Next generation cosmological analysis with nested sampling

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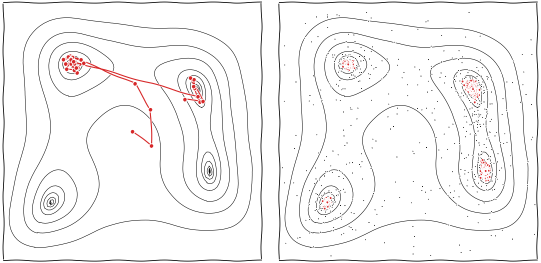
8th September 2022

Overview

- DiRAC 2020 RAC allocation of 30MCPUh
- Main goal: Planck Legacy Archive equivalent
- Parameter estimation $\to$ Model comparison
- MCMC $\to$ Nested sampling
- Planck $\to$ $\{\text{Planck}, \text{DESY1}, \text{BAO}, \ldots\}$
- Pairwise combinations
- Suite of tools for processing these
    - `unimpeded` 1.0
    - `margarine` 1.0
    - `anesthetic` 2.0
    - `zenodo` archive
- MCMC chains also available.
- Work in progress, but β-testers requested (email wh260@cam.ac.uk)



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

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

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

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_*:

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

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

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

- Natural regularisation which penalises models with too many parameters.

Kullback Liebler divergence

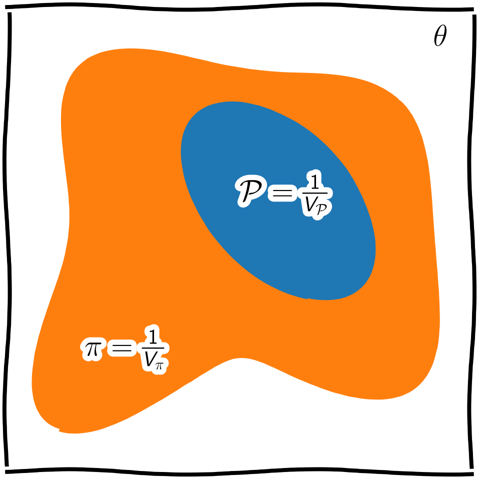
- The KL divergence between prior π and posterior $\mathcal{P}$ is is defined as:

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

- 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":

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

(this is exact for top-hat distributions).

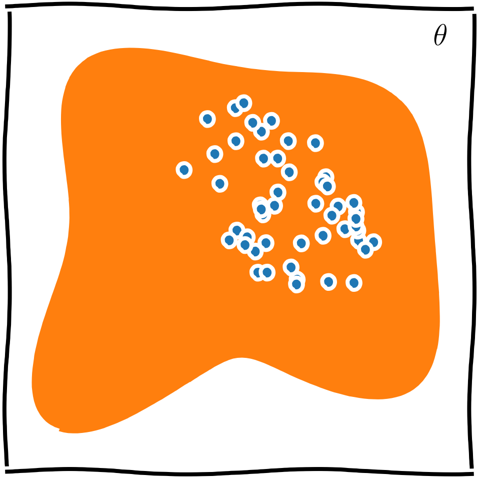


Why do sampling?

- The cornerstone of numerical Bayesian inference is working with **samples**.
- Generate a set of representative parameters drawn in proportion to the posterior $\theta\sim\mathcal{P}$.
- The magic of marginalisation $\Rightarrow$ perform usual analysis on each sample in turn.
- The golden rule is stay in samples until the last moment before computing summary statistics/triangle plots because

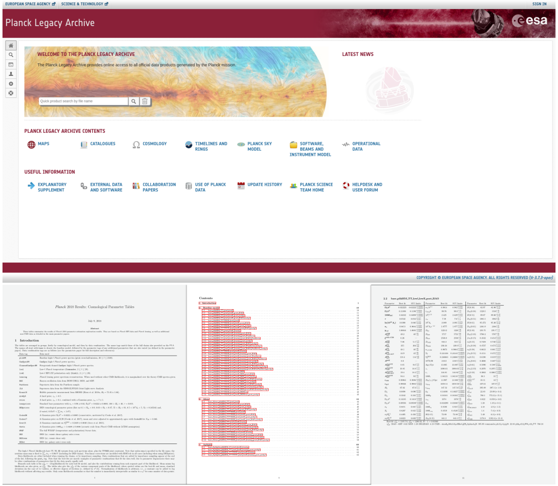
$$\boxed{f(\,\langle X\rangle\,) \ne \langle\, f(X)\,\rangle}$$

- Generally need $\sim\mathcal{O}(12)$ independent samples to compute a value and error bar.

