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

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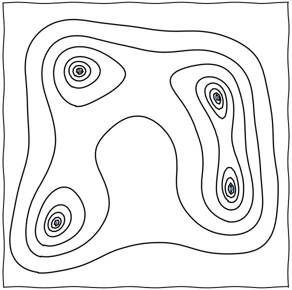
What is Nested Sampling?

- 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:

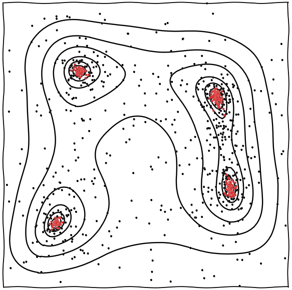
Optimisation

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



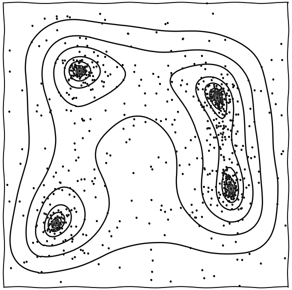
Exploration

$$\text{draw/sample} \quad \theta \sim f$$



Integration

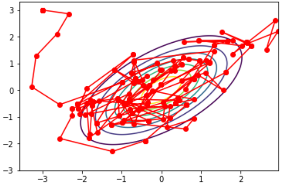
$$\int f(\theta) dV$$

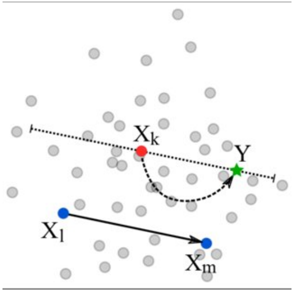


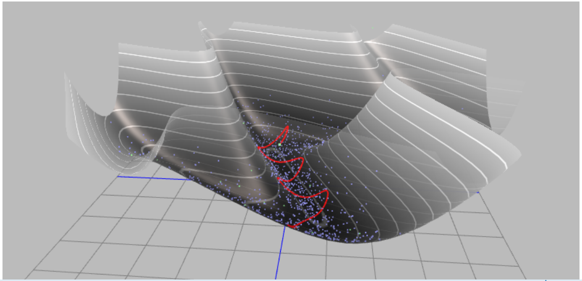
Where is Nested Sampling?

- 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

emcee
the mcmc hammer







Integration in Physics

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

Partition functions

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

Path integrals

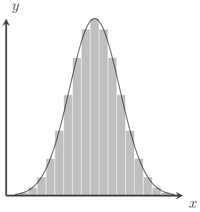
$$\Psi = \int e^{iS} \mathcal{D}x$$

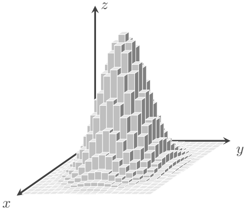
Bayesian marginals

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

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

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





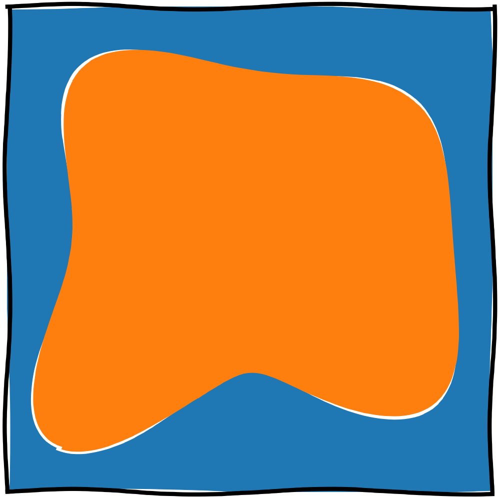
- Curse of dimensionality $\Rightarrow$ exponential scaling.

Probabalistic volume estimation

- Key idea in NS: estimating volumes probabilistically

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

- 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
- Basis of all Monte-Carlo integration
- Nested Sampling uniquely uses a nested framework to couple together MC integrals in a robust, scalable manner.



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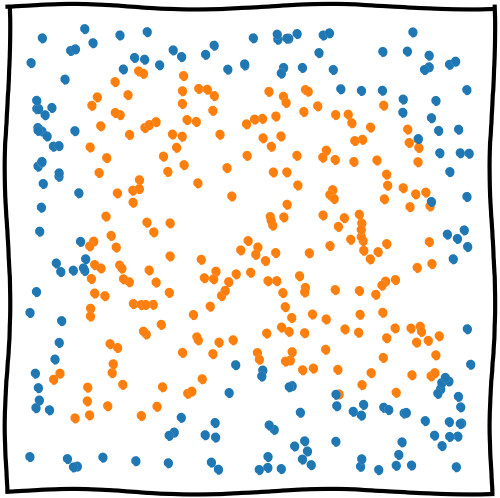
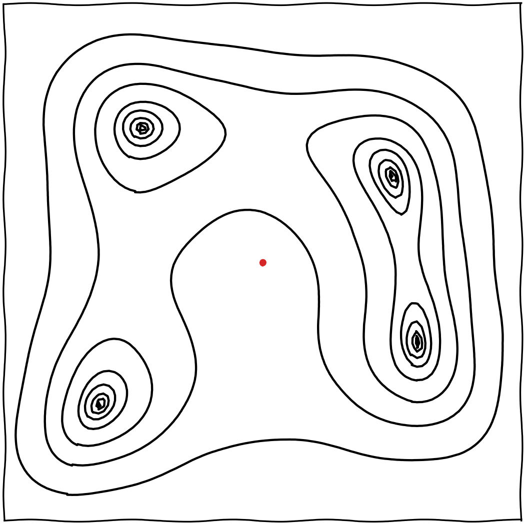


MCMC



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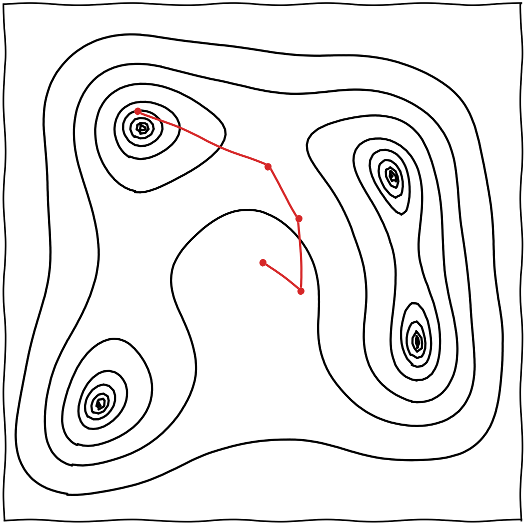

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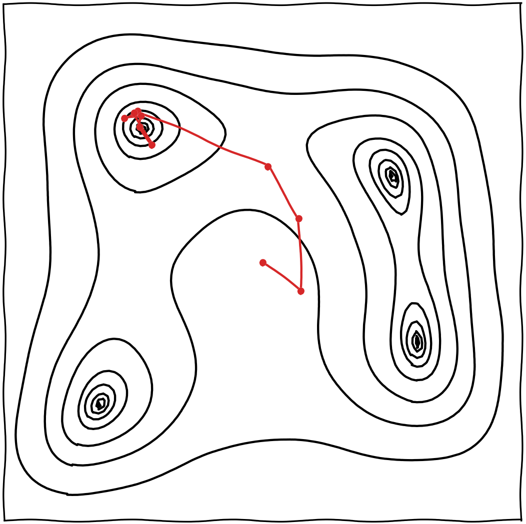

