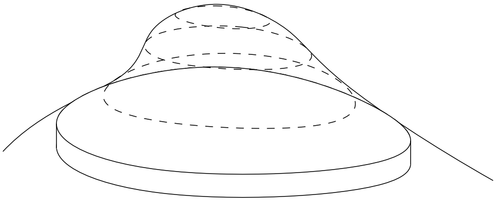

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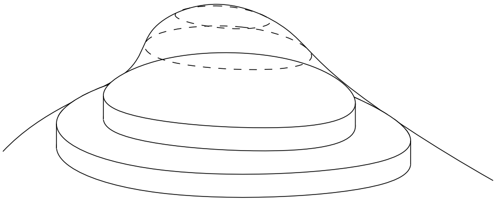

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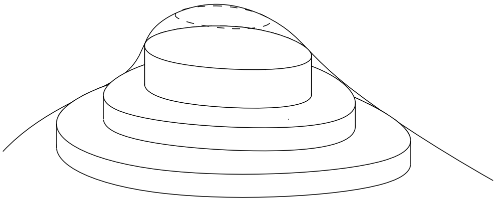

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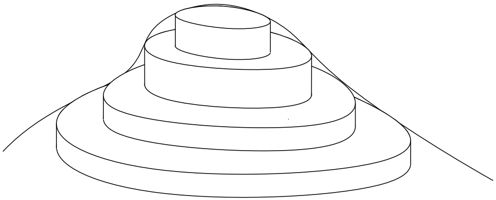

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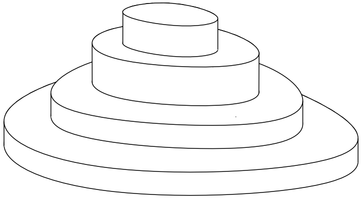

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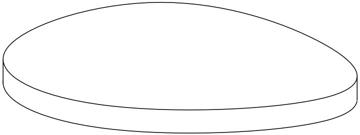

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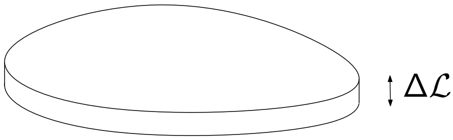

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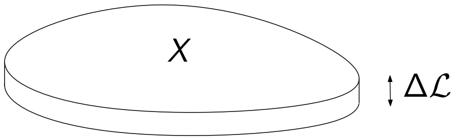

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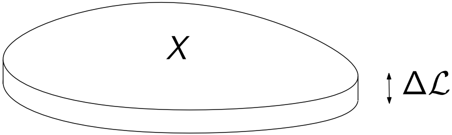

Volume $= X\Delta\mathcal{L}$

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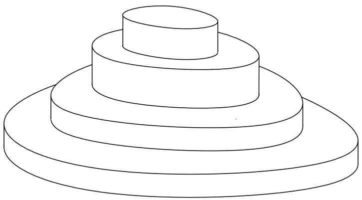

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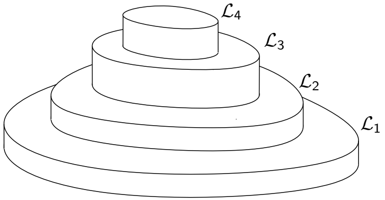

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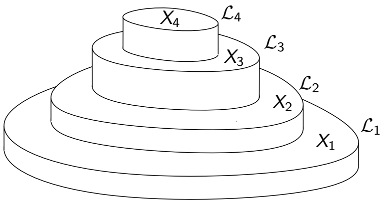

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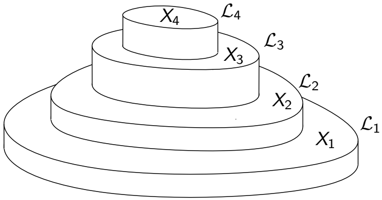
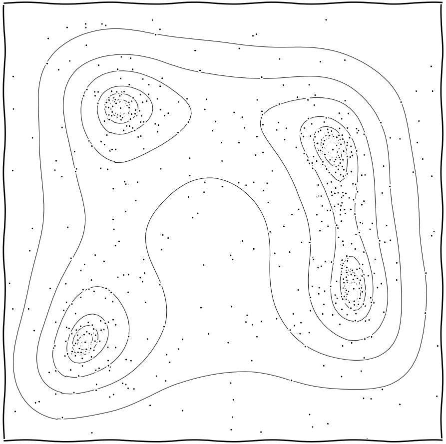


