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

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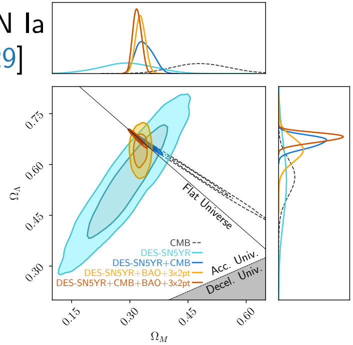
LBI: Likelihood-based inference

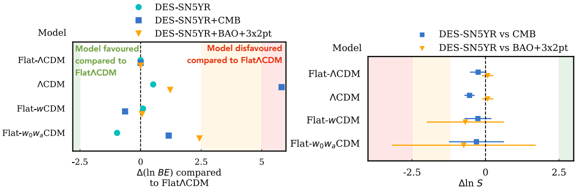
The standard approach if you are fortunate enough to have a likelihood function $P(D|\theta)$:

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

1. Define prior $\pi(\theta)$
   - spend some time being philosophical
2. Sample posterior $\mathcal{P}(\theta|D)$
   - use out-of-the-box MCMC tools such as `emcee` or `MultiNest`
   - make some triangle plots
3. Optionally compute evidence $\mathcal{Z}(D)$
   - e.g. nested sampling or parallel tempering
   - do some model comparison (i.e. science)
   - talk about tensions

DES Y5 SN Ia [2401.02929]





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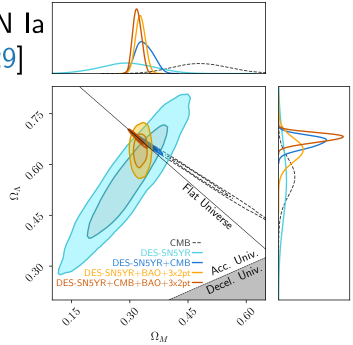

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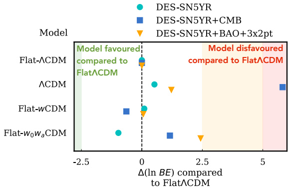

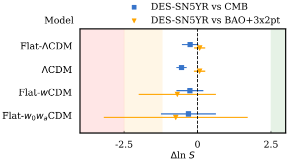

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The standard approach if you are fortunate enough to have a likelihood function $\mathcal{L}(D|\theta)$:

$$\mathcal{P}(\theta|D) = \frac{\mathcal{L}(D|\theta)\pi(\theta)}{\mathcal{Z}(D)} \qquad \text{Posterior} = \frac{\text{Likelihood} \times \text{Prior}}{\text{Evidence}}$$

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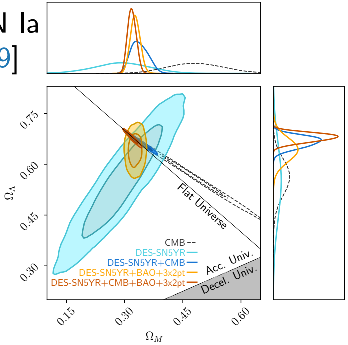

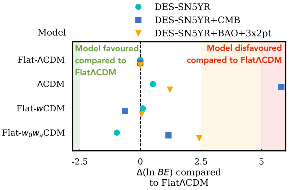

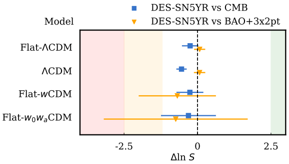

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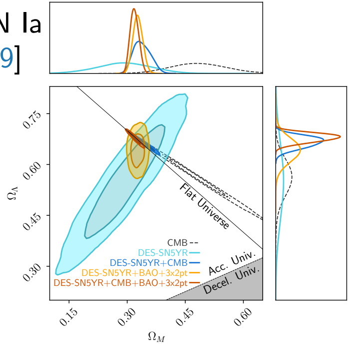

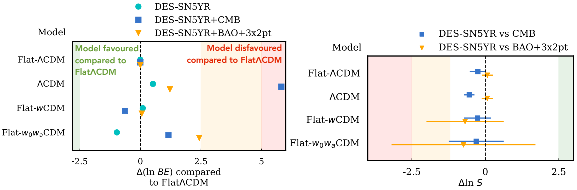

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$$\mathcal{P} \times \mathcal{Z} = \mathcal{J} = \mathcal{L} \times \pi, \qquad \text{Joint} = \mathcal{J} = P(\theta, D)$$

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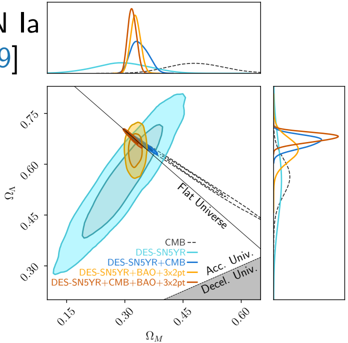
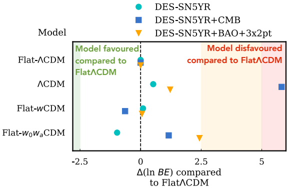
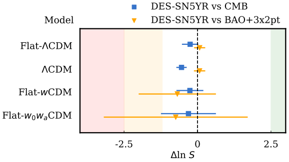






The three pillars of Bayesian inference

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*

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

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

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

Tension quantification

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

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

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

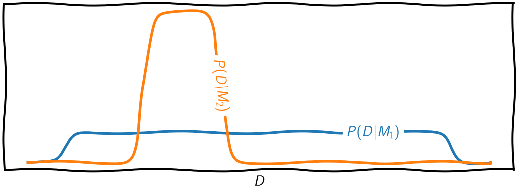
Model comparison $\mathcal{Z} = P(D|M)$

- Bayesian model comparison allows mathematical derivation of key philosophical principles.

Viewed from data-space D:

Popper's falsificationism

- Prefer models that make bold predictions.
- if proven true, model more likely correct.



- Falsificationism comes from normalisation

Viewed from parameter-space θ:

Occam's razor

- Models should be as simple as possible
- ...but no simpler

- Occam's razor equation:

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

- "Occam penalty": KL divergence between prior π and posterior $\mathcal{P}$.

$$\mathcal{D}_{\text{KL}} \sim \log \frac{\text{Prior volume}}{\text{Posterior volume}}$$

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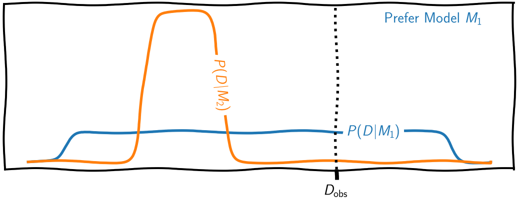

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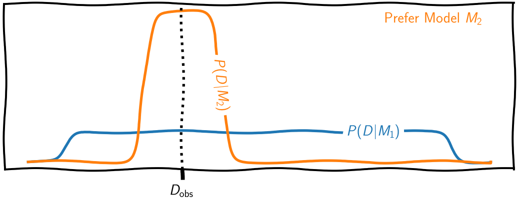

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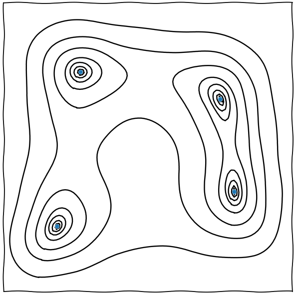
What is Nested Sampling?

- 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:

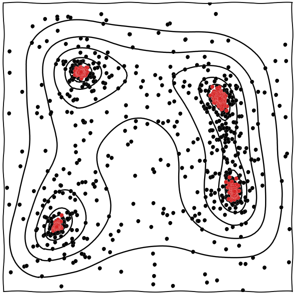
Optimisation

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



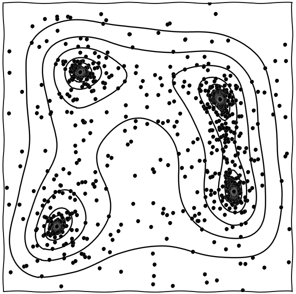
Exploration

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



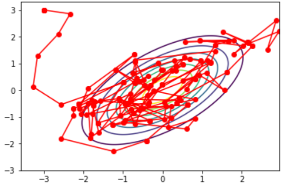
Integration

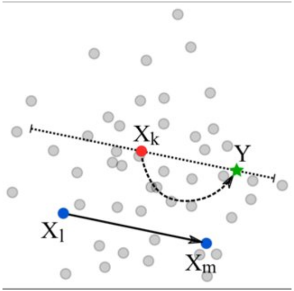
$$\int f(\theta) dV$$

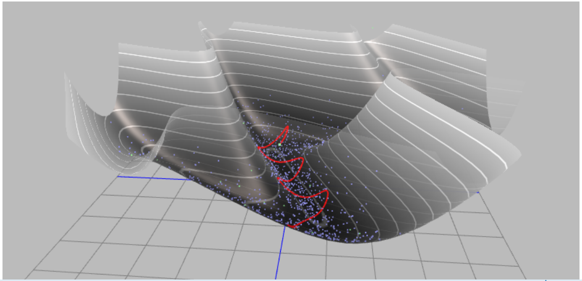


- For many purposes, in your Neural Net you should group Nested Sampling with (MCMC) techniques such as:
  - Metropolis-Hastings (PyMC, MontePython)
  - Hamiltonian Monte Carlo (Stan, blackjax)
  - Ensemble sampling (emcee, zeus).
  - Variational Inference (Pyro)
  - Sequential Monte Carlo
  - Thermodynamic 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

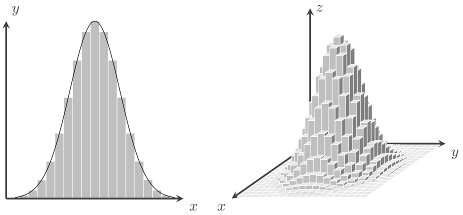
$$\Psi = \int e^{iS} \mathcal{D}x$$

Bayesian marginals

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

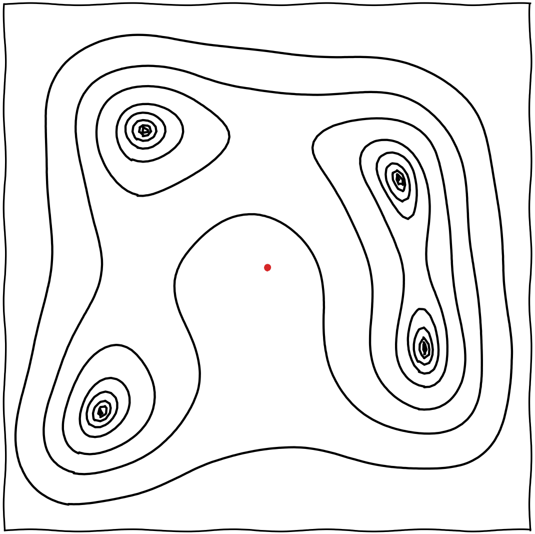
- Need numerical tools if analytic solution unavailable.
- High-dimensional numerical integration is hard.
- Riemannian strategy estimates volumes geometrically:

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



- Curse of dimensionality $\Rightarrow$ exponential scaling.