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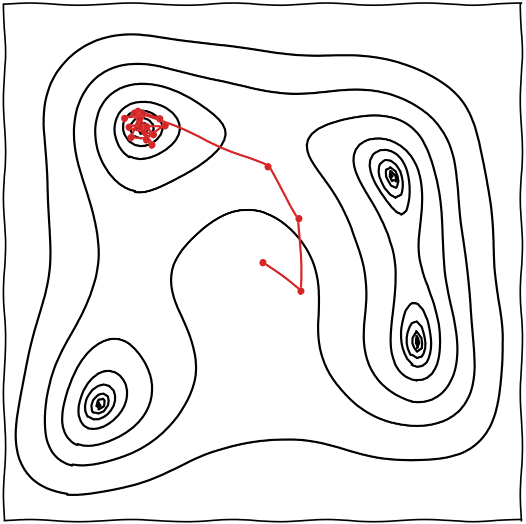
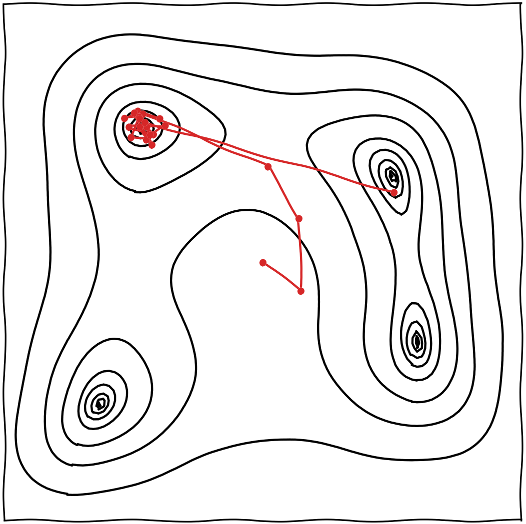
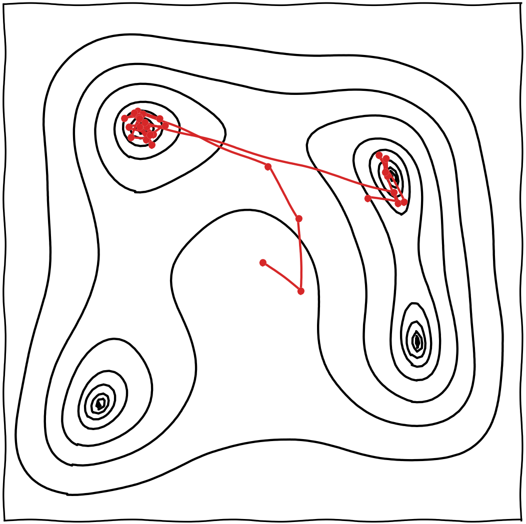


MCMC



MCMC



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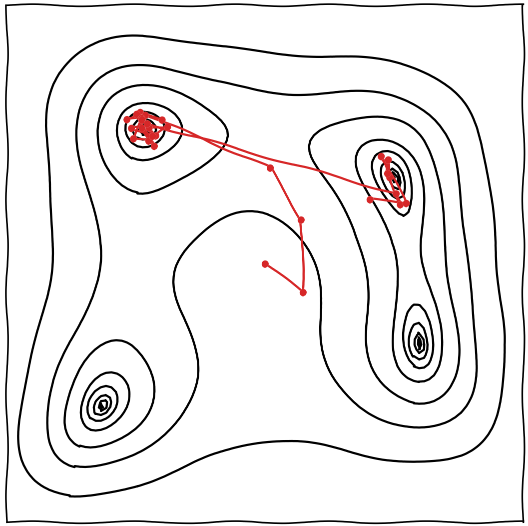
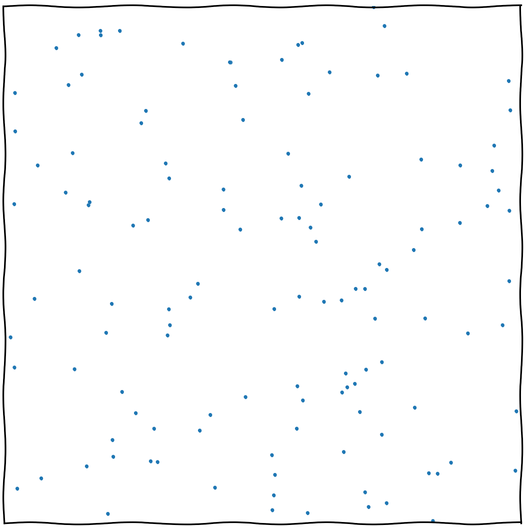
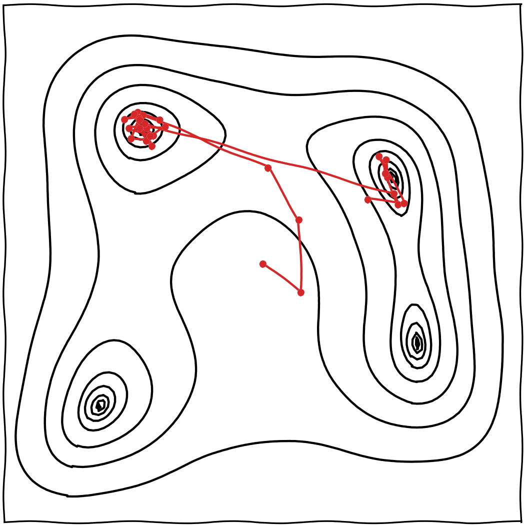


Nested sampling



MCMC



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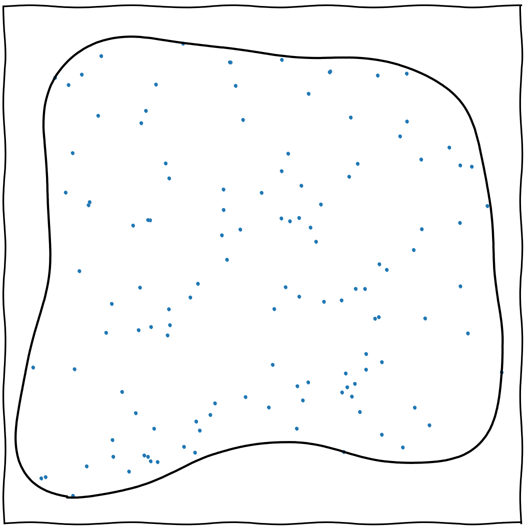

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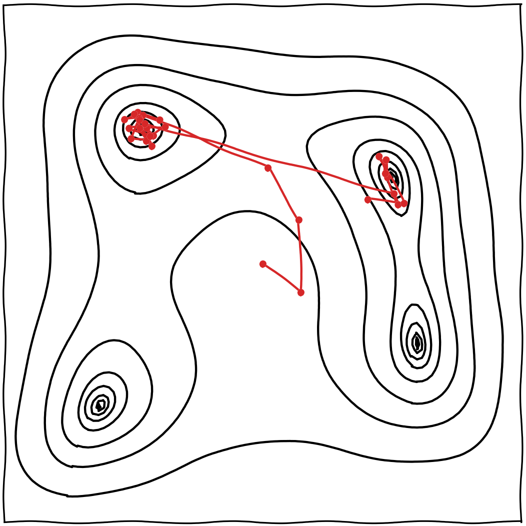

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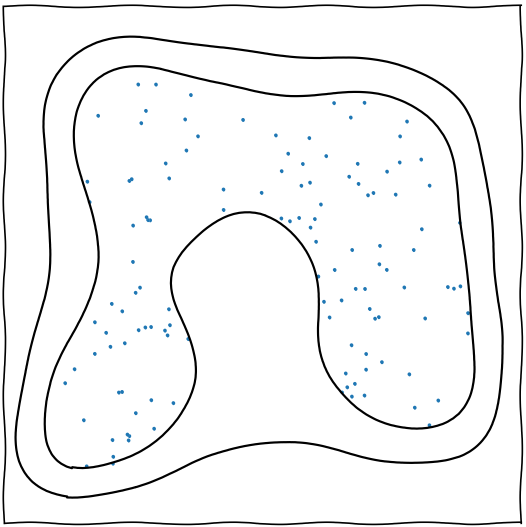

