Nested Sampling: a multi-purpose numerical tool for particle physics and cosmology

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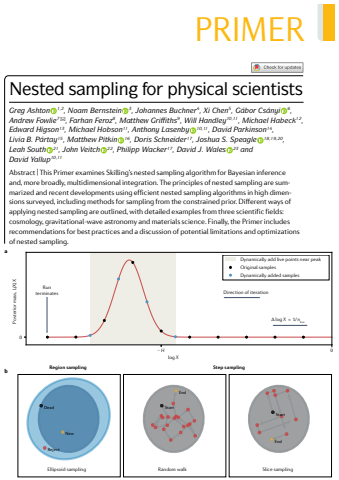
Highlight: state-of-the-art Nature review [NatRev]

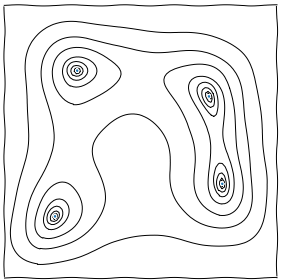
- Invented by John Skilling in 2004.
- Recent Nature review primer on nested sampling led by Andrew Fowlie and assembled by the community.
- Showcases the current set of tools, and applications from chemistry to cosmology.
- In this talk
  - User guide to nested sampling
  - Particle physics applications
  - Cosmology applications

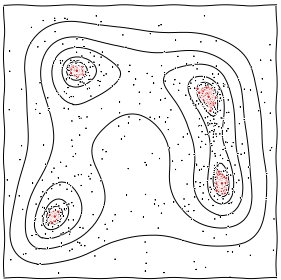


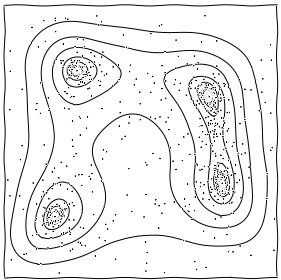
What is Nested Sampling?

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

Optimisation	Sampling	Integration
$\theta_{\max} = \max_{\theta} f(\theta)$	draw $\theta \sim f$	$\int f(\theta) dV$







MCMC sampling

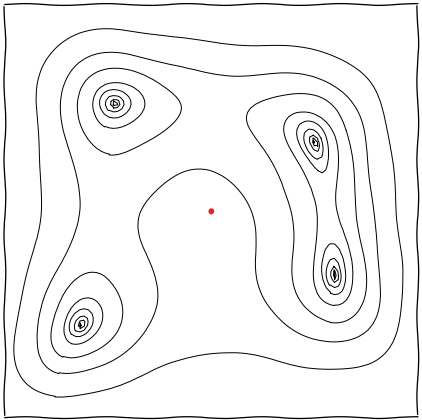
- Markov chain based methods generate samples from distribution by a stepping procedure.
- This can get stuck in local peaks.
- Cannot compute normalisation $\mathcal{Z}$ of Bayes theorem:

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

$$\mathcal{P} = \frac{\mathcal{L}\times\pi}{\mathcal{Z}}, \qquad \text{posterior} = \frac{\text{likelihood}\times\text{prior}}{\text{evidence}}.$$

- We generally want the evidence $\mathcal{Z} = P(D|M)$ for the second stage of inference: model comparison:

$$P(M|D) = \frac{P(D|M)P(M)}{P(D)}, \qquad \text{Science}(M) = \frac{\mathcal{Z}_M\Pi_M}{\sum_m \mathcal{Z}_m\Pi_m}.$$



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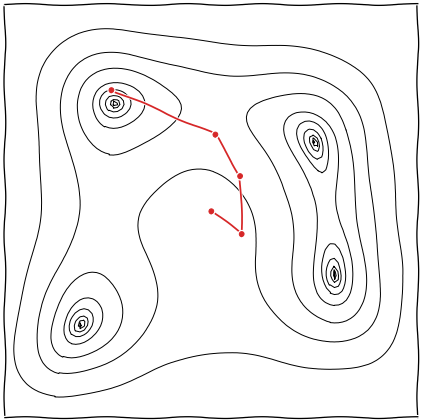

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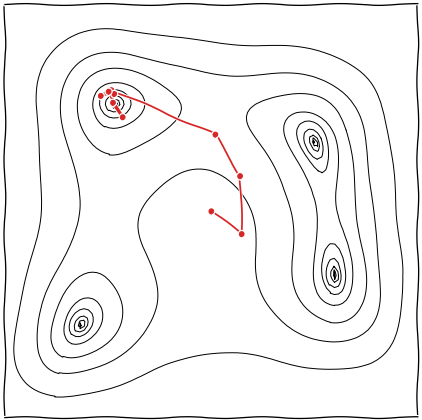

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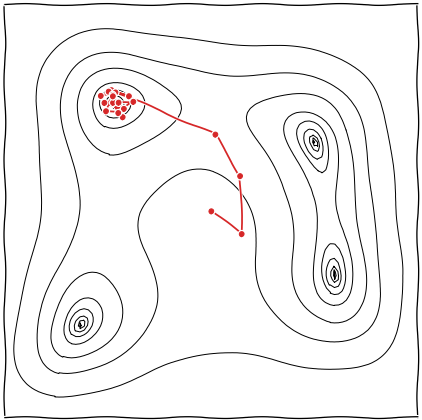

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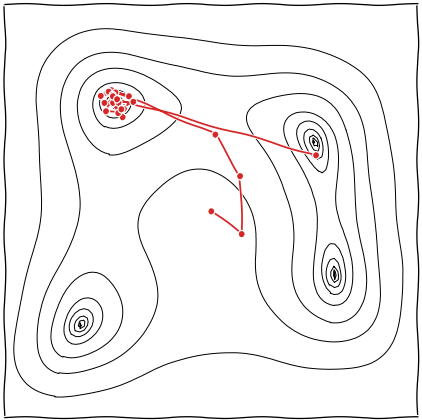

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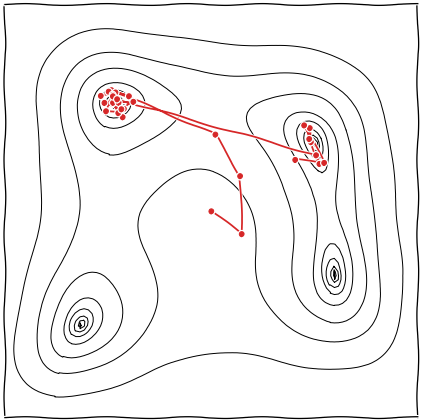