MCMC



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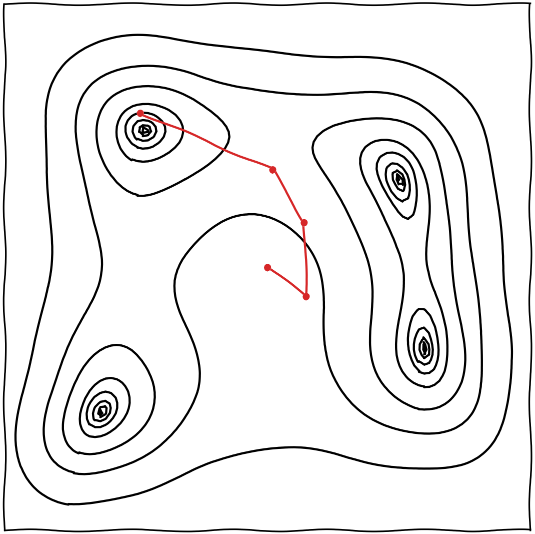

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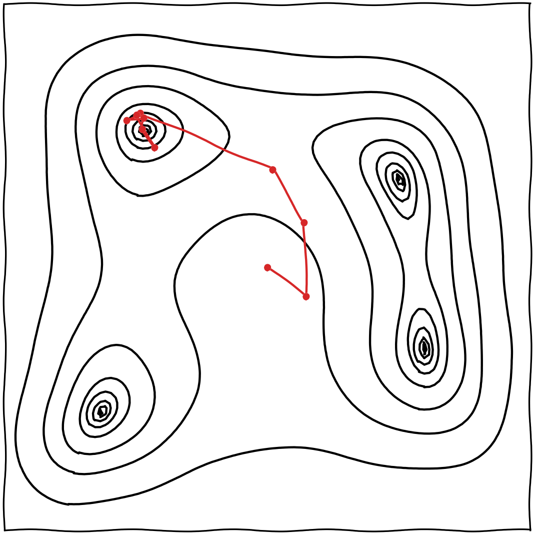

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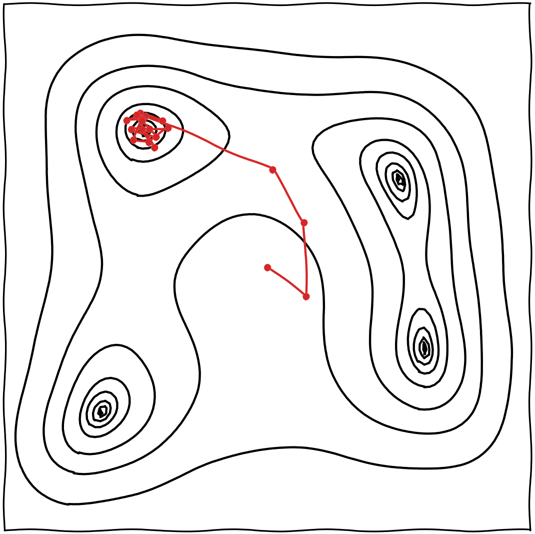

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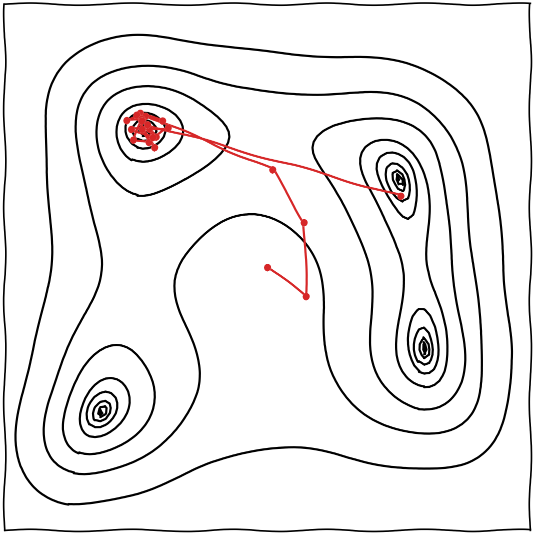

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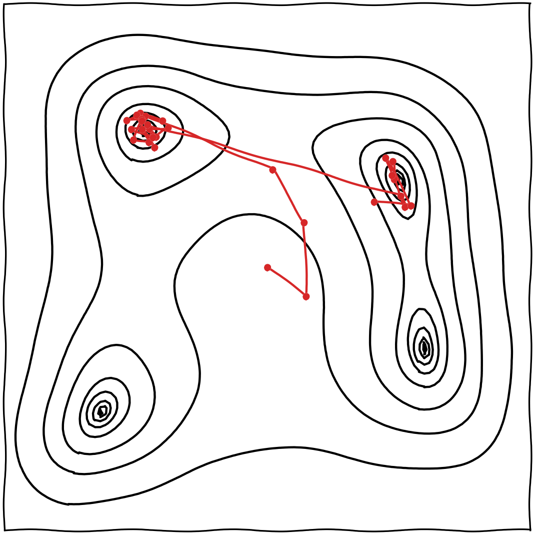

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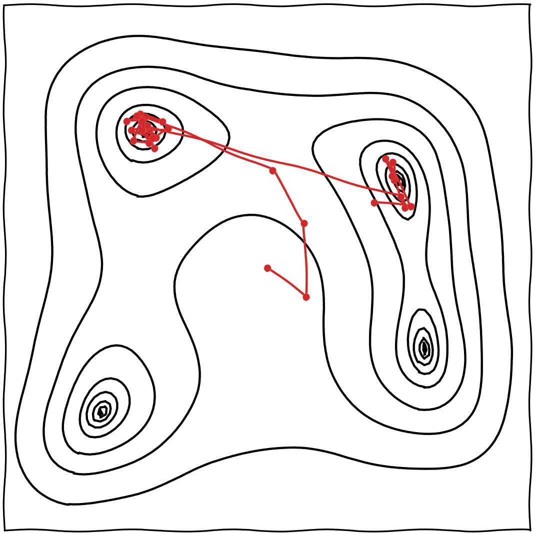

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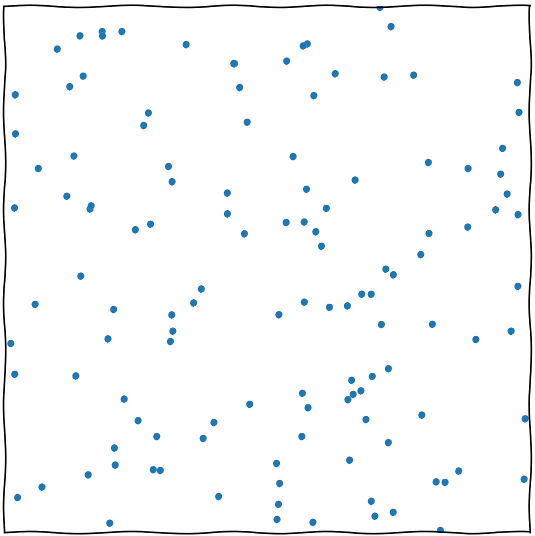

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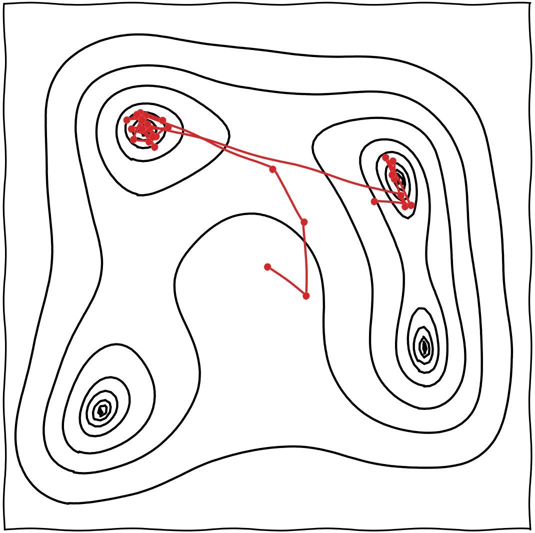

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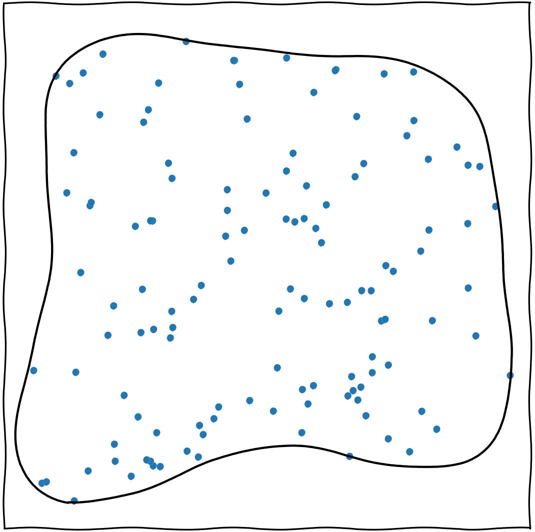

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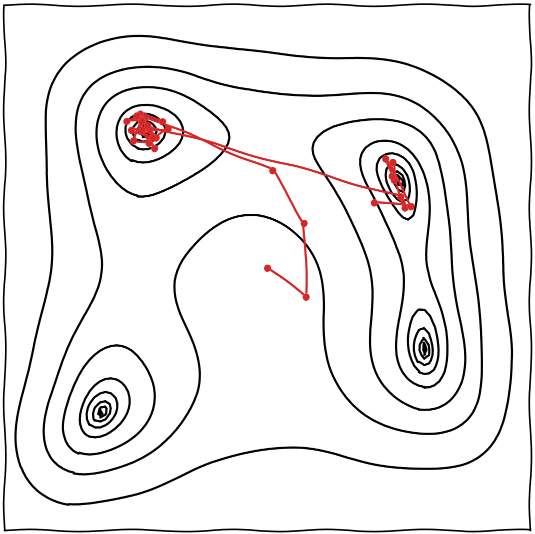