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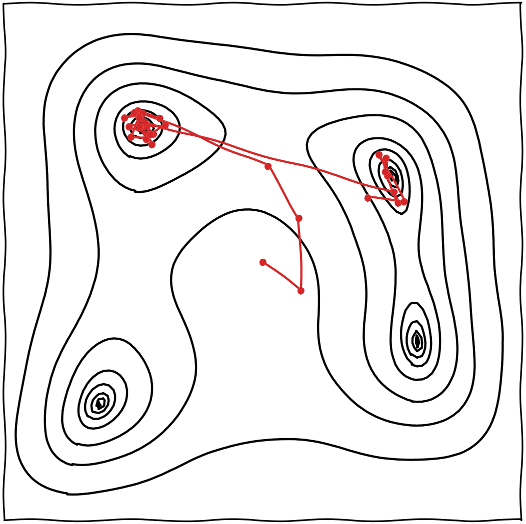

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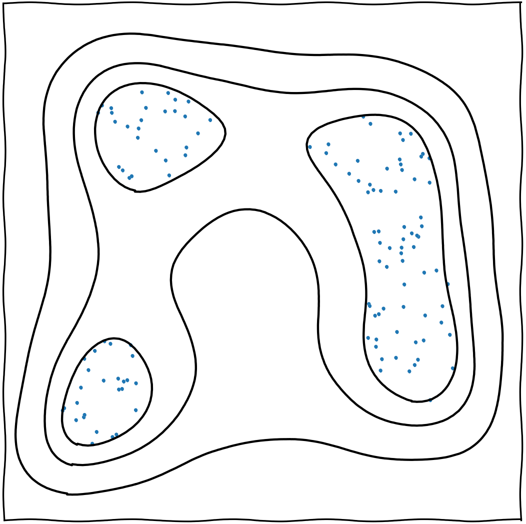
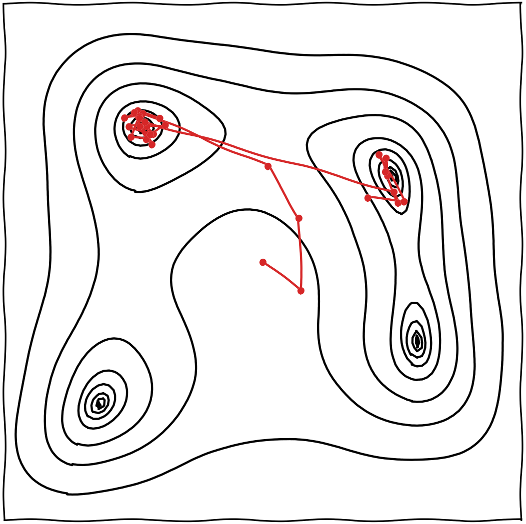


MCMC



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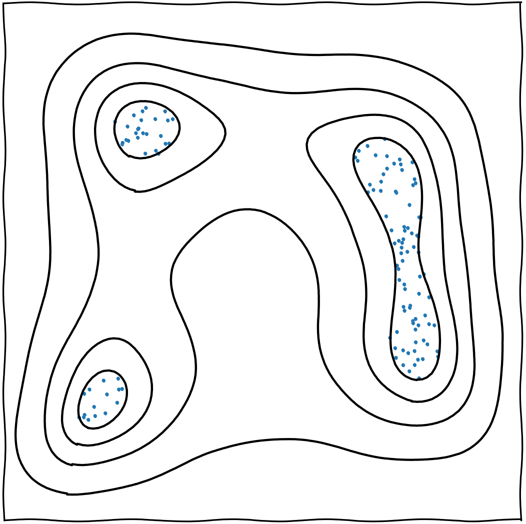

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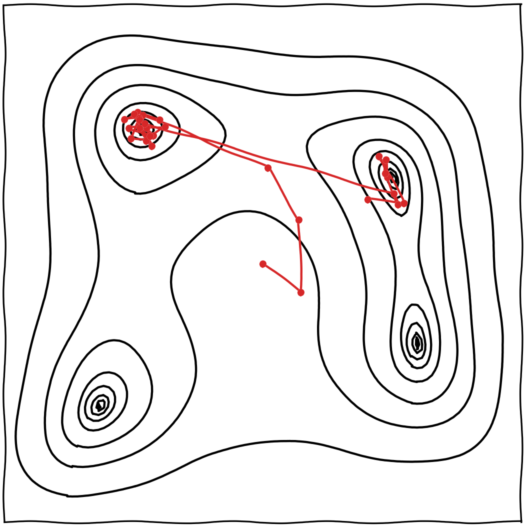

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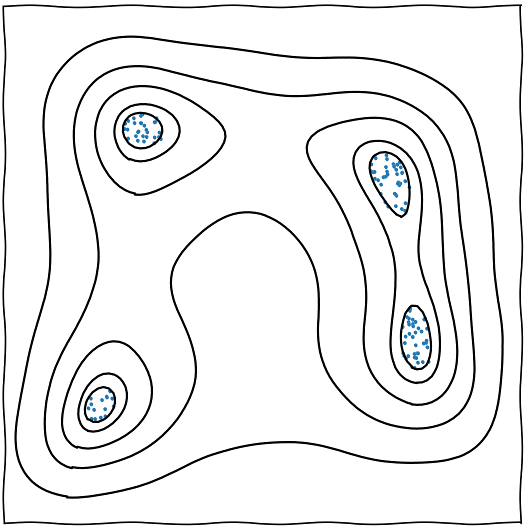

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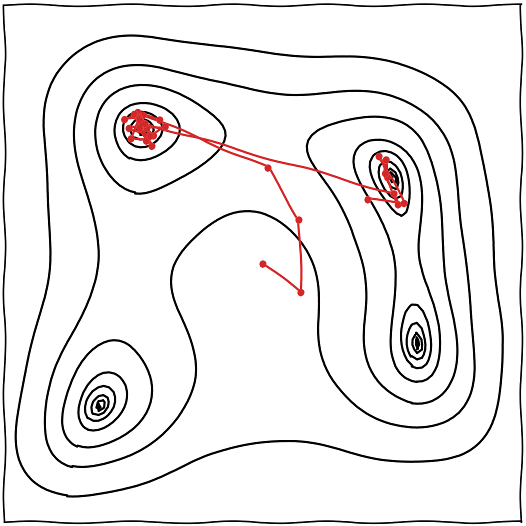

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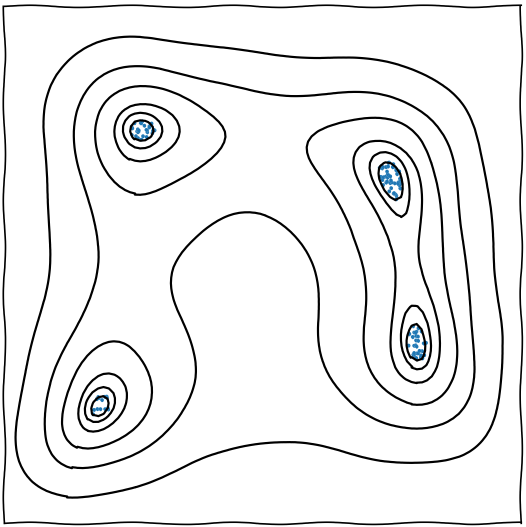

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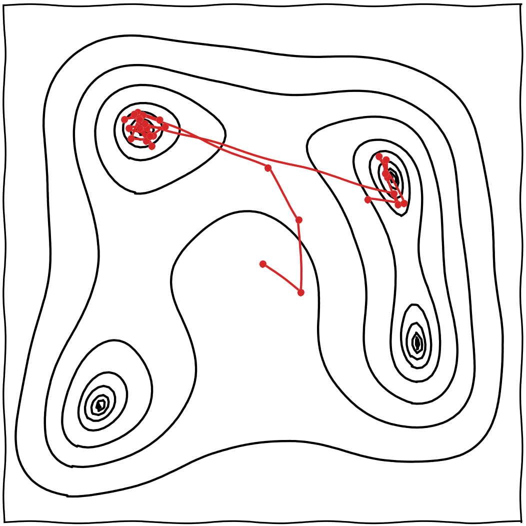