Dead points: posteriors & evidences

- At the end, one is left with a set of discarded points.
- These may be weighted to form weighted posterior samples using $w_i = \mathcal{L}_i \Delta X_i$.
- They can also be used to calculate the integral $\mathcal{Z} = \sum \mathcal{L}_i \Delta X_i$, or more generally $\sum_i f(\mathcal{L}_i) \Delta X_i$.
  - Nested sampling probabilistically estimates the volume of the parameter space

$$X_i \approx \left(\frac{n}{n+1}\right) X_{i-1} \quad \Rightarrow \quad X_i \approx \left(\frac{n}{n+1}\right)^i \approx e^{-i/n},$$

  - Nested sampling thus estimates the density of states,
  - it is therefore a partition function calculator $Z(\beta) = \sum_i \mathcal{L}_i^\beta \Delta X_i$.
- The evolving ensemble of live points allows algorithms to perform self-tuning and mode clustering.



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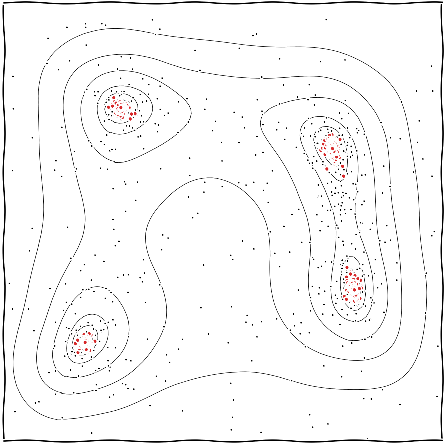
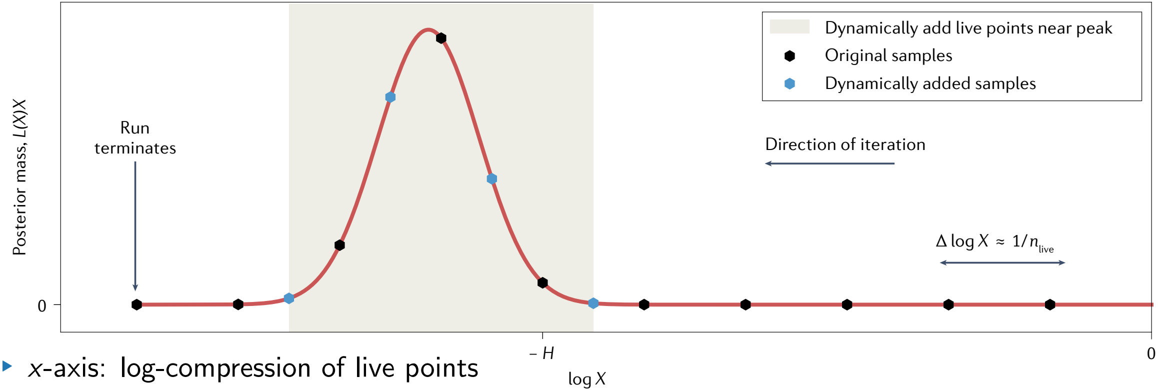


Time complexity of nested sampling



- x-axis: log-compression of live points
- Area $\propto$ posterior mass
- Shows Bayesian balance of likelihood vs prior
- Run proceeds right to left
- Run finishes after bump (typical set)

- Time complexity

$$\boxed{T = n_{\mathrm{live}} \times T_{\mathcal{L}} \times T_{\mathrm{sampler}} \times \mathcal{D}_{\mathrm{KL}}(\mathcal{P}||\pi)}$$

- Error complexity $\boxed{\sigma \propto \sqrt{\mathcal{D}_{\mathrm{KL}}(\mathcal{P}||\pi)/n_{\mathrm{live}}}}$

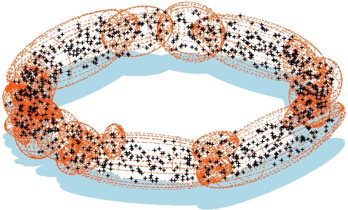
Sampling from a hard likelihood constraint

