Gradients and Nested Sampling

The present state of the art

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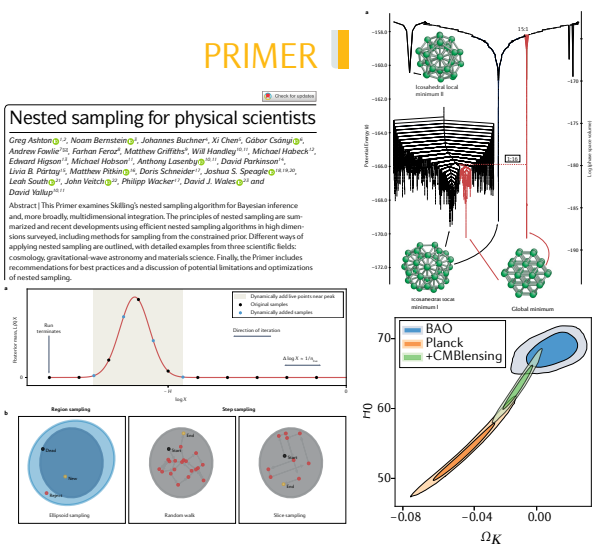
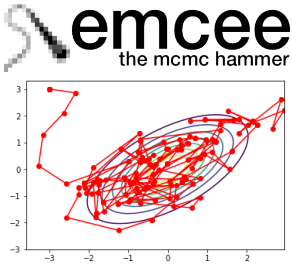
Highlight: state-of-the-art Nature review primer [2205.15570]

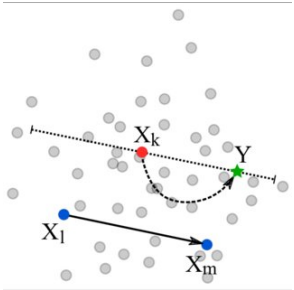
- Invented by John Skilling in 2004.
- Recent Nature review primer on nested sampling led by Andrew Fowlie and assembled by the community.
- Showcases the current set of tools, and applications from chemistry to cosmology.
- Buchner technical review [2101.09675]
- In this talk
  - What is nested sampling?
  - How can it use gradients?

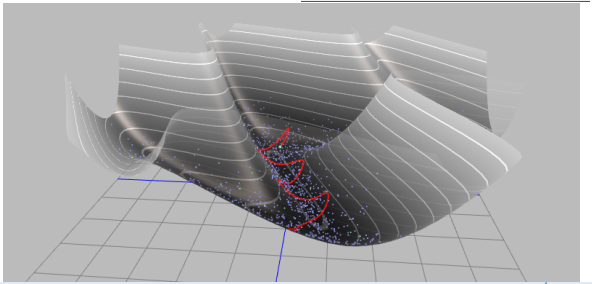


Where is Nested Sampling?

- 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





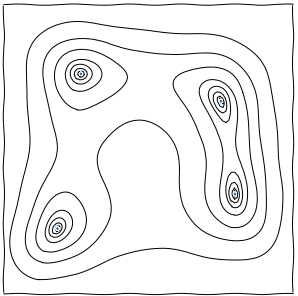


What is Nested Sampling?

- 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:

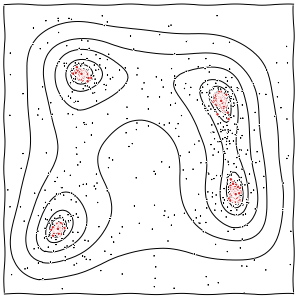
Optimisation

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



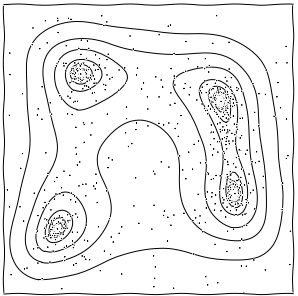
Exploration

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

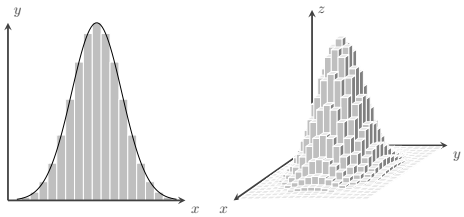
$$\Psi = \int e^{iS} \mathcal{D}x$$

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:

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



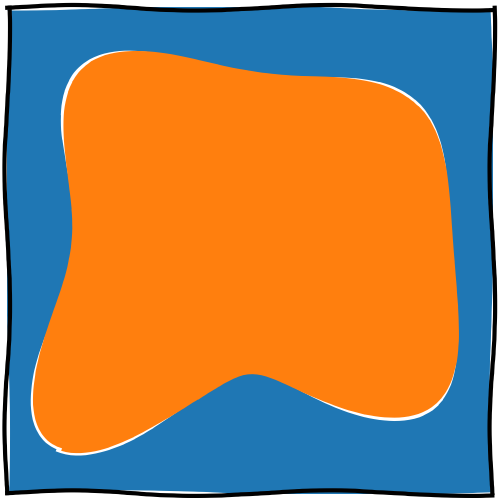
- Curse of dimensionality $\Rightarrow$ exponential scaling.
- Nested sampling integrates **probabilistically**.

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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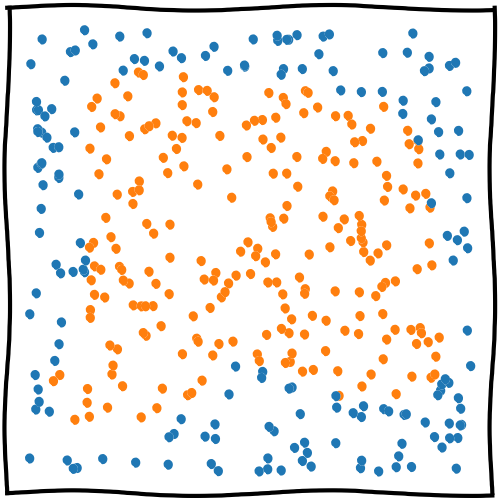

Probabalistic volume estimation

- 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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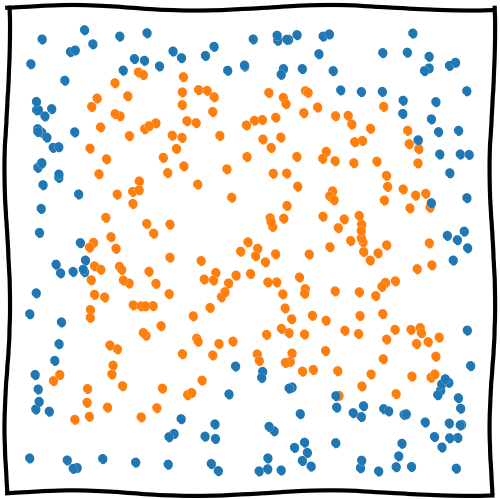