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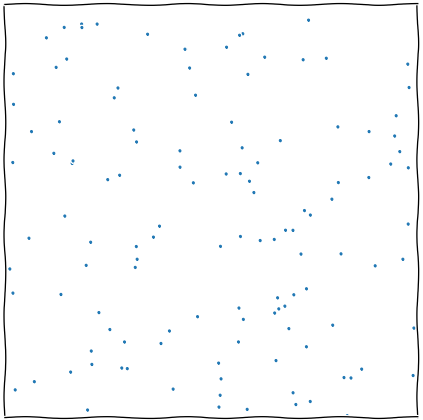
- Nested sampling: completely different way to scan.
- Ensemble sampling compresses entire space→peak(s).
- Sequentially update a set S of n samples:
  - S_0: Generate n samples uniformly over the space (from a measure π).
  - S_{i+1}: Delete the lowest likelihood sample in S_i, and replace it with a new uniform sample with higher likelihood.
- Requires one to be able to sample uniformly within a region, subject to a *hard constraint*:

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

- This procedure optimises (multimodally), and can calculate the evidence/integral of function & posterior/sample weights.



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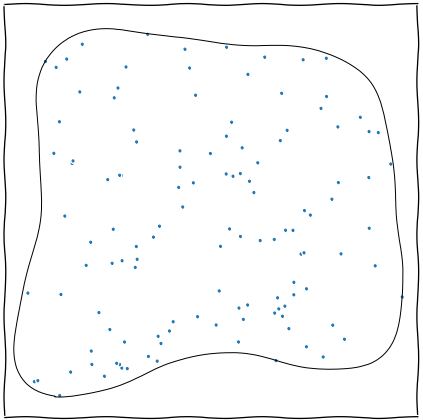

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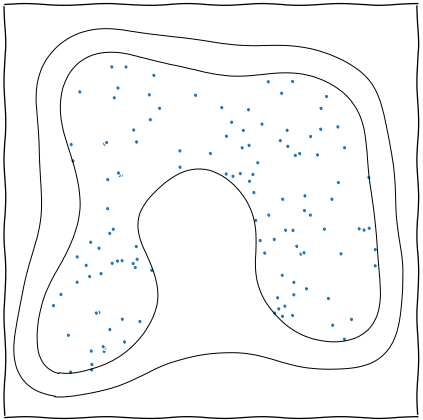

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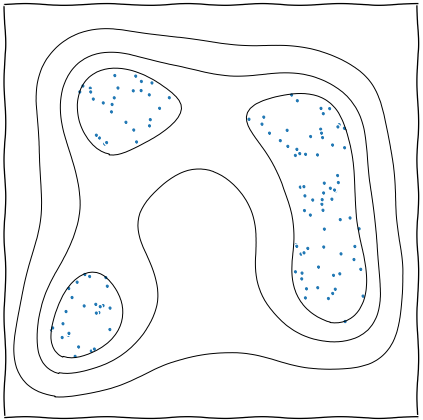

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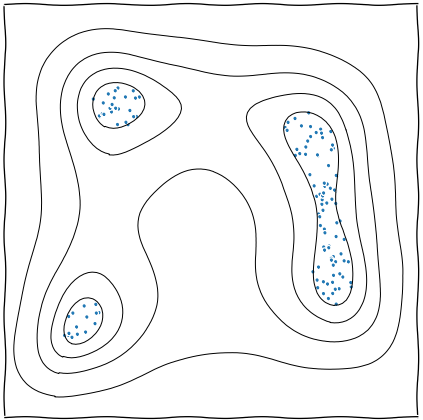

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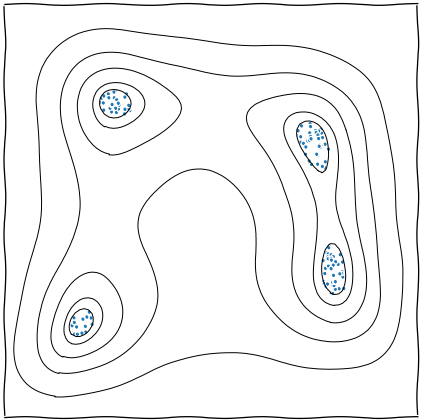

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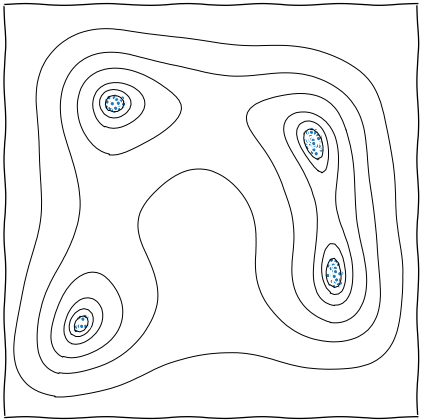

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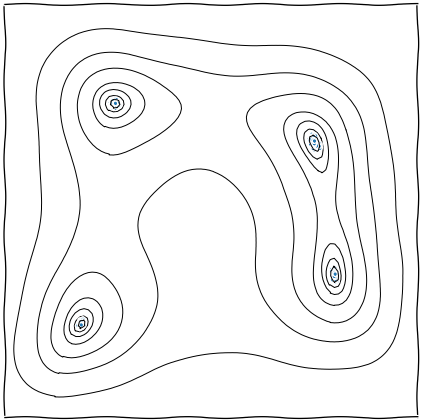
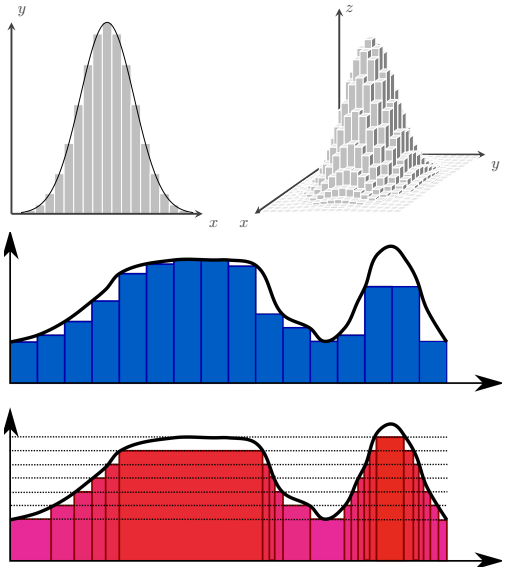


Integration in high dimensions

- Numerical integration $\int f(x)dV$ in high dimensions is hard.
- `scipy.integrate(...)` is unusable in more than four dimensions.
- This is due to the curse of dimensionality: need to sum $\sim N^d$ units to compute $\approx \sum_i f(x_i)\Delta V_i$.
- Additionally, estimating volumes with geometry becomes exponentially hard as d increases.
- *Aside:* **Riemannian integration** *(blue) is taught as standard. An orthogonal approach (red) [usually theoretical] is* **Lesbesgue integration**.