> *"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*

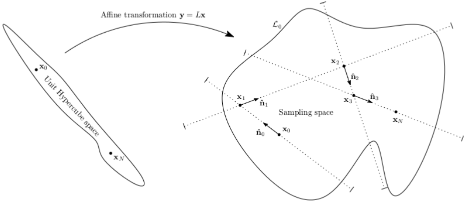
- A large fraction of the work in NS to date has been in attempting to implement a hard-edged sampler in the NS meta-algorithm $\{\theta \sim \pi : \mathcal{L}(\theta) > \mathcal{L}_*\}$.
- `https://projecteuclid.org/euclid.ba/1340370944`.
- There has also been much work beyond this (see "Frontiers of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

Implementations of Nested Sampling [2205.15570](NatReview)

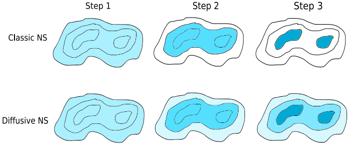
MultiNest [0809.3437]



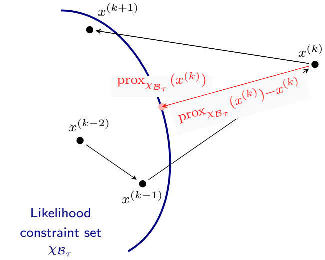
PolyChord [1506.00171]



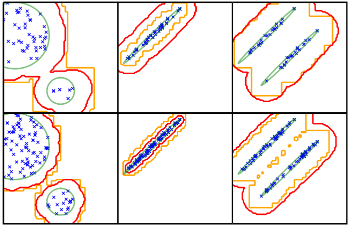
DNest [1606.03757]



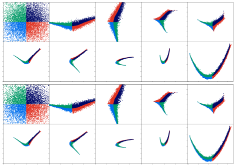
ProxNest [2106.03646]

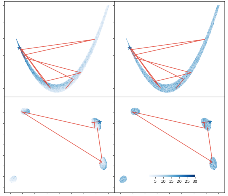


UltraNest [2101.09604]



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 $d > d_0 \sim 10$.

Chain-based samplers

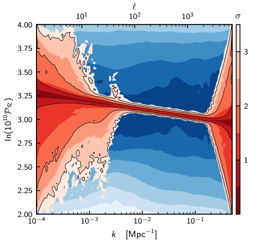
- e.g. `PolyChord`, `ProxNest`.
- Run Markov chain starting at a live point, generating many valid (correlated) points.
- Linear $\sim \mathcal{O}(d)$ penalty in decorrelating new live point from the original seed point.

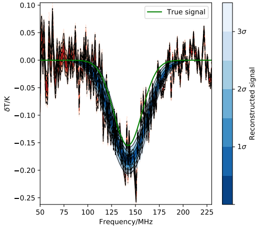
- Nested samplers usually come with:
  - *resolution* parameter n_live (which improve results as $\sim \mathcal{O}(n_\mathrm{live}^{-1/2})$.
  - set of *reliability* parameters [2101.04525], which don't improve results if set arbitrarily high, but introduce systematic errors if set too low.
  - e.g.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

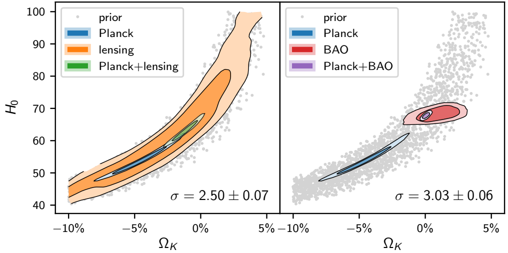
Applications of nested sampling

Cosmology

- Battle-tested in Bayesian cosmology on
  - Parameter estimation: multimodal alternative to MCMC samplers.
  - Model comparison: using integration to compute the Bayesian evidence
  - Tension quantification: using deep tail sampling and suspiciousness computations.
- Plays a critical role in major cosmology pipelines: Planck, DES, KiDS, BAO, SNe.
- The default ΛCDM cosmology is well-tuned to have Gaussian-like posteriors for CMB data.
- Less true for alternative cosmologies/models and orthogonal datasets, so nested sampling crucial.