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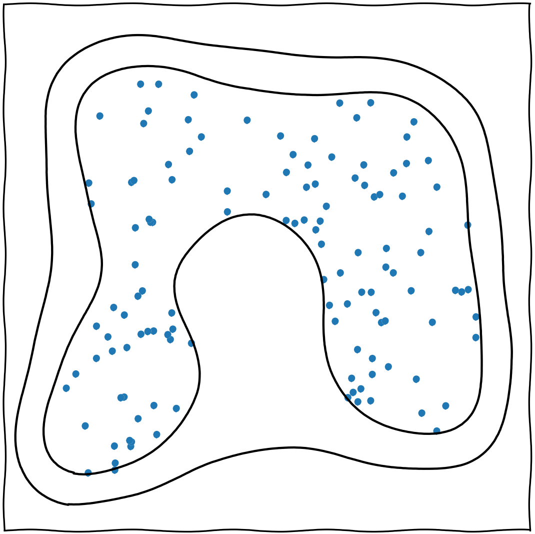

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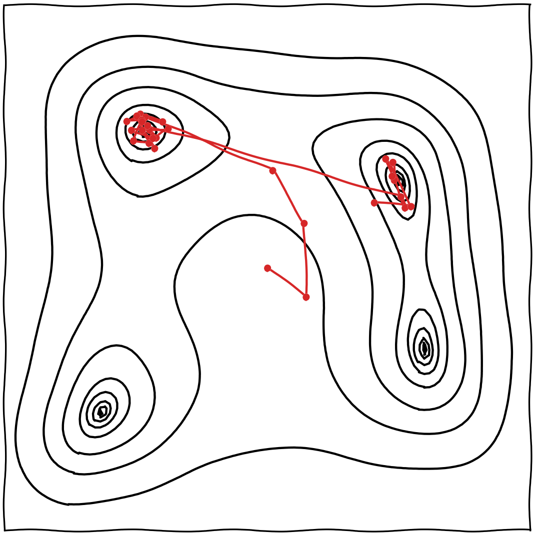

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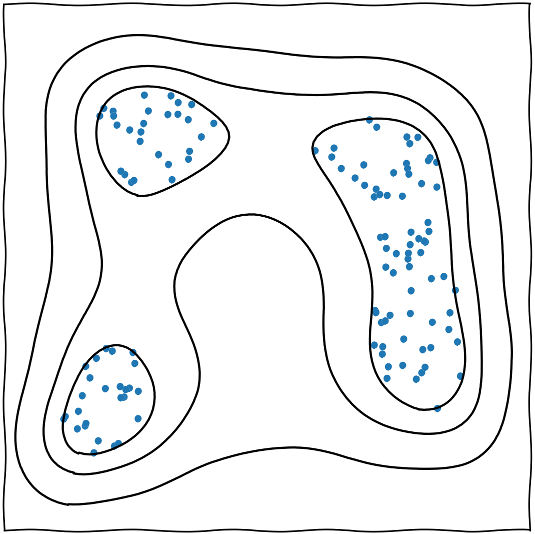

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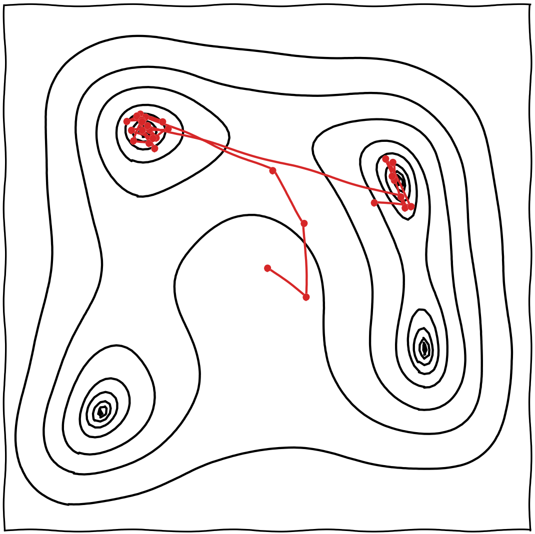

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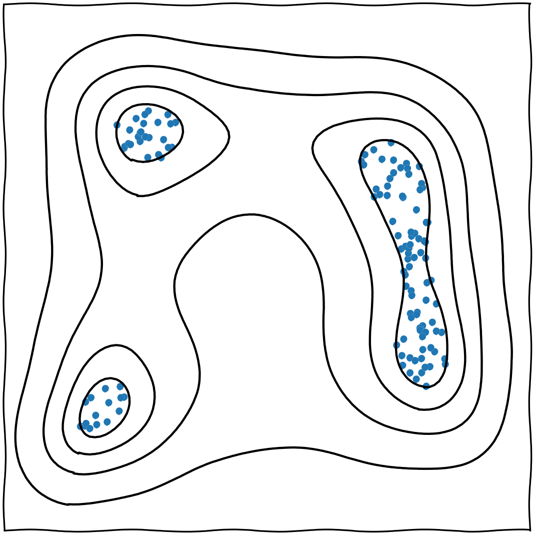

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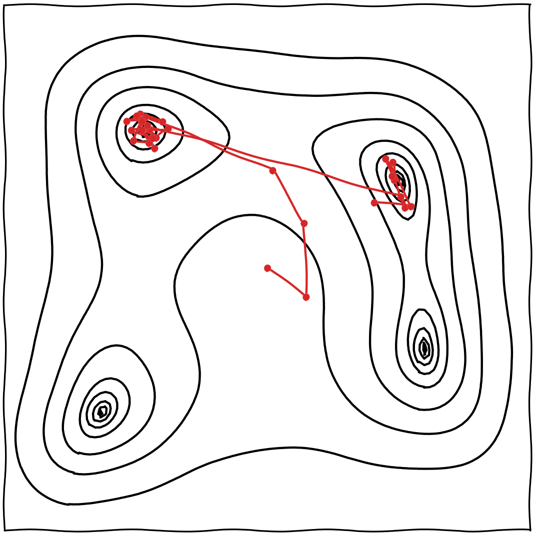

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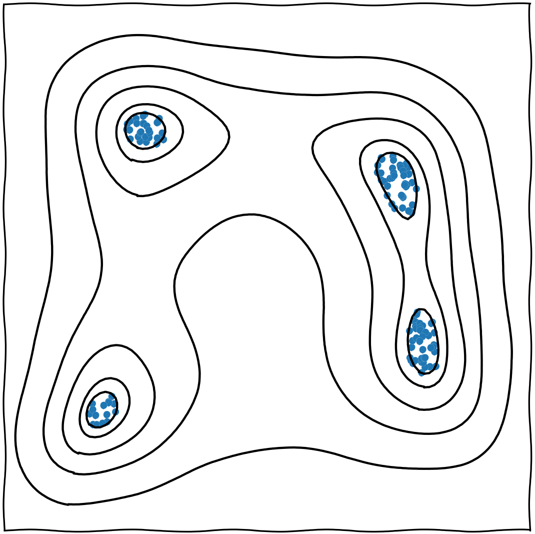

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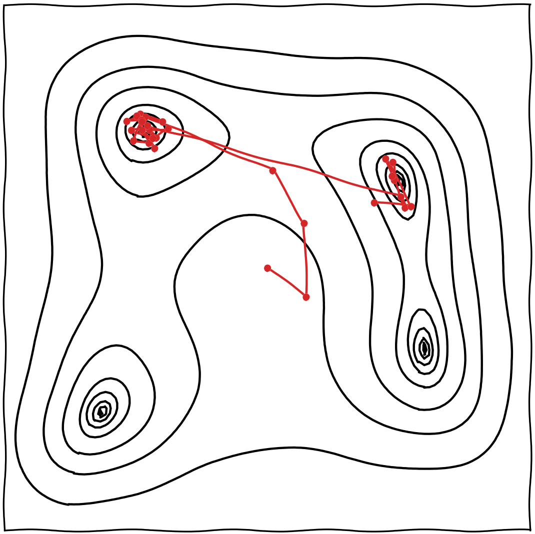

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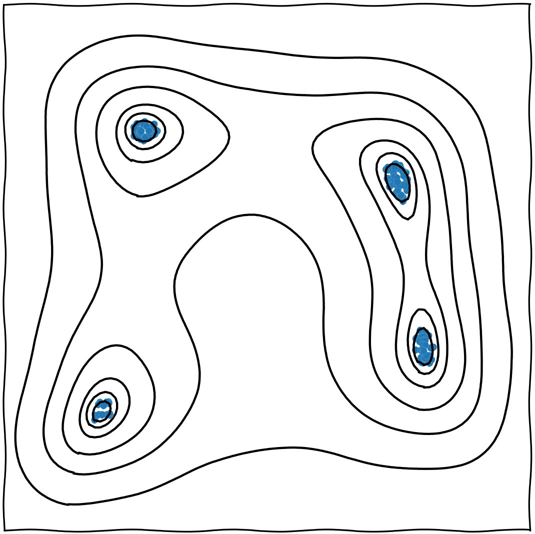

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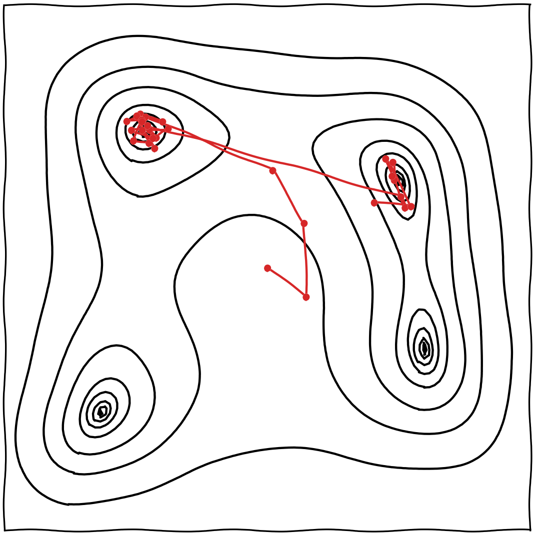