Probabalistic volume estimation

- 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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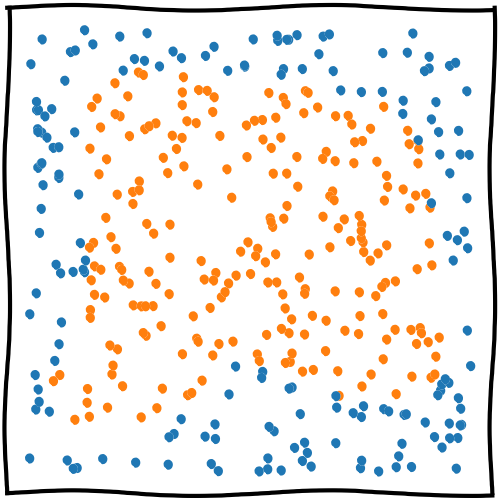
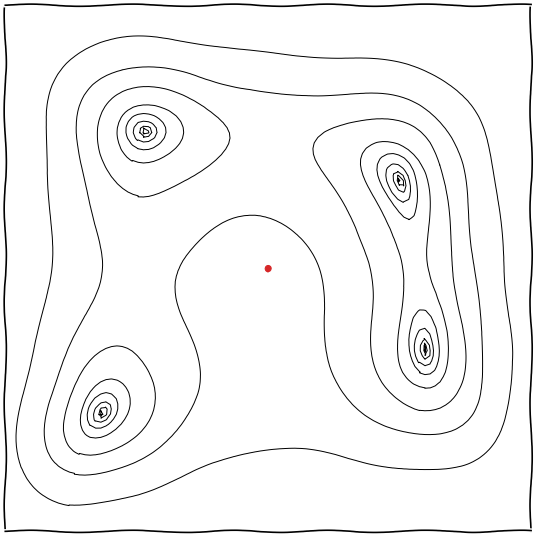


MCMC



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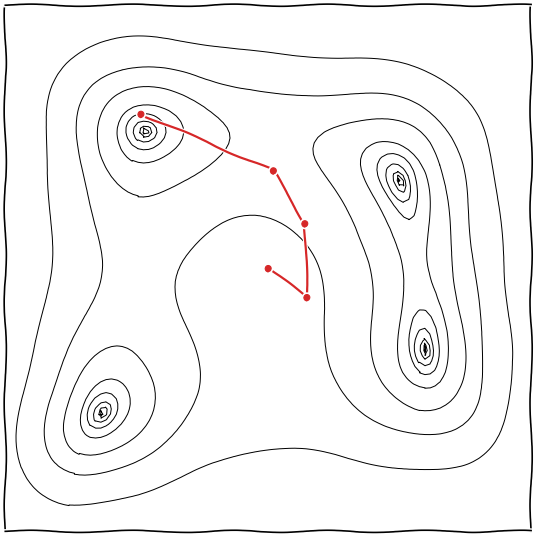

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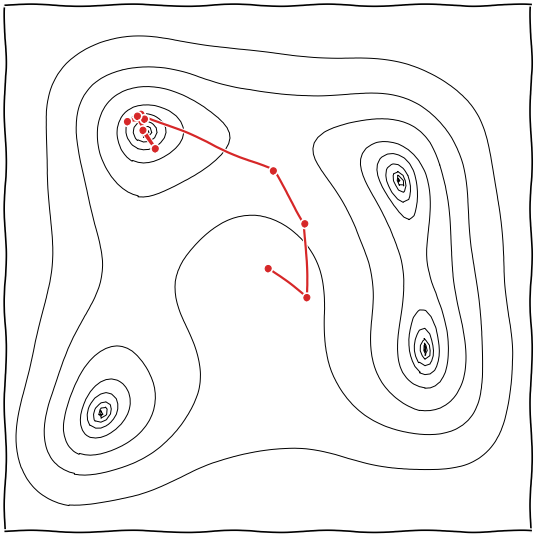

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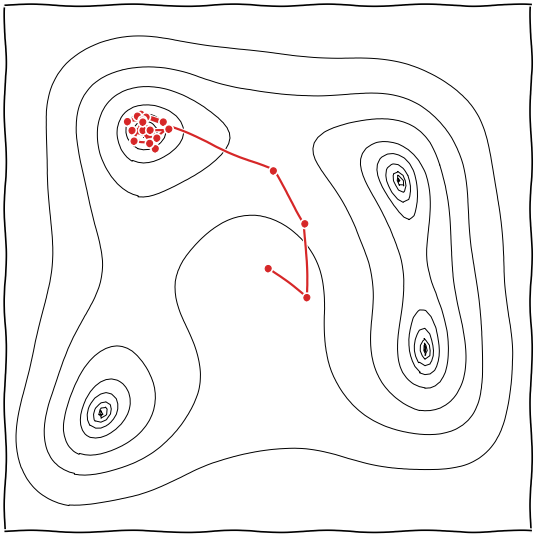

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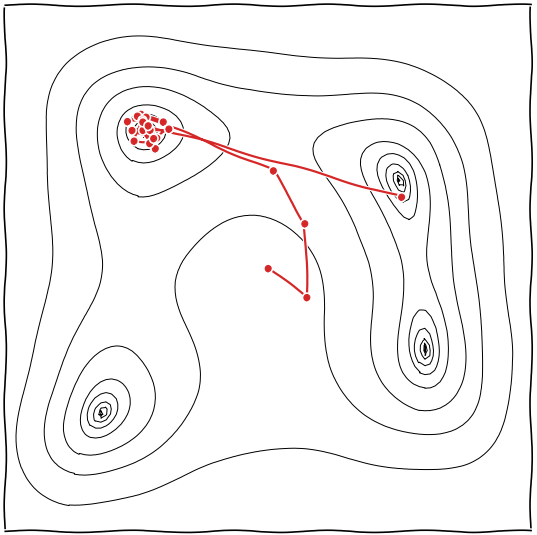

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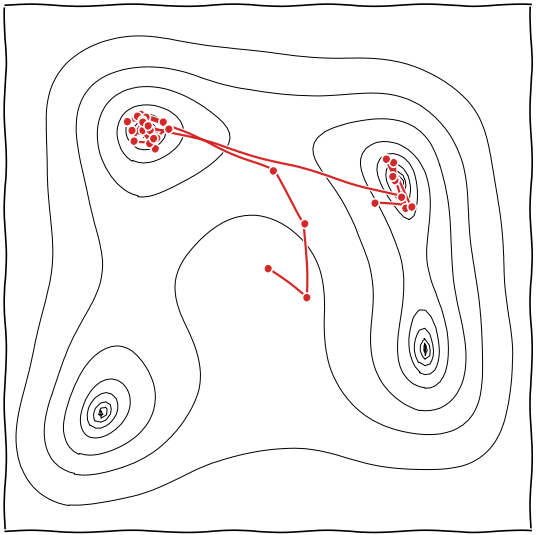

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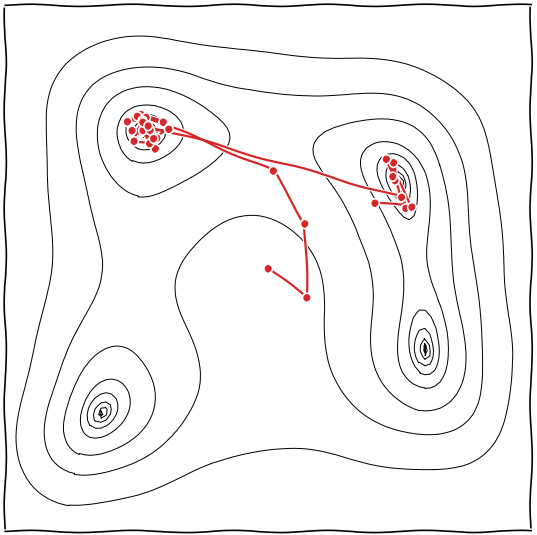
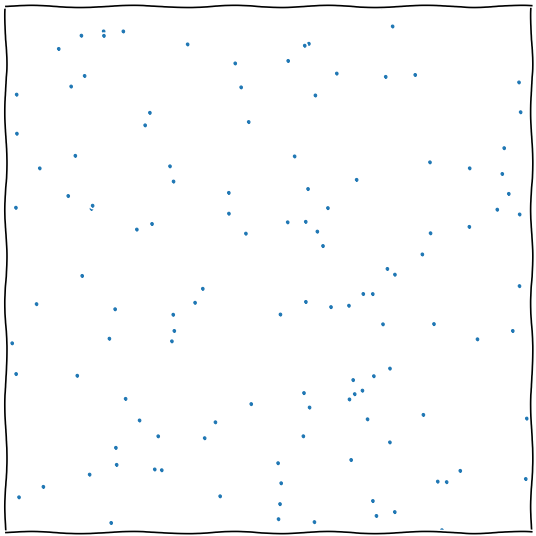


