

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

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The
Alan Turing
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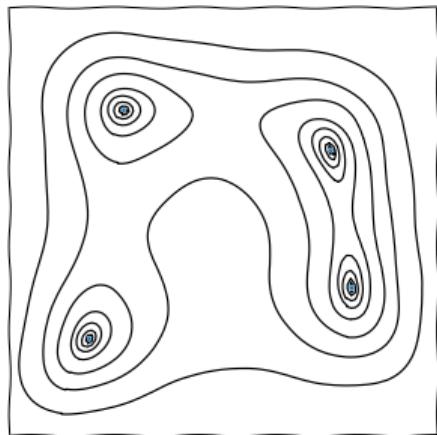


What is Nested Sampling?

- ▶ 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:

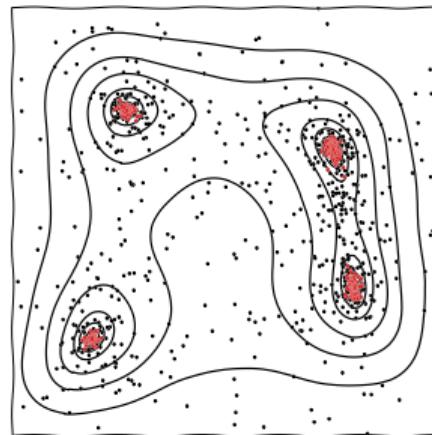
Optimisation

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



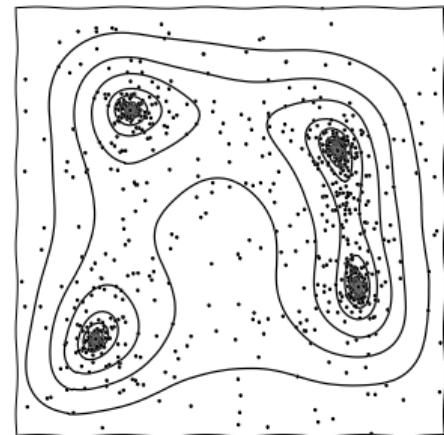
Exploration

draw/sample $\theta \sim f$



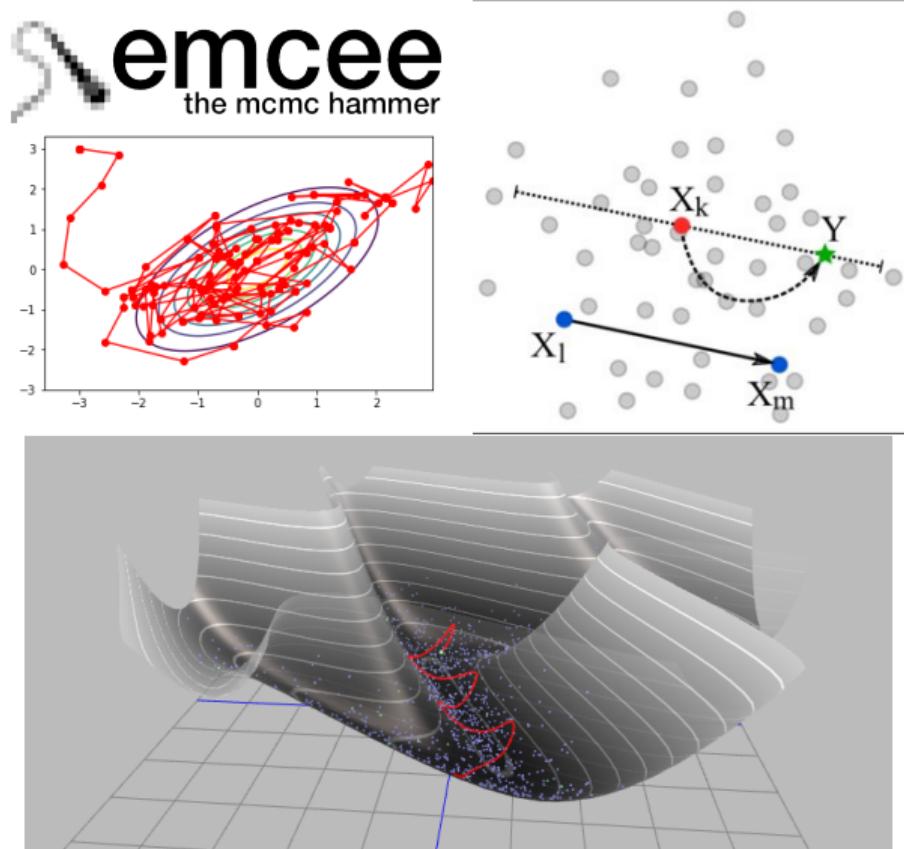
Integration

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



Where is Nested Sampling?

- ▶ For many purposes, in your Neural Net you should group Nested Sampling with (MCMC) techniques such as:
 - ▶ Metropolis-Hastings (PyMC, MontePython)
 - ▶ Hamiltonian Monte Carlo (Stan, blackjax)
 - ▶ Ensemble sampling (emcee, zeus).
 - ▶ Variational Inference (Pyro)
 - ▶ Sequential Monte Carlo
 - ▶ Thermodynamic integration
 - ▶ Genetic algorithms
- ▶ You may have heard of it branded form:
 - ▶ MultiNest
 - ▶ PolyChord
 - ▶ dynesty
 - ▶ ultranest



Integration in Physics

- ▶ Integration is a fundamental concept in physics, statistics and data science:

Partition functions

$$Z(\beta) = \int e^{-\beta H(q,p)} dq dp$$

Path integrals

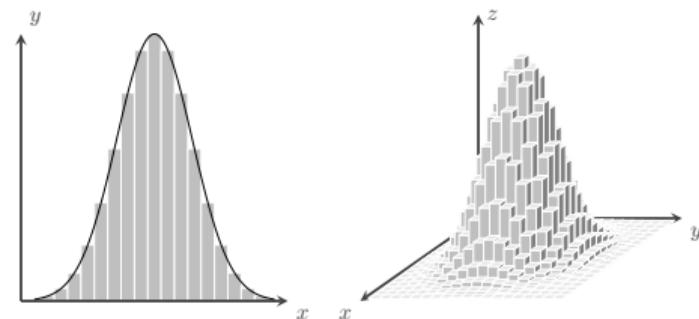
$$\Psi = \int e^{iS} \mathcal{D}x$$

Bayesian marginals

$$\mathcal{Z}(D) = \int \mathcal{L}(D|\theta) \pi(\theta) d\theta$$

- ▶ Need numerical tools if analytic solution unavailable.
- ▶ High-dimensional numerical integration is hard.
- ▶ Riemannian strategy estimates volumes geometrically:

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



- ▶ Curse of dimensionality \Rightarrow exponential scaling.

Probabalistic volume estimation

- ▶ Key idea in NS: estimating volumes probabilistically

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

- ▶ This is the **only** way to calculate volume in high dimensions $d > 3$.
 - ▶ Geometry is exponentially inefficient.
- ▶ This estimation process does not depend on geometry, topology or dimensionality
- ▶ Basis of all Monte-Carlo integration
- ▶ Nested Sampling uniquely uses a nested framework to couple together MC integrals in a robust, scalable manner.

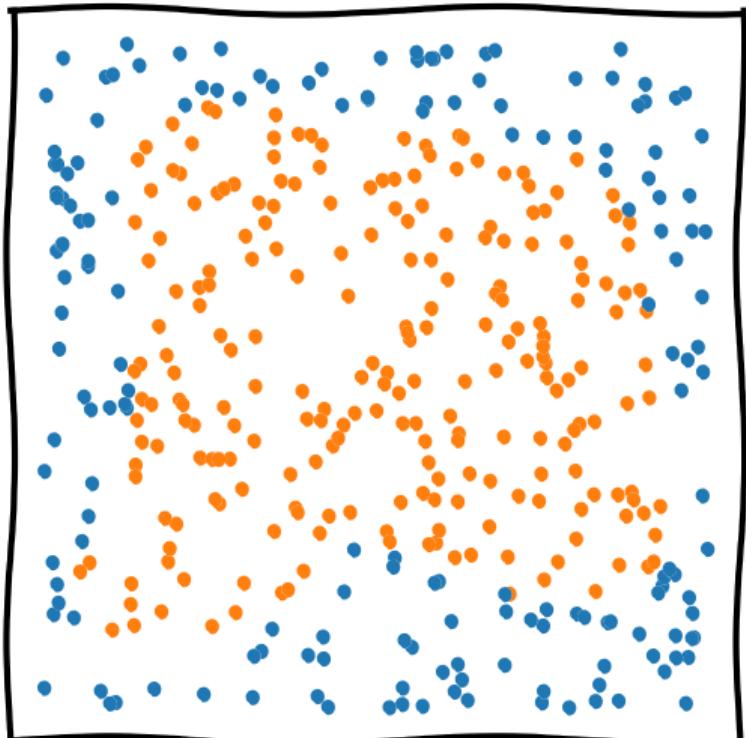


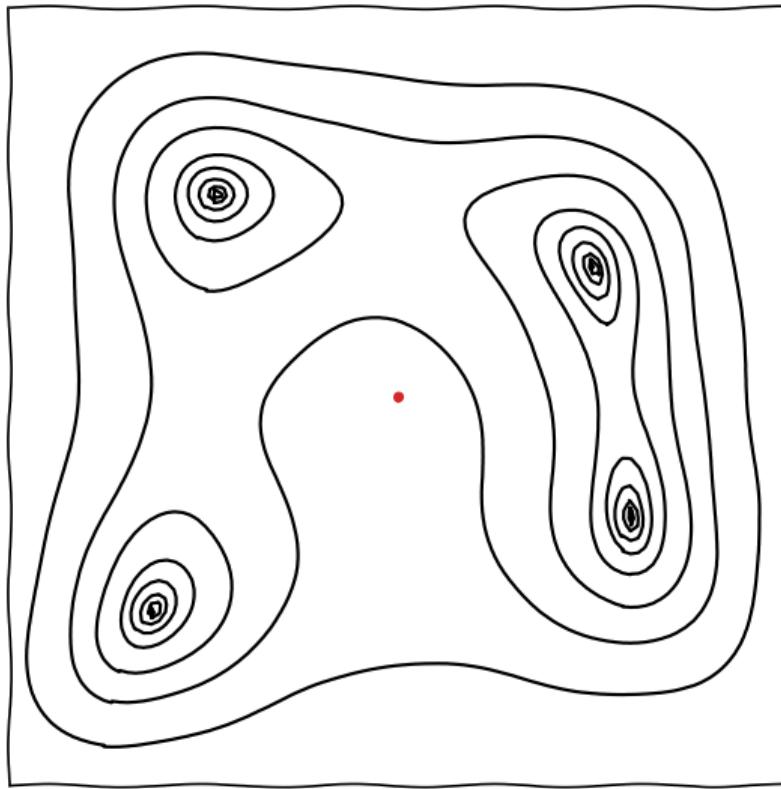
Probabalistic volume estimation

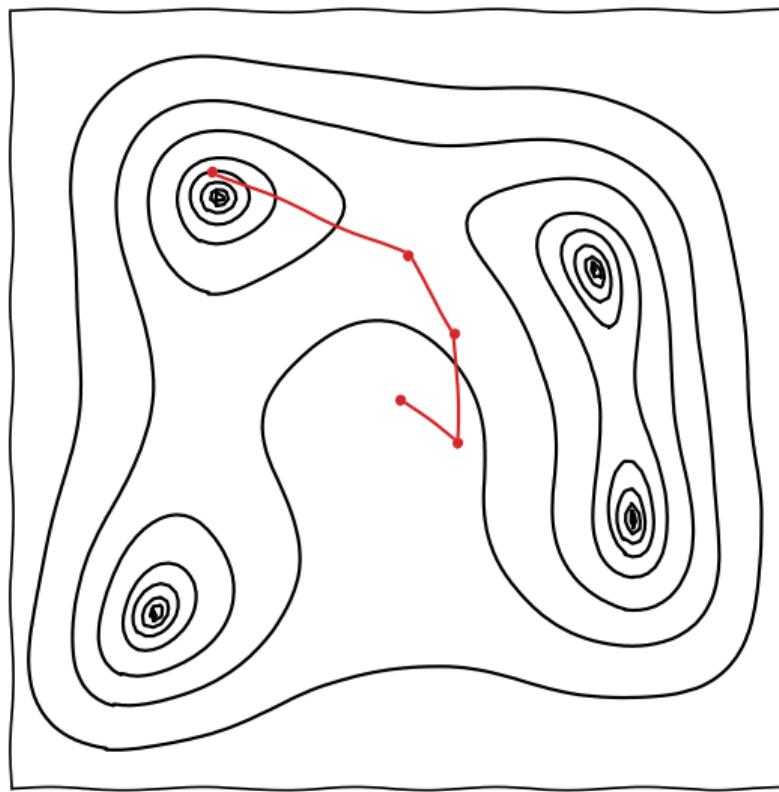
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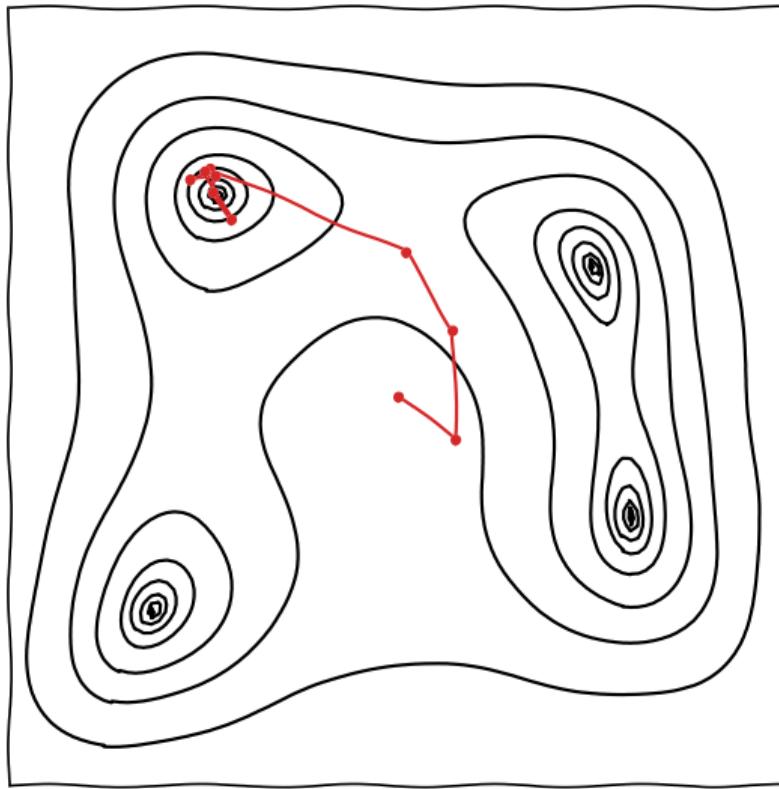
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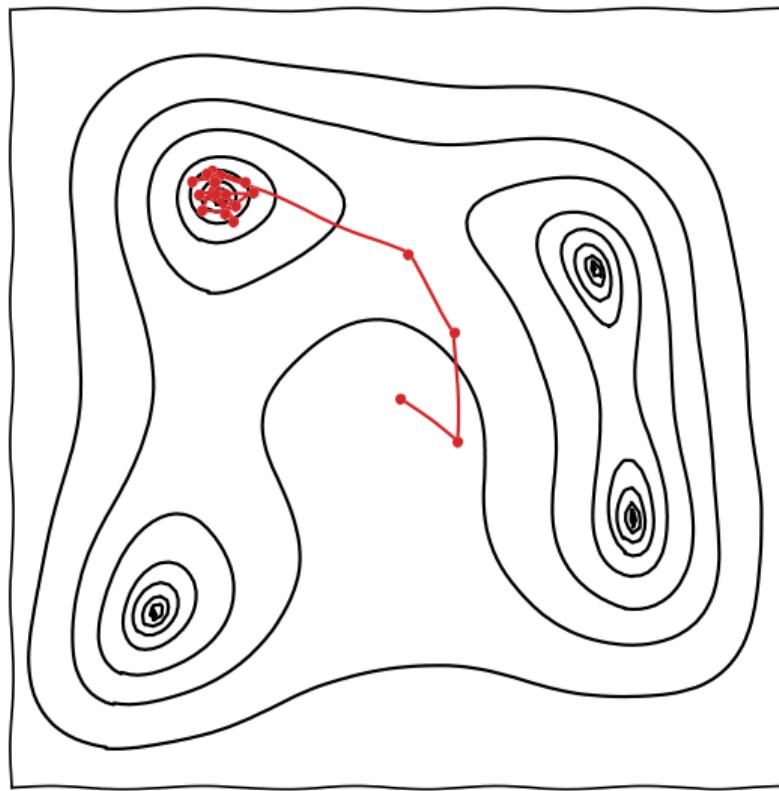
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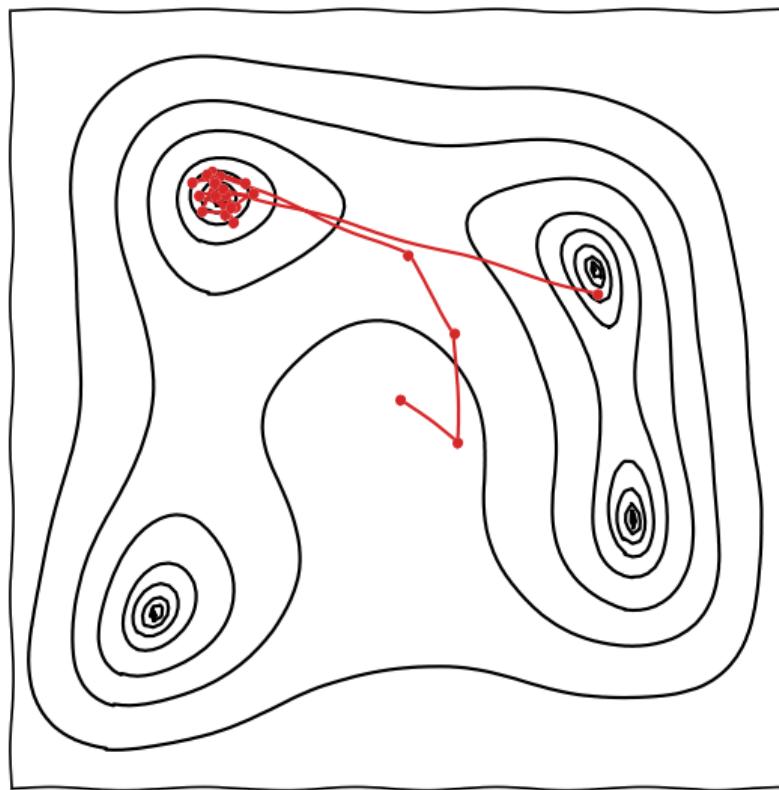