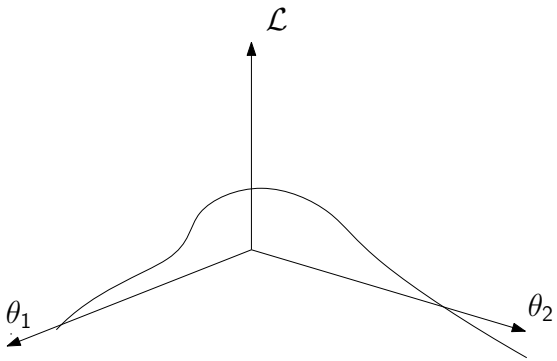
(Lesbesgue) Integrating with nested sampling

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

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

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

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



- Integral can be discretised in several ways

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

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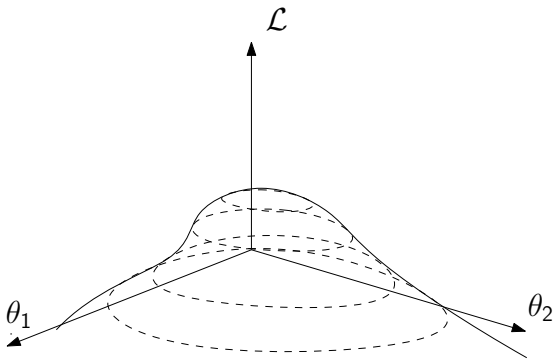

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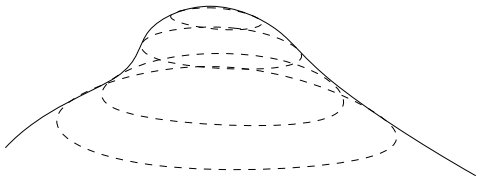

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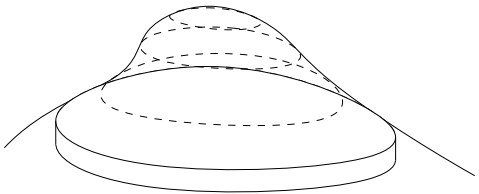

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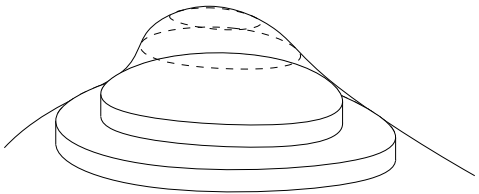

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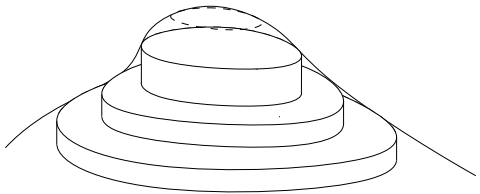

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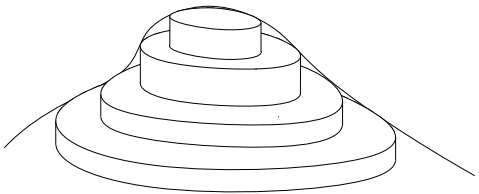

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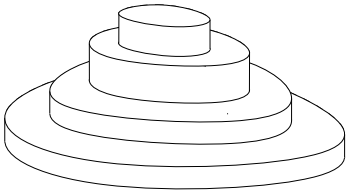

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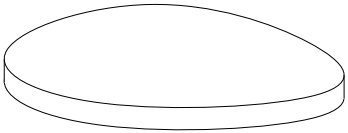

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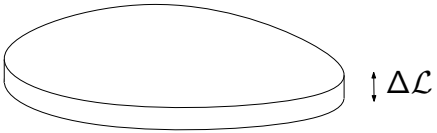

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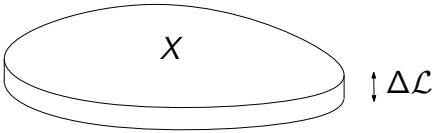

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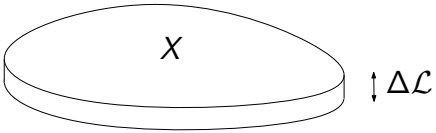

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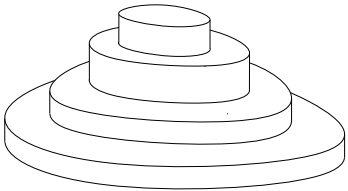

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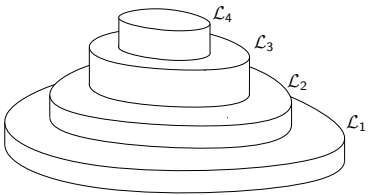

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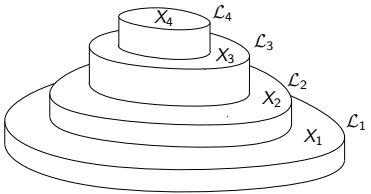

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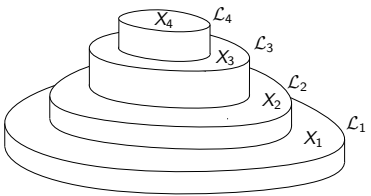
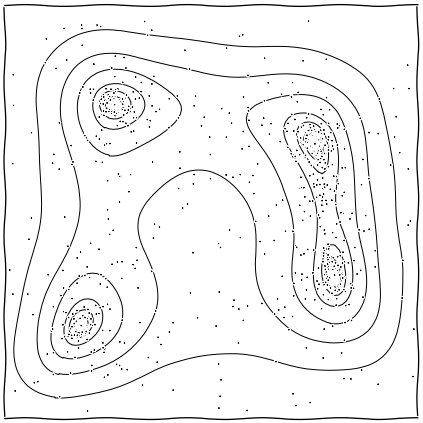