Nested sampling



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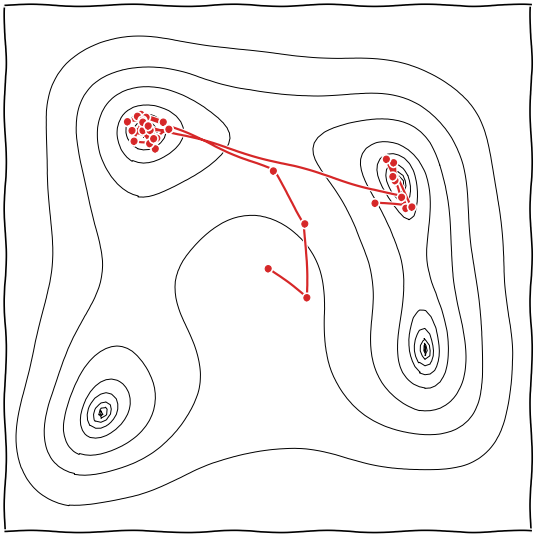

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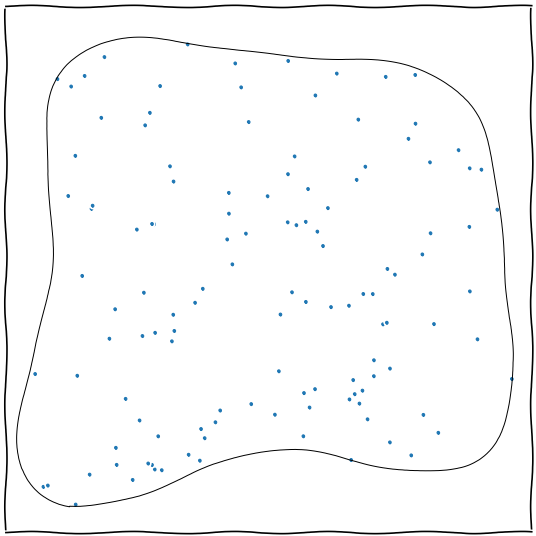

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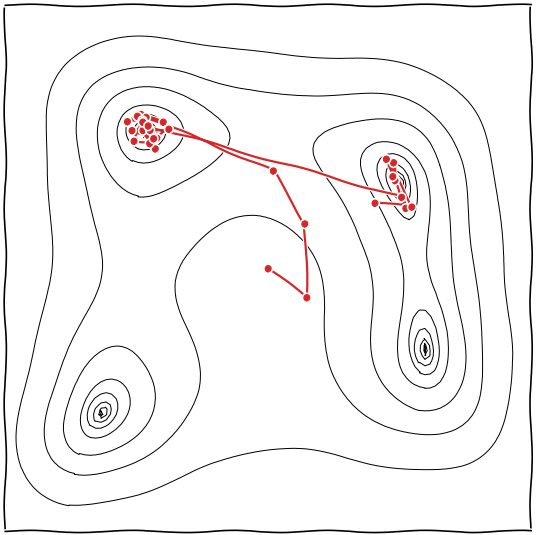

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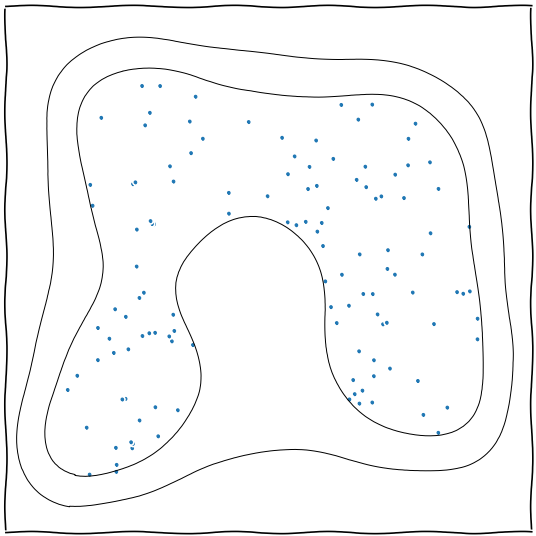

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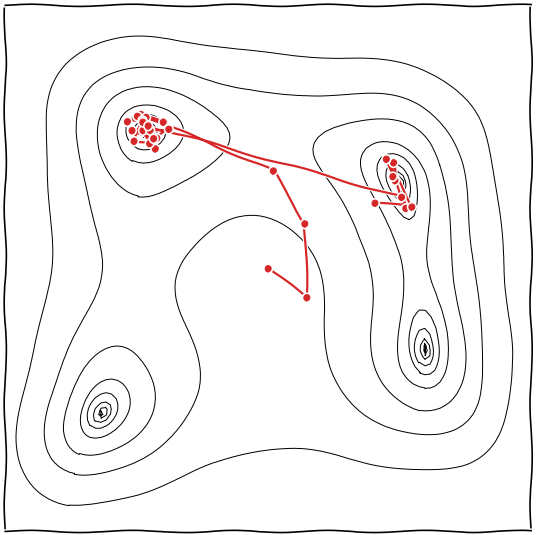

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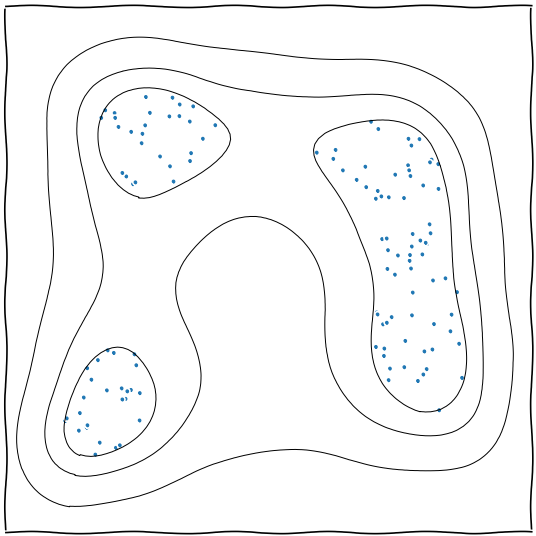

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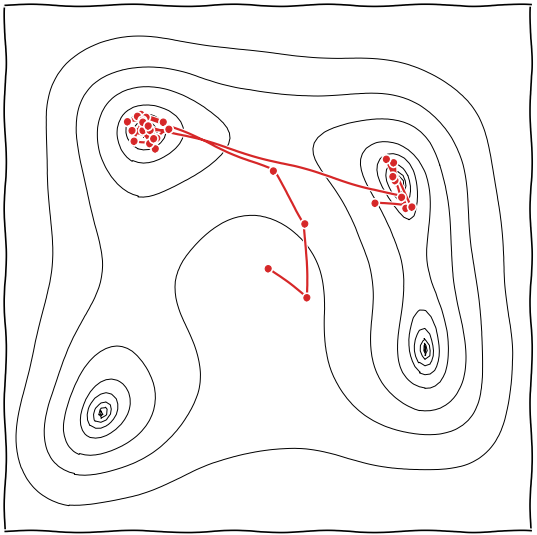