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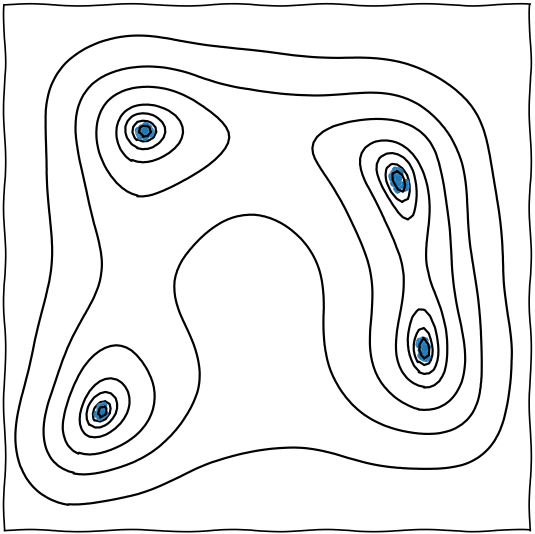

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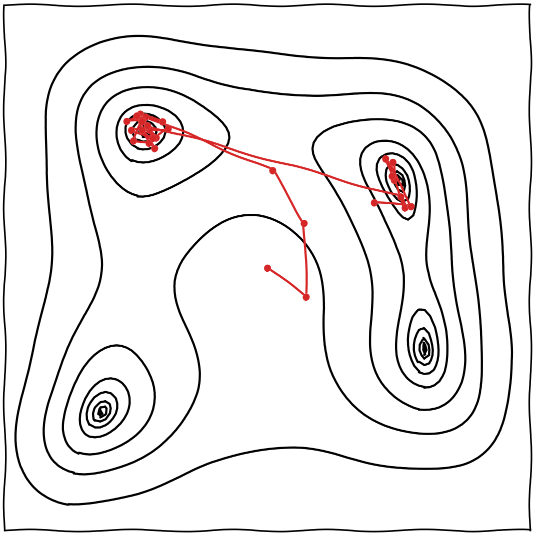

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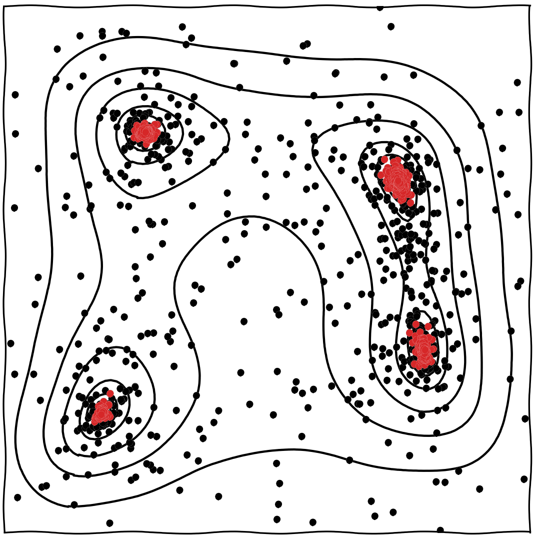
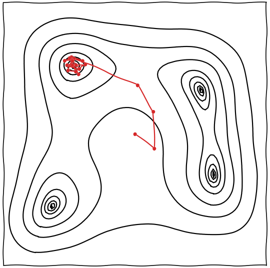


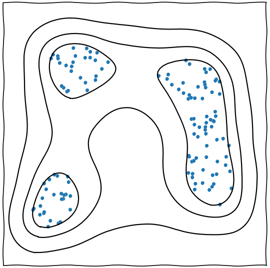
MCMC

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



Nested sampling

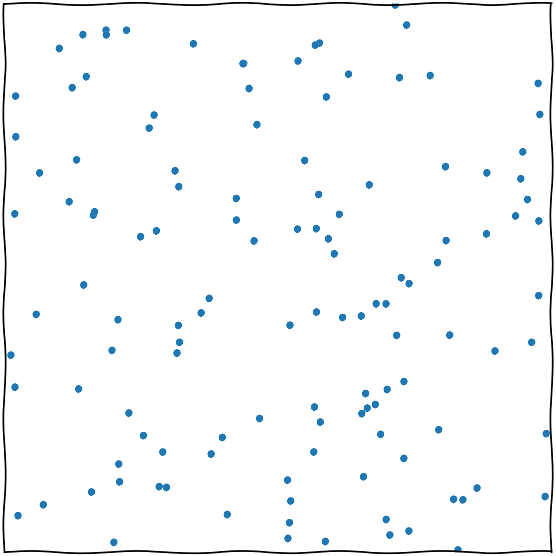
- Ensemble of "live points"
- Scans from prior to peak of likelihood
- Slower, no tuning required
- Parameter estimation, model comparison, tension quantification
- Channel capacity optimised for computing partition function



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

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



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.
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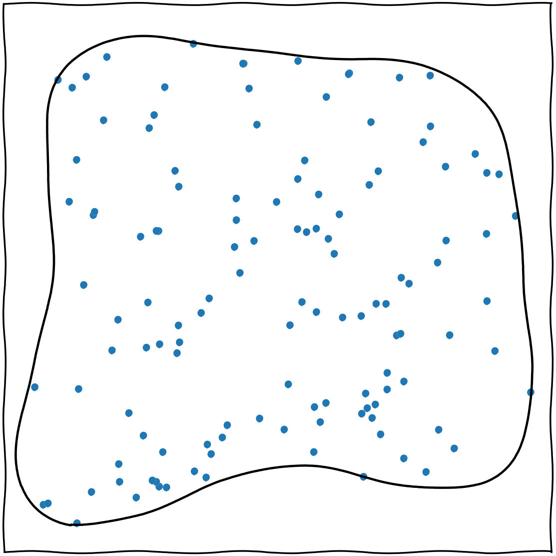

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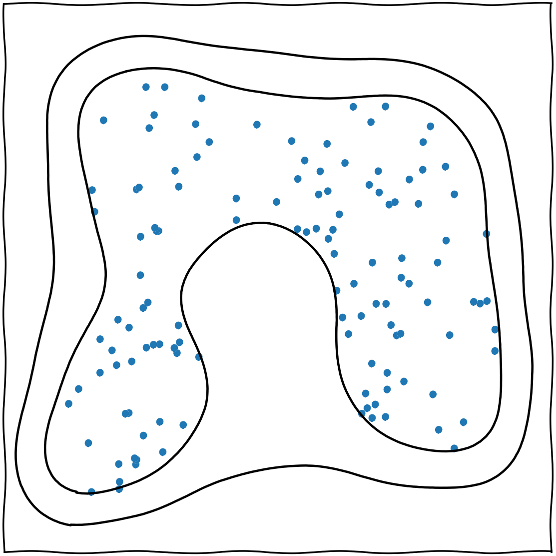

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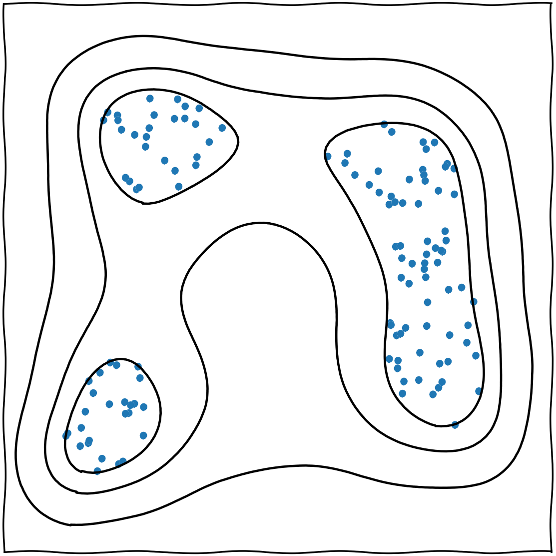

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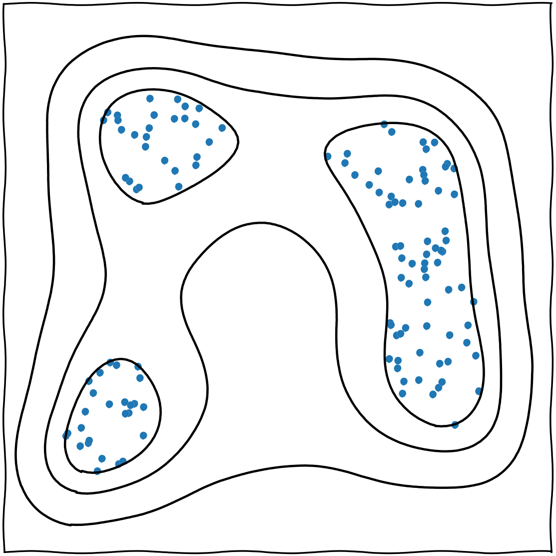
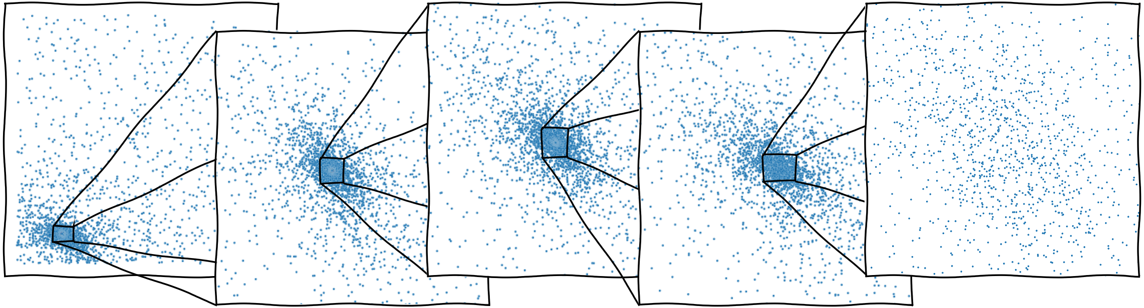
- We can use this evolution to estimate volume *probabilistically*.
- At each iteration, the contours contract by $\sim \frac{1}{n} \pm \frac{1}{n}$ of their volume.
- This is an exponential contraction, so

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



The nested sampling meta-algorithm: dead points



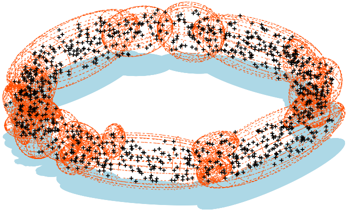
- At the end, one is left with a set of discarded "dead" points.
- Dead points have a unique scale-invariant distribution $\propto \frac{dV}{V}$.
- Uniform over original region, exponentially concentrating on region of interest (until termination volume).
- Good for training emulators (HERA [2108.07282]).