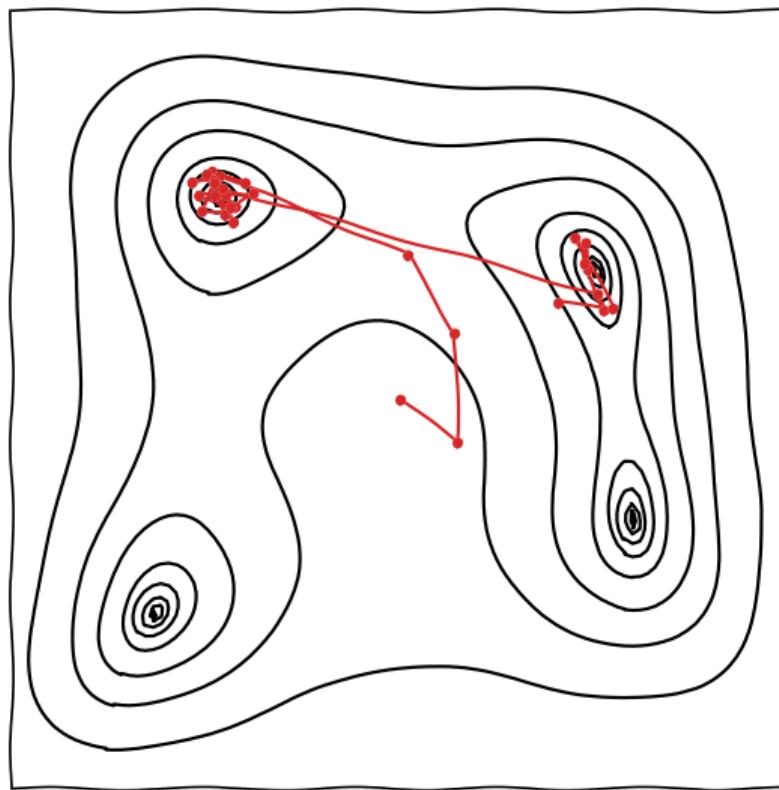




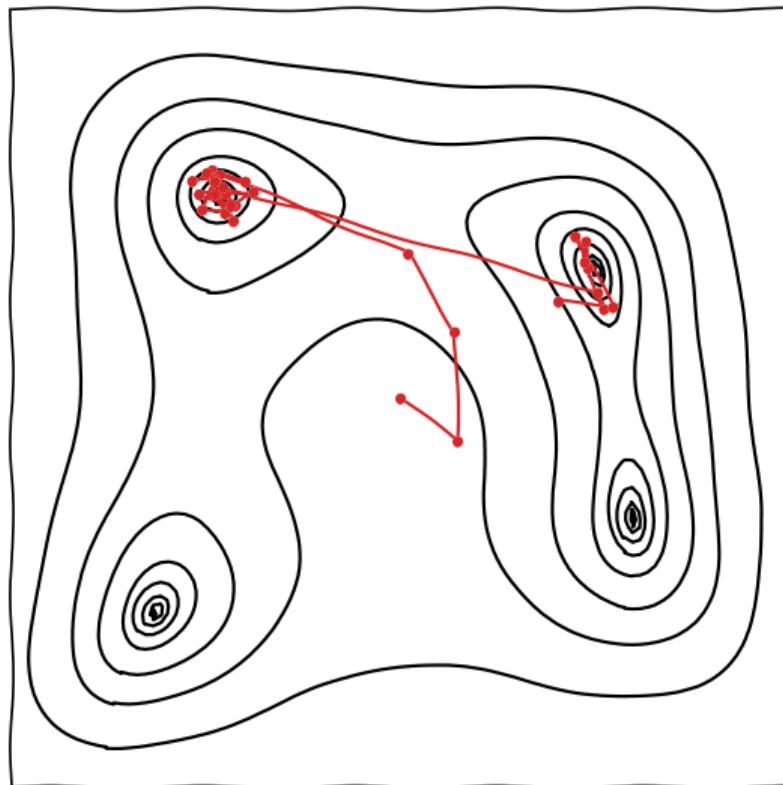




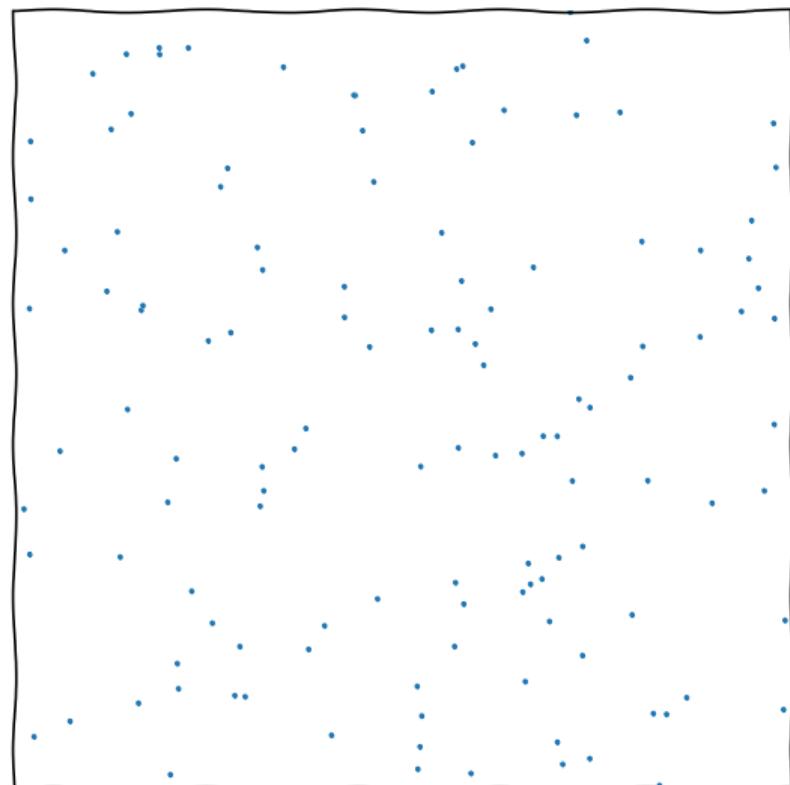




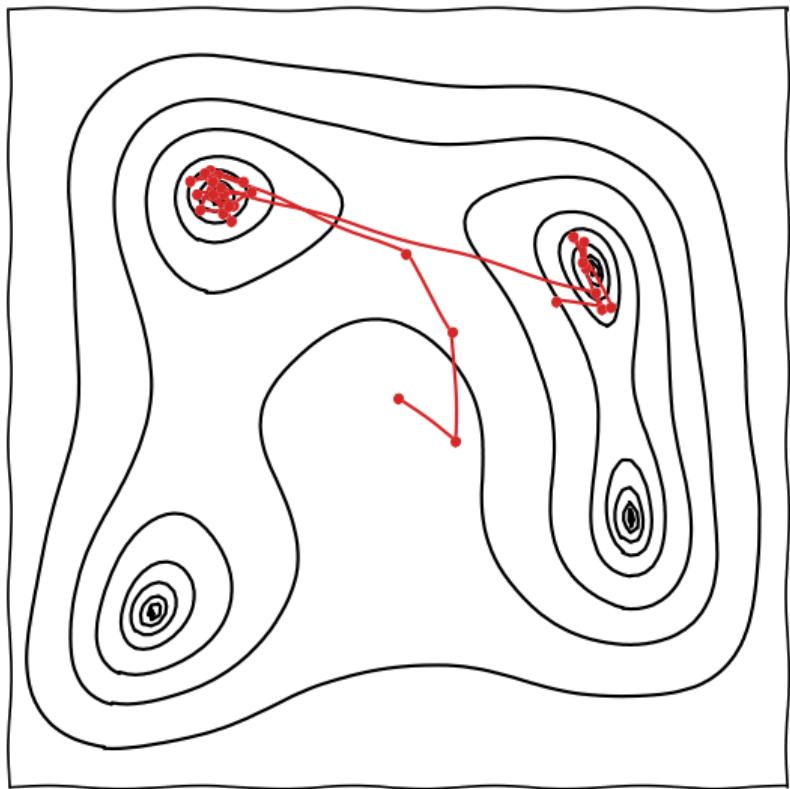
MCMC



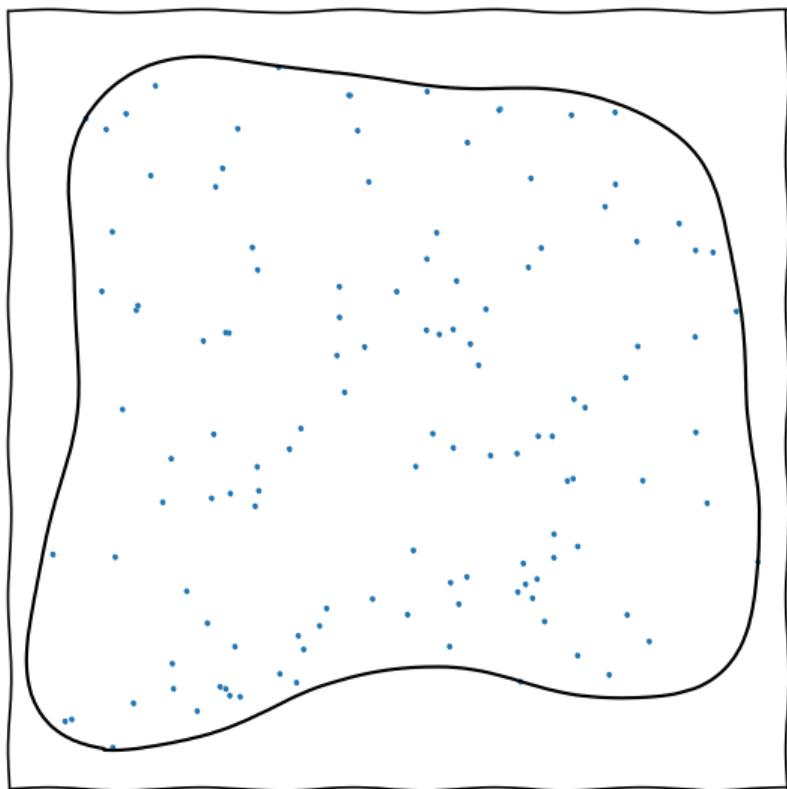
Nested sampling



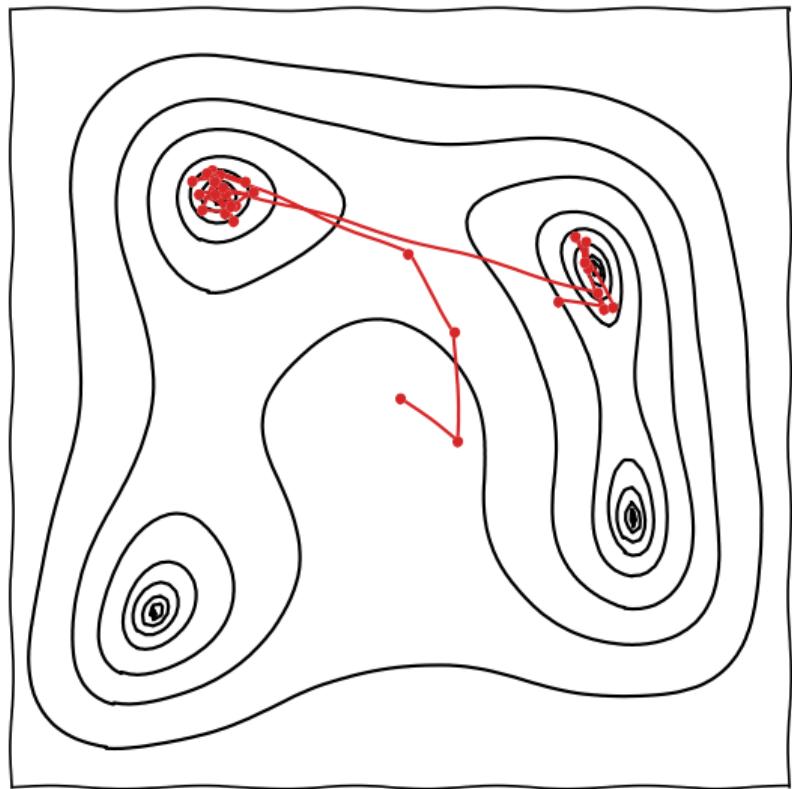
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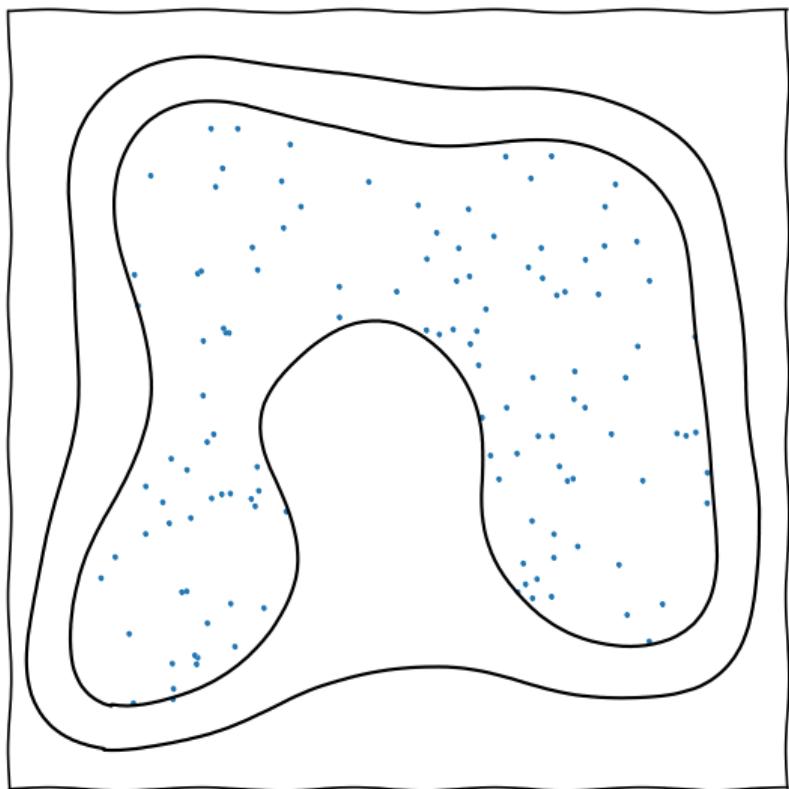
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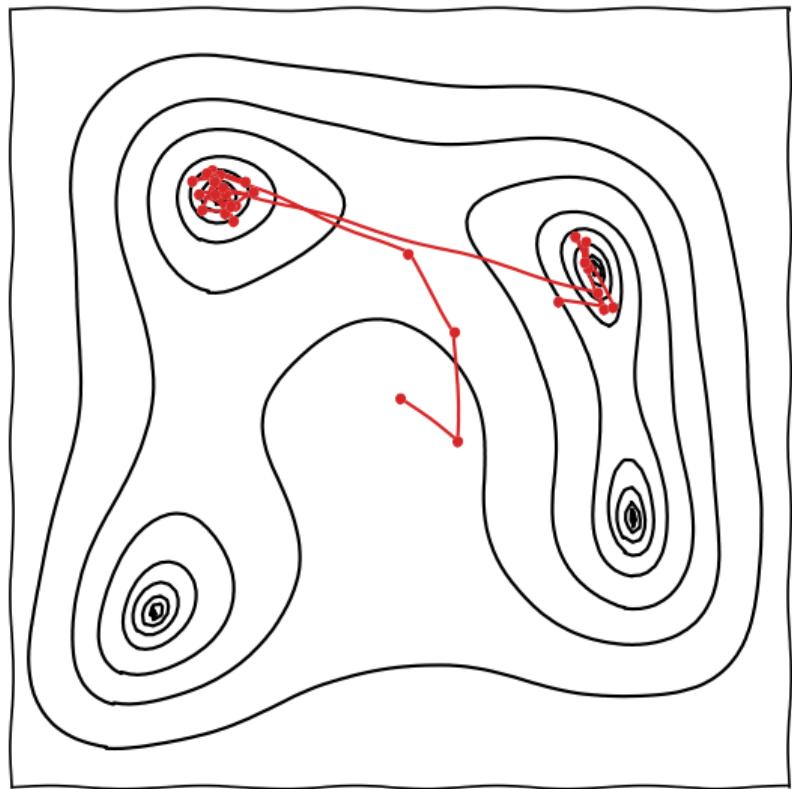
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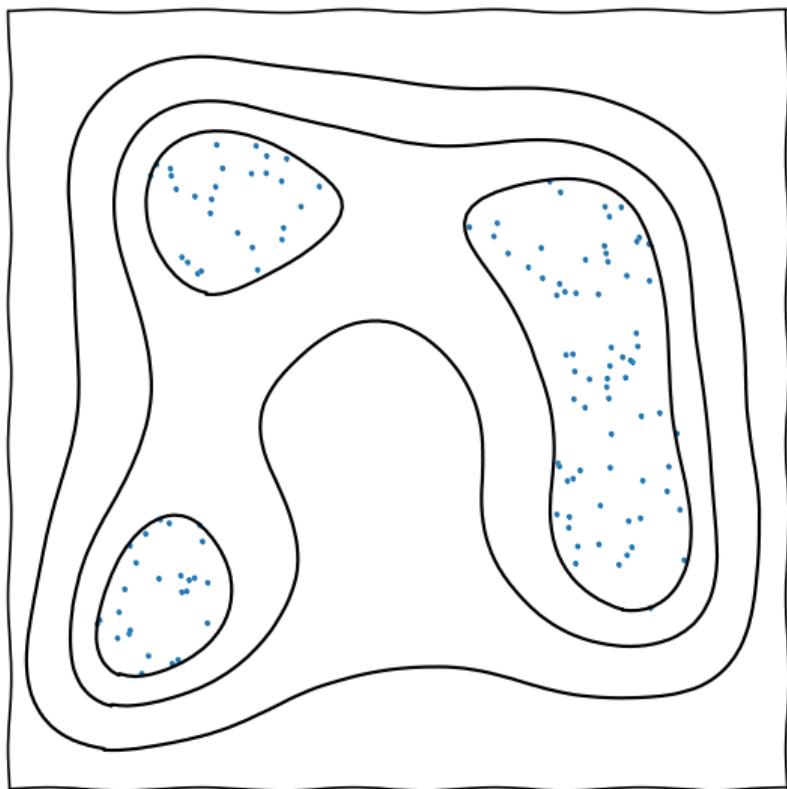
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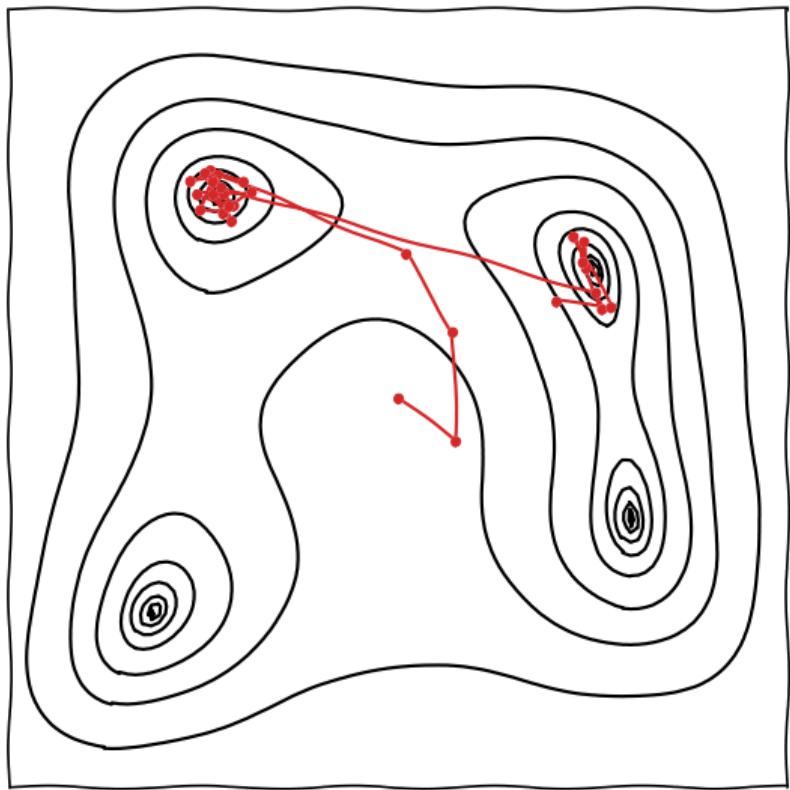