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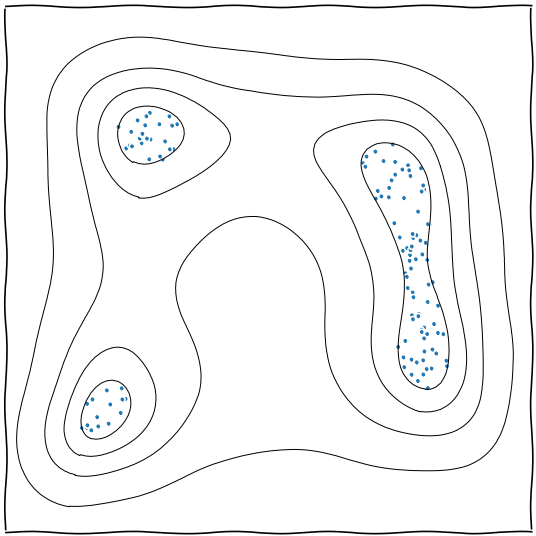

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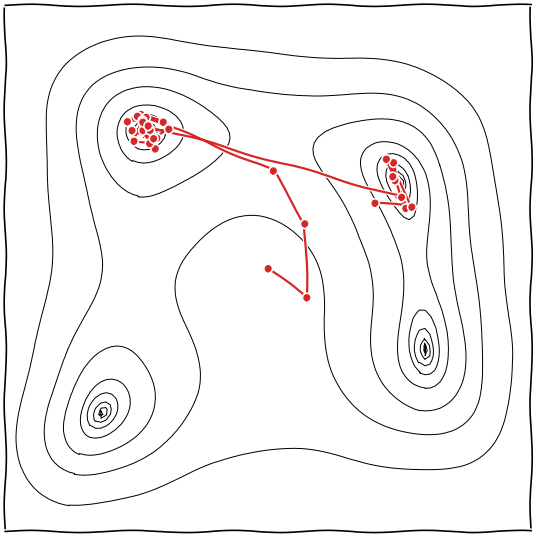

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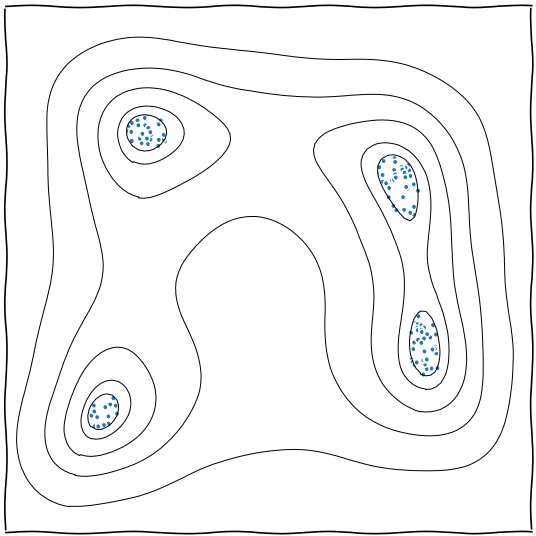

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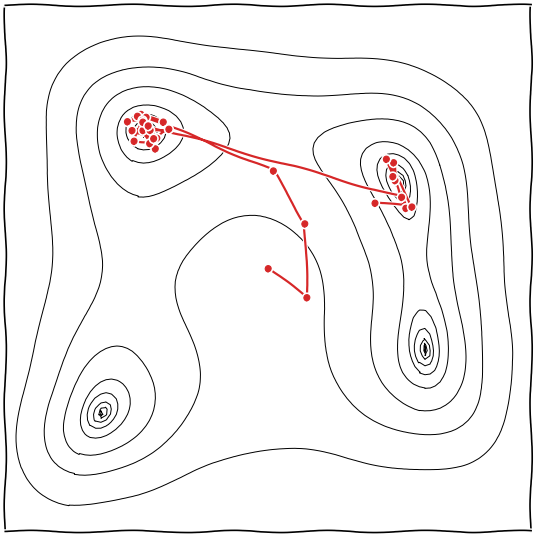

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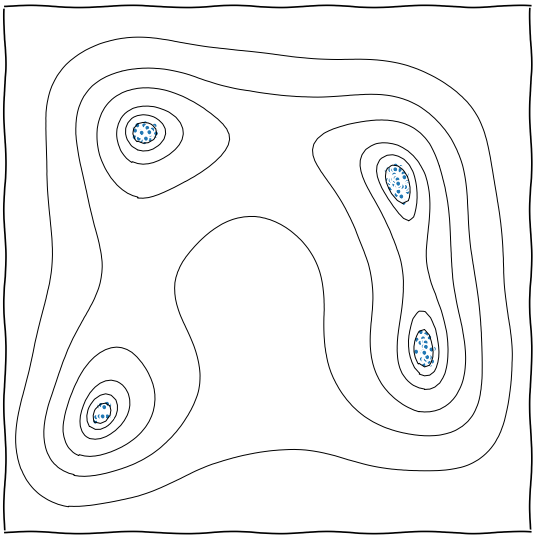

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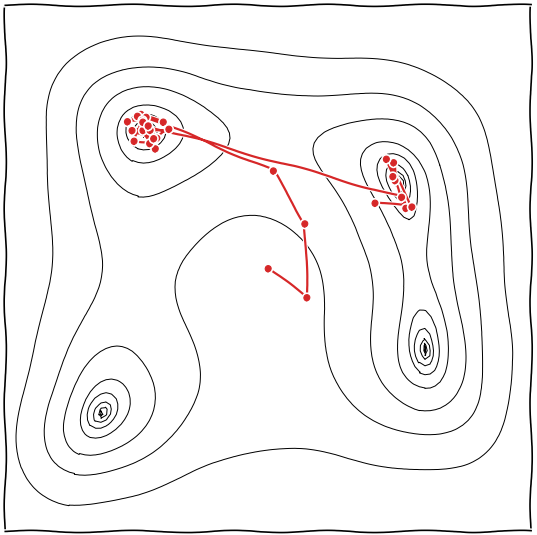

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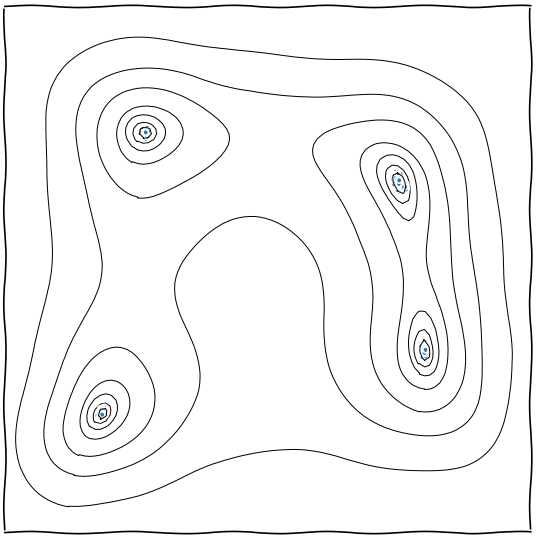