Applications

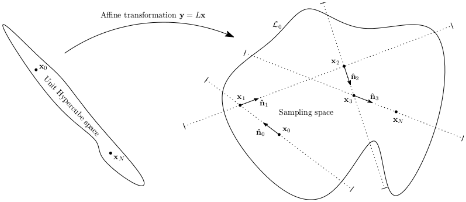
- training emulators.
- gridding simulations
- beta flows
- "dead measure"

Implementations of Nested Sampling [2205.15570](NatReview)

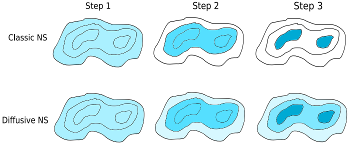
MultiNest [0809.3437]



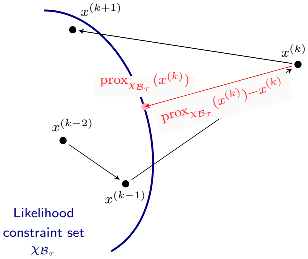
PolyChord [1506.00171]



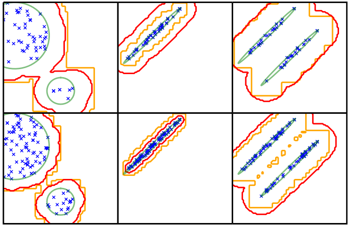
DNest [1606.03757]



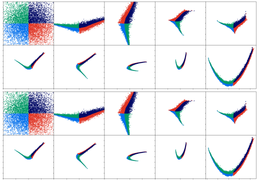
ProxNest [2106.03646]

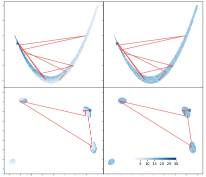


UltraNest [2101.09604]



NeuralNest [1903.10860]





nautilus [2306.16923]

nessai [2102.11056]

nora [2305.19267]

jaxnest [2012.15286]

dynesty [1904.02180]

Types of nested sampler

- Broadly, most nested samplers can be split into how they create new live points.
- i.e. how they sample from the hard likelihood constraint $\{\theta \sim \pi : \mathcal{L}(\theta) > \mathcal{L}_*\}$.

Rejection samplers

- e.g. `MultiNest`, `UltraNest`.
- Constructs bounding region and draws many invalid points until $\mathcal{L}(\theta) > \mathcal{L}_*$.
- Efficient in low dimensions, exponentially inefficient $\sim \mathcal{O}(e^{d/d_0})$ in high $d > d_0 \sim 10$.

Chain-based samplers

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

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

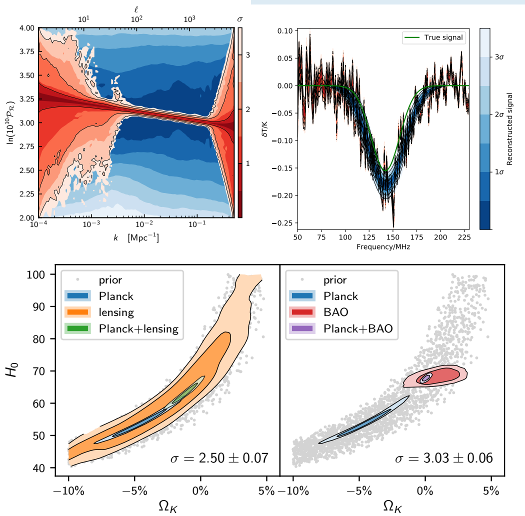
Applications of nested sampling

Cosmology

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.



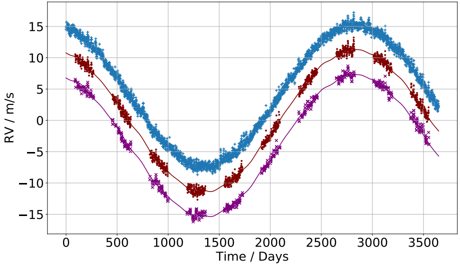
Applications of nested sampling

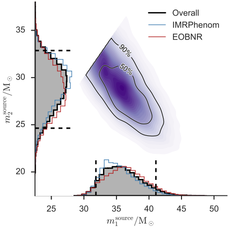
Astrophysics

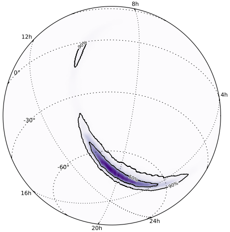
Metha Prathaban

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



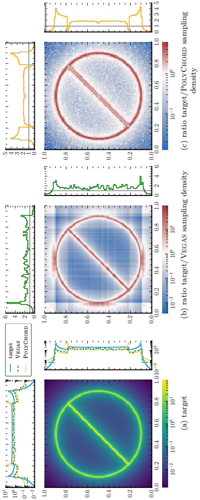


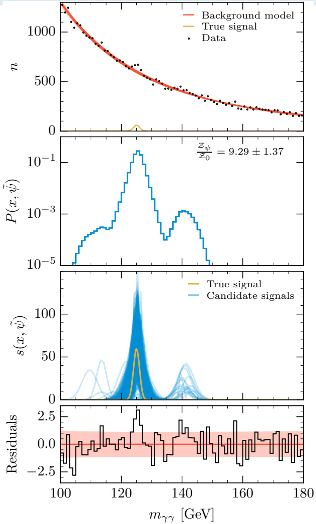


David Yallup

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

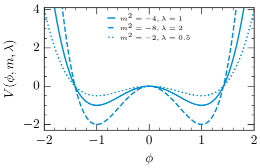
Lattice field theory

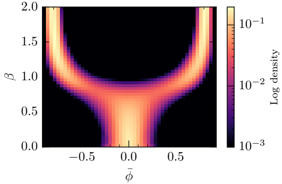
David Yallup
PDRA

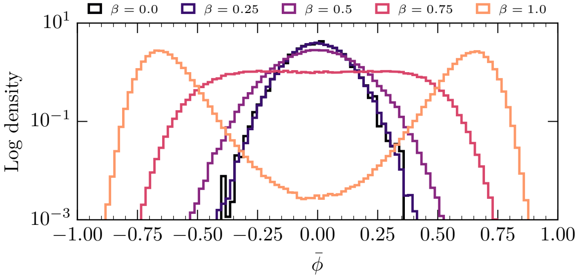
- Consider standard field theory Lagrangian:

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

- 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



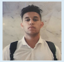




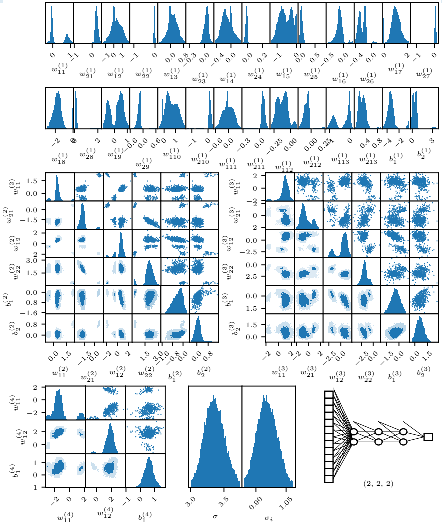
Applications of nested sampling

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]



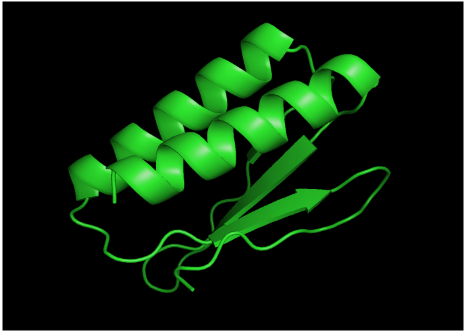
Applications of nested sampling

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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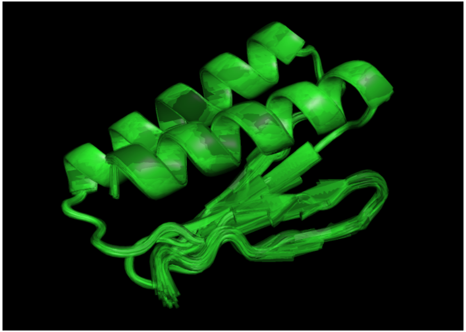

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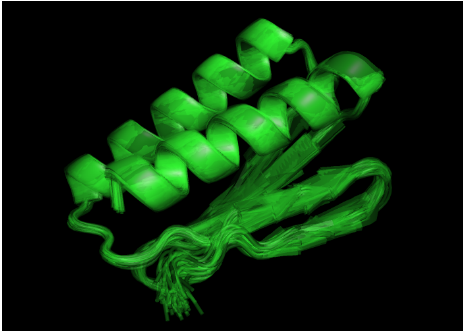

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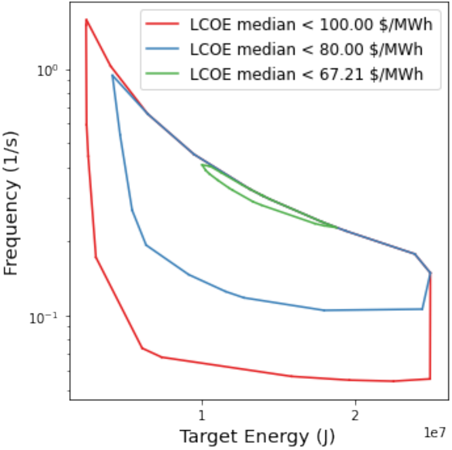

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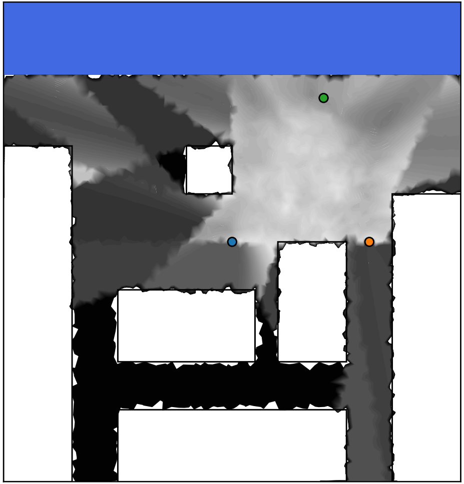

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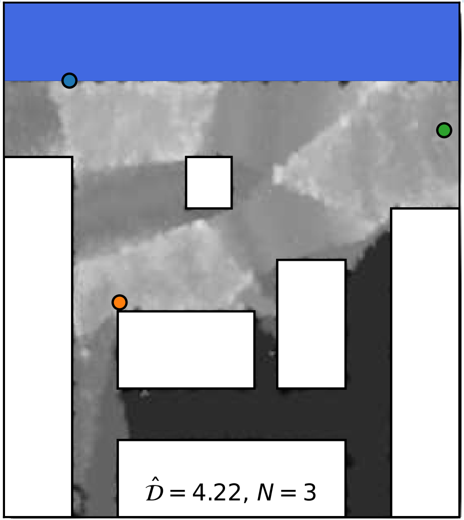