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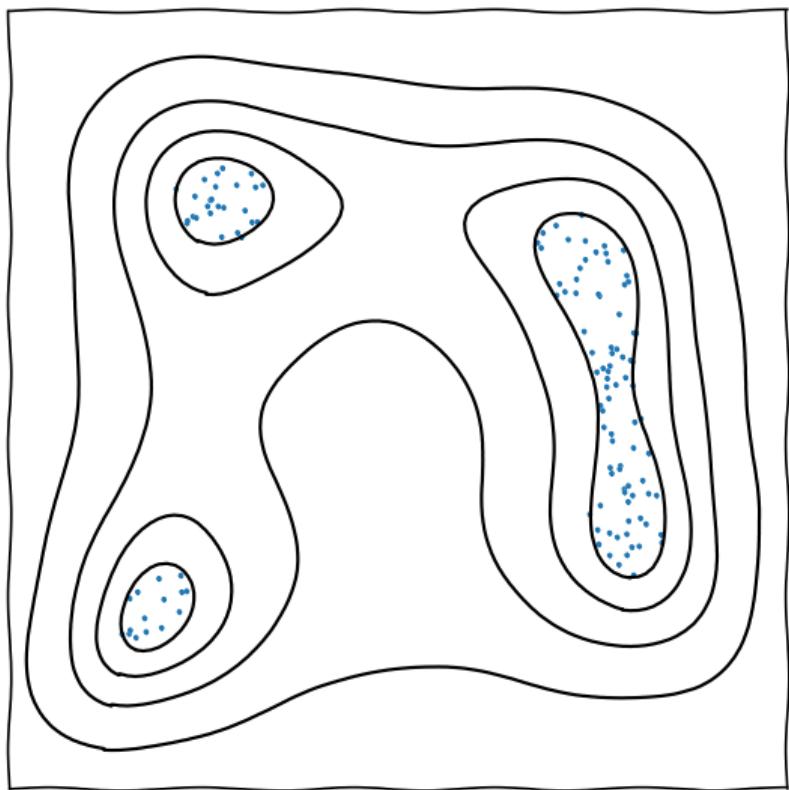
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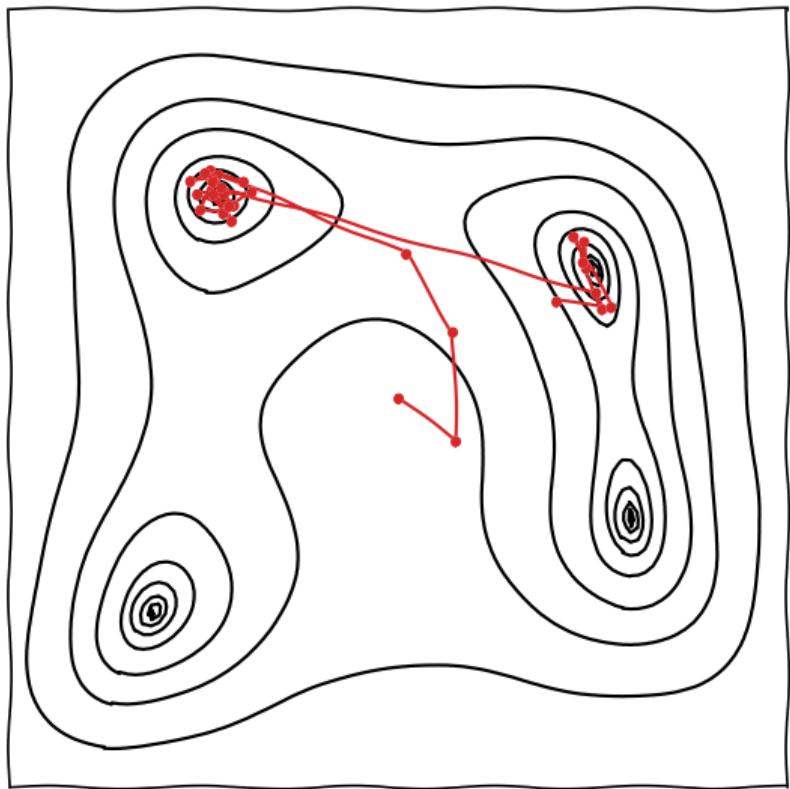
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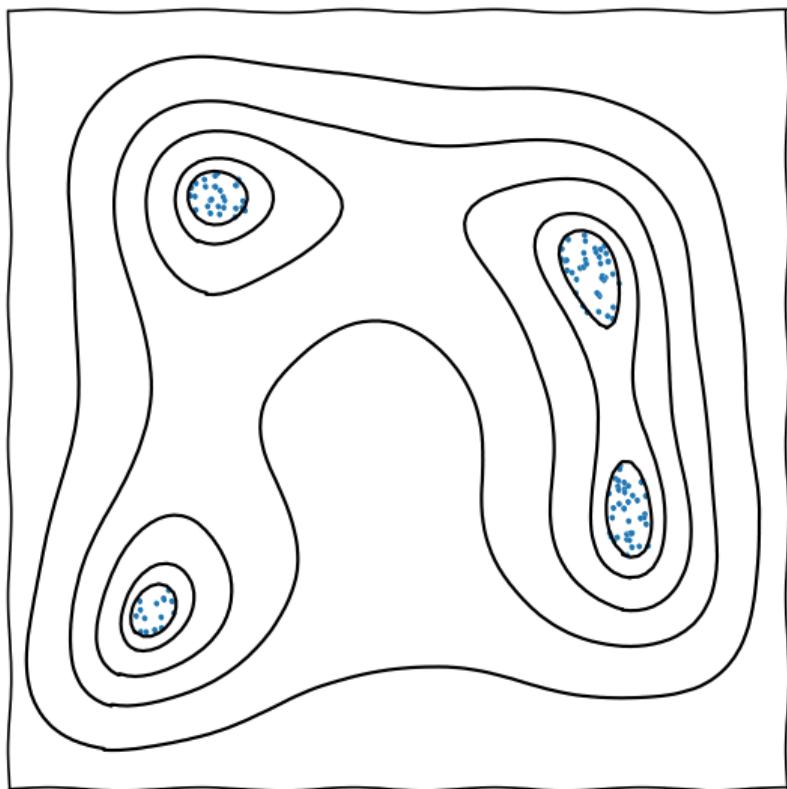
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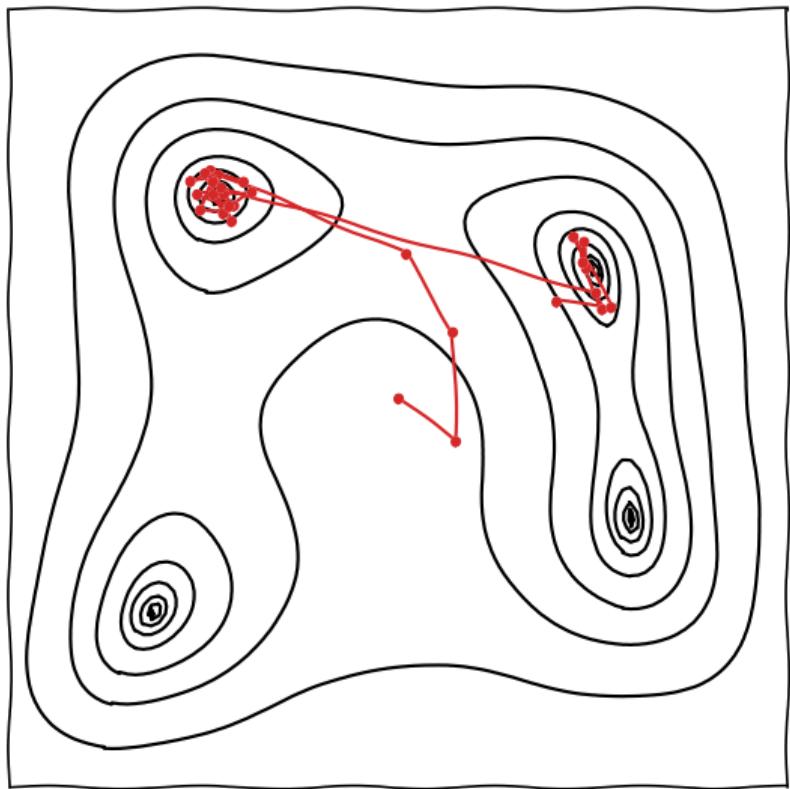
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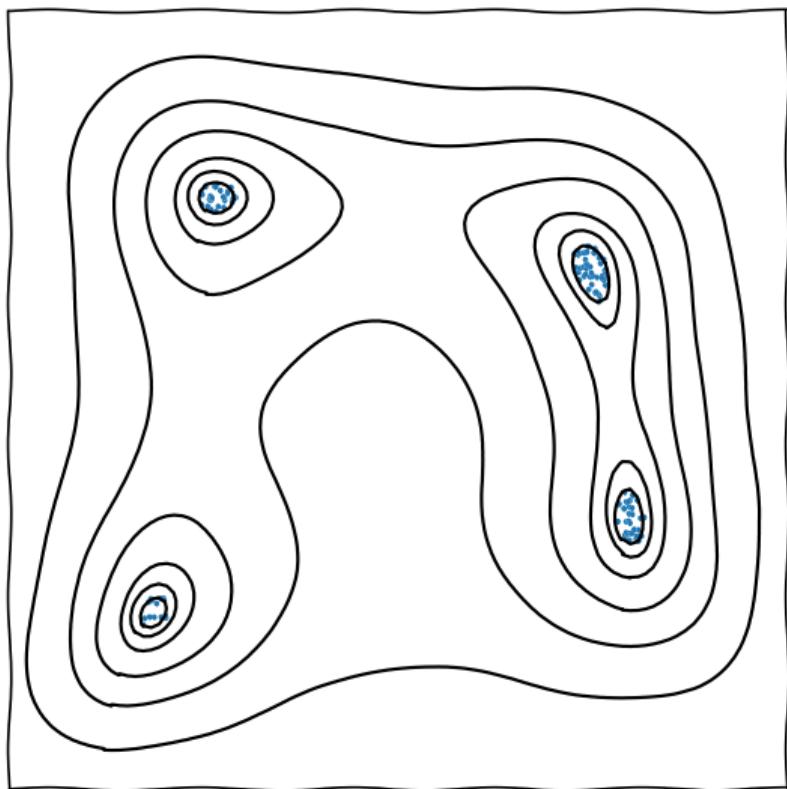
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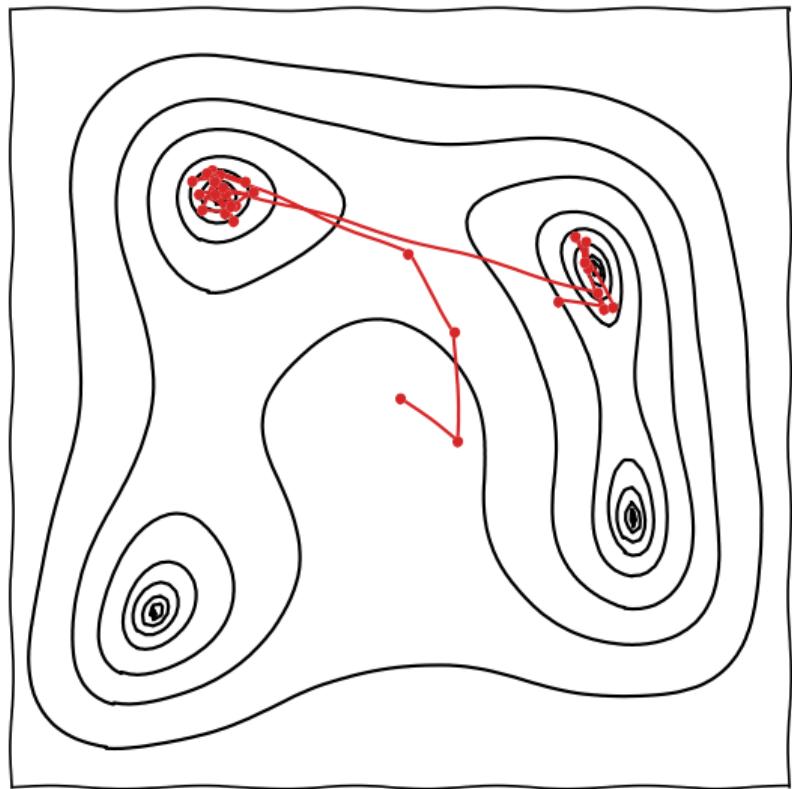
MCMC