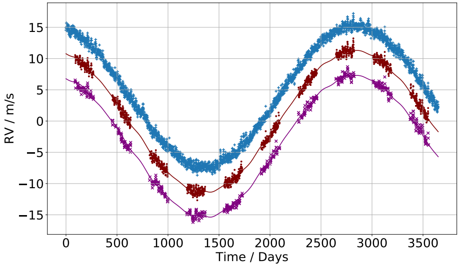


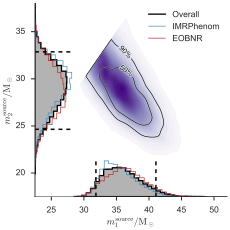


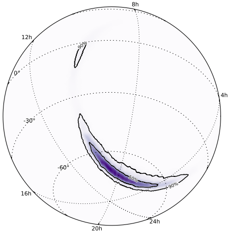
Applications of nested sampling

Astrophysics

- 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



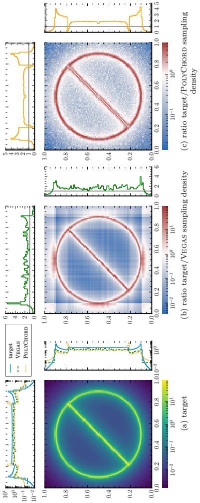


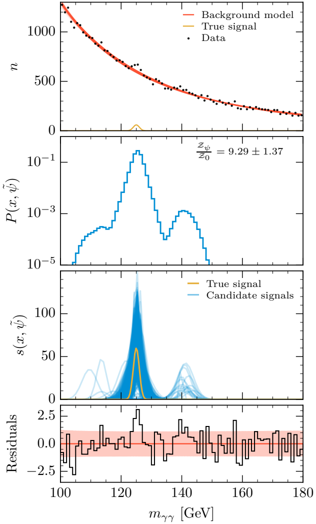


Applications of nested sampling

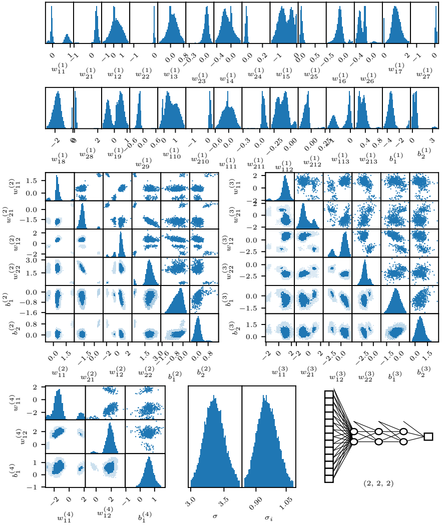
Particle physics

- 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





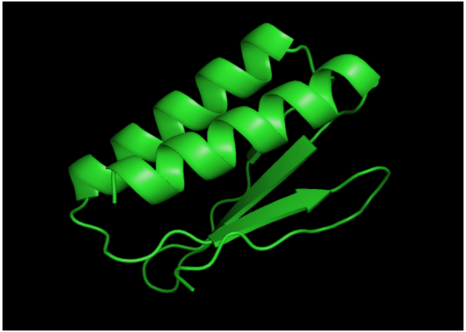
- Machine learning requires:
  - Training to find weights
  - Choice of architecture/topology/hyperparameters
- Bayesian NNs treat training as a model fitting problem
- Compute posterior of weights (parameter estimation), rather than optimisation (gradient descent)
- Use evidence to determine best architecture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

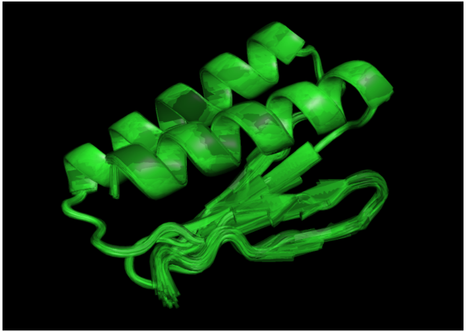
- Techniques have been spun-out (PolyChord Ltd) to:
- Protein folding
  - Navigating free energy surface.
  - Computing misfolds.
  - Thermal motion.
- Nuclear fusion reactor optimisation
  - multi-objective.
  - uncertainty propagation.
- Telecoms & DSTL research (MIDAS)
  - Optimising placement of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



Applications of nested sampling

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.