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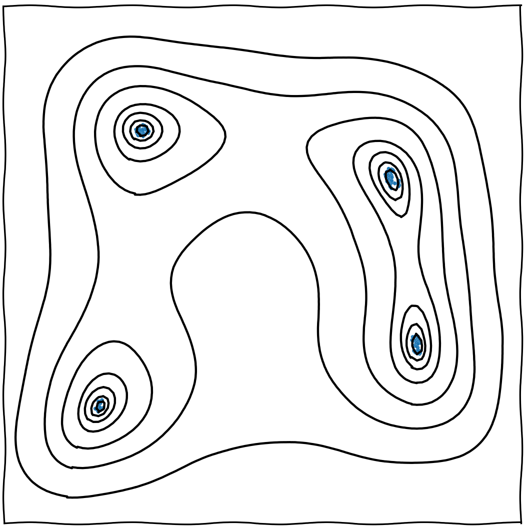

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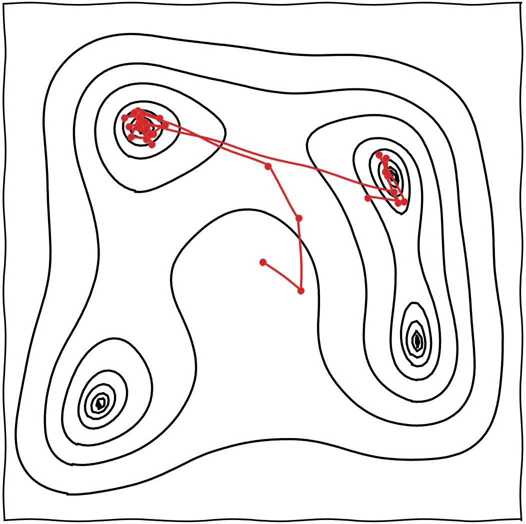

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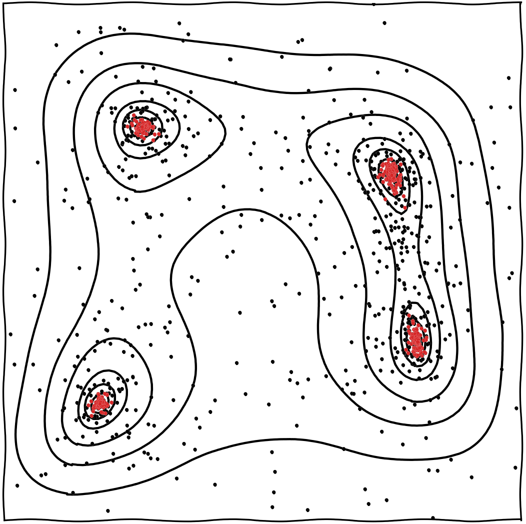
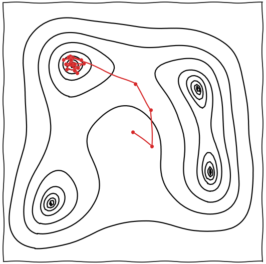


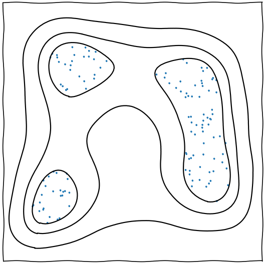
MCMC

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



Nested sampling

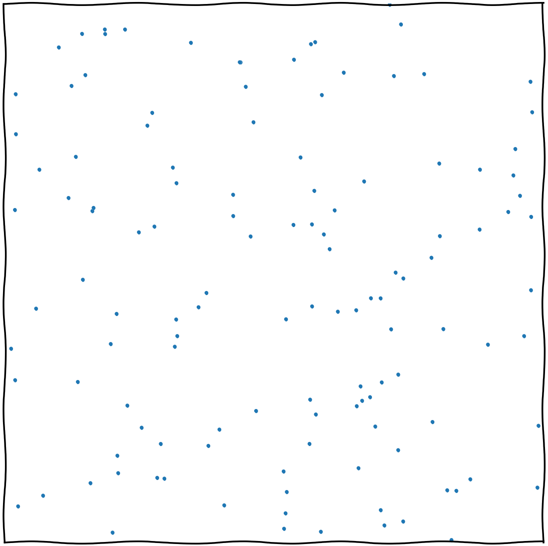
- Ensemble of "live points"
- Scans from prior to peak of likelihood
- Slower, no tuning required
- Parameter estimation, model comparison, tension quantification
- Channel capacity optimised for computing partition function



The nested sampling meta-algorithm: live points

- 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

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



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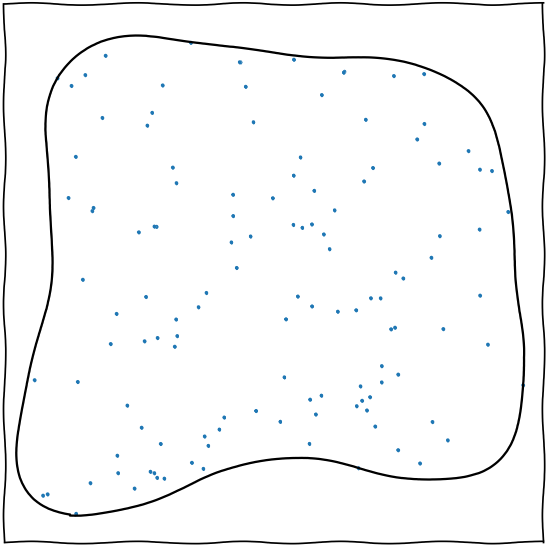

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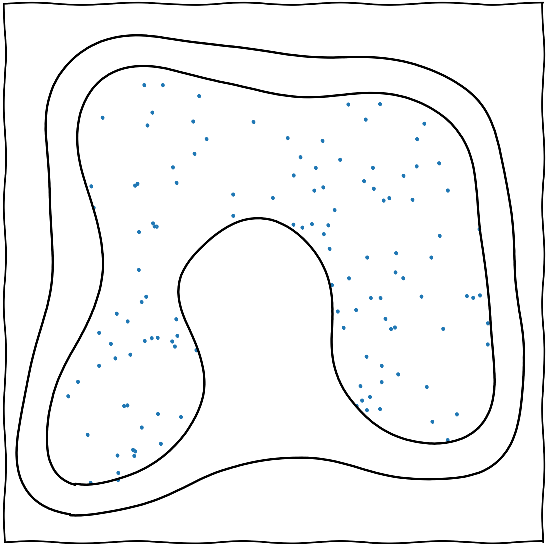

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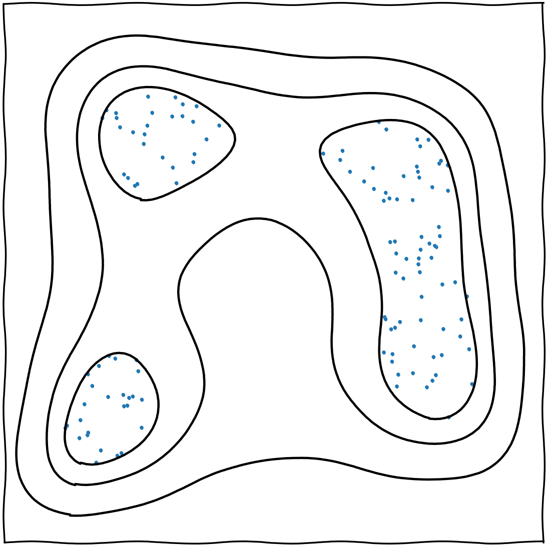