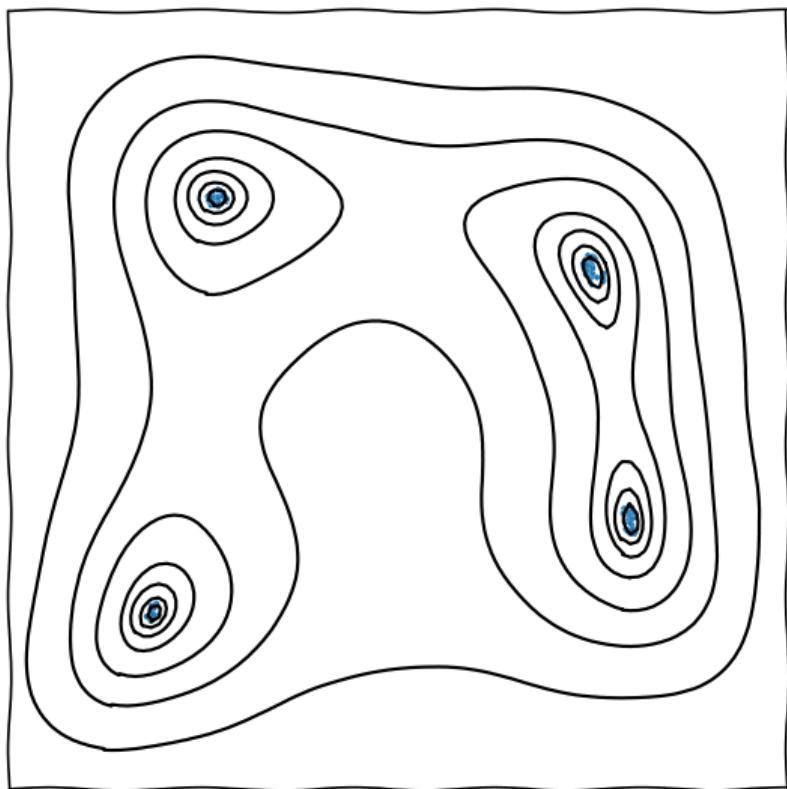
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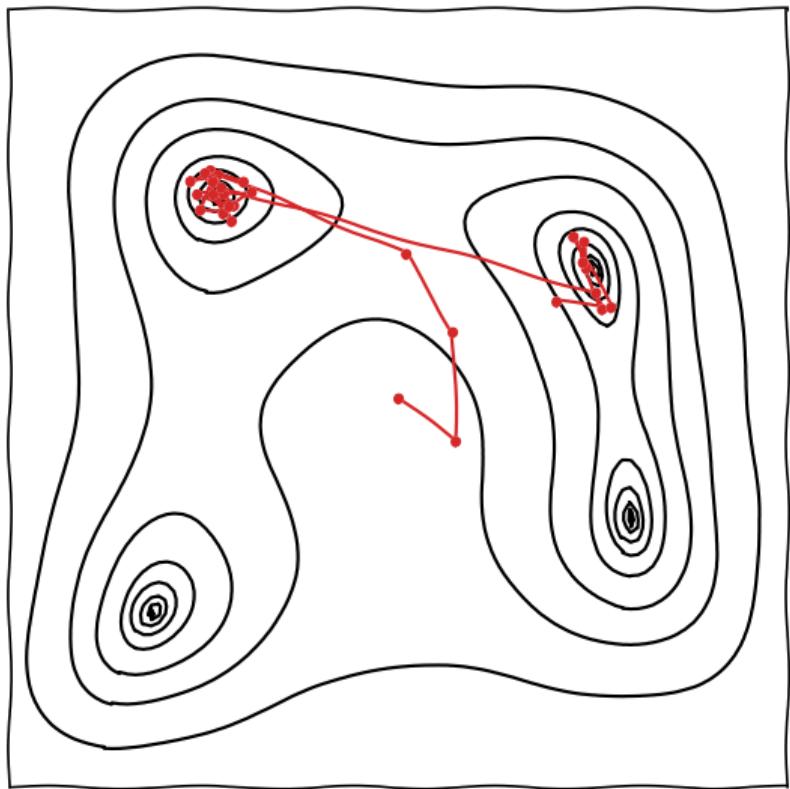
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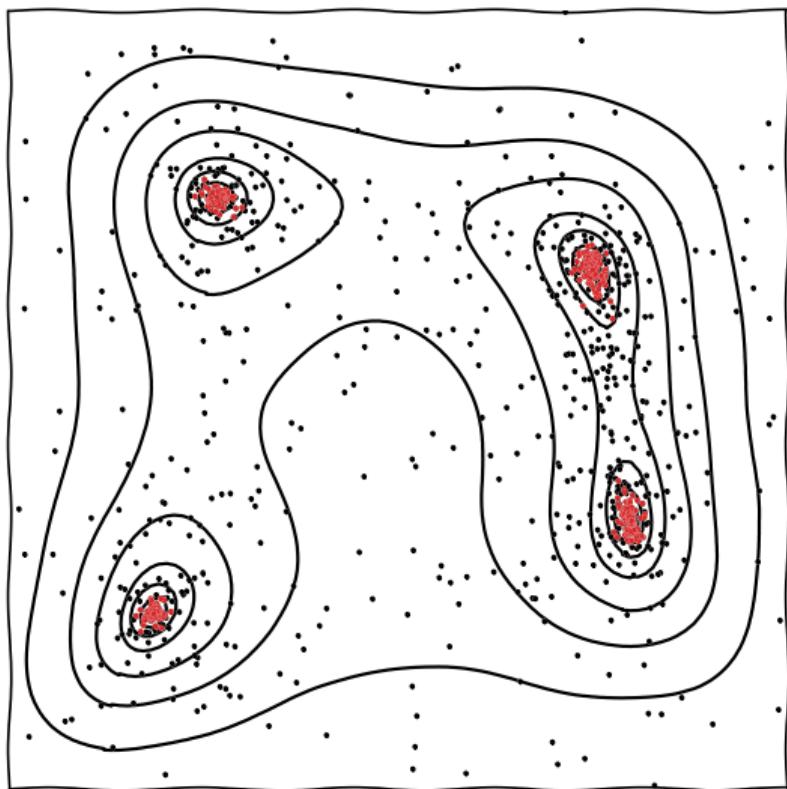
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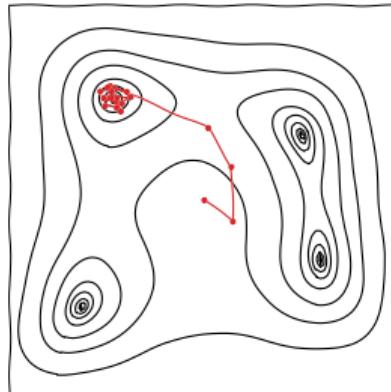


Nested sampling



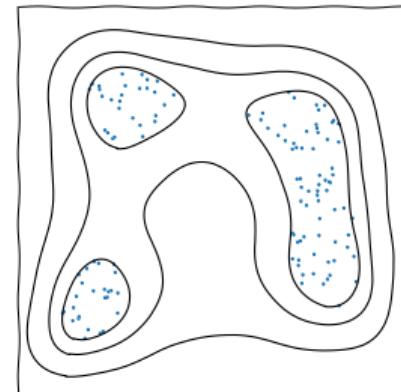
MCMC

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



Nested sampling

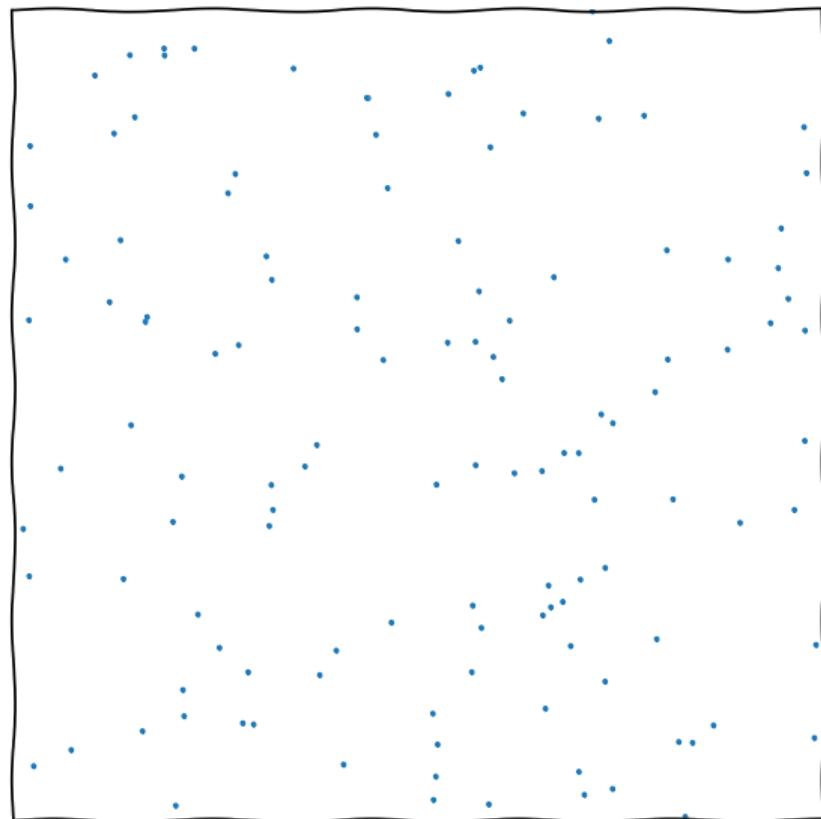
- ▶ Ensemble of “live points”
- ▶ Scans from prior to peak of likelihood
- ▶ Slower, no tuning required
- ▶ Parameter estimation, model comparison, tension quantification
- ▶ Channel capacity optimised for computing partition function



The nested sampling meta-algorithm

- ▶ Start with n random samples over the space.
- ▶ Delete outermost sample, and replace with a new random one at higher integrand value.
- ▶ The “live points” steadily contract around the peak(s) of the function.
- ▶ We can use this evolution to estimate volume *probabilistically*.
- ▶ At each iteration, the contours contract by $\sim \frac{1}{n}$ of their volume.
- ▶ This is an exponential contraction, so