Dead points: posteriors & evidences

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

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

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



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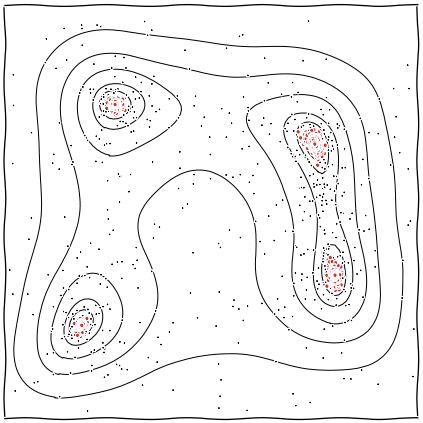


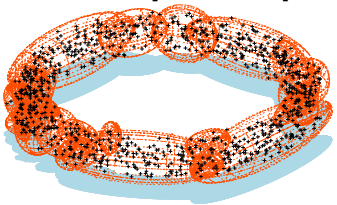
Sampling from a hard likelihood constraint

> *"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*

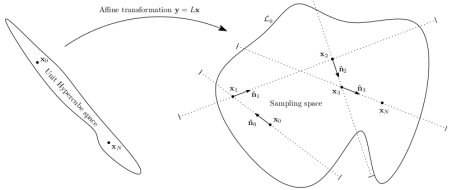
- A large fraction of the work in NS to date has been in attempting to implement a hard-edged sampler in the NS meta-algorithm $\{\theta \sim \pi : \mathcal{L}(\theta) > \mathcal{L}_*\}$.
- `https://projecteuclid.org/euclid.ba/1340370944`.
- There has also been much work beyond this (focus of this talk).

Implementations of Nested Sampling

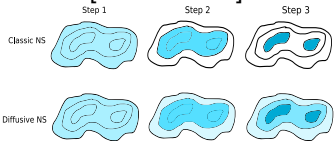
MultiNest [0809.3437]



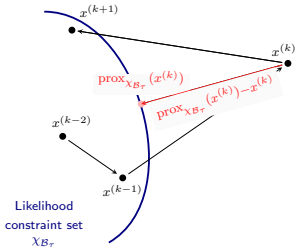
PolyChord [1506.00171]



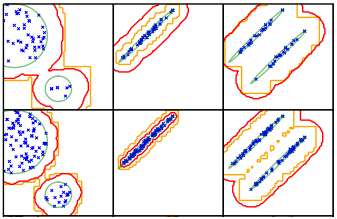
DNest [1606.03757]



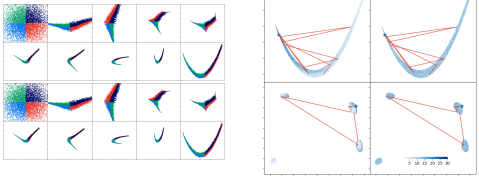
ProxNest [2106.03646]



UltraNest [2101.09604]



NeuralNest [1903.10860]



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 one is found within L_*.
- Efficient in low dimensions, exponentially inefficient $\sim \mathcal{O}(e^{d/d_0})$ in high $d > d_0 \sim 10$.

Chain-based samplers

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

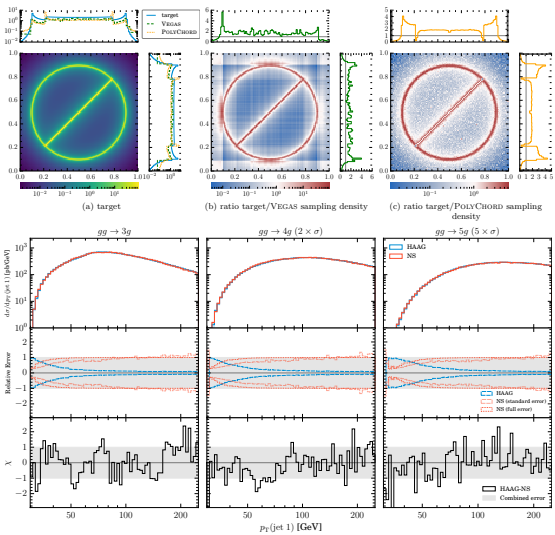
- Nested samplers usually come with:
  - *resolution* parameter n_{live} (which improve results as $\sim \mathcal{O}(n_{\text{live}}^{-1/2})$.
  - set of *reliability* parameters [2101.04525], which don't improve results if set arbitrarily high, but introduce systematic errors if set too low.
  - e.g.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

Exploration of phase space [2106.02056]

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

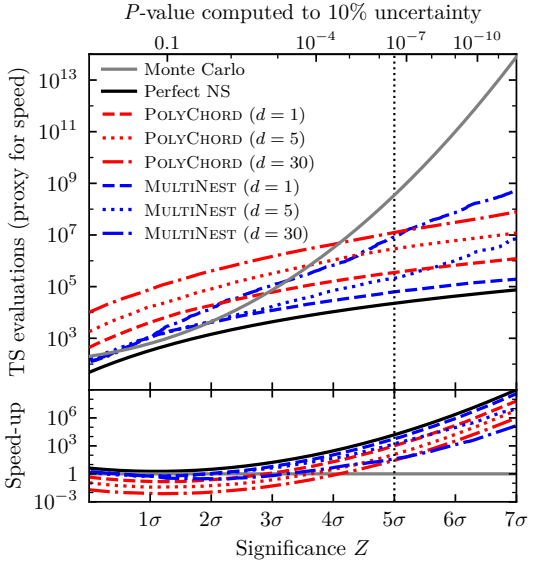
$$\sigma = \int_{\Omega} d\Phi |\mathcal{M}|^2,$$

  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.



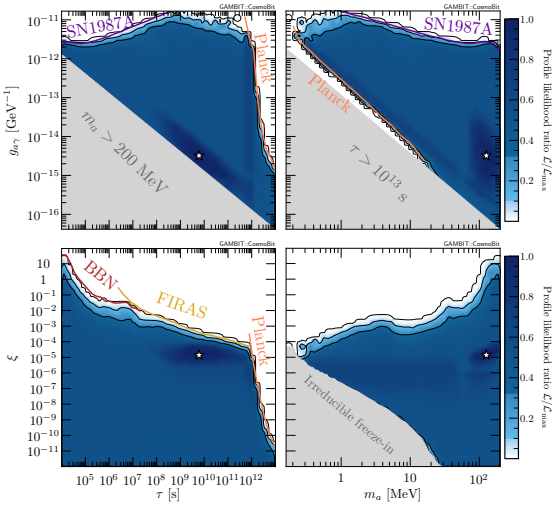
Statistics: fast estimation of small p-values [2106.02056](PRL)

- 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.