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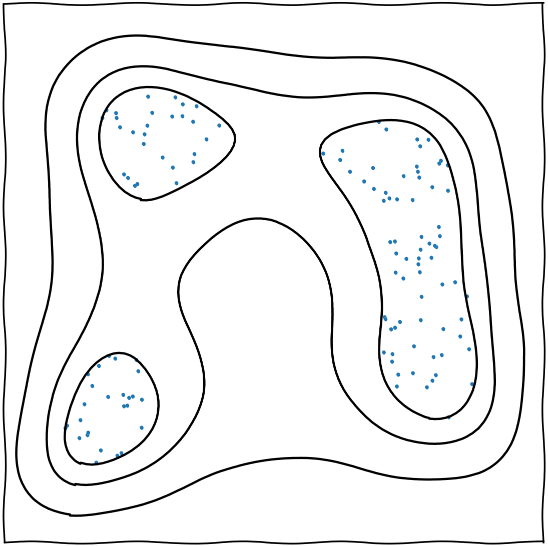
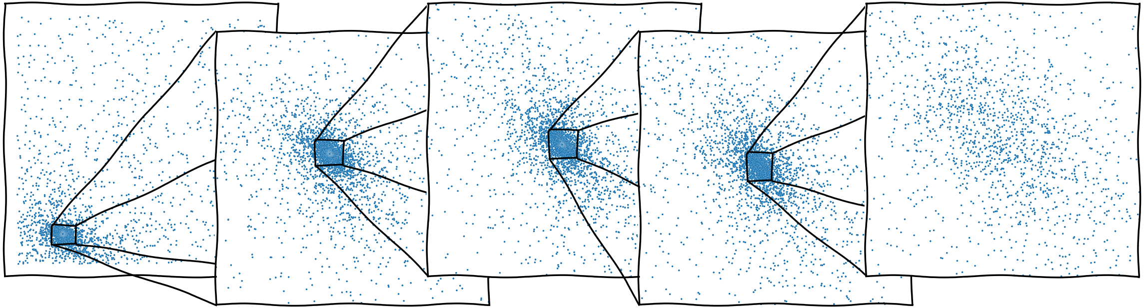


The nested sampling meta-algorithm: dead points



- At the end, one is left with a set of discarded "dead" points.
- Dead points have a unique scale-invariant distribution $\propto \frac{dV}{V}$.
- Uniform over original region, exponentially concentrating on region of interest (until termination volume).
- Good for training emulators (HERA [2108.07282]).

Applications

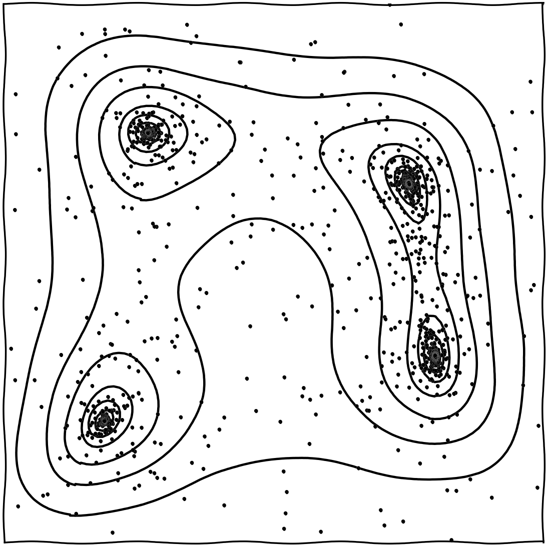
- training emulators.
- gridding simulations
- beta flows
- "dead measure"

The nested sampling meta-algorithm: Lebesgue integration

- Full dead-point coverage of tails enables integration.
- 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

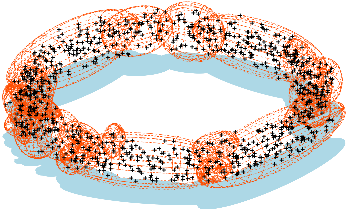
"It is not the purpose of this introductory paper to develop the technology of navigation within such a volume. We merely note that exploring a hard-edged likelihood-constrained domain should prove to be neither more nor less demanding than exploring a likelihood-weighted space."

— *John Skilling*

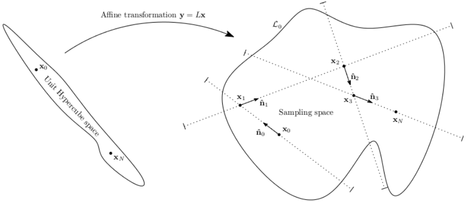
- A large fraction of the work in NS to date has been in attempting to implement a hard-edged sampler in the NS meta-algorithm $\{\theta \sim \pi : \mathcal{L}(\theta) > \mathcal{L}_*\}$.
- `https://projecteuclid.org/euclid.ba/1340370944`.
- There has also been much work beyond this (see 'Frontiers of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

Implementations of Nested Sampling [2205.15570](NatReview)

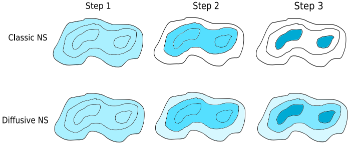
MultiNest [0809.3437]



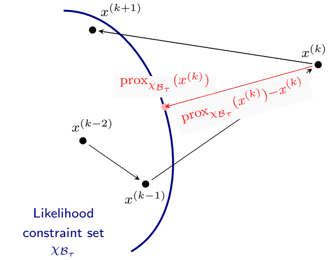
PolyChord [1506.00171]



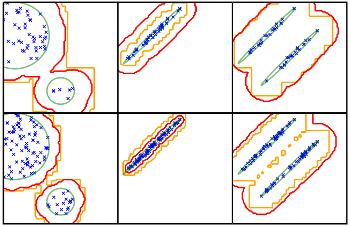
DNest [1606.03757]



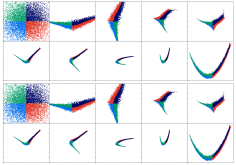
ProxNest [2106.03646]

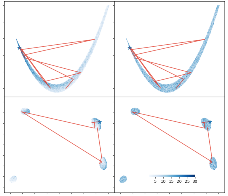


UltraNest [2101.09604]



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 $d > d_0 \sim 10$.

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: 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 ΛCDM 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. ΛCDM vs a dynamic dark energy cosmology*

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

$$\frac{\mathcal{Z}_\mathcal{M}\Pi_\mathcal{M}}{\sum_m Z_m\Pi_m}$$

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

Tension quantification

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

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

$$\log\mathcal{S} = \langle\log\mathcal{L}_{AB}\rangle_{\mathcal{P}_{AB}} - \langle\log\mathcal{L}_A\rangle_{\mathcal{P}_A} - \langle\log\mathcal{L}_B\rangle_{\mathcal{P}_B}$$

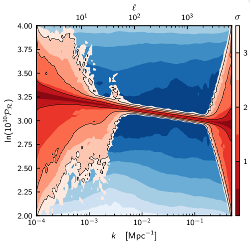
Applications of nested sampling

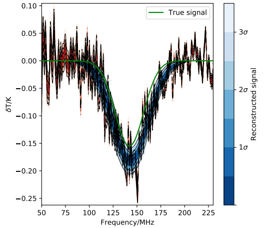
Cosmology

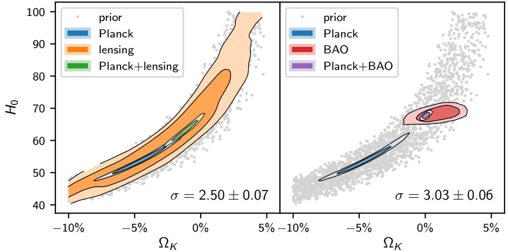
Adam Ormondroyd

PhD

- 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.







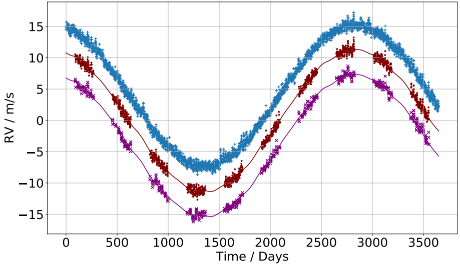
Applications of nested sampling

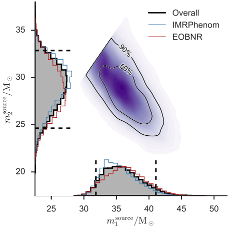
Astrophysics

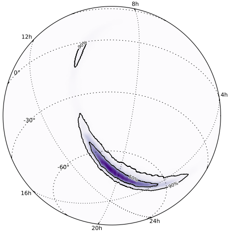
Metha Prathaban

PhD

- 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



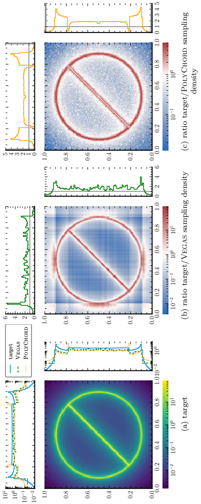


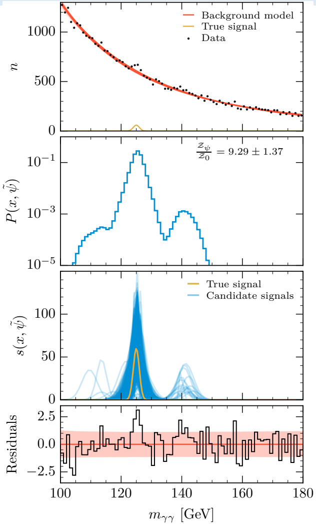


David Yallup

PDRA

- 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: $X \leftrightarrow p$, $\mathcal{L} \leftrightarrow \lambda$, $\theta \leftrightarrow x$.