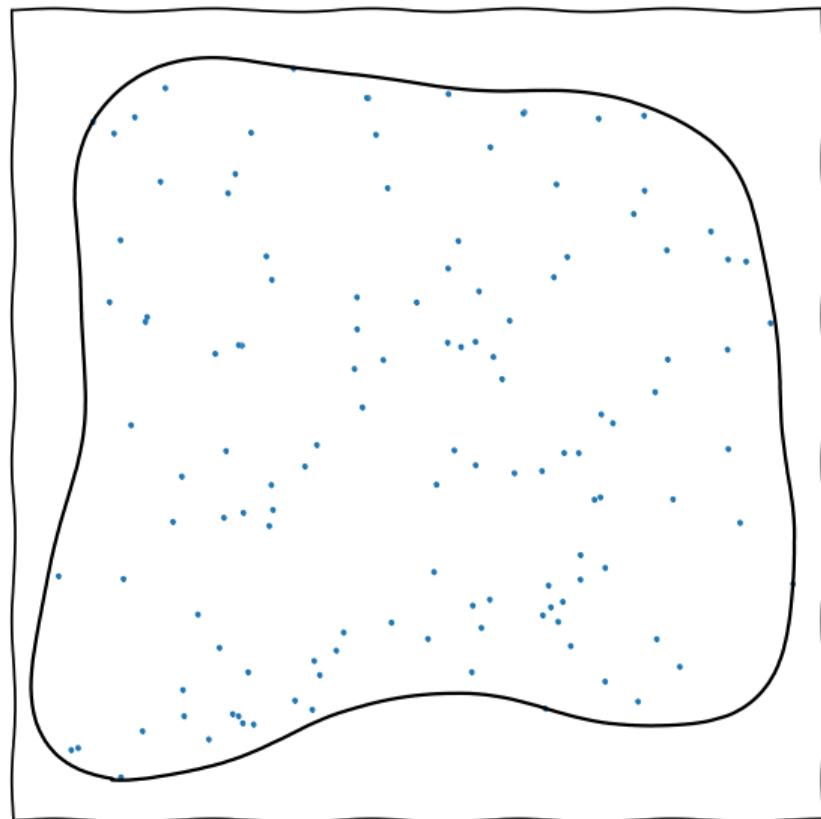
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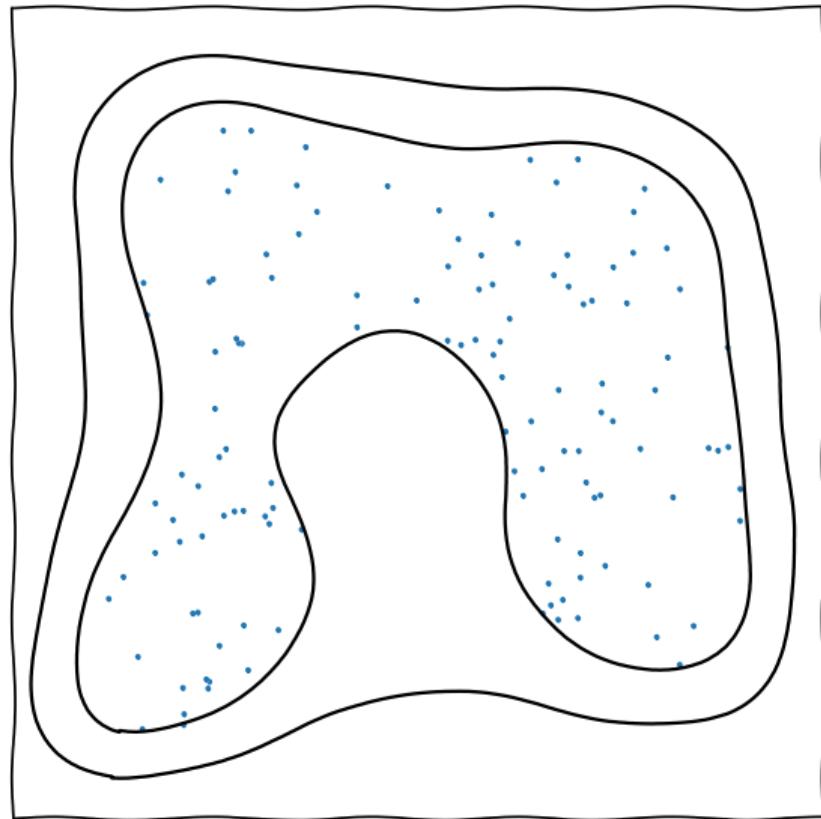
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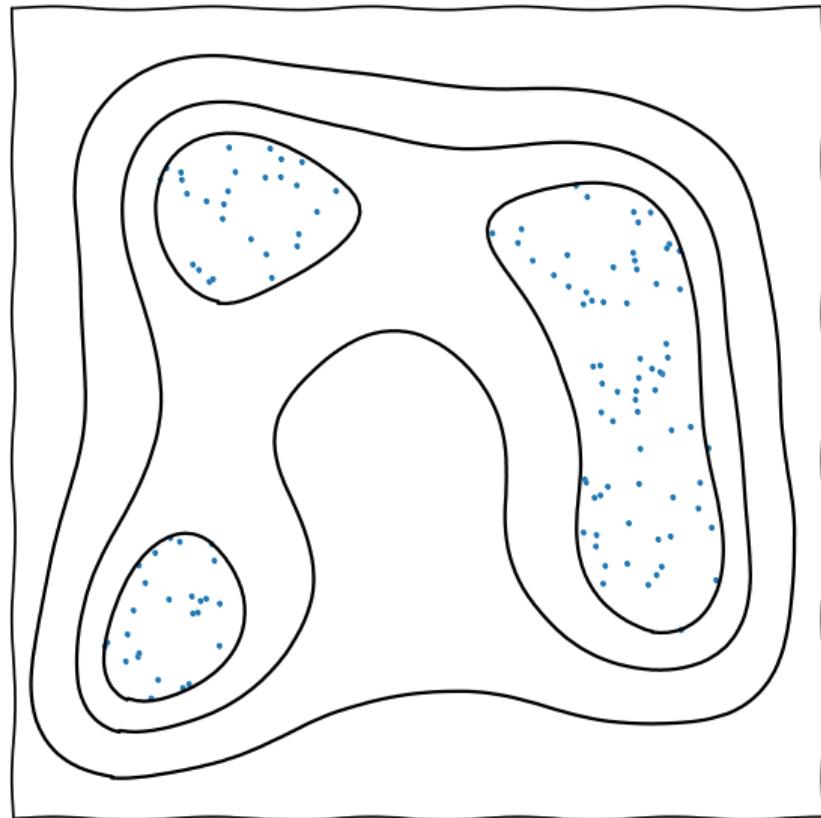
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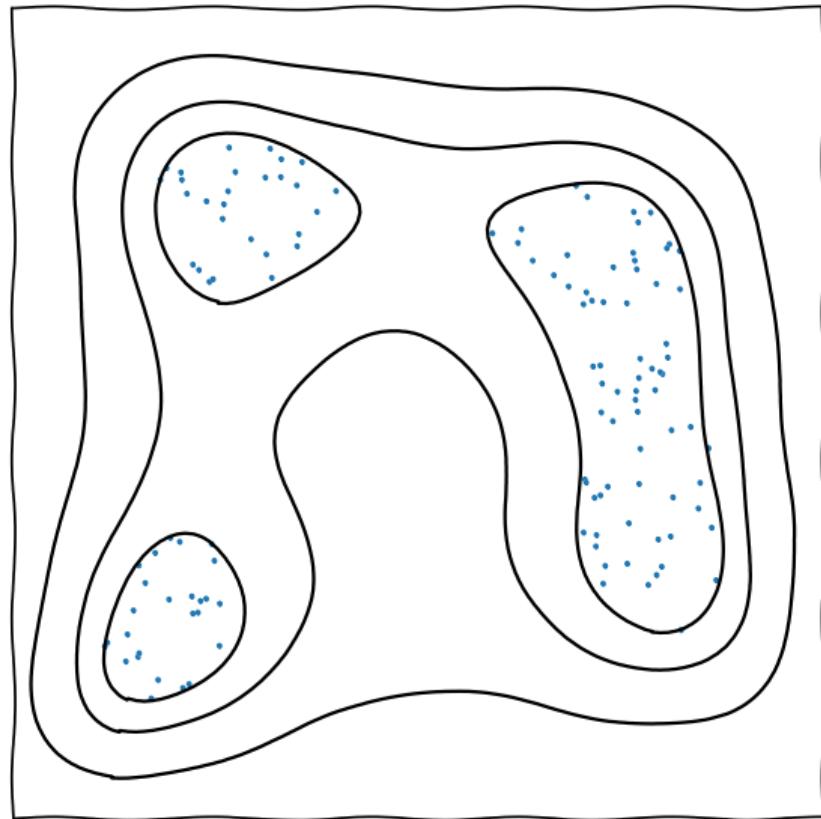
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$$\int f(x)dV \approx \sum_i f(x_i)\Delta V_i, \quad V_i = V_0 e^{-(i \pm \sqrt{i})/n}$$

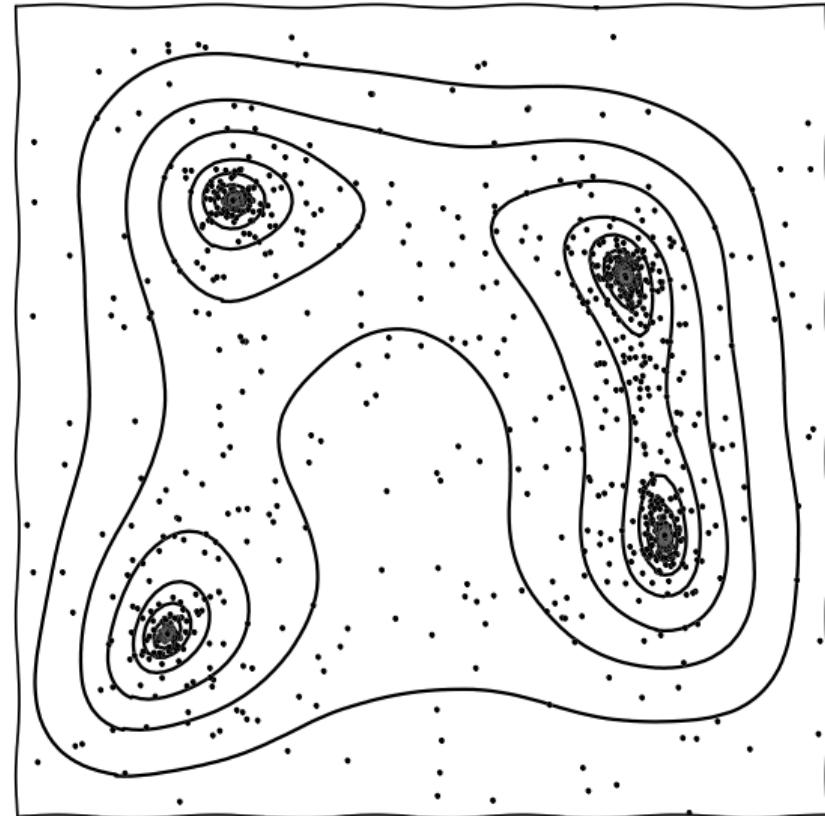


The nested sampling meta-algorithm: Lebesgue integration

- ▶ At the end, one is left with a set of discarded “dead” points.
- ▶ Can be weighted to form posterior samples, prior samples, or anything in between.
- ▶ Nested sampling estimates the **density of states** and calculates partition functions

$$Z(\beta) = \sum_i f(x_i)^\beta \Delta V_i.$$

- ▶ The evolving ensemble of live points allows:
 - ▶ implementations to self-tune
 - ▶ exploration of multimodal functions
 - ▶ global and local optimisation



Sampling from a hard likelihood constraint

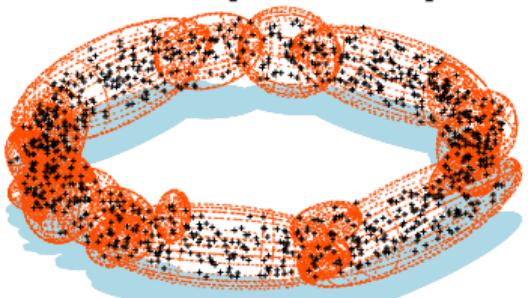
"It is not the purpose of this introductory paper to develop the technology of navigation within such a volume. We merely note that exploring a hard-edged likelihood-constrained domain should prove to be neither more nor less demanding than exploring a likelihood-weighted space."

— John Skilling

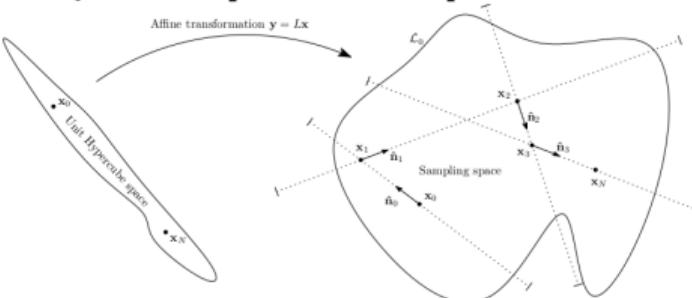
- ▶ A large fraction of the work in NS to date has been in attempting to implement a hard-edged sampler in the NS meta-algorithm $\{\theta \sim \pi : \mathcal{L}(\theta) > \mathcal{L}_*\}$.
- ▶ <https://projecteuclid.org/euclid.ba/1340370944>.
- ▶ There has also been much work beyond this (see 'Frontiers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

Implementations of Nested Sampling [2205.15570](NatReview)

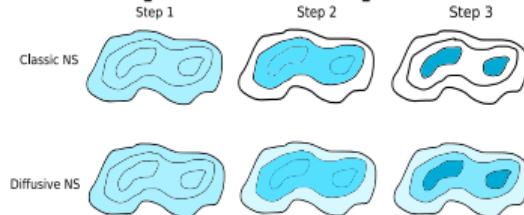
MultiNest [0809.3437]



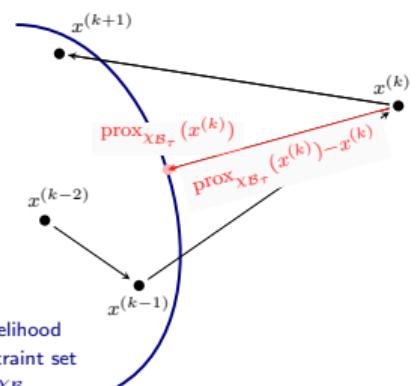
PolyChord [1506.00171]



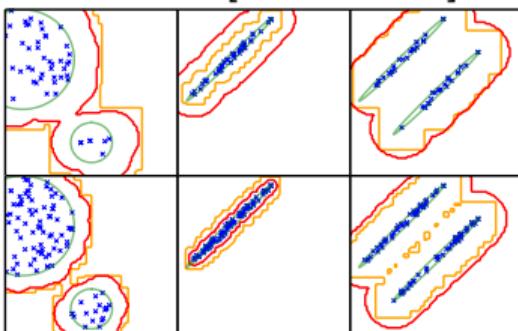
DNest [1606.03757]



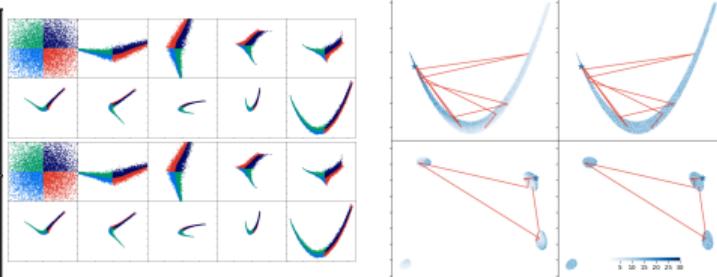
ProxNest [2106.03646]



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: The three pillars of Bayesian inference

Parameter estimation

What do the data tell us about the parameters of a model?
e.g. the size or age of a Λ CDM universe

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

$$\mathcal{P} = \frac{\mathcal{L} \times \pi}{\mathcal{Z}}$$

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

Model comparison

How much does the data support a particular model?
e.g. Λ CDM vs a dynamic dark energy cosmology

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

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

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

Tension quantification

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

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

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

Applications of nested sampling

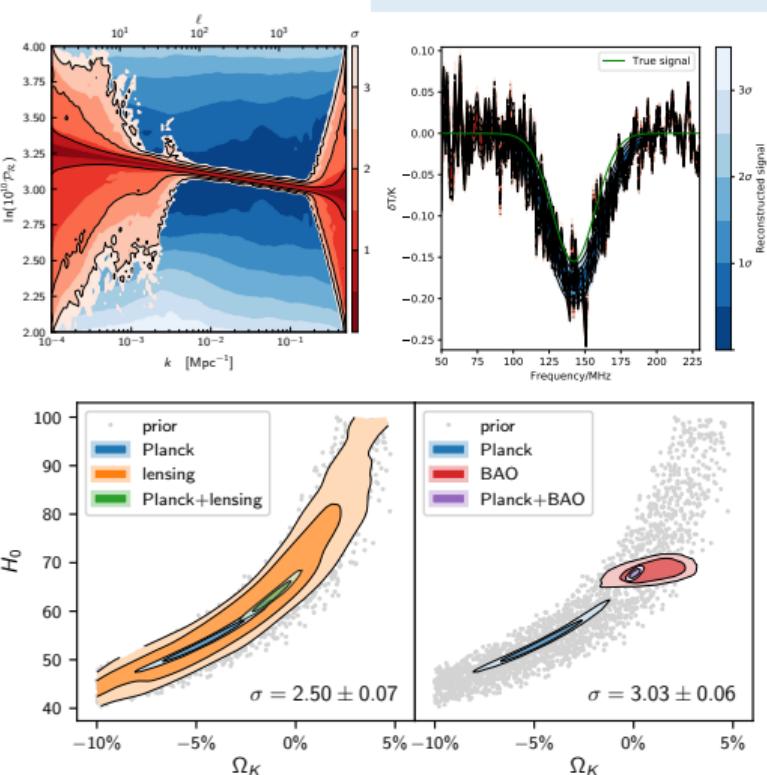
Adam Ormondroyd



PhD

Cosmology

- ▶ Battle-tested in Bayesian cosmology on
 - ▶ Parameter estimation: multimodal alternative to MCMC samplers.
 - ▶ Model comparison: using integration to compute the Bayesian evidence
 - ▶ Tension quantification: using deep tail sampling and suspiciousness computations.
- ▶ Plays a critical role in major cosmology pipelines: Planck, DES, KiDS, BAO, SNe.
- ▶ The default 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