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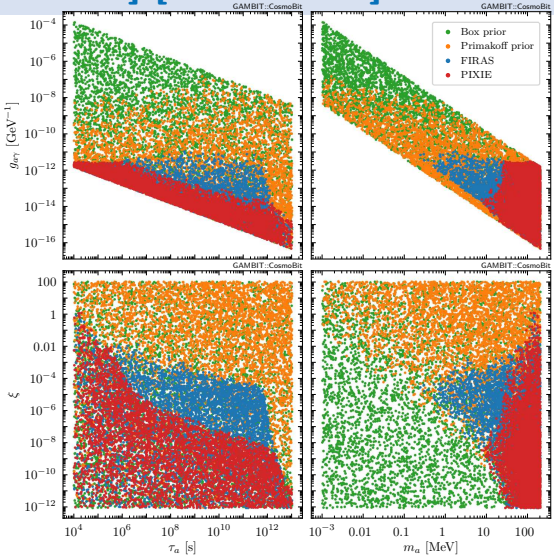
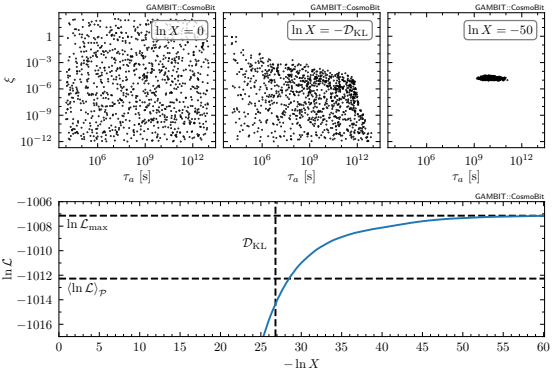
- Nested sampling scan:
  - Quantifies amount of parameter space ruled out with Kullback-Liebler divergence $\mathcal{D}_{\mathrm{KL}}$.
  - Identifies best fit region as statistically irrelevant from information theory/Bayesian.
  - No evidence for decaying ALPs. Fit the data equally well: but more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



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.
- Nested sampling scan:
  - 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.

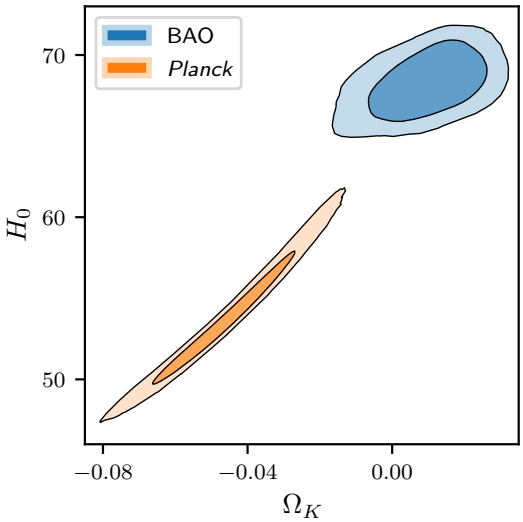


What is a model?

- Model comparison in its purest form answers question such as:
  - "Is the universe ΛCDM?"
  - "Are neutrinos in a normal or inverted hierarchy?"
  - "Is there a detectable global signal in this data?"
- However model $\mathcal{M}$ is likelihood $\mathcal{L} = P(D|\theta, M)$ and priors $\pi = P(\theta|M)$, $\Pi = P(M)$.
- Can use the evidence $\mathcal{Z}$ to decide on which out of a set of likelihoods best describe data (e.g. Gaussian, Cauchy, Poisson, radiometric).
- Can also use it for antenna selection [2106.10193] [2109.10098].
- In principle can use it to decide between theoretically motivated priors (care needed).
- It can also be used for non-parametric reconstruction:
  - "How many polynomial terms best describe the data?"
  - "How complicated a sky model do I need?"
  - "Which is the best sky model?"

Model comparison and parameter estimation [1908.09139]

- If you allow $\Omega_K \neq 0$, *Planck* (`plikTTTEEE`) has a moderate preference for closed universes (50:1 betting odds on), $\Omega_K = -4.5 \pm 1.5\%$.
- *Planck*+lens+BAO strongly prefer $\Omega_K = 0$.
- But, *Planck* vs lensing is 2.5σ in tension, and Planck vs BAO is 3σ.
- Reduced if `plik` $\rightarrow$ `camspec` [2002.06892]
- BAO and lensing summary assume ΛCDM.
- Doing this properly with BAO retains preference for closed universe (though closer to flat $\Omega_K = -0.4 \pm 0.2\%$) [2205.05892]
- Present-day curvature has profound consequences for inflation [2205.07374]



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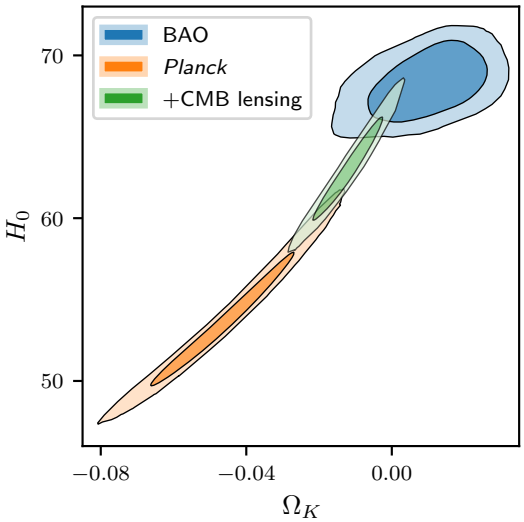