Applications of nested sampling

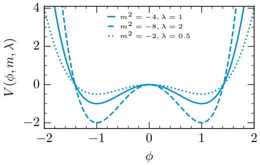
Lattice field theory

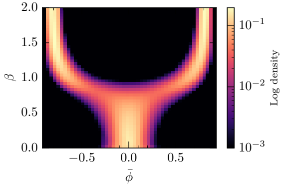
David Yallup
PDRA

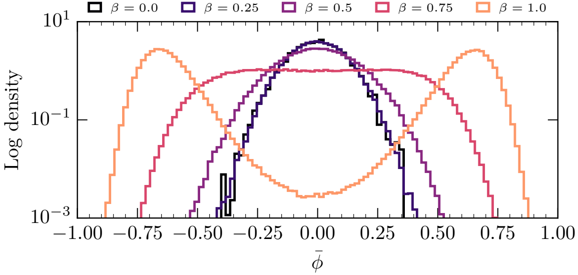
- Consider standard field theory Lagrangian:

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

- 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)





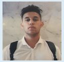


Applications of nested sampling

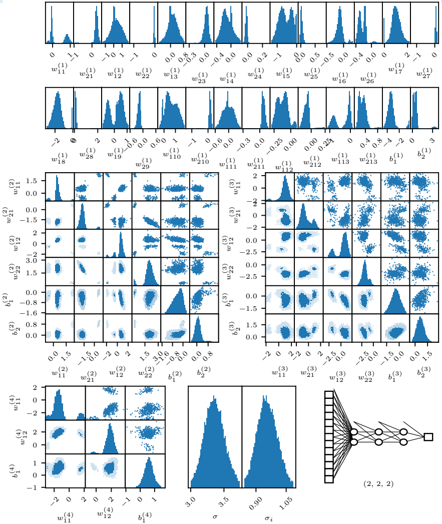
Machine learning

Kamran Javid

PDRA



- 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]



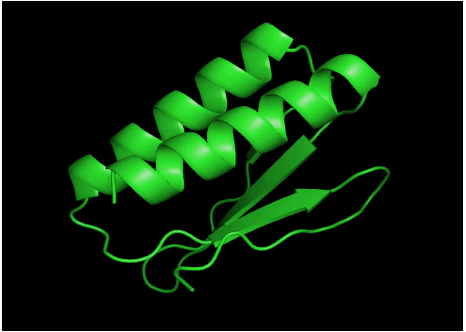
Applications of nested sampling

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.



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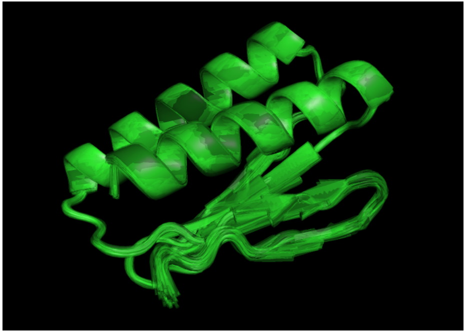

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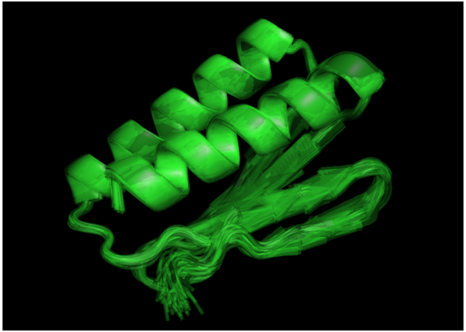

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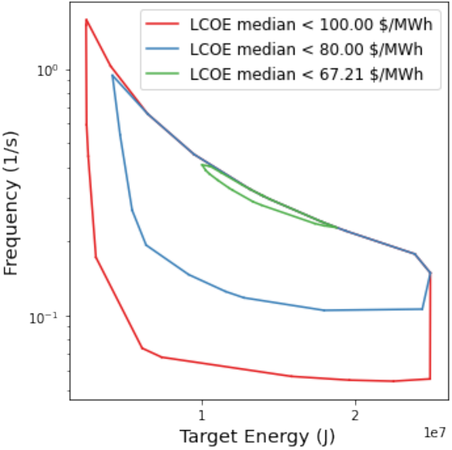

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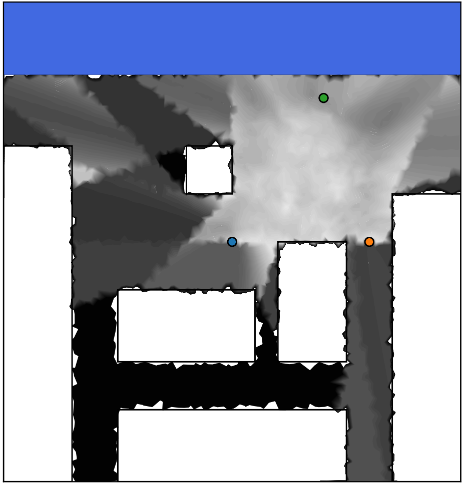

Applications of nested sampling

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PhD → Data Scientist

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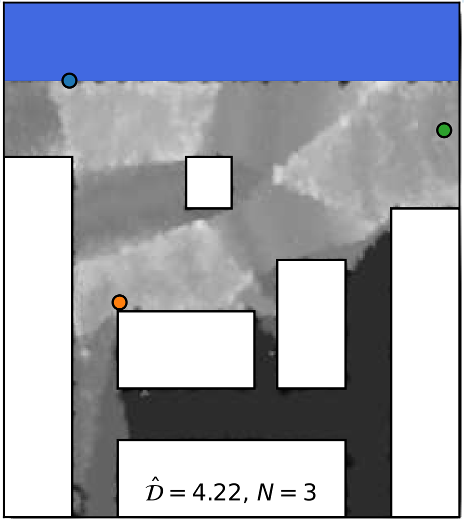

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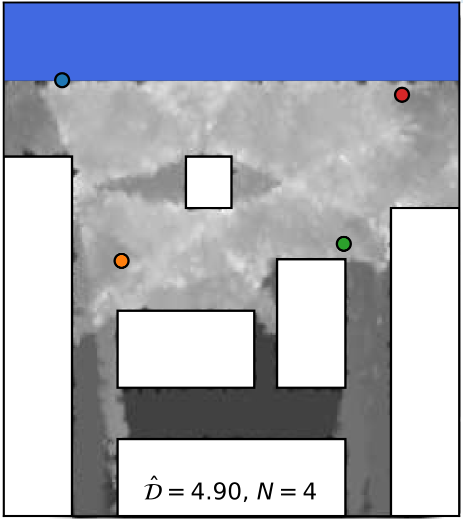