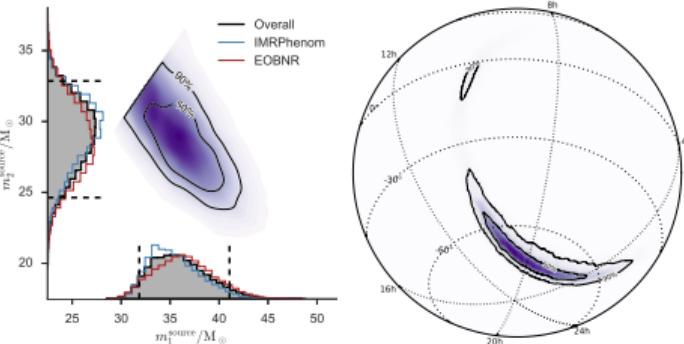
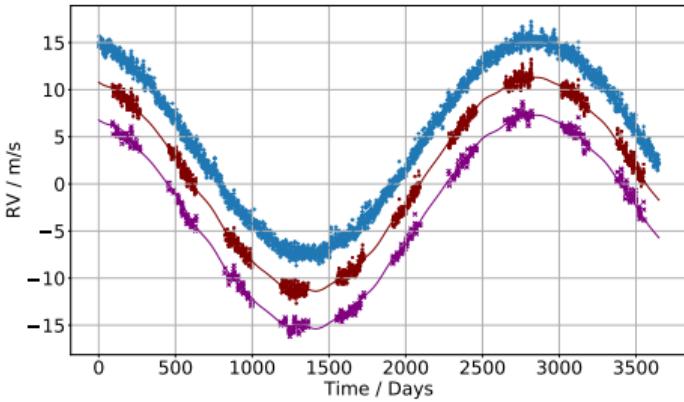
Metha Prathaban

PhD



Astrophysics

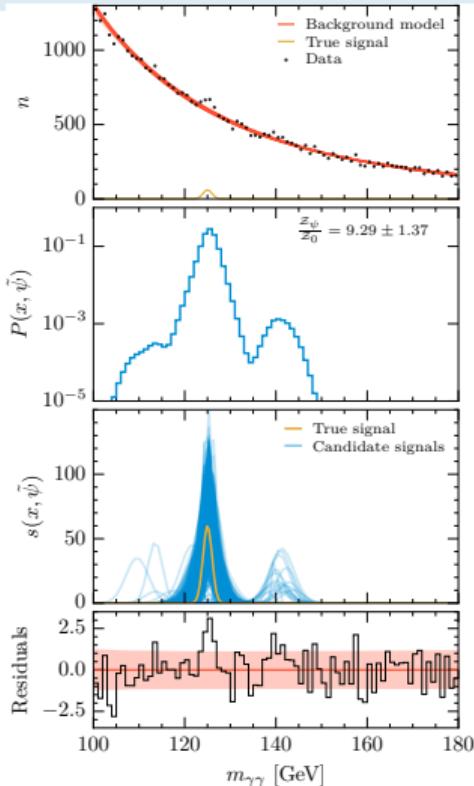
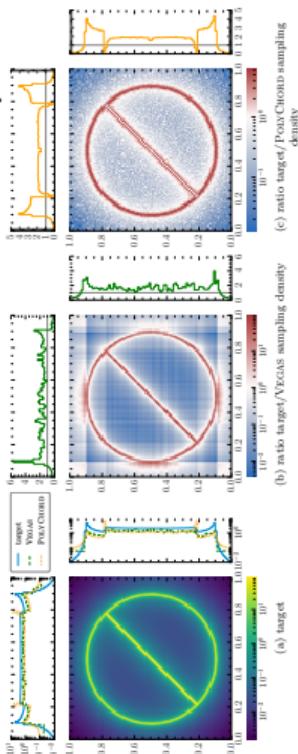
- ▶ In exoplanets [1806.00518]
 - ▶ Parameter estimation: determining properties of planets.
 - ▶ Model comparison: how many planets? Stellar modelling [2007.07278].
 - ▶ exoplanet problems regularly have posterior phase transitions [2102.03387]
- ▶ In gravitational waves
 - ▶ Parameter estimation: Binary merger properties
 - ▶ Model comparison: Modified theories of gravity, selecting phenomenological parameterisations [1803.10210]
 - ▶ Likelihood reweighting: fast slow properties



Applications of nested sampling

Particle physics

- ▶ 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].
- ▶ Fine tuning quantification
- ▶ Fast estimation of small p -values [2106.02056](PRL), just make switch:
 $X \leftrightarrow p, \mathcal{L} \leftrightarrow \lambda, \theta \leftrightarrow x.$



David Yallup

PDRA



Applications of nested sampling

Lattice field theory

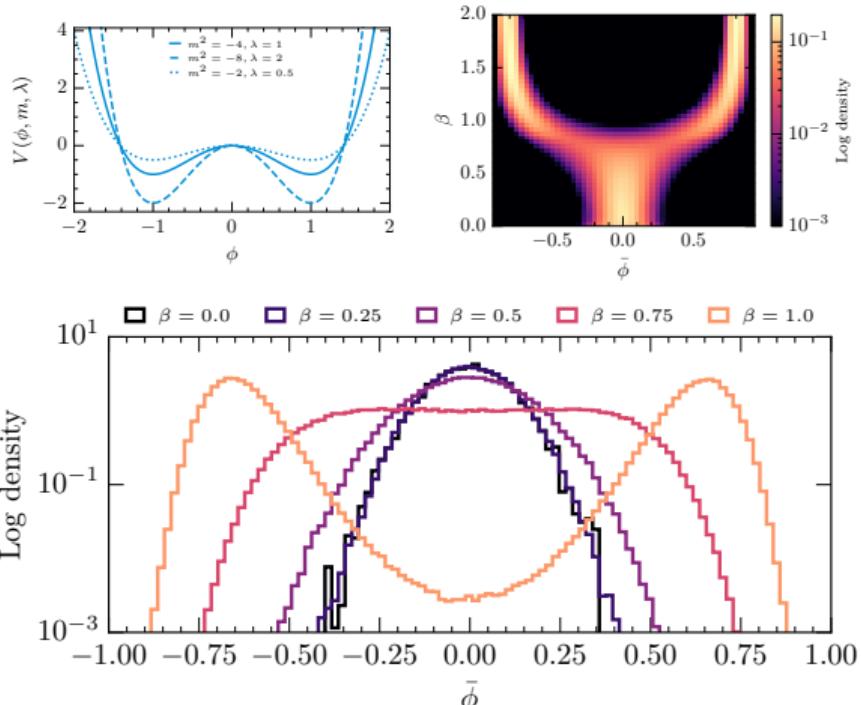
- ▶ Consider standard field theory Lagrangian:

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

- ▶ Discretize onto spacetime grid.
- ▶ Compute partition function
- ▶ NS unique traits:
 - ▶ Get full partition function for free
 - ▶ allows for critical tuning
 - ▶ avoids critical slowing down
- ▶ Applications in lattice gravity, QCD, condensed matter physics
- ▶ Publication imminent (next week)

David Yallup

PDRA

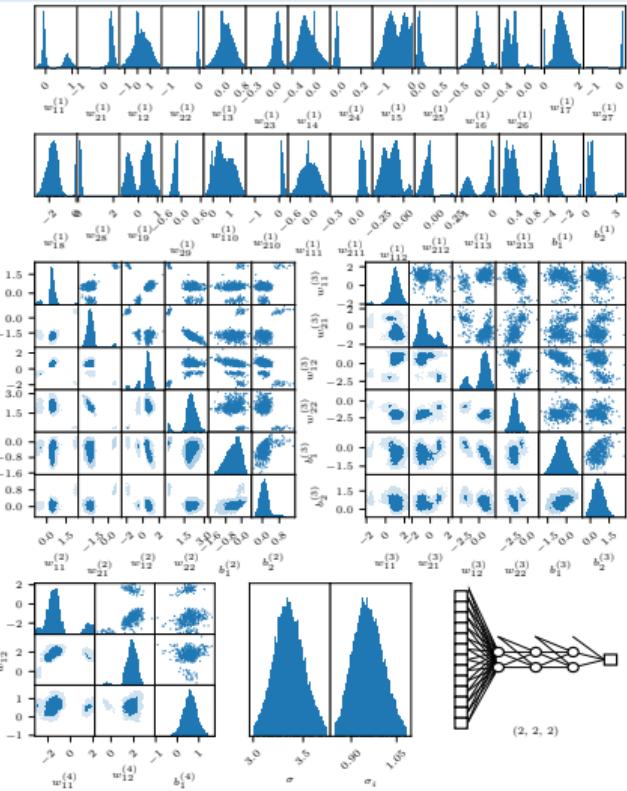




Applications of nested sampling

Machine learning

- ▶ Machine learning requires:
 - ▶ Training to find weights
 - ▶ Choice of architecture/topology/hyperparameters
- ▶ Bayesian NNs treat training as a model fitting problem
- ▶ Compute posterior of weights (parameter estimation), rather than optimisation (gradient descent)
- ▶ Use evidence to determine best architecture (model comparison), correlates with out-of-sample performance!
- ▶ Solving the full “shallow learning” problem without compromise [2004.12211][2211.10391].
 - ▶ Promising work ongoing to extend this to transfer learning and deep nets.
- ▶ More generally, dead points are optimally spaced for training traditional ML approaches e.g. [2309.05697]



Applications of nested sampling

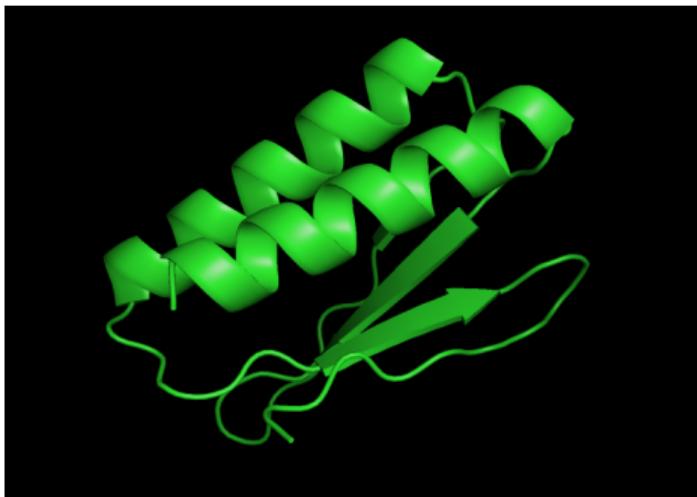
And beyond...

Catherine Watkinson

Senior Data Scientist



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



Applications of nested sampling

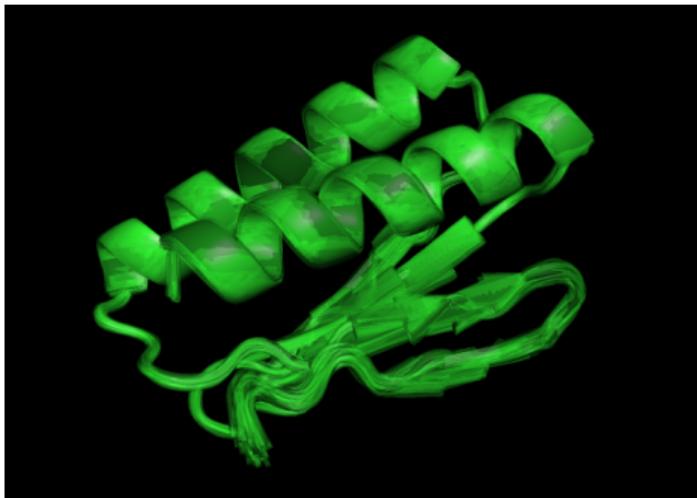
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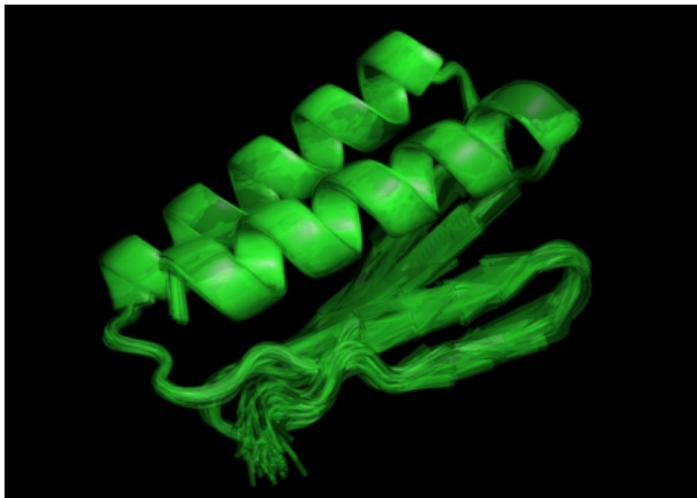
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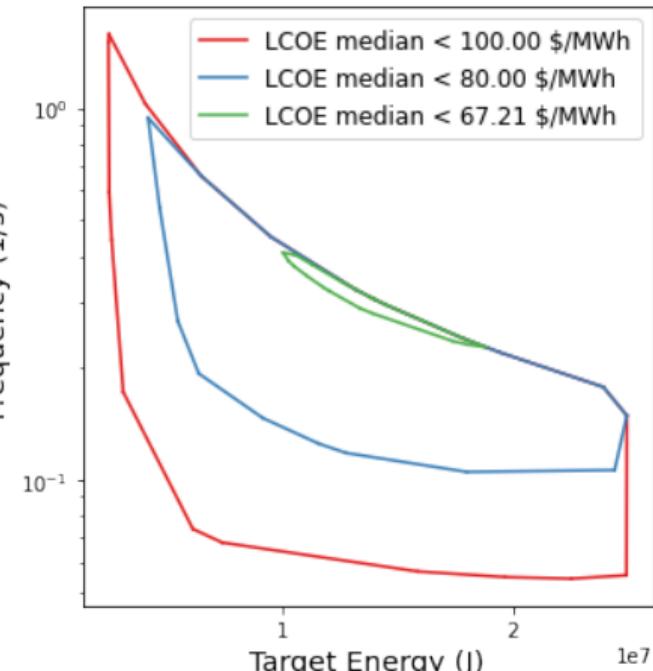
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Applications of nested sampling