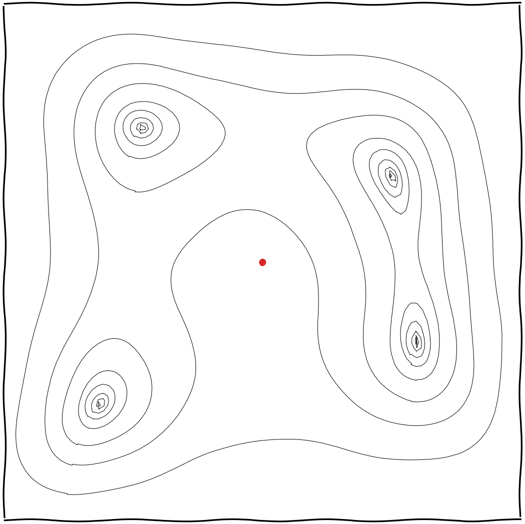


The Planck legacy archive

- *Planck* collaboration science products
- distributed cosmology inference results as MCMC chains
- Across a grid of:
  - subsets/combinations of *Planck* data
    - TT, lowl, lowE, lensing
  - ΛCDM extensions
    - base, mnu, nrun, omegak, r
- importance sampling across some other likelihoods (BAO, JLA,. . .)
- Cannot compute evidences in high dimensions from MCMC chains
  - Only parameter estimation
  - no model comparison



MCMC



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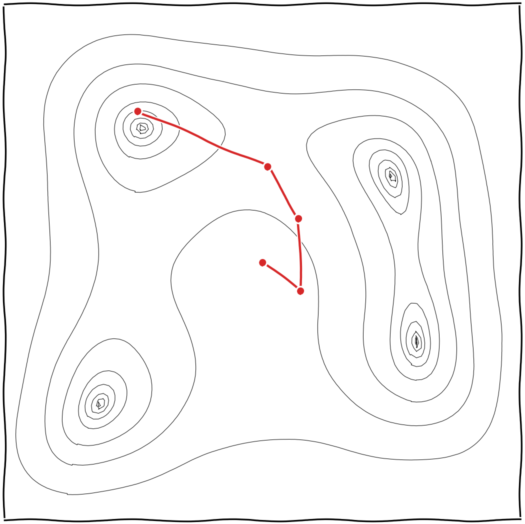

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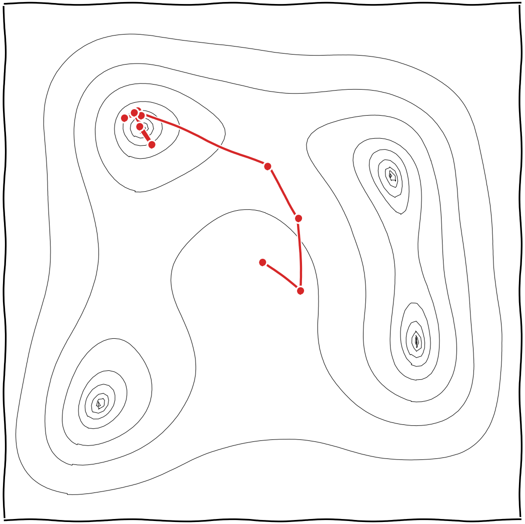

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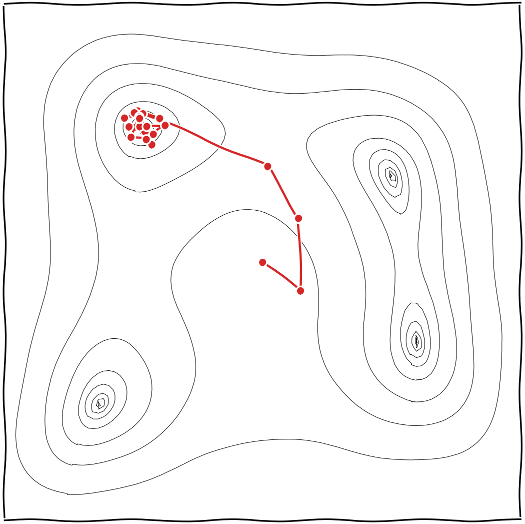