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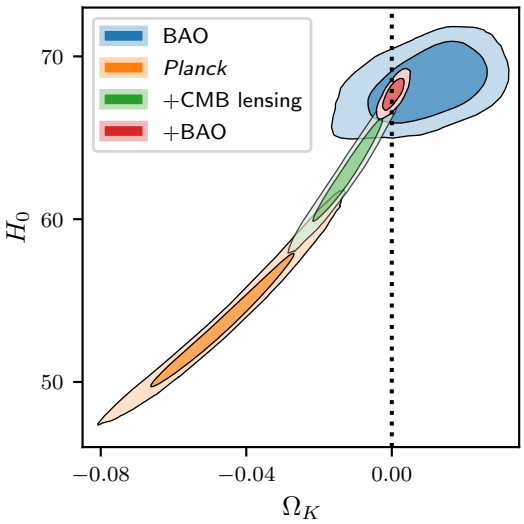
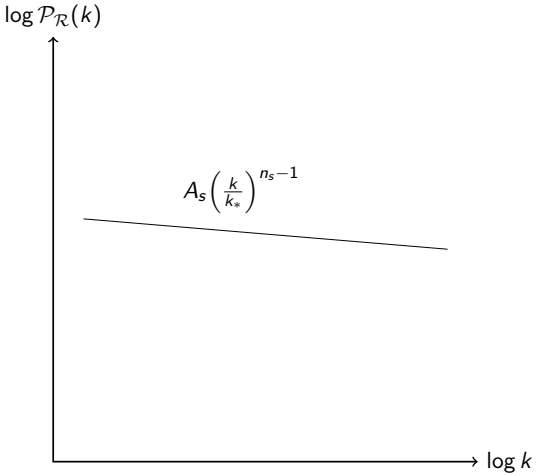


Primordial power spectrum $\mathcal{P}_\mathcal{R}(k)$ reconstruction [1908.00906]

- Traditionally parameterise the primordial power spectrum with (A_s, n_s)

$$\mathcal{P}_\mathcal{R}(k) = A_s \left(\frac{k}{k_*}\right)^{n_s - 1}$$

- To add more degrees of freedom, can add "running" parameters n_{run} (higher order polynomial in index)
- Alternative non-parametric technique introduces a more flexible phenomenological parameterisation: "FlexKnots"
- Let the Bayesian evidence decide when you've introduced too many parameters



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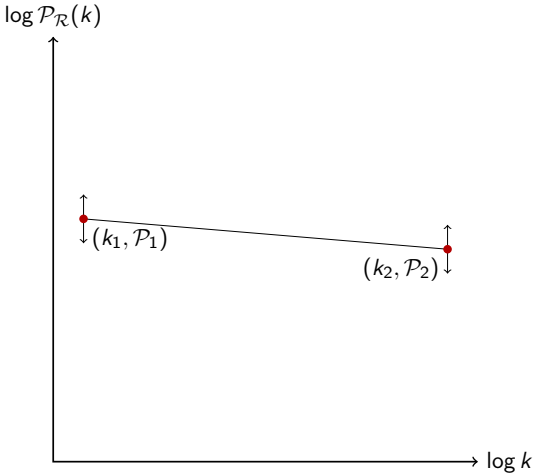

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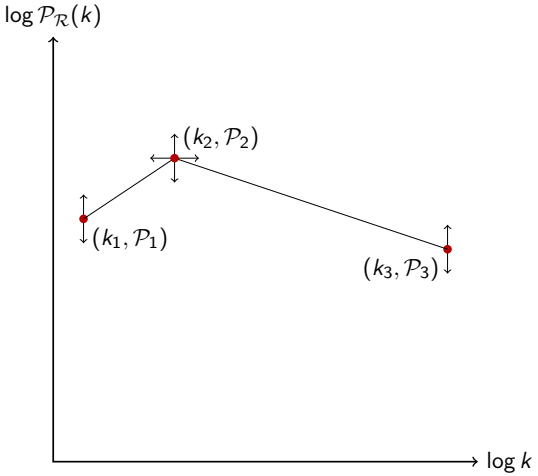

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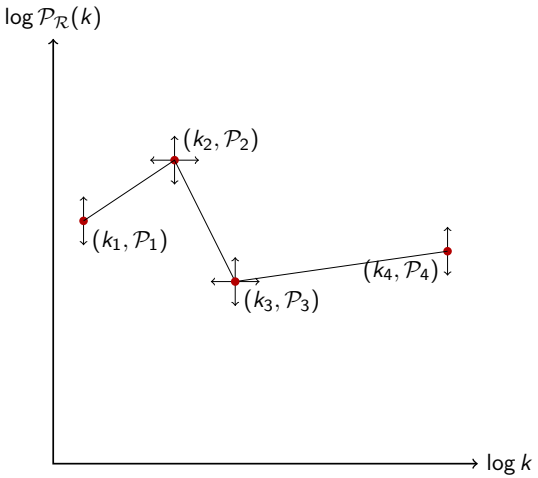

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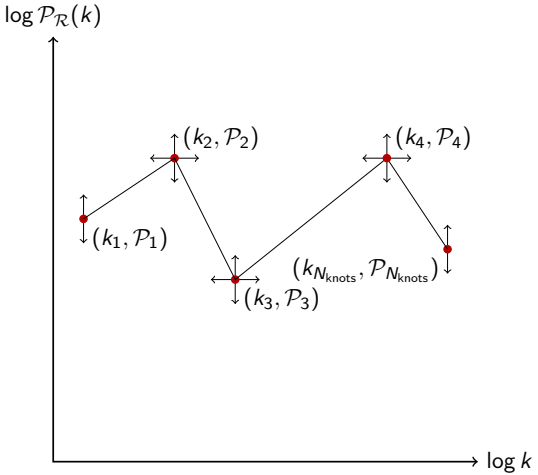

0 internal knots

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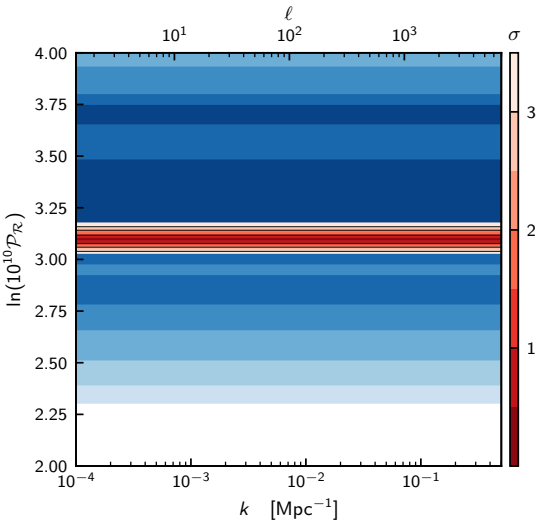