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PhD → Data Scientist



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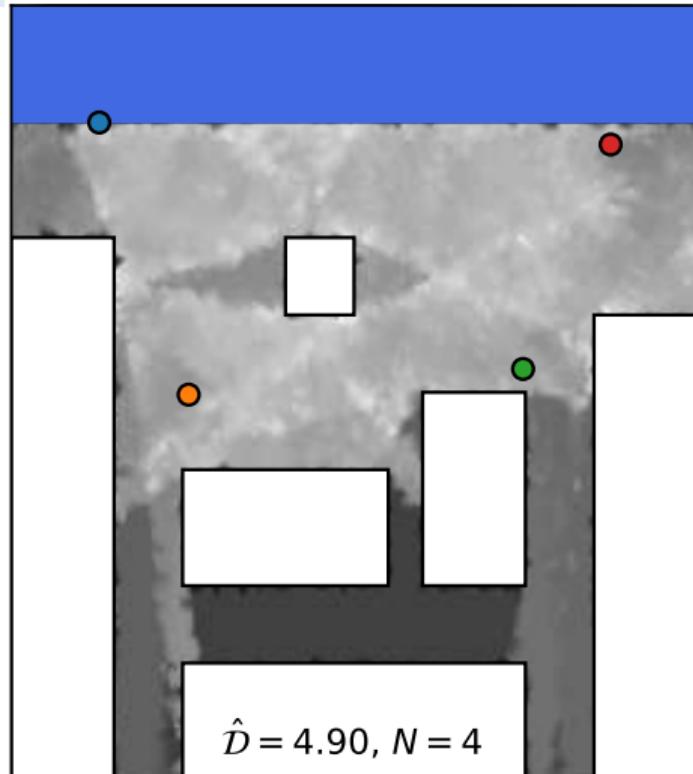
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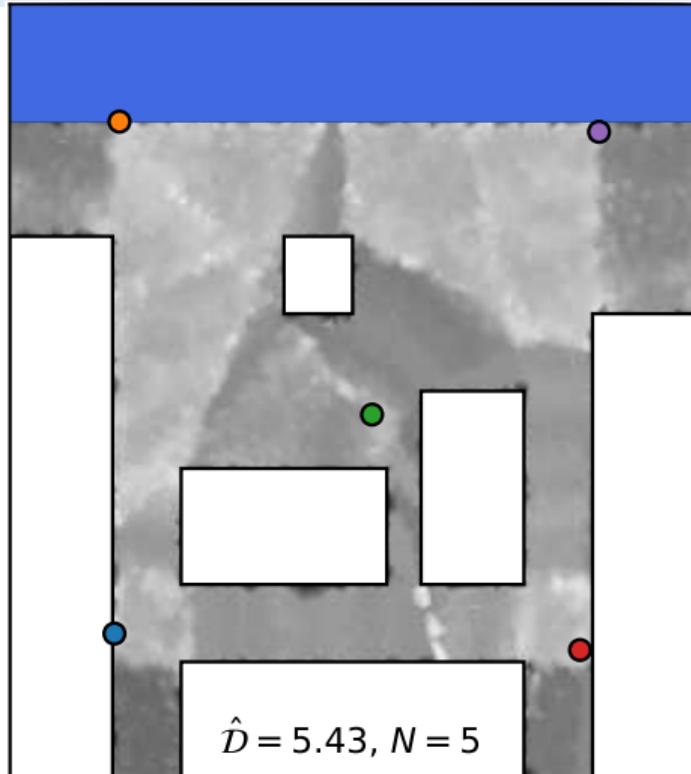
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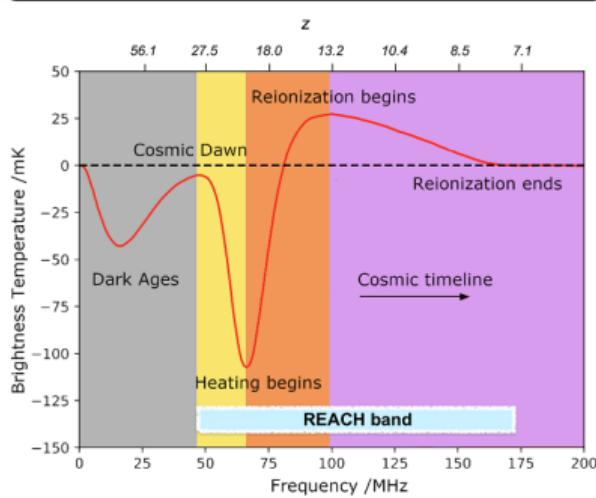
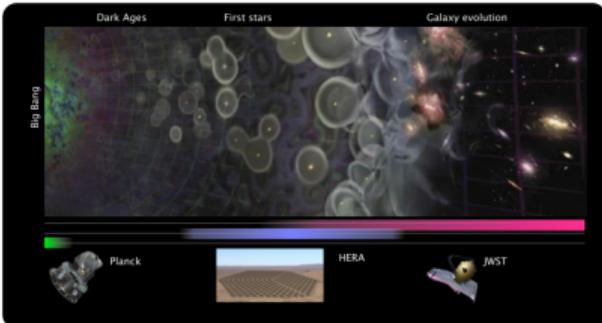
REACH: Global 21cm cosmology [2210.07409](NatAstro)

Ian Roque

PhD

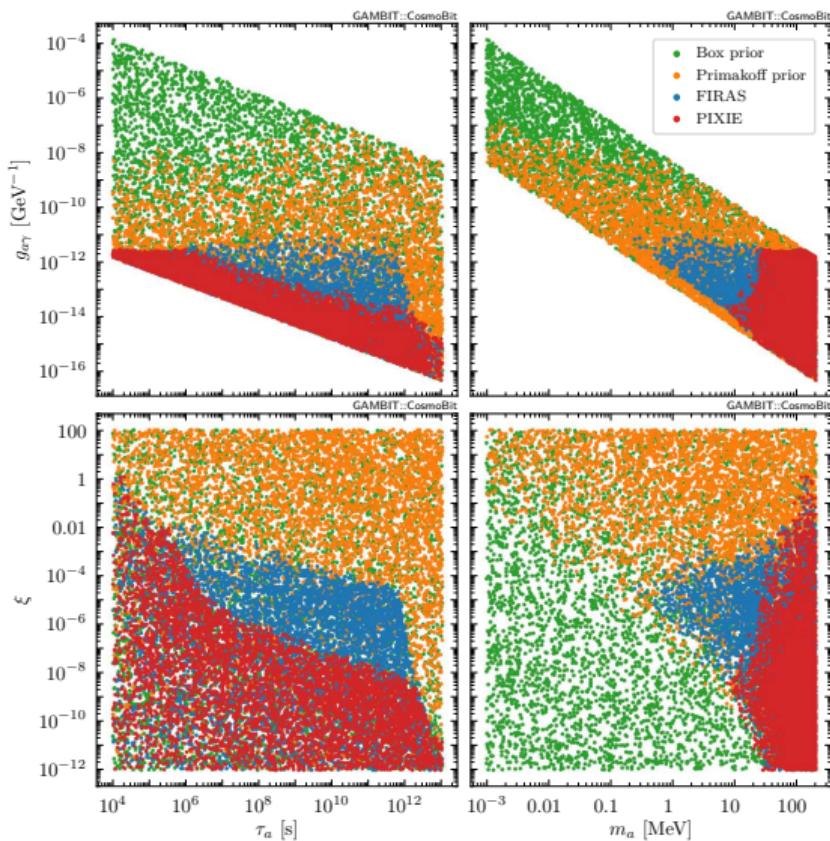


- ▶ Imaging the universal dark ages using CMB backlight.
- ▶ 21cm hyperfine line emission from neutral hydrogen.
- ▶ Global experiments measure monopole across frequency.
- ▶ Challenge: science hidden in foregrounds $\sim 10^4 \times$ signal.
- ▶ Lead data analysis team (REACH first light in January)
- ▶ Nested sampling woven in from the ground up (calibrator, beam modelling, signal fitting, likelihood selection).
- ▶ All treated as parameterised model comparison problems.



GAMBIT: combining particle physics & cosmological data

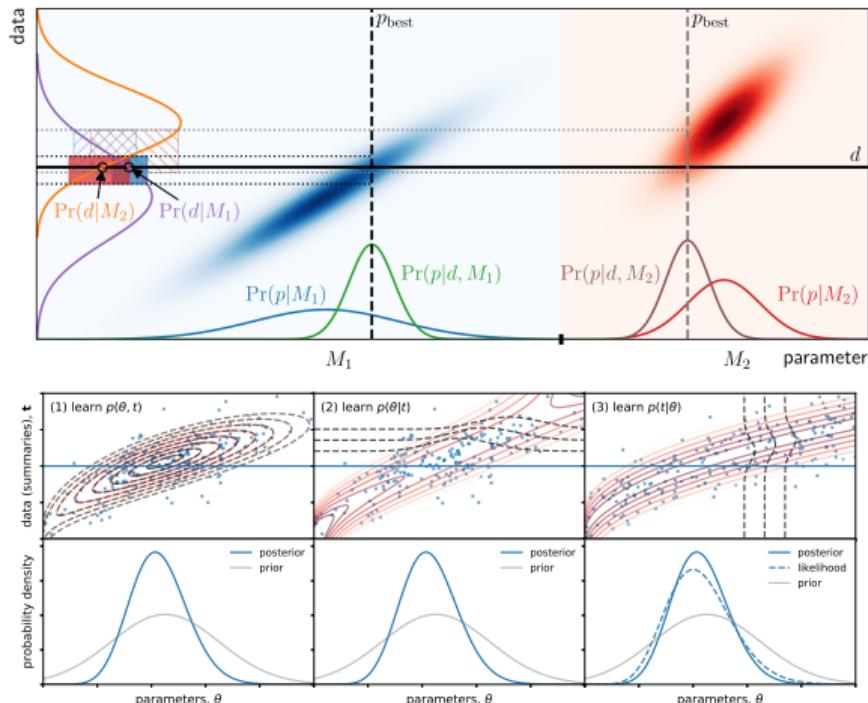
- ▶ Multinational team of particle physicists, cosmologists and statisticians.
- ▶ Combine cosmological data, particle colliders, direct detection, & neutrino detectors in a statistically principled manner [2205.13549].
- ▶ Lead Cosmo/Dark Matter working group [2009.03286].
- ▶ Nested sampling used for global fitting, and fine-tuning quantification [2101.00428]





Likelihood-free inference (aka SBI)

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



unimpeded: PLA for the next generation

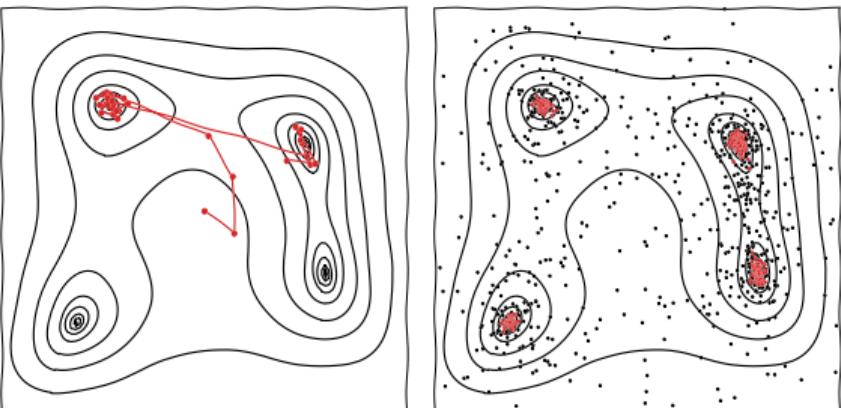
Harry Bevins



PhD→JRF

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

DiRAC



CosmoTension

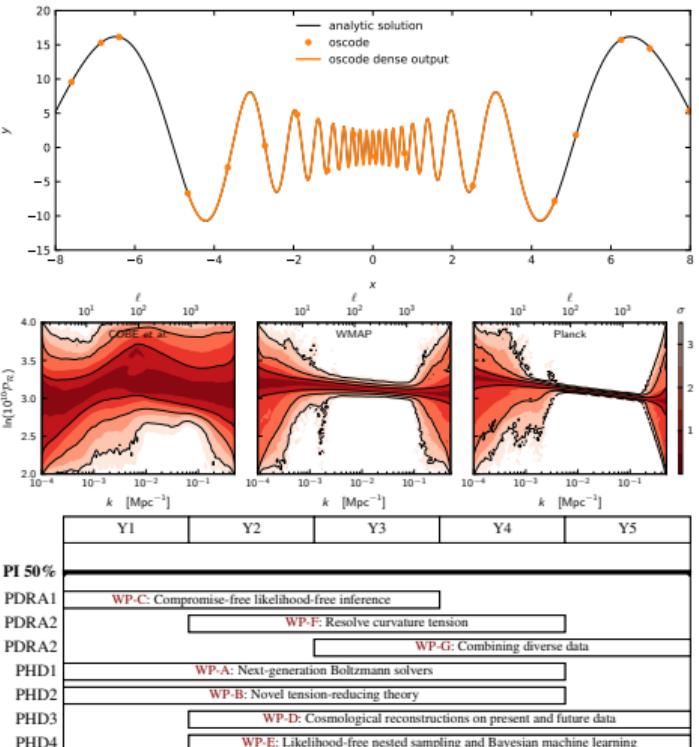
Resolving cosmological tensions with diverse data, novel theories and Bayesian machine learning

Will Barker

PhD→JRF



- ▶ ERC grant ⇒ UKRI Frontier, commencing 2023.
- ▶ Funds 3 PDRAs and 4 PhDs over 5 years.
- ▶ Research programme centered around combining novel theories of gravity, Boltzmann solvers [1906.01421], reconstruction [1908.00906], nested sampling & likelihood free inference.
- ▶ Aims to disentangle cosmological tensions H_0 , σ_8 , Ω_K with next-generation data analysis techniques.



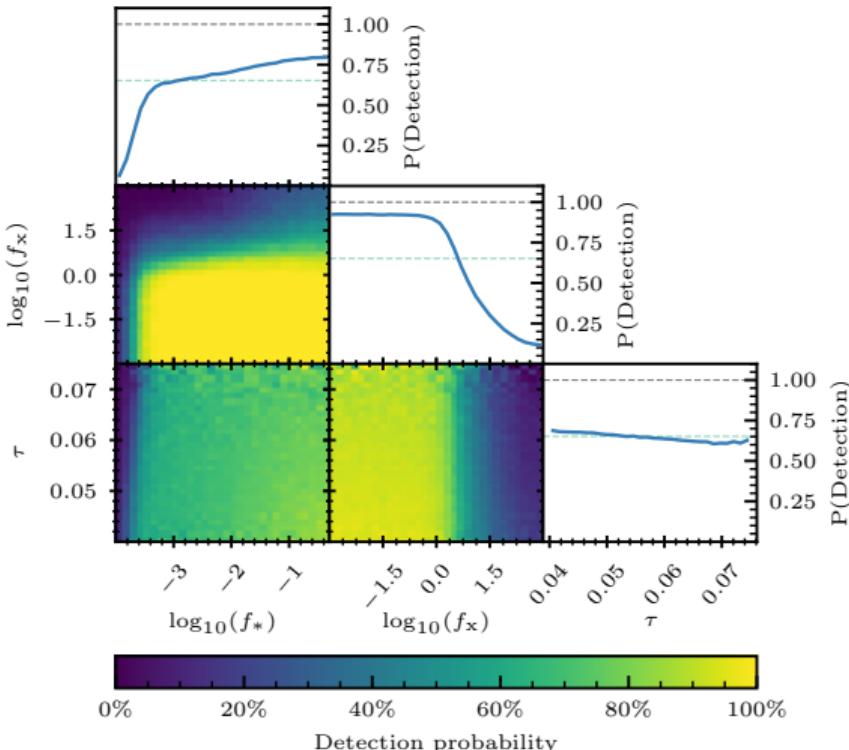
Fully Bayesian Forecasting [2309.06942]

Thomas Gessey-Jones



PhD

- ▶ Experimental design necessitates forecasting the constraints that future data might give.
- ▶ Have you ever done a Fisher forecast, and then felt Bayesian guilt?
- ▶ Simulation based inference gives us the language to marginalise over parameters θ and possible future data D .
- ▶ Evidence networks [2305.11241] (Jeffreys & Wandelt) give us the ability to do this at scale in the case of forecasting.
- ▶ Can answer questions such as “Given current knowledge/theoretical uncertainty $\pi(\theta)$, how probable is a detection?”
- ▶ Re-usable package: prescience

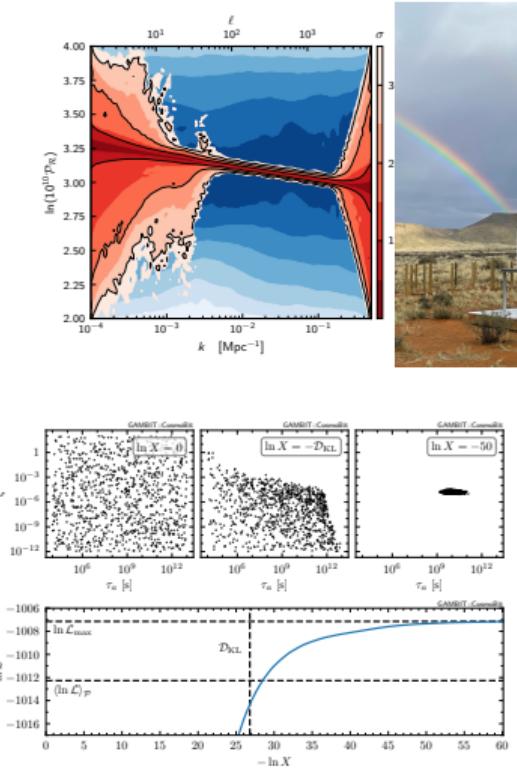
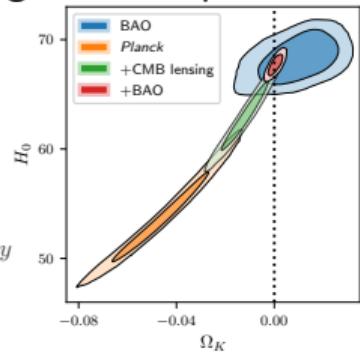
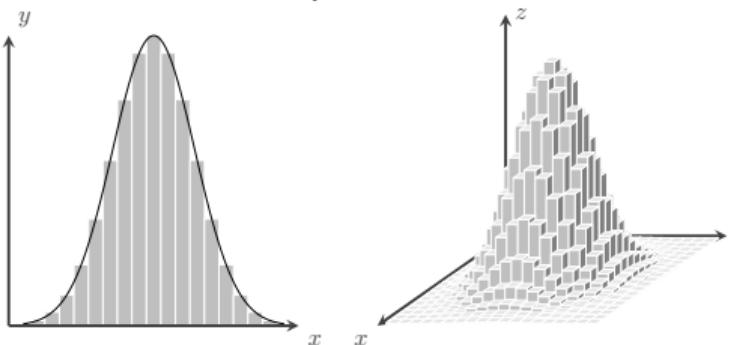


Conclusions

github.com/handley-lab



- ▶ Nested sampling is a multi-purpose numerical tool for:
 - ▶ Numerical integration $\int f(x)dV$,
 - ▶ Exploring/scanning/optimising *a priori* unknown functions,
 - ▶ Performing Bayesian inference and model comparison.
- ▶ It is applied widely across cosmology, particle physics & machine learning.
- ▶ It's unique traits as the only numerical Lebesgue integrator mean with compute it will continue to grow in importance.