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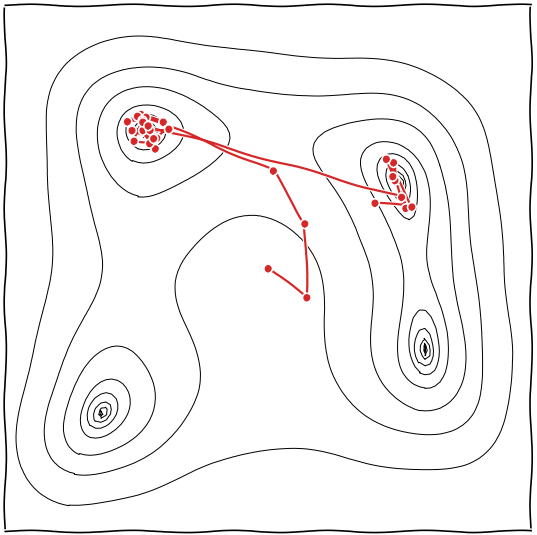

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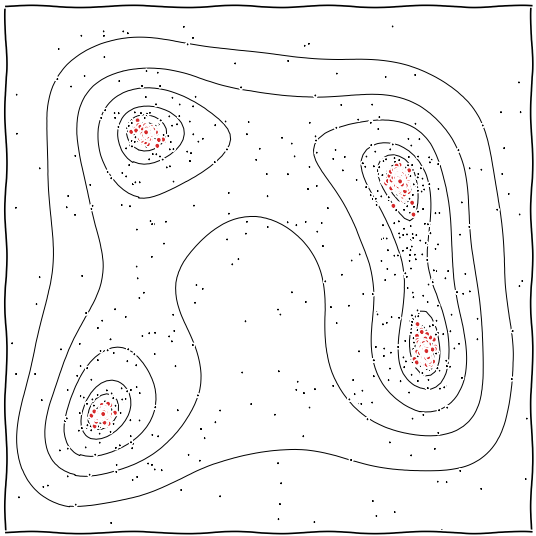
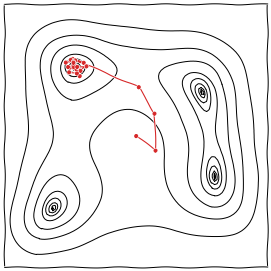


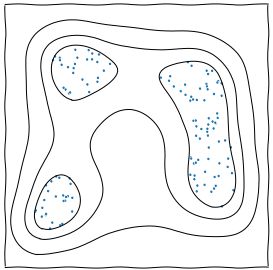
MCMC

- 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:

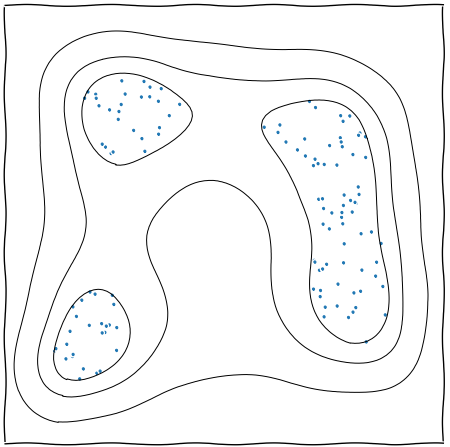
  S_0: Generate n samples uniformly over the space (from the prior π).

  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.

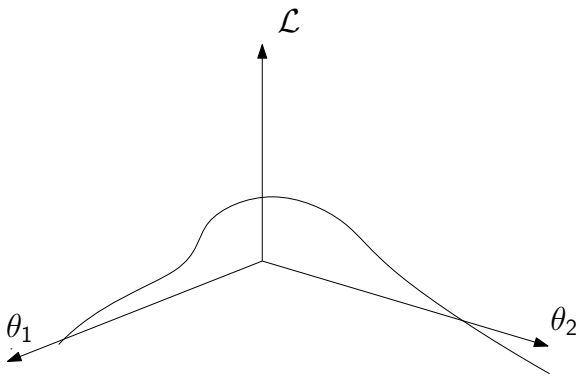


(Lesbesgue) Integrating with nested sampling

- 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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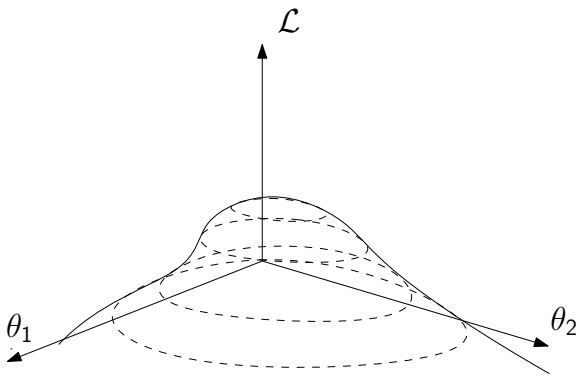

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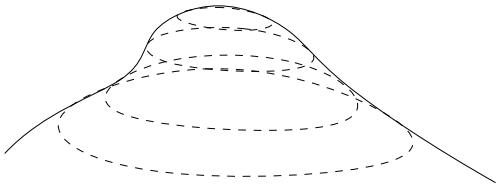

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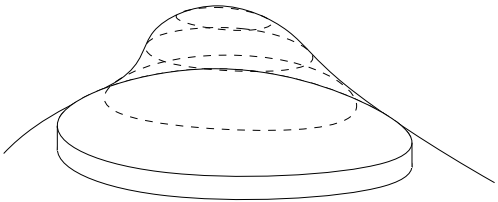

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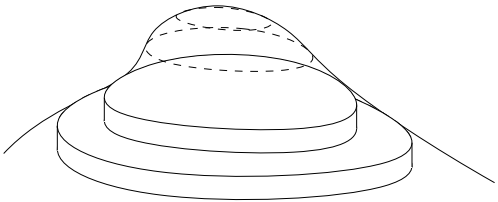

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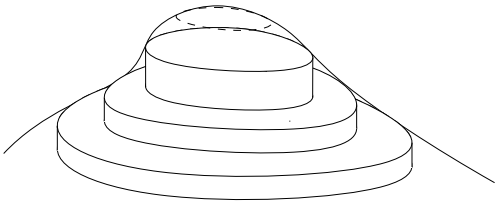

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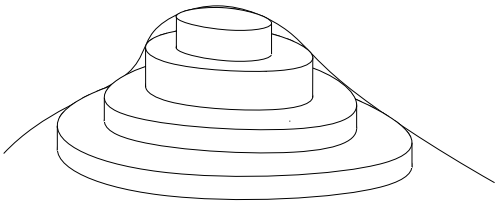

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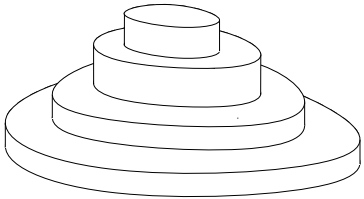

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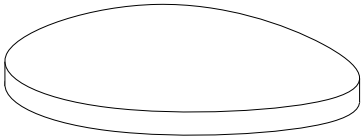

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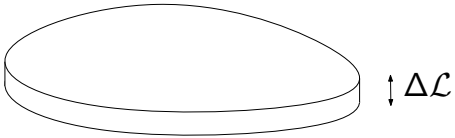

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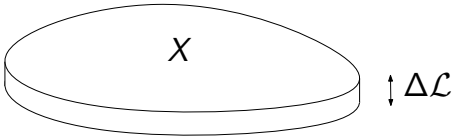