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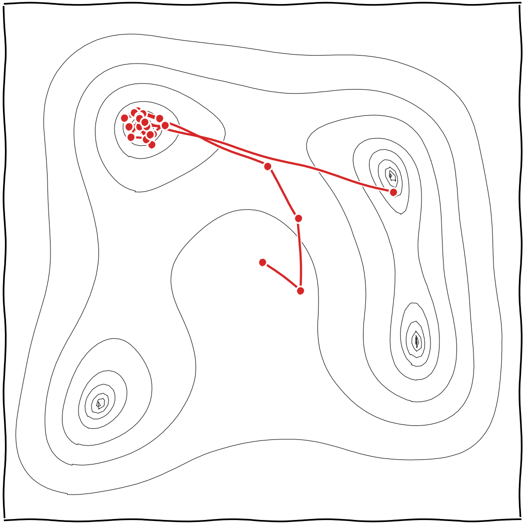

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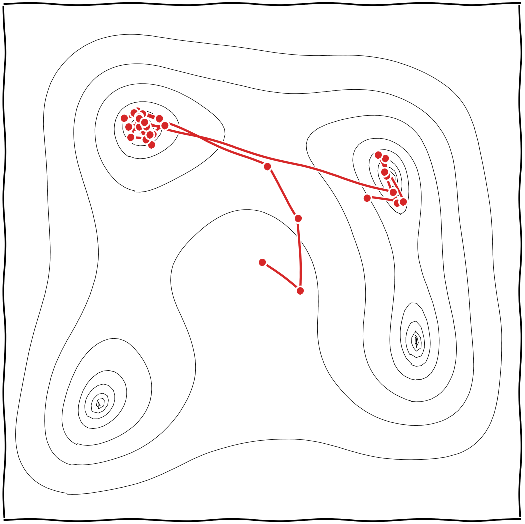

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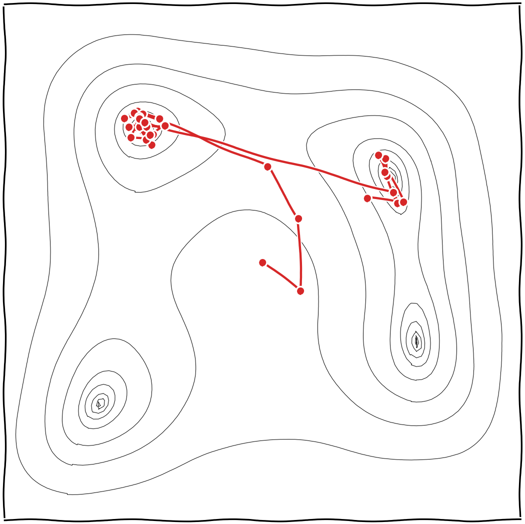

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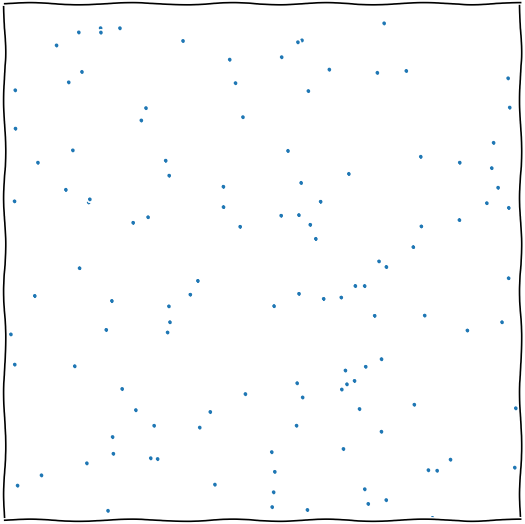

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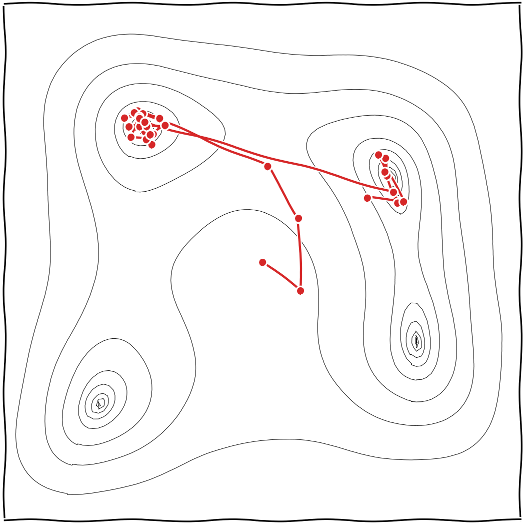

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