How does Nested Sampling compare to other approaches?

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

Optimisation

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

Sampling

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

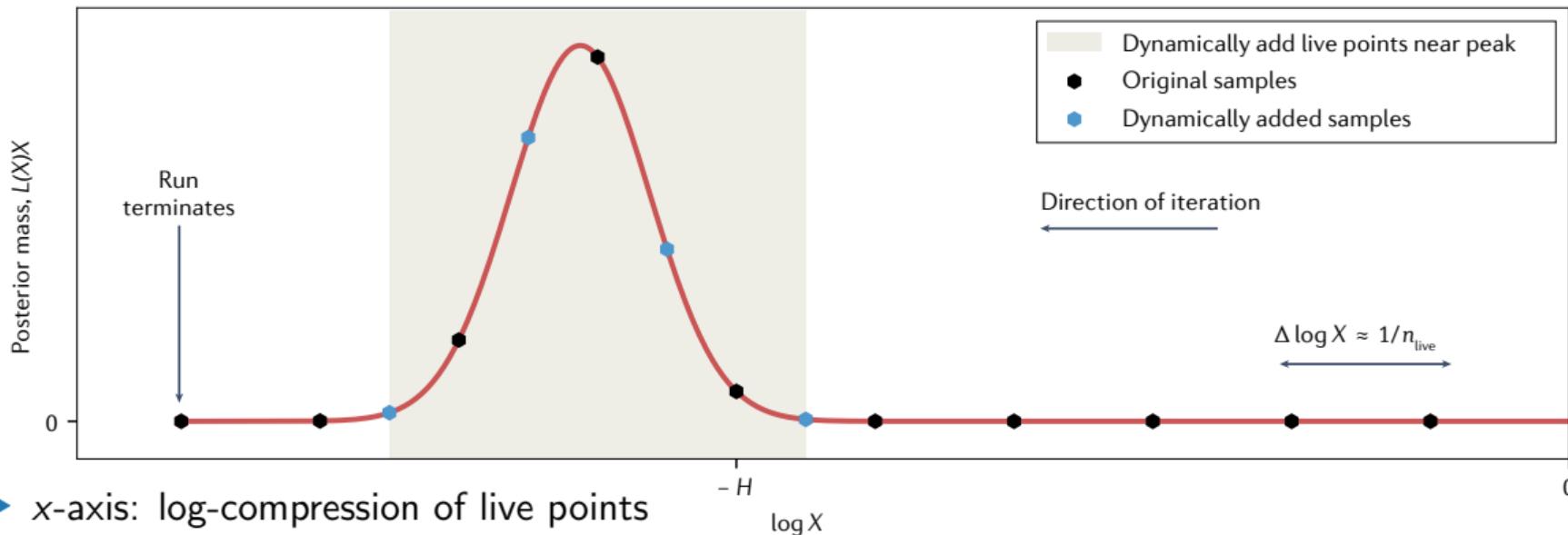
Integration

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

Nested Sampling: a user's guide

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

Time complexity of nested sampling



► Time complexity

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

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

Occam's Razor [2102.11511]

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

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

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

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

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

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

Kullback Liebler divergence

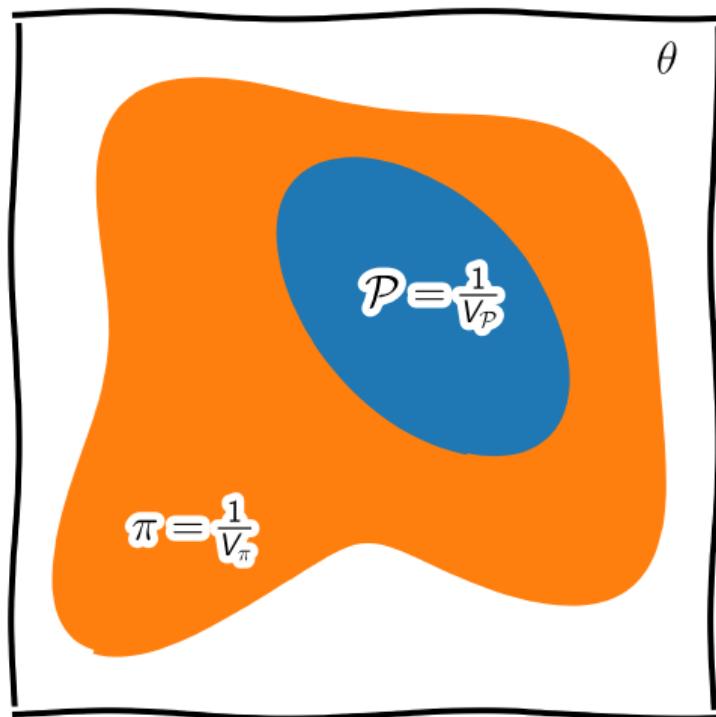
- The KL divergence between prior π and posterior \mathcal{P} is defined as:

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

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

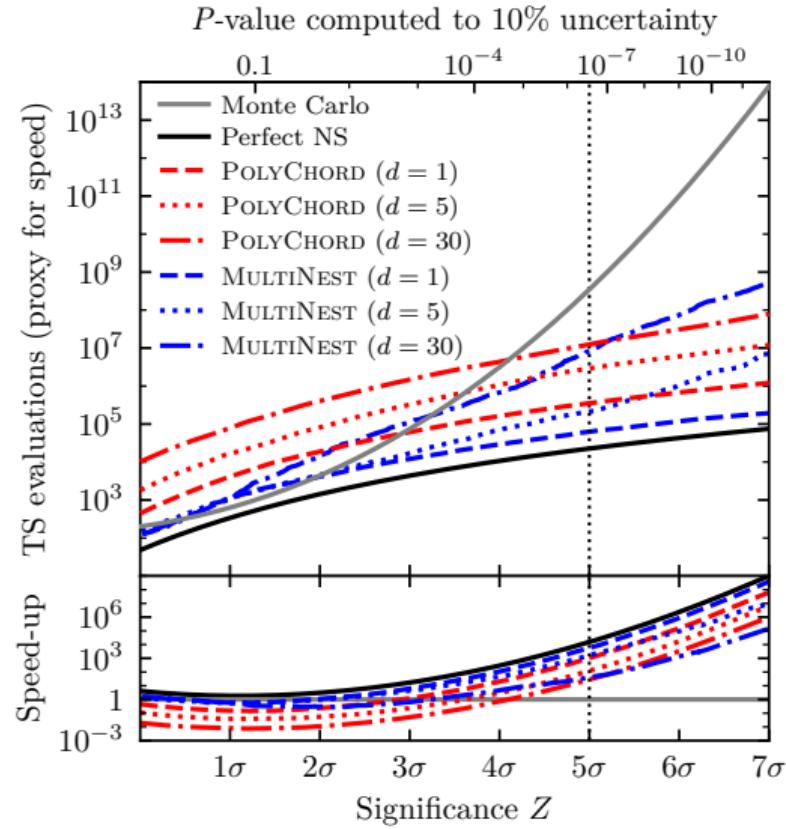
$$\mathcal{D}_{\text{KL}} \approx \log \frac{V_\pi}{V_{\mathcal{P}}}.$$

(this is exact for top-hat distributions).



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

- ▶ Nested sampling for frequentist computation!?
- ▶ p -value: $P(\lambda > \lambda^* | H_0)$ – probability that test statistic λ is at least as great as observed λ^* .
- ▶ Computation of a tail probability from sampling distribution of λ under H_0 .
- ▶ For gold-standard 5σ , this is very expensive to simulate directly ($\sim 10^9$ by definition).
- ▶ Need insight/approximation to make efficient.
- ▶ Nested sampling is tailor-made for this, just make switch: $X \leftrightarrow p$, $\mathcal{L} \leftrightarrow \lambda$, $\theta \leftrightarrow x$.
- ▶ The only real conceptual shift is switching the integrator from parameter- to data-space.



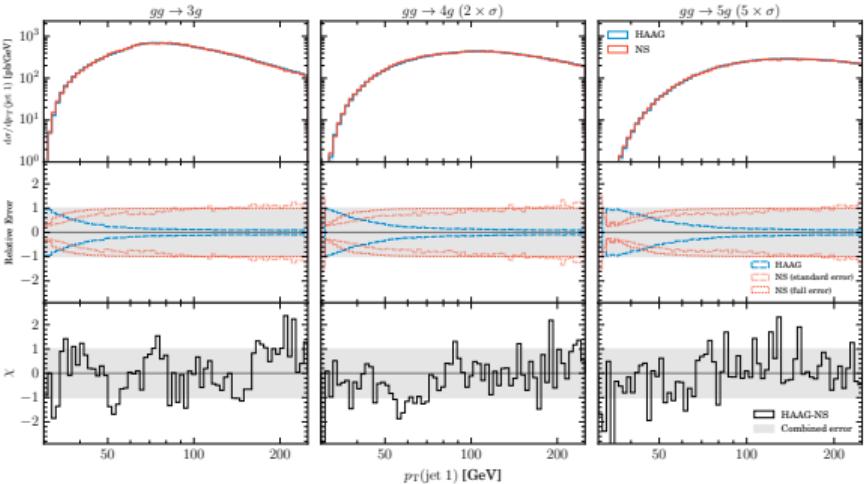
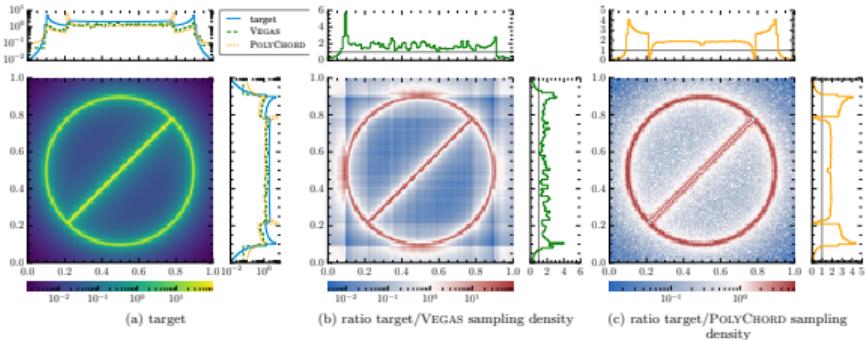
Exploration of phase space [2106.02056]

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

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

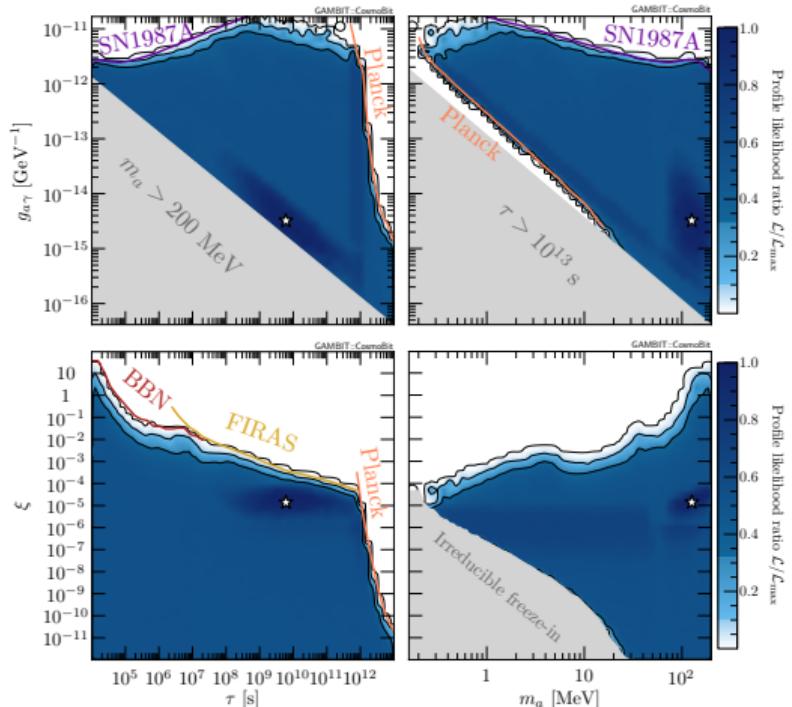
Ω phase space of kinematic configurations Φ , each with matrix element $\mathcal{M}(\Phi)$.

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



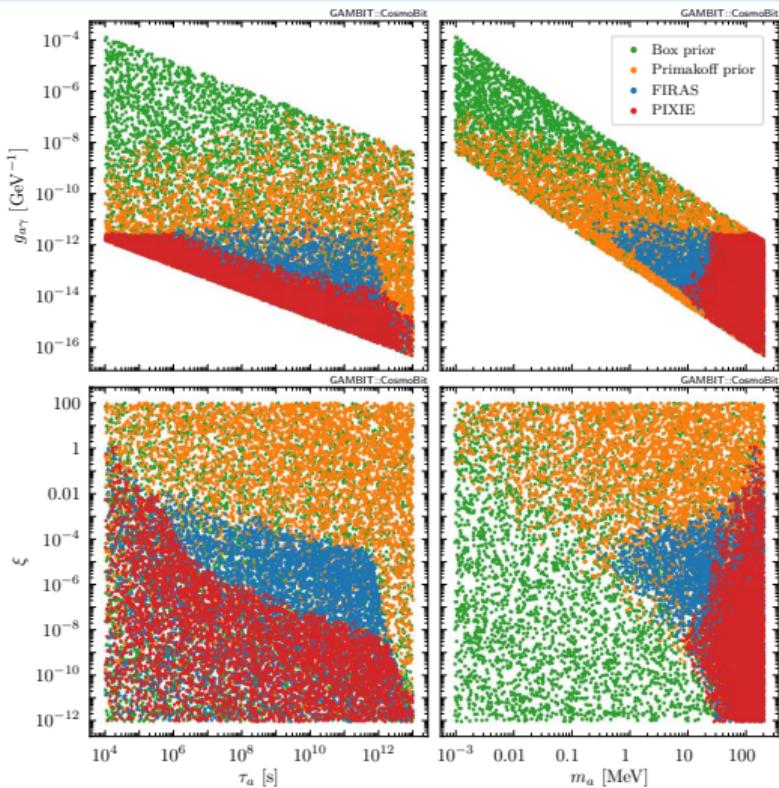
Quantification of fine tuning [2101.00428] [2205.13549]

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



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