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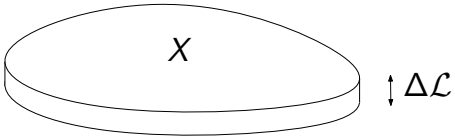

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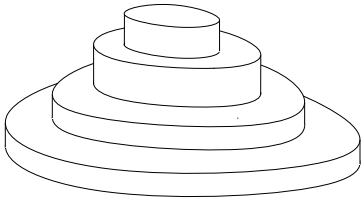

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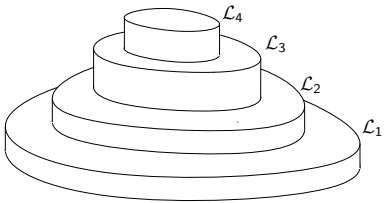

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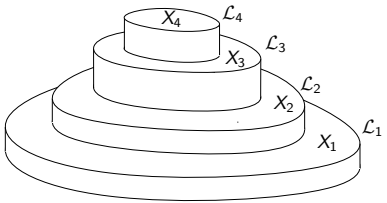

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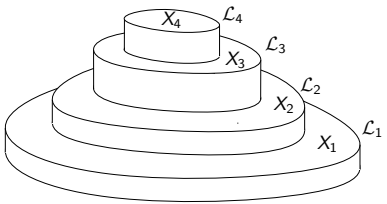

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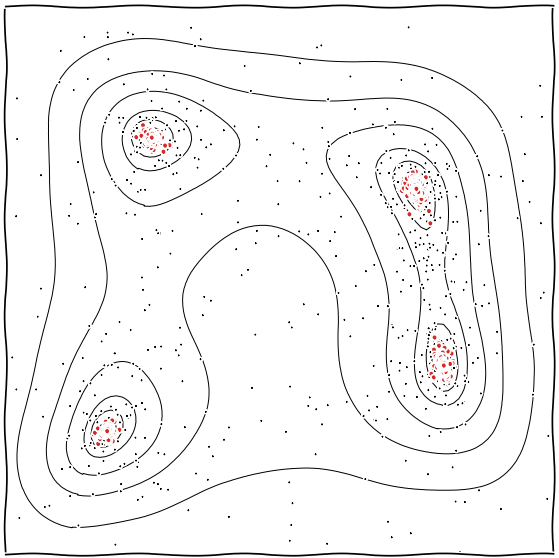


Sampling from a hard likelihood constraint

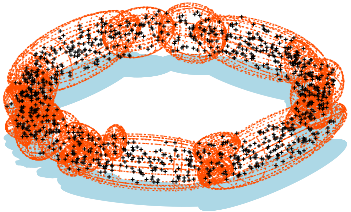
"It is not the purpose of this introductory paper to develop the technology of navigation within such a volume. We merely note that exploring a hard-edged likelihood-constrained domain should prove to be neither more nor less demanding than exploring a likelihood-weighted space."

— *John Skilling*

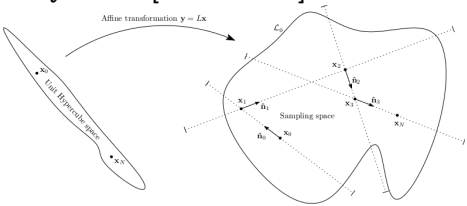
- A large fraction of the work in NS to date has been in attempting to implement a hard-edged sampler in the NS meta-algorithm $\{\theta \sim \pi : \mathcal{L}(\theta) > \mathcal{L}_*\}$.
- `https://projecteuclid.org/euclid.ba/1340370944`.
- There has also been much work beyond this (see "Frontiers of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

Implementations of Nested Sampling [2205.15570](NatReview)

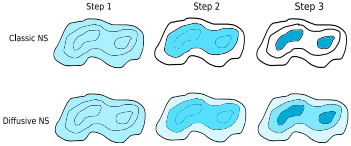
MultiNest [0809.3437]



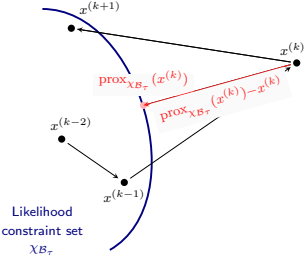
PolyChord [1506.00171]



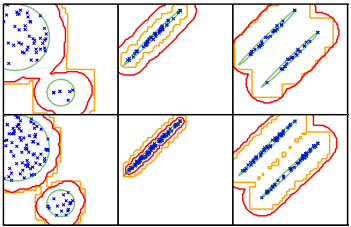
DNest [1606.03757]



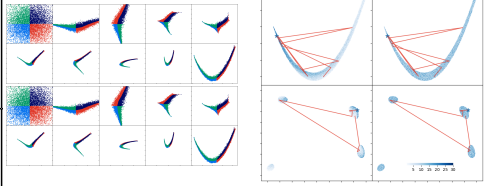
ProxNest [2106.03646]



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 $d > d_0 \sim 10$.

Chain-based samplers

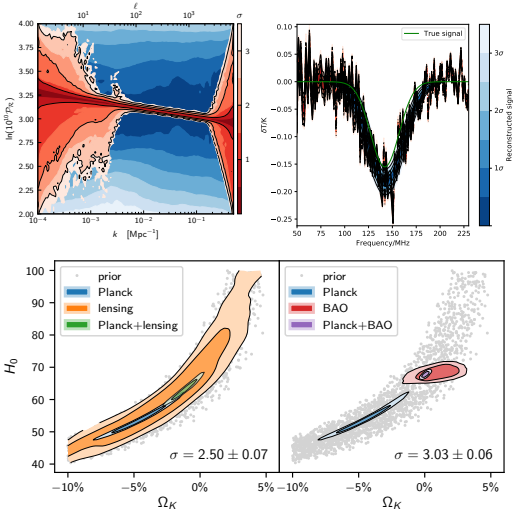
- e.g. `PolyChord`, `ProxNest`.
- Run Markov chain starting at a live point, generating many valid (correlated) points.
- Linear $\sim \mathcal{O}(d)$ penalty in decorrelating new live point from the original seed point.

- Nested samplers usually come with:
  - *resolution* parameter n_{live} (which improve results as $\sim \mathcal{O}(n_{\text{live}}^{-1/2})$.
  - 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}.

Applications of nested sampling

Cosmology

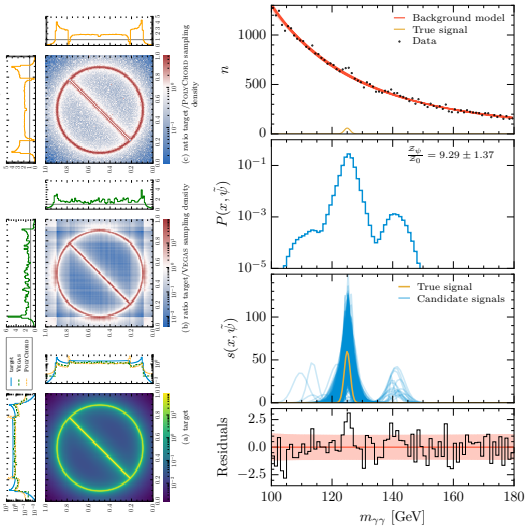
- Battle-tested in Bayesian cosmology on
  - Parameter estimation: multimodal alternative to MCMC samplers.
  - Model comparison: using integration to compute the Bayesian evidence
  - Tension quantification: using deep tail sampling and suspiciousness computations.
- Plays a critical role in major cosmology 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