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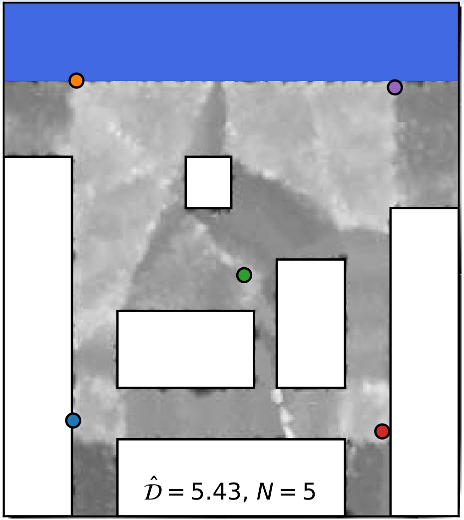
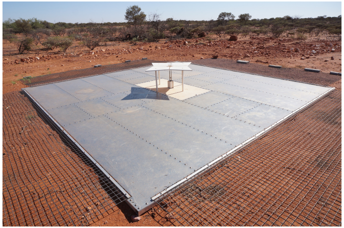
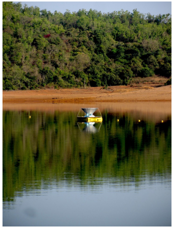


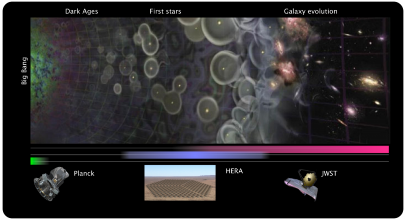
REACH: Global 21cm cosmology [2210.07409](NatAstro)

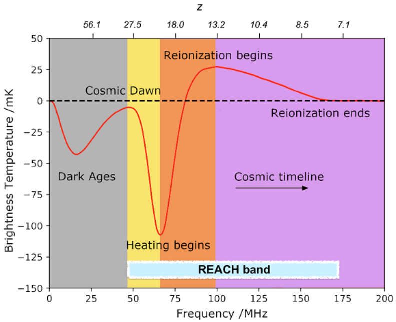
Ian Roque
PhD

- 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.



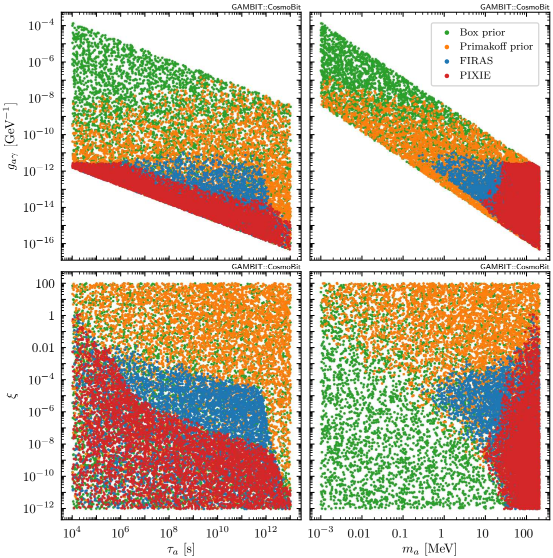






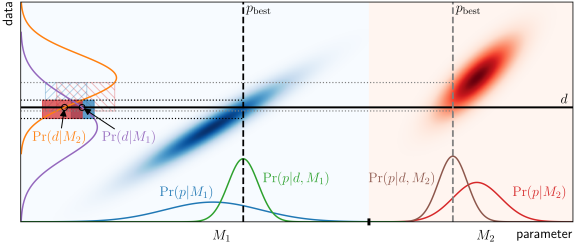
GAMBIT: combining particle physics & cosmological data

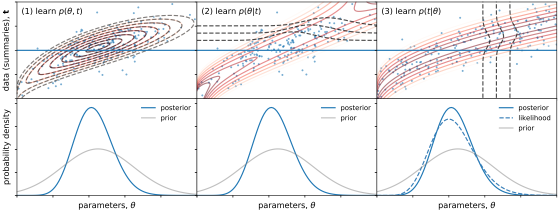
- Multinational team of particle physicists, cosmologists and statisticians.
- Combine cosmological data, particle colliders, direct detection, & neutrino detectors in a statistically principled manner [2205.13549].
- Lead Cosmo/Dark Matter working group [2009.03286].
- Nested sampling used for global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



Kilian Scheutwinkel
PhD

- 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 $\theta \to D$, 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.



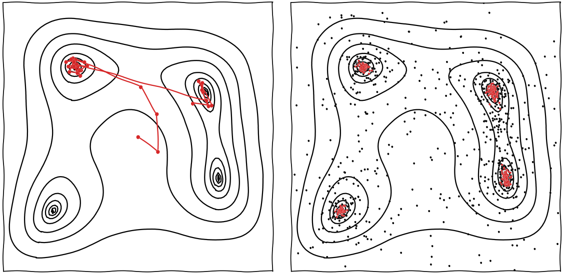


Harry Bevins

PhD→JRF

- DiRAC 2020 RAC allocation of 30MCPUh
- Main goal: Planck Legacy Archive equivalent
- Parameter estimation → Model comparison
- MCMC → Nested sampling
- Planck → $\{\text{Planck}, \text{DESY1}, \text{BAO}, \ldots\}$
- 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



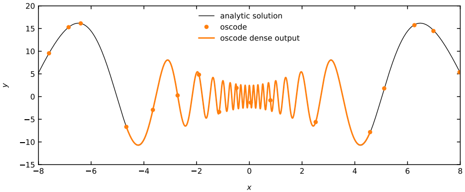
CosmoTension

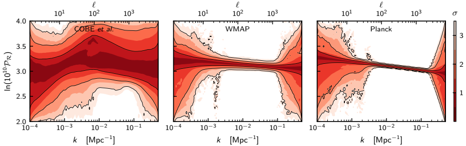
Will Barker

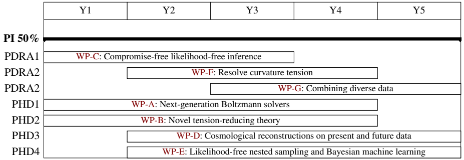
PhD→JRF

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

- 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.

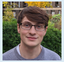




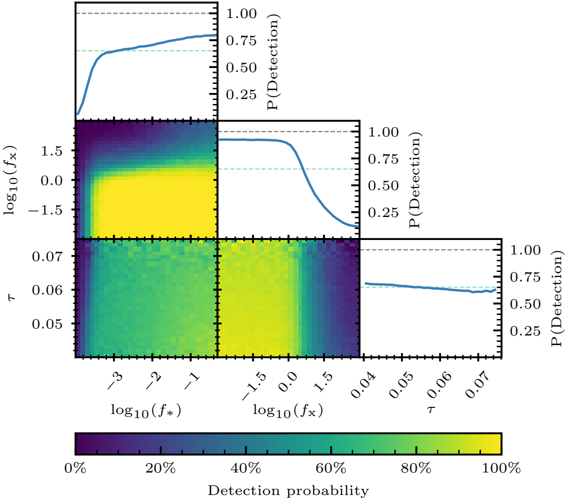


Fully Bayesian Forecasting [2309.06942]

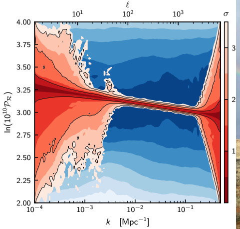
Thomas Gessey-Jones
PhD

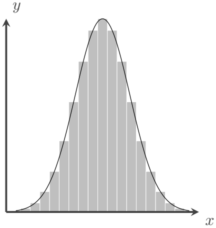


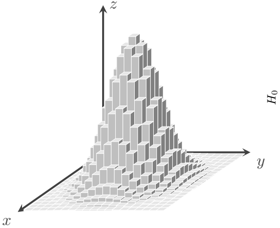
- Experimental design necessitates forecasting the constraints that future data might give.
- Have you ever done a Fisher forecast, and then felt Bayesian guilt?
- Simulation based inference gives us the language to marginalise over parameters θ and possible future data D.
- Evidence networks [2305.11241] (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`