1 internal knot

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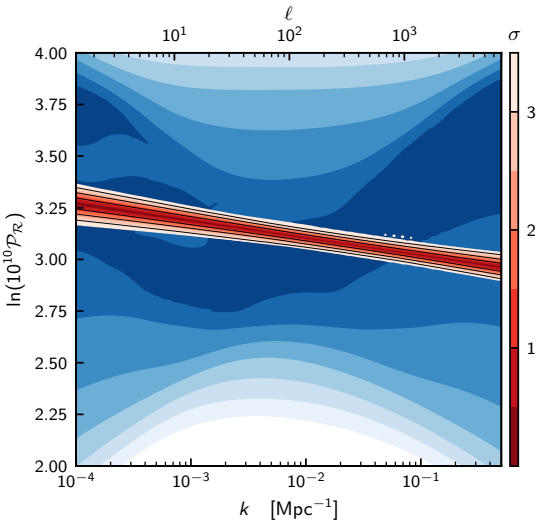

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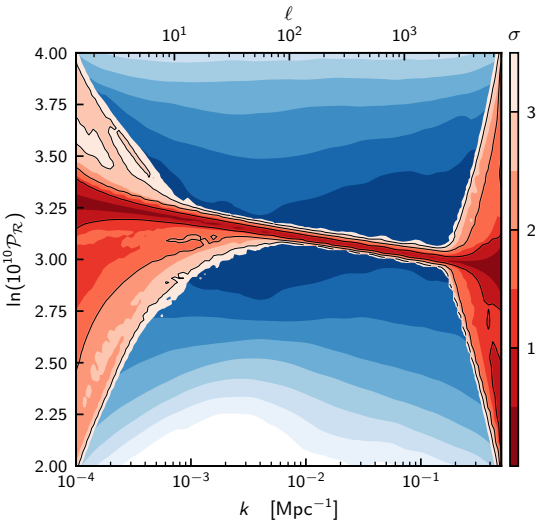

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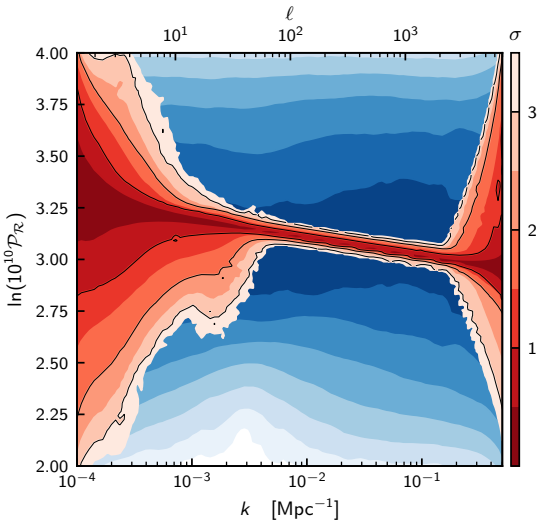

4 internal knots

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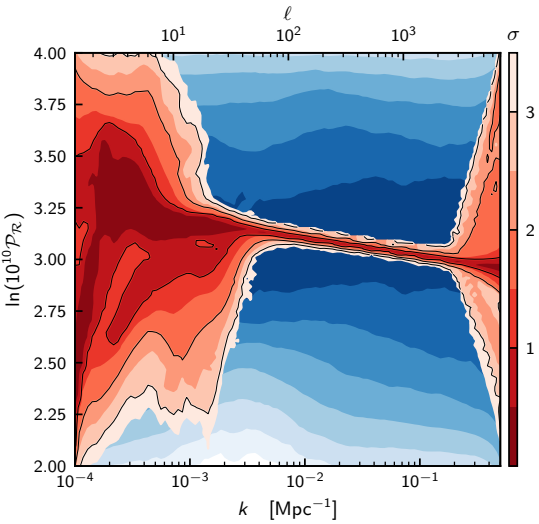

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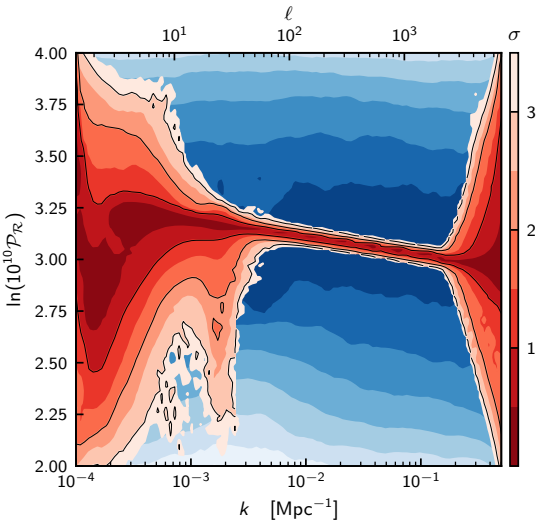

6 internal knots

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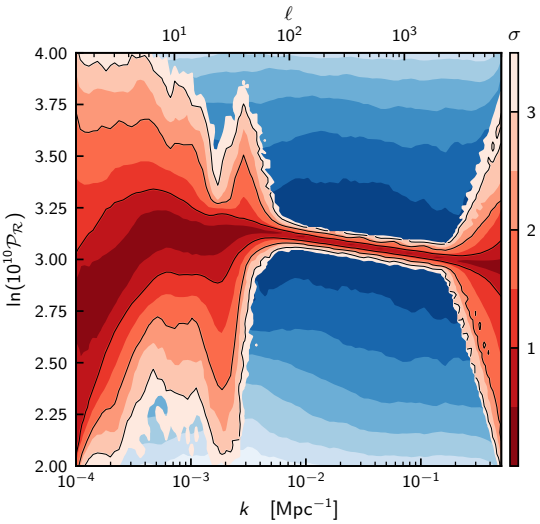

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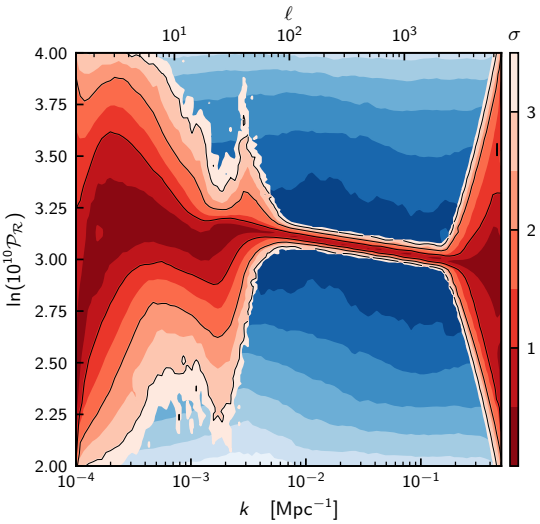