Particle physics

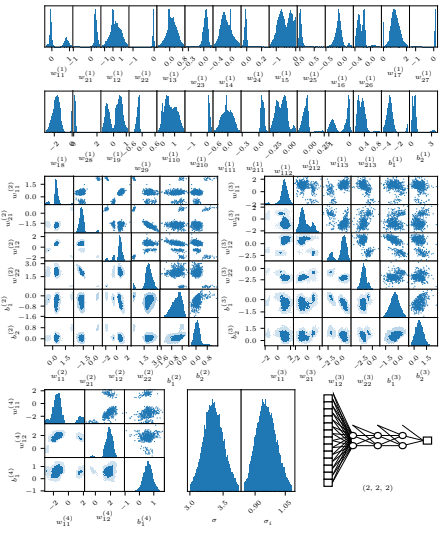
- Nested sampling for cross section computation/event generation $\sigma = \int_\Omega d\Phi |\mathcal{M}|^2.$
- Nested sampling can explore the phase space Ω and compute integral blind with comparable efficiency to HAAG/RAMBO [2205.02030].
- Bayesian sparse reconstruction [1809.04598] applied to bump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

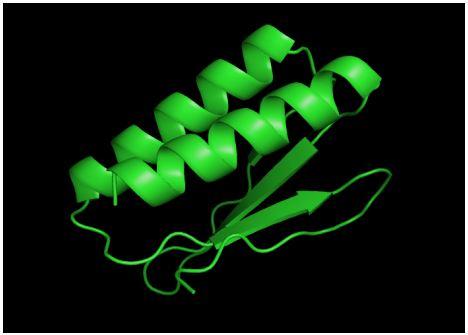
- Machine learning requires:
  - Training to find weights
  - Choice of architecture/topology/hyperparameters
- Bayesian NNs treat training as a model fitting problem
- Compute posterior of weights (parameter estimation), rather than optimisation (gradient descent)
- Use evidence to determine best architecture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



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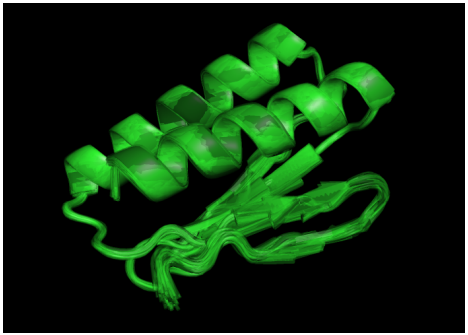
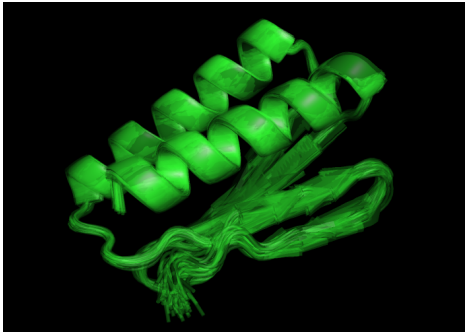


Applications of nested sampling

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.



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, entropies and evidences
- Athermal evolution
- Order statistics

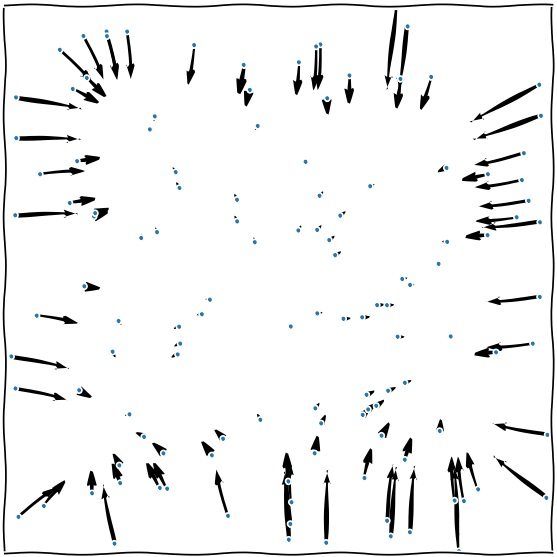
The main goal of using gradients is to improve dimensionality scaling/reliability

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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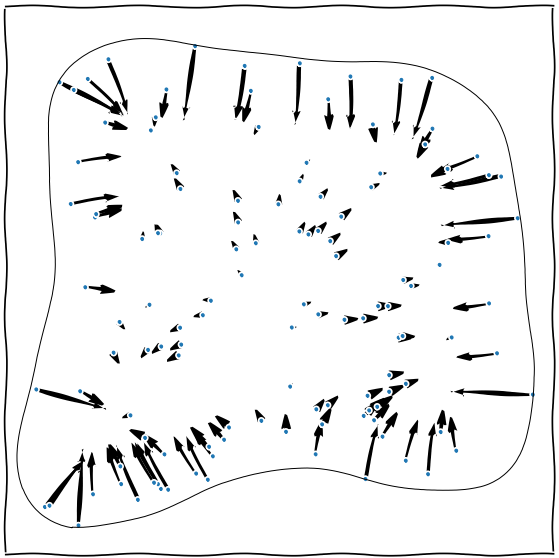

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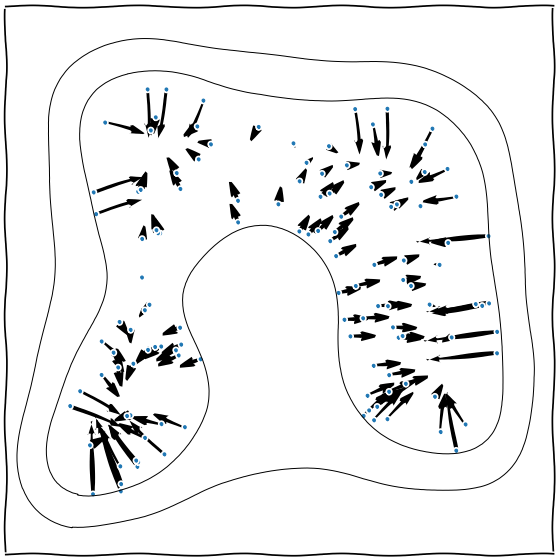


Why doesn't HMC work?

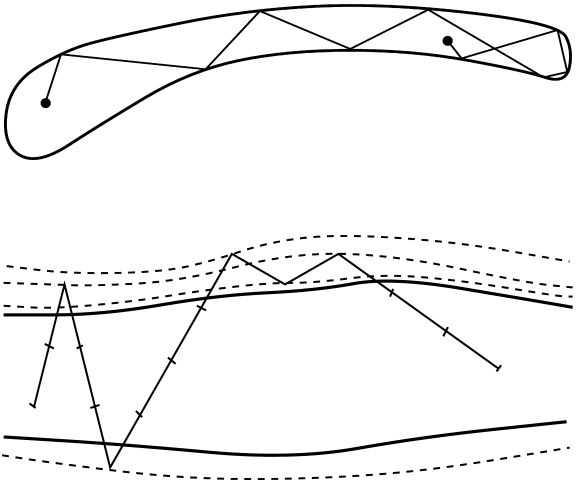
"Tabletop" distributions are difficult to sample!