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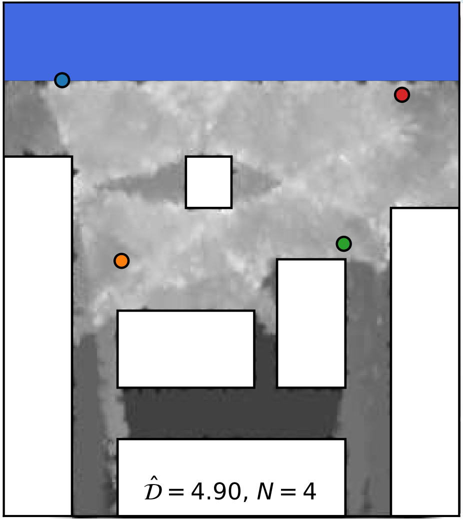

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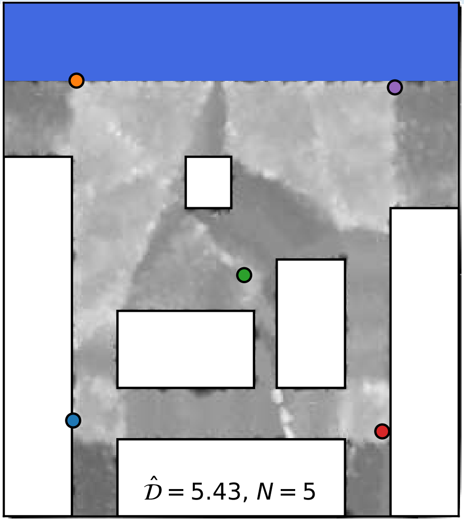
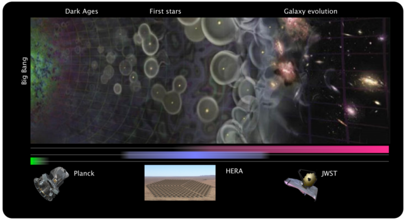
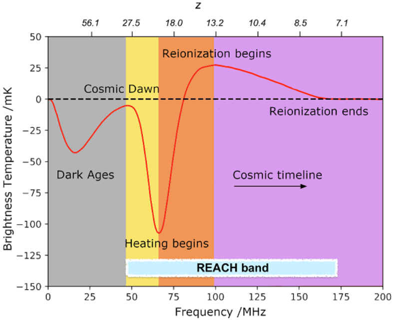


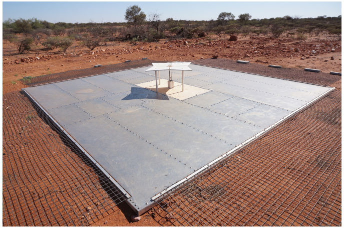
REACH: Global 21cm cosmology [2210.07409](NatAstro)

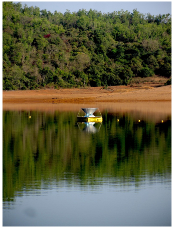
Ian Roque
PhD

- 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

Interdisciplinary case studies

- GAMBIT is an interdisciplinary community and software framework.
- Like `CosmoMC`/`Cobaya`/`Bilby`, an organiser of data, likelihoods & theory, including:
  - Collider data (e.g. LHC)
  - Direct detections (e.g. XENON1T)
  - Cosmology (`MontePython`)
  - Astrophysics (e.g. Bullet Cluster, Supernovae)
  - Pulsar timing
  - ... & much more
- `GravBit` and `LowEnergyBit` arising from GAMBIT@KICC workshop

Felix Kahlhoefer et al

GAMBIT cosmo/DM working group

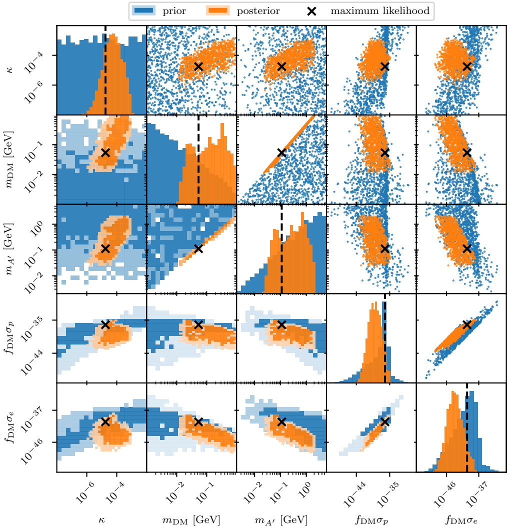
- Physical model of sub-GeV thermal dark matter with a dark photon mediator A:

$$\mathcal{L}_{\text{int}} = -\frac{1}{2}m_{A'}^2 A'^{\mu} A'_{\mu} - \frac{1}{4}A'^{\mu\nu}A'_{\mu\nu} - \kappa e A'^{\mu}\sum_f q_f \bar{f}\gamma_\mu f\,,$$

- Constrain using cosmological, astrophysical, accelerator & direct detection data.
- Bayesian Model comparison of Fermion ψ vs scalar Φ models (scalar preferred).

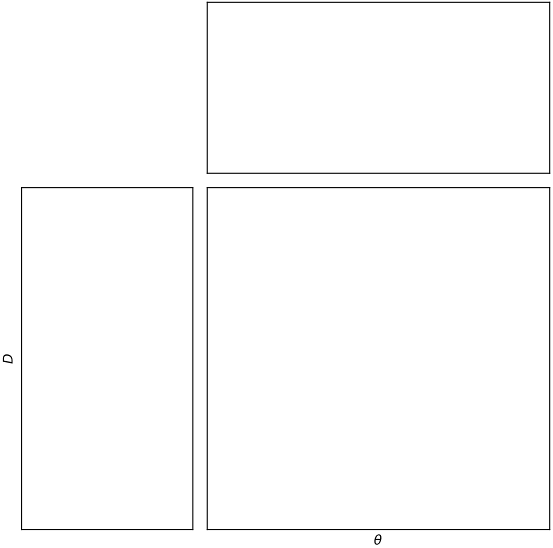
$$\mathcal{L}_\psi = \bar{\psi}(i\not{\partial} - m_{\text{DM}})\psi + g_{\text{DM}}A'^{\mu}\bar{\psi}\gamma_\mu\psi\,,$$

$$\mathcal{L}_\Phi = |\partial_\mu\Phi|^2 - m_{\text{DM}}^2|\Phi|^2 - g_{\text{DM}}^2 A'_\mu A'^\mu|\Phi|^2 + ig_{\text{DM}}A'^{\mu}\left[\Phi^*(\partial_\mu\Phi) - (\partial_\mu\Phi^*)\Phi\right]\,,$$



SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \rightarrow D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$ *the "probability of everything"*.
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$ and evidence $\mathcal{Z}(D)$ and possibly likelihood $\mathcal{L}(D|\theta)$.
- Present state of the art achieves this using *machine learning* (neural networks).
  - My group's research tries to removes machine learning `github.com/handley-lab/lsbi`.



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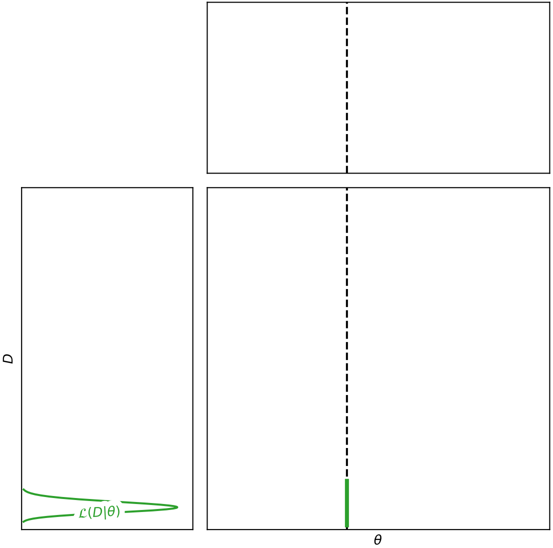

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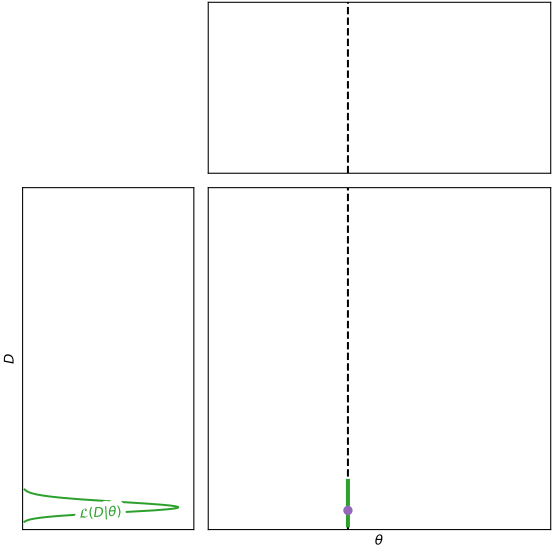

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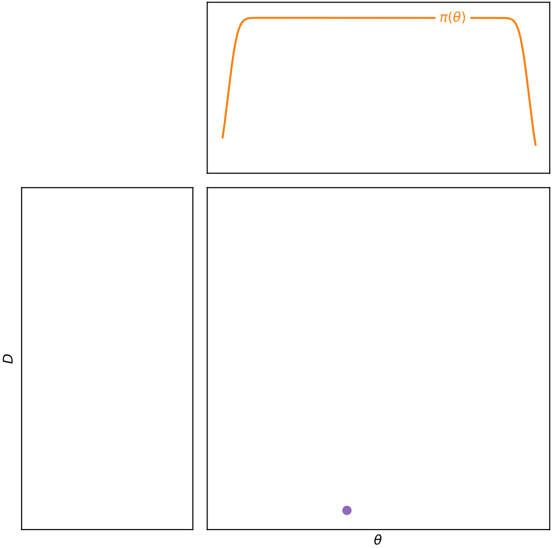