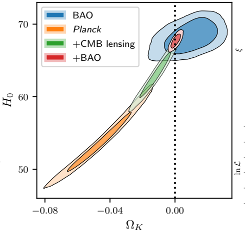


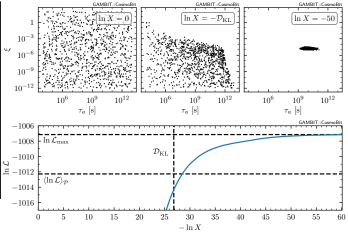
- Nested sampling is a multi-purpose numerical tool for:
  - Numerical integration $\int f(x) dV$,
  - Exploring/scanning/optimising *a priori* unknown functions,
  - Performing Bayesian inference and model comparison.
- It is applied widely across cosmology, particle physics & machine learning.
- It's 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

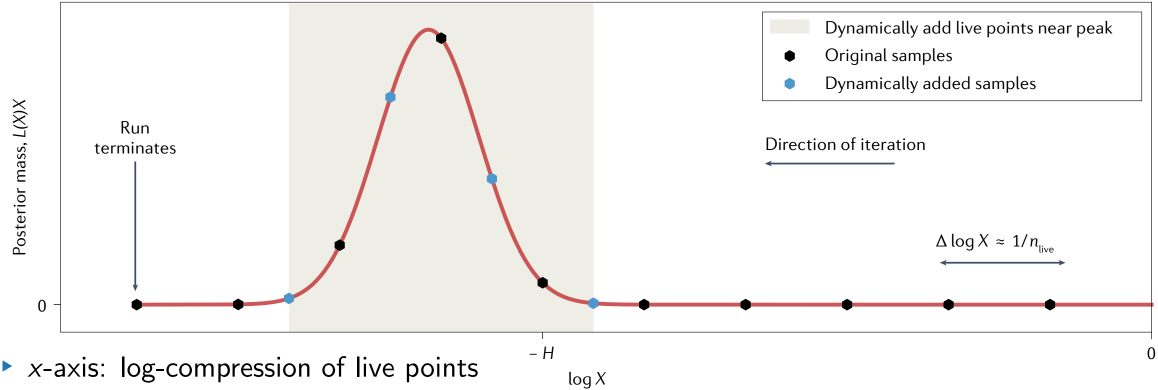
Integration

- Thermodynamic integration
  - $+$ protective against phase trasitions
  - $+$ 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 $\frac{1}{\sqrt{n_{\mathrm{live}}}}$.
   - 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



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

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

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

- Evidence is composed of a "goodness of fit" term and "Occam Penalty".

- RHS true for all θ. Take max likelihood value θ_*:

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

- Be more Bayesian and take posterior average to get the "Occam's razor equation"

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

- Natural regularisation which penalises models with too many parameters.

Kullback Liebler divergence

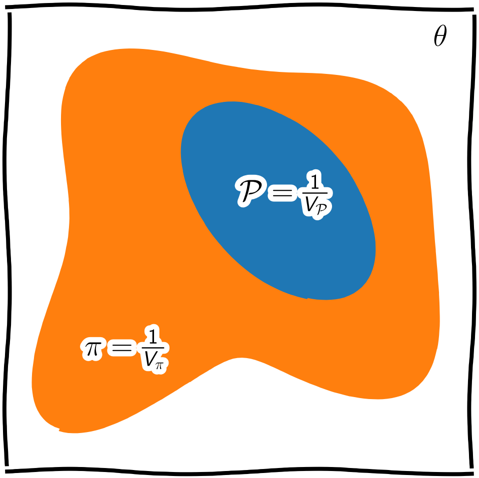
- The KL divergence between prior π and posterior $\mathcal{P}$ is is defined as:

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

- 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":

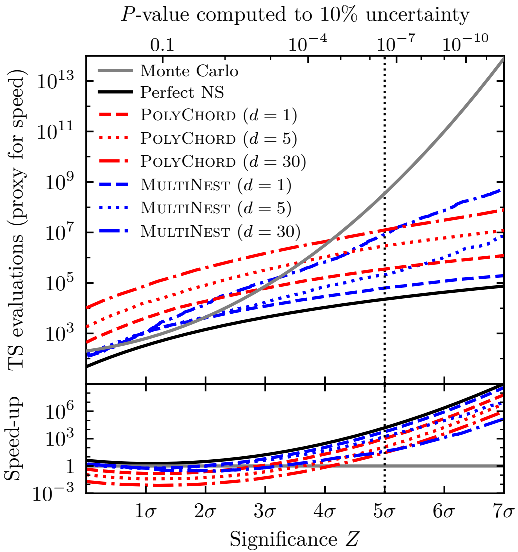
$$\mathcal{D}_{\mathrm{KL}} \approx \log \frac{V_\pi}{V_{\mathrm{P}}}.$$

(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.

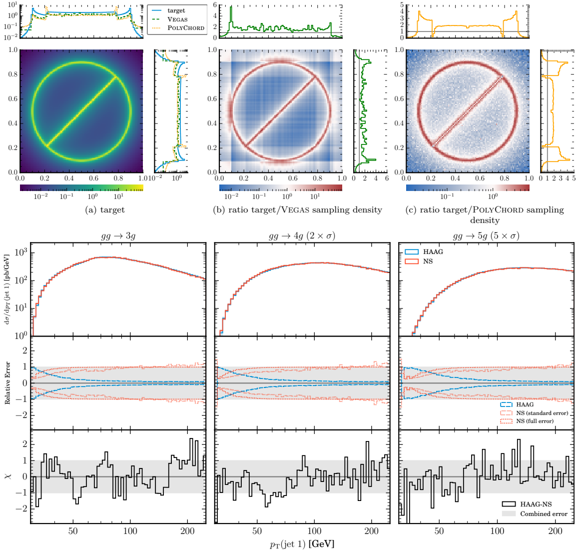


Exploration of phase space [2106.02056]

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

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

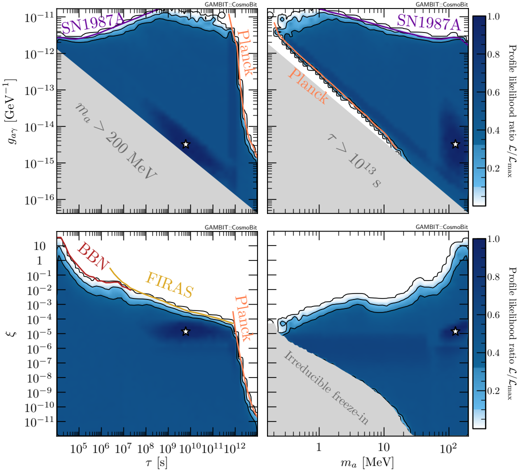
  Ω phase space of kinematic configurations Φ, each with matrix element $\mathcal{M}(\Phi)$.
- Current state of the art e.g. HAAG (improvement on RAMBO) requires knowledge of $\mathcal{M}(\Phi)$.
- Nested sampling can explore the phase space and compute integral blind with comparable efficiency.



(a) target (b) ratio target/VEGAS sampling density (c) ratio target/POLYCHORD sampling density

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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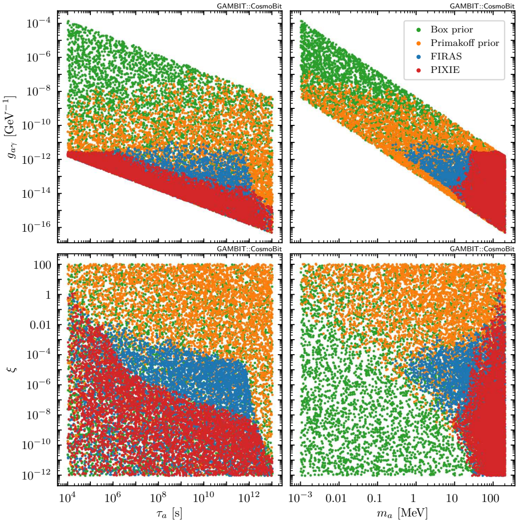
  - Quantifies amount of parameter space ruled out with Kullback-Liebler divergence $\mathcal{D}_{\mathrm{KL}}$.
  - Identifies best fit region as statistically irrelevant from information theory/Bayesian.
  - No evidence for decaying ALPs. Fit the data equally well: but more constrained parameters create Occam penalty.



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