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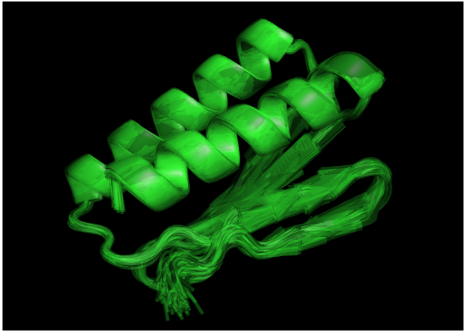


How does Nested Sampling compare to other approaches?

- 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 trasitions
  - + 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
- Athermal evolution
- Order statistics

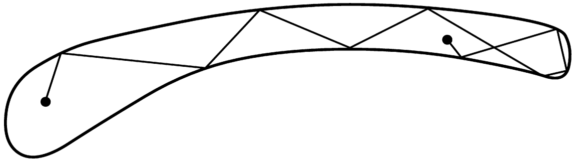
Why doesn't HMC work?

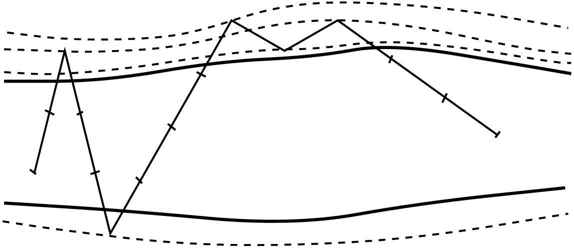
- Nested sampling requires you to sample from the truncated *prior*, not the likelihood
- Other than at the boundaries, it is not obvious how to use a likelihood gradient to navigate the prior.
- In addition, since nested sampling begins in the tails, proceeding through the typical set and onto the peak,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

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 $\hat{n}$: $v \to v - 2(v \cdot \hat{n})\hat{n}$
  - 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.



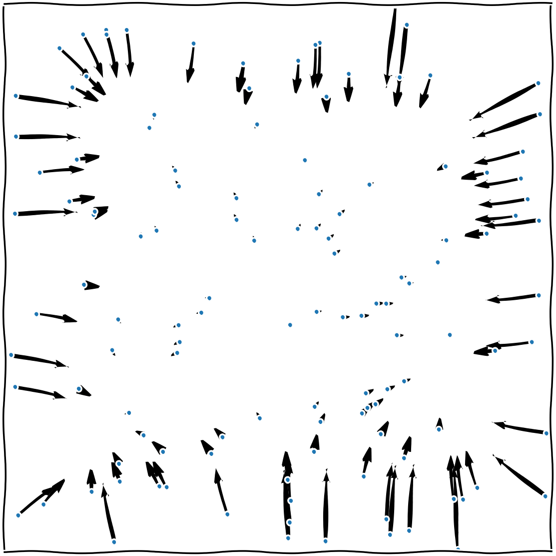


Historical attempts

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, incoporating momenta in a more HMC like way, but specialised to materials science [1710.11085].
Cai	ProxNest for high-dimensional convex imaging problems [2106.03646].

Nested sampling with gradients

- Existing 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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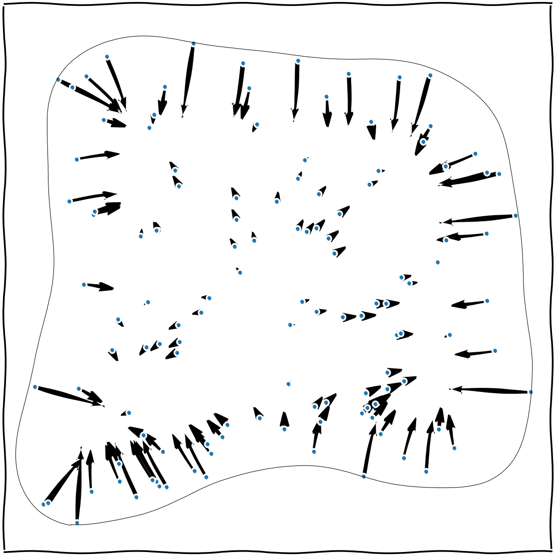