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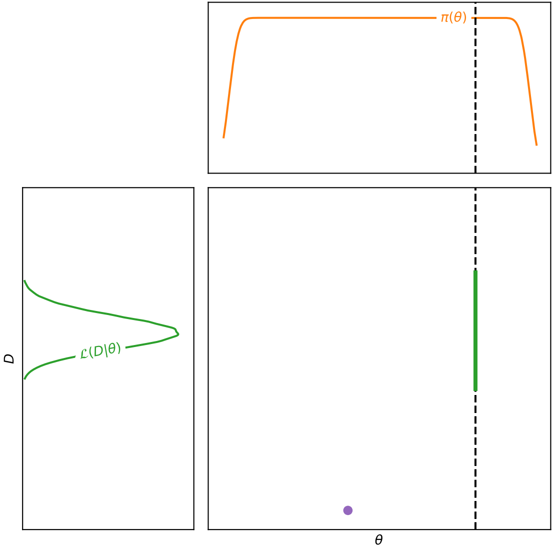

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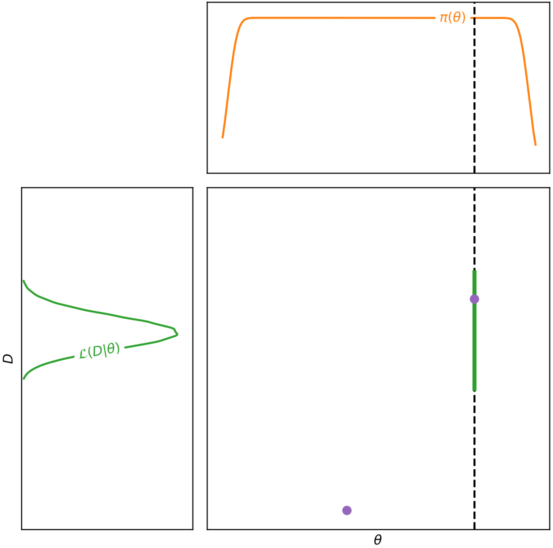

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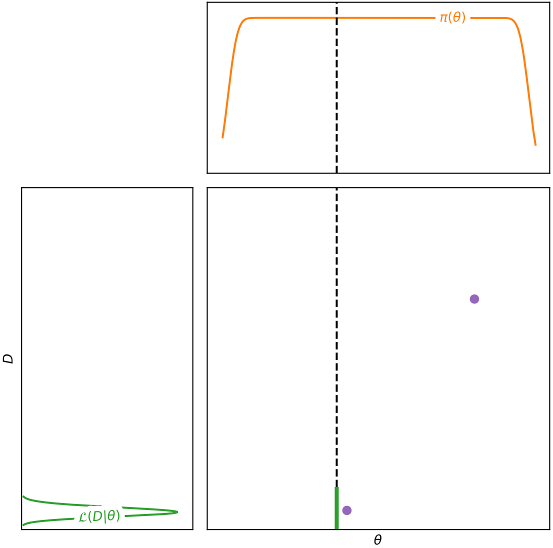

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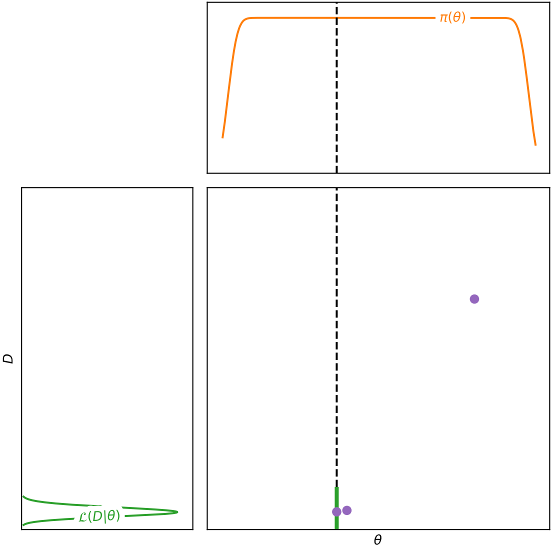

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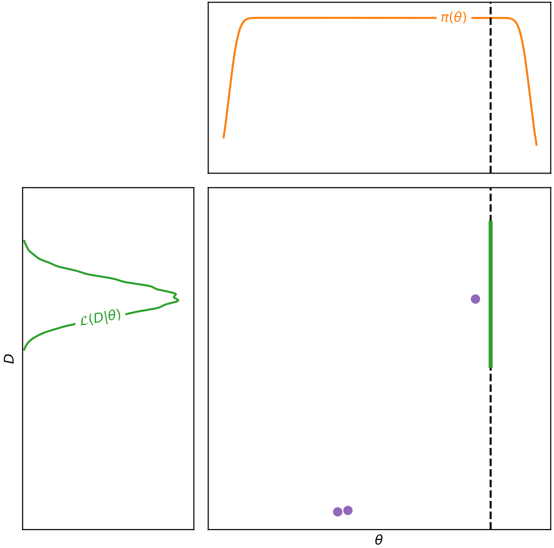

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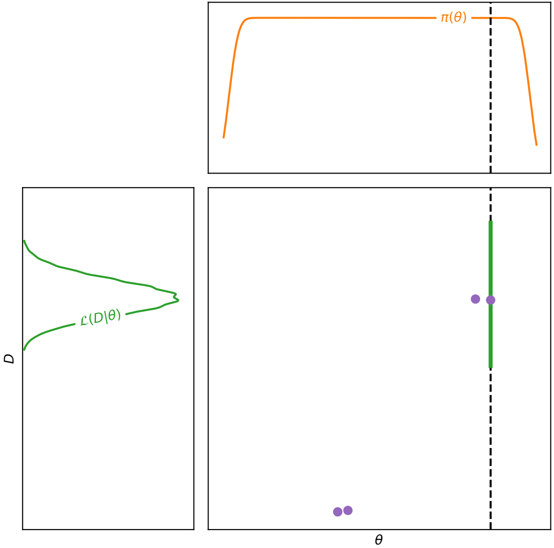

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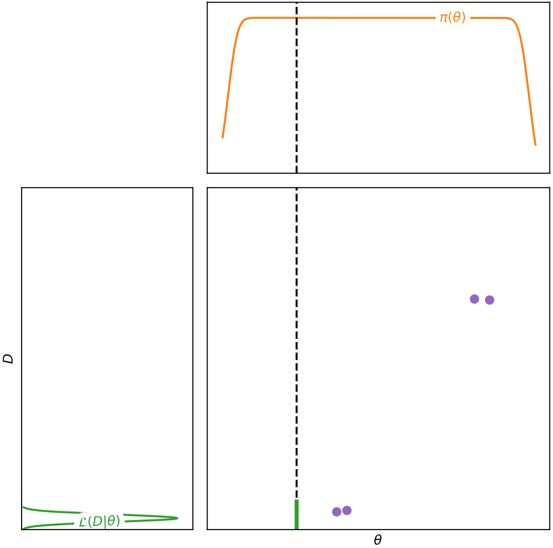

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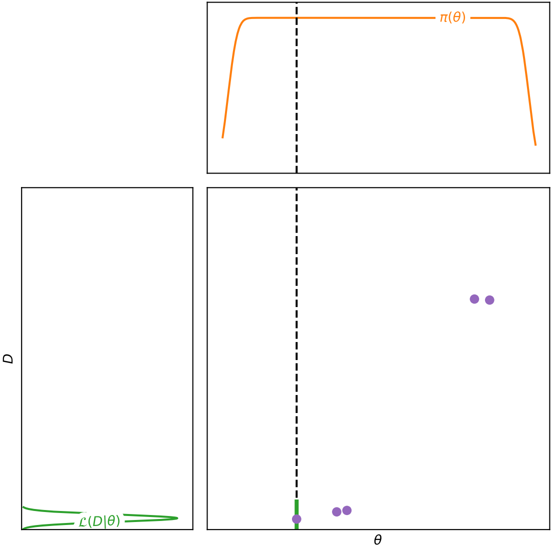

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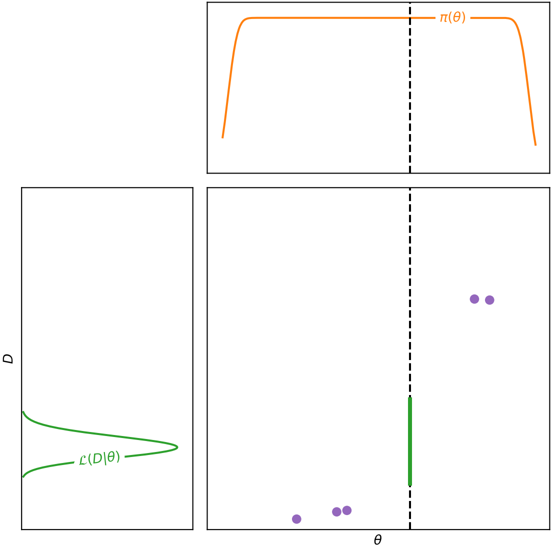

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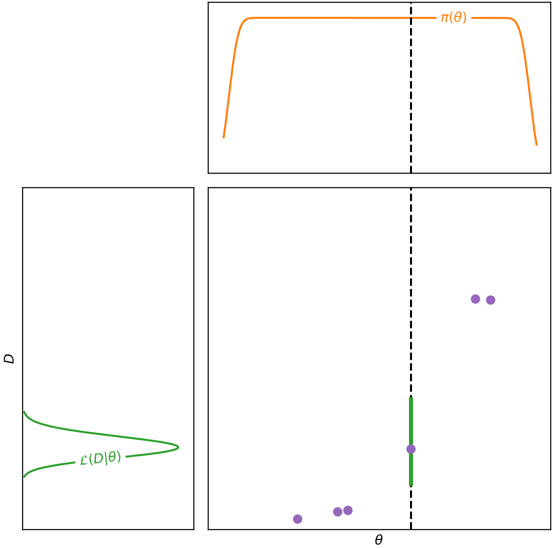

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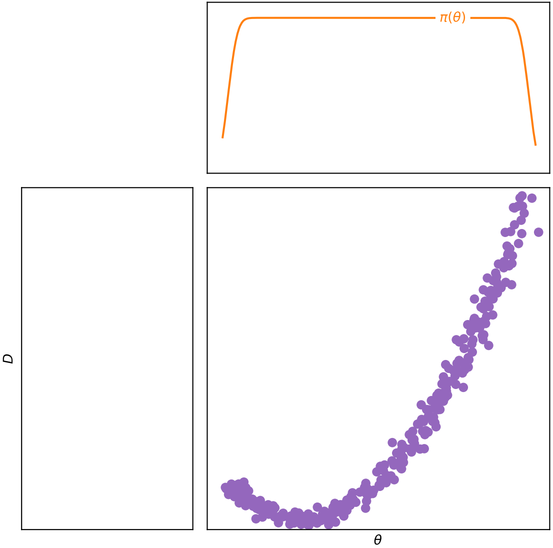