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

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

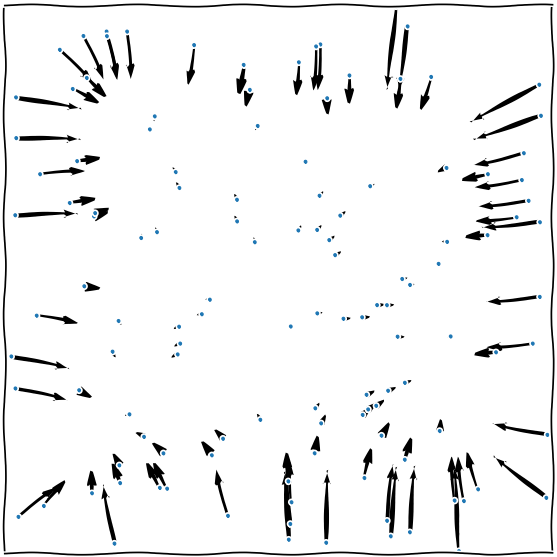
Stephen Thorpe Curved slice sampling.

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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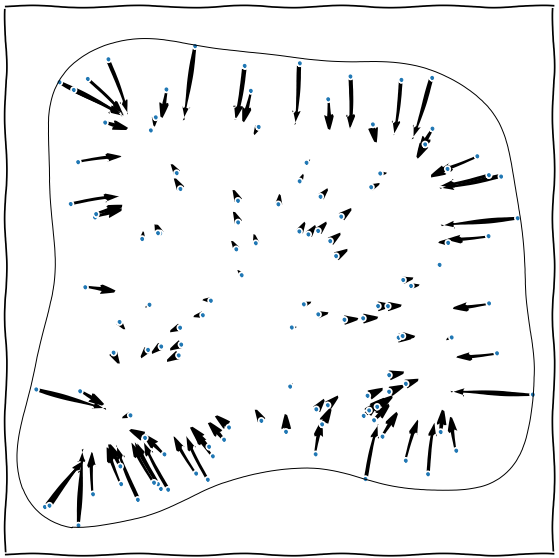

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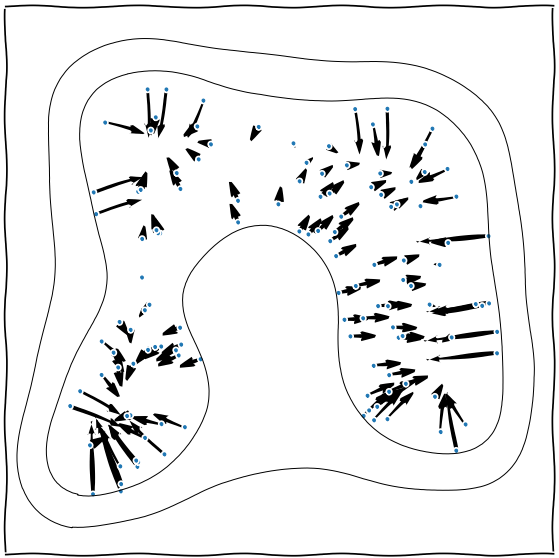

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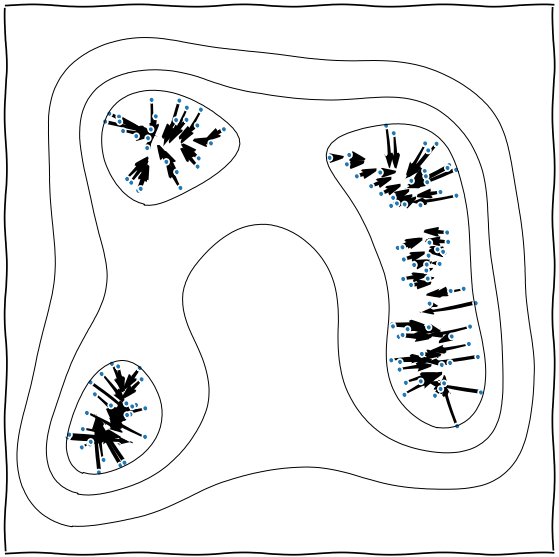

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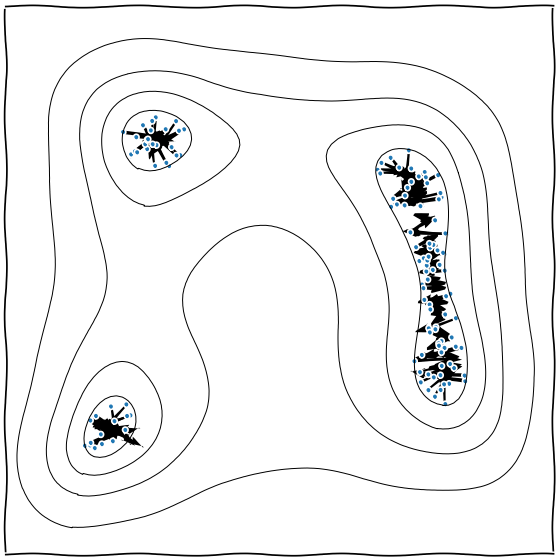

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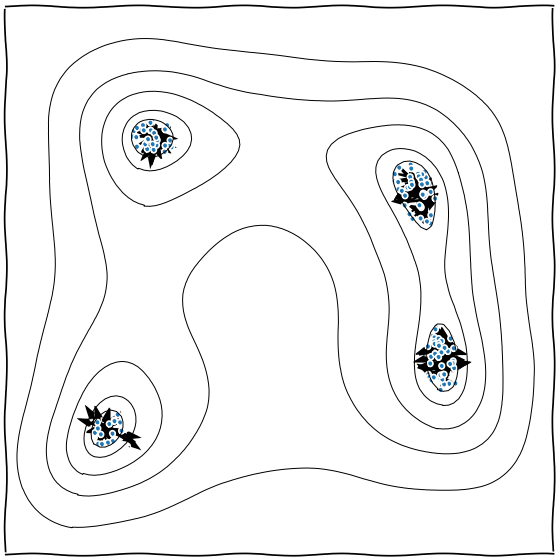
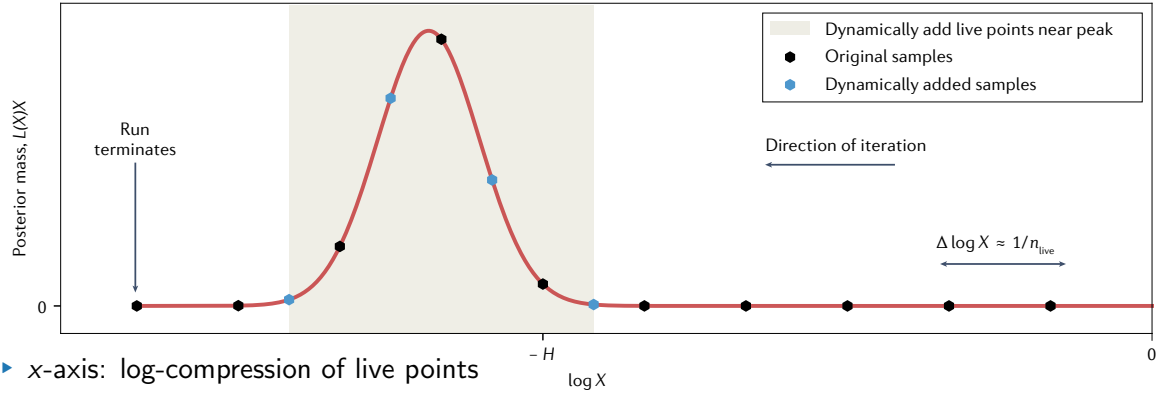


Conclusions

- 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 we can reasonably expect most codes to be able to provide them
- One of my main aims this week is to find ideas from other fields which NS could use.

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

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

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