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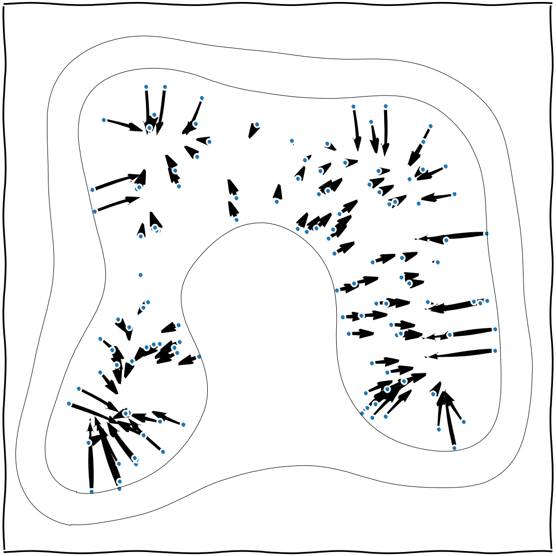

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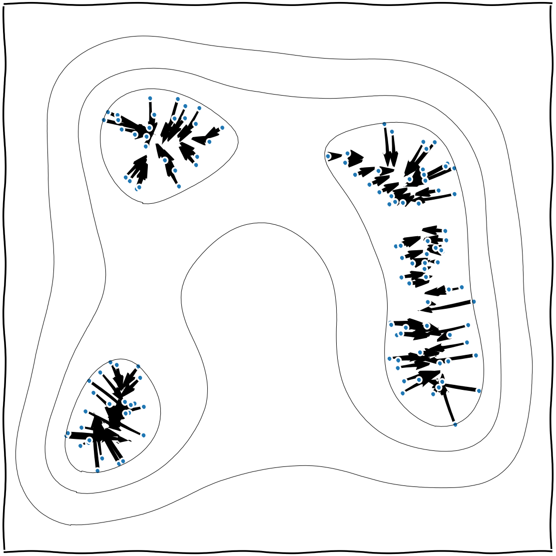

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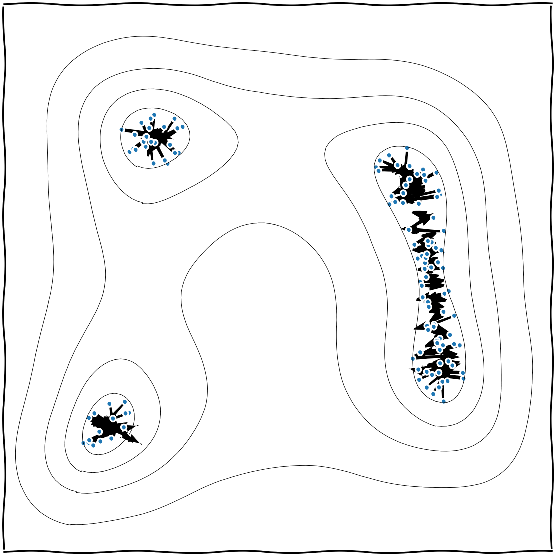

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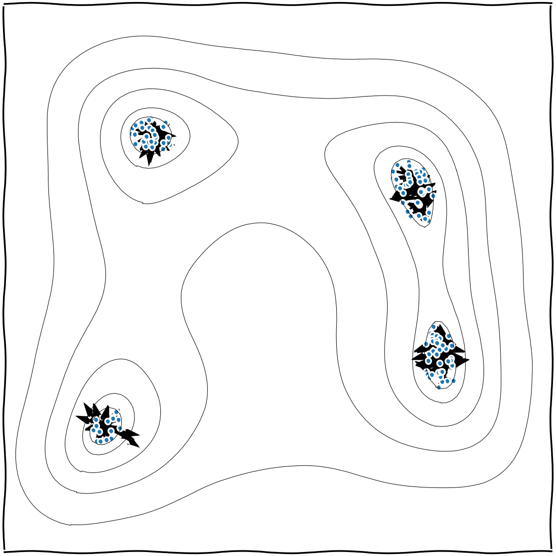

Conclusions

- 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, probababilistic programming means there are a lot of analyses which would benefit.