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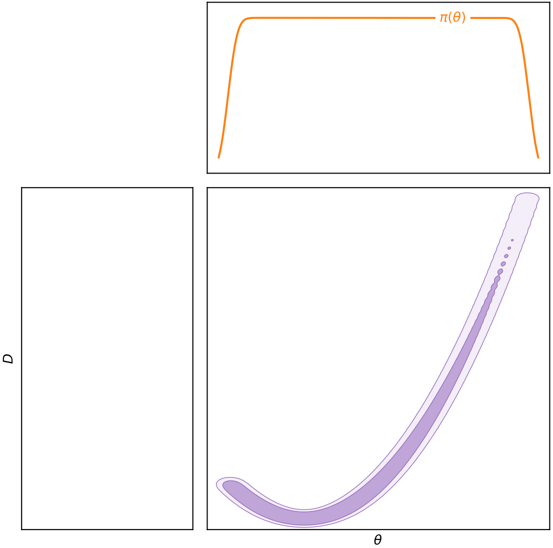

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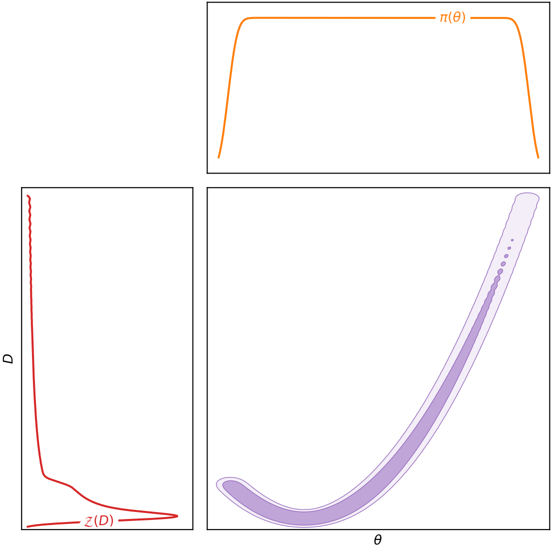

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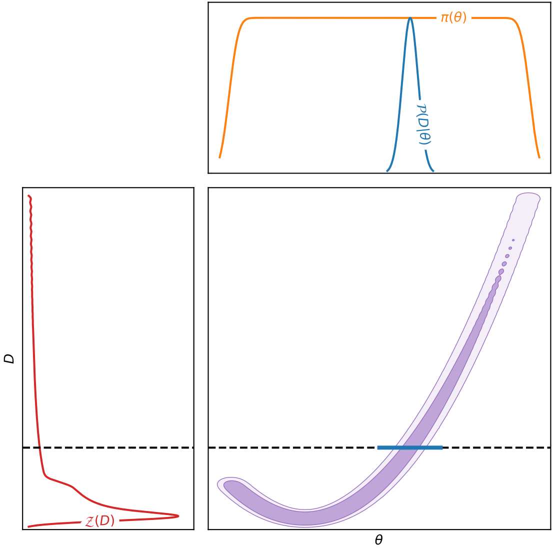

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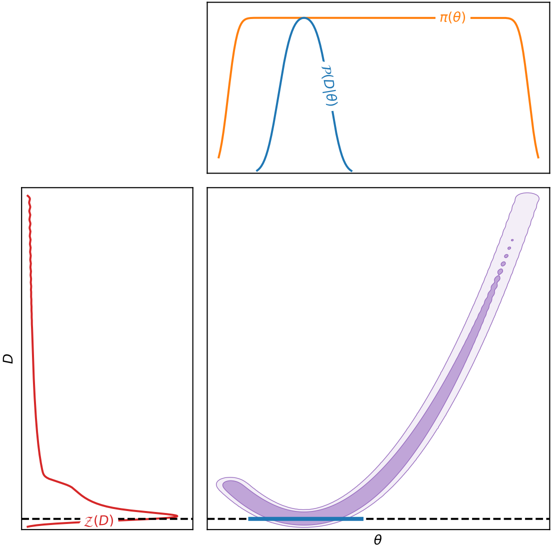

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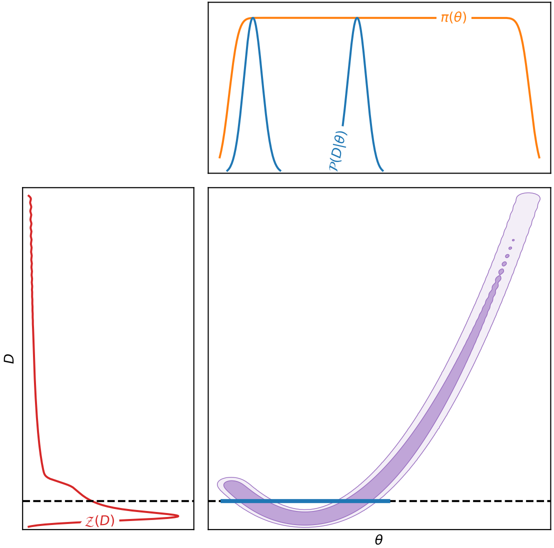

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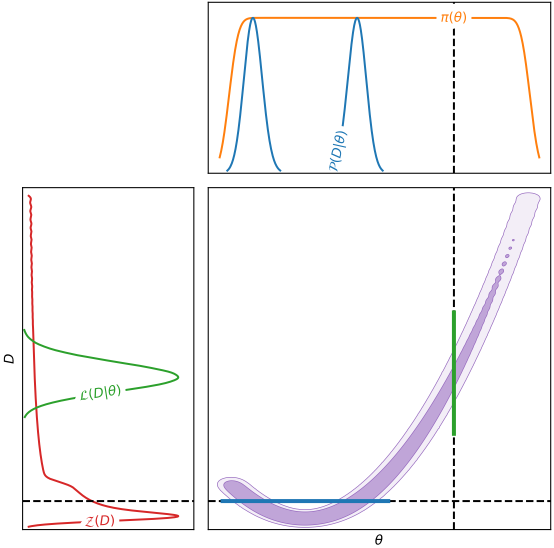
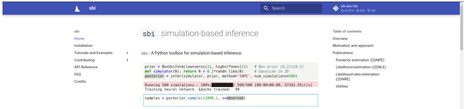


Why SBI?

SBI is useful because:

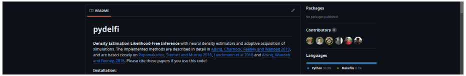
1. If you don't have a likelihood, you can still do inference
   - This is the usual case beyond CMB cosmology
2. Faster than LBI
   - emulation – also applies to LBI in principle
3. No need to pragmatically encode fiducial cosmologies
   - Covariance computation implicitly encoded in simulations
   - Highly relevant for disentangling tensions & systematics
4. Equips AI/ML with Bayesian interpretability
5. Lower barrier to entry than LBI
   - Much easier to forward model a systematic
   - Emerging set of plug-and-play packages
   - For this reason alone, it will come to dominate scientific inference



github.com/sbi-dev

github.com/undark-lab/swyft

github.com/florent-leclercq/pyselfi



github.com/justinalsing/pydelfi

SBI in cosmology

- 2024 has been the year it has started to be applied to real data.
- Mostly for weak lensing
- However: SBI requires mock data generation code
- Most data analysis codes were built before the generative paradigm.
- It's still a lot of work to upgrade cosmological likelihoods to be able to do this (e.g. `plik` & `camspec`).

Investigating the turbulent hot gas in X-COP galaxy clusters

S. Dupourqué[1], N. Clerc[1], E. Pointecouteau[1], D. Eckert[2], S. Ettori[3], and F. Vazza[4,5,6]

Dark Energy Survey Year 3 results: simulation-based cosmological inference with wavelet harmonics, scattering transforms, and moments of weak lensing mass maps II. Cosmological results

M. Gatti,[1,*] G. Campailla,[2] N. Jeffrey,[3] L. Whiteway,[3] A. Porredon,[4] J. Prat,[5] J. Williamson,[3] M. Raveri,[2] B.

Neural Posterior Estimation with guaranteed exact coverage: the ringdown of GW150914

Marco Crisostomi[1,2], Kallol Dey[3], Enrico Barausse[1,2], Roberto Trotta[1,2,4,5]

Applying Simulation-Based Inference to Spectral and Spatial Information from the Galactic Center Gamma-Ray Excess

Katharena Christy,[a] Eric J. Baxter,[b] Jason Kumar[a]

KiDS-1000 and DES-Y1 combined: Cosmology from peak count statistics

Joachim Harnois-Déraps[1⋆], Sven Heydenreich[2], Benjamin Giblin[3], Nicolas Martinet[4], Tilman Tröster[5], Marika Asgari[1,6,7], Pierre Burger[8,9,10], Tiago Castro[11,12,13,14], Klaus Dolag[15], Catherine Heymans[3,16], Hendrik Hildebrandt[16], Benjamin Joachimi[17] & Angus H. Wright[16]

KiDS-SBI: Simulation-Based Inference Analysis of KiDS-1000 Cosmic Shear

Maximilian von Wietersheim-Kramsta[1,2,3], Kiyam Lin[1], Nicolas Tessore[1], Benjamin Joachimi[1], Arthur Loureiro[4,5], Robert Reischke[6,7], and Angus H. Wright[7]

Simulation-based inference of deep fields: galaxy population model and redshift distributions

Beatrice Moser,[a,1] Tomasz Kacprzak,[a,b] Silvan Fischbacher,[a] Alexandre Refregier,[a] Dominic Grimm,[a] Luca Tortorelli[c]

SimBIG: Cosmological Constraints using Simulation-Based Inference of Galaxy Clustering with Marked Power Spectra

Elena Massara[1,2,*], ChangHoon Hahn[3], Michael Eickenberg,[4] Shirley Ho,[5] Jiamin Hou,[6,7] Pablo Lemos,[8,9,5] Chirag Modi,[4,5] Azadeh Moradinezhad Dizgah[10,11], Liam Parker,[5,12] and Bruno Régaldo-Saint Blancard[4]

- 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.
- It's unique traits as the only numerical Lebesgue integrator mean with compute it will continue to grow in importance.
- SBI represents the future of inference beyond LBI.