Bayes Factors

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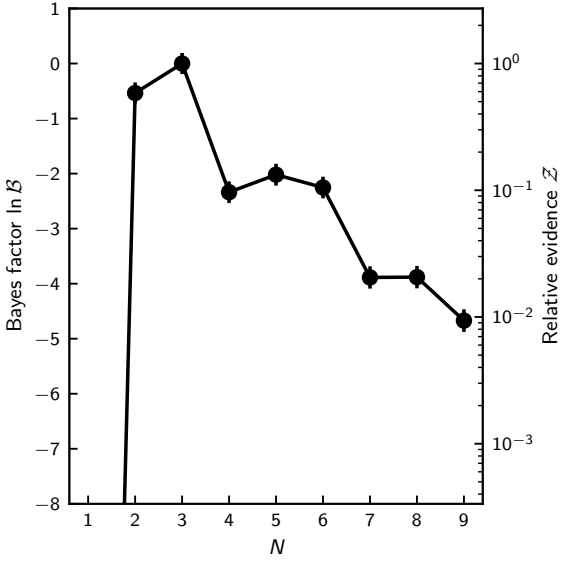

Marginalised plot

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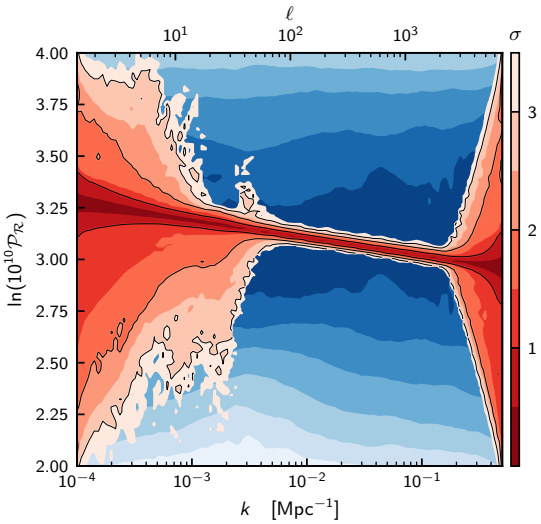

Kullback-Liebler divergences

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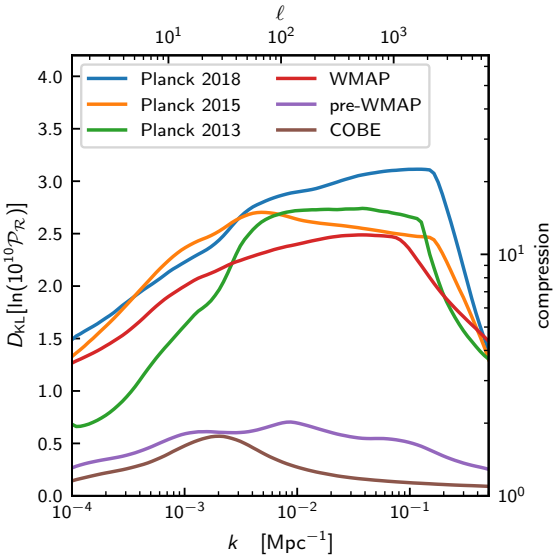
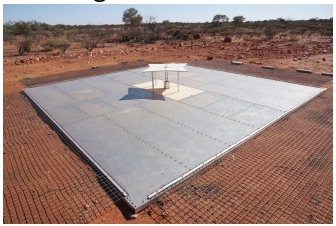
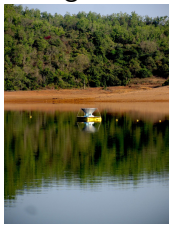
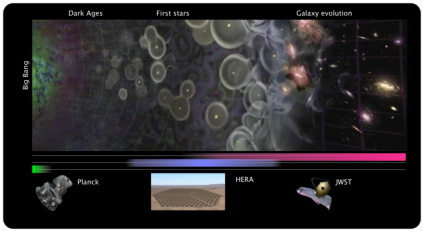
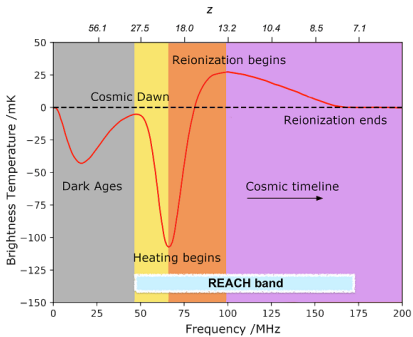


REACH: Global 21cm cosmology [NatAstro]

- Imaging the universal dark ages using CMB backlight.
- 21cm hyperfine line emission from neutral hydrogen.
- Global experiments measure monopole across frequency.
- Gives a specific absorption trough, which if detected allows constraints on the physics of the dark ages decade(s) before SKA.
- Challenge: science hidden in foregrounds $\sim 10^4 \times$signal.

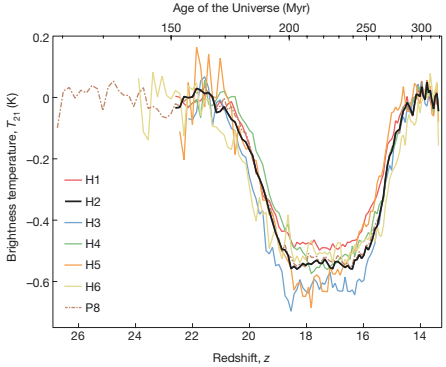





REACH: Global 21cm cosmology [NatAstro]

- EDGES [Nat] claimed a controversial 2019 detection.
- SARAS3 [NatAstro] would have detected this by 2021.
- REACH [NatAstro] aims to settle the debate.
  - Broader band,
  - Honesty about systematic modelling,
  - State of the art inference.
- Create parameterised models of sky, beam and signal, breaking degeneracy with a time-dependent likelihood to measure all three simultaneously.
- Use model comparison based reconstruction to determine complexity of parameterisation.
- Use model comparison to select likelihoods.
- A collaboration powered by nested sampling.



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 does not require gradients
- Genetic algorithms
  - \+ NS discarded points have statistical meaning

Sampling

- Metropolis-Hastings?
  - – Very little beats a 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
  - – Some people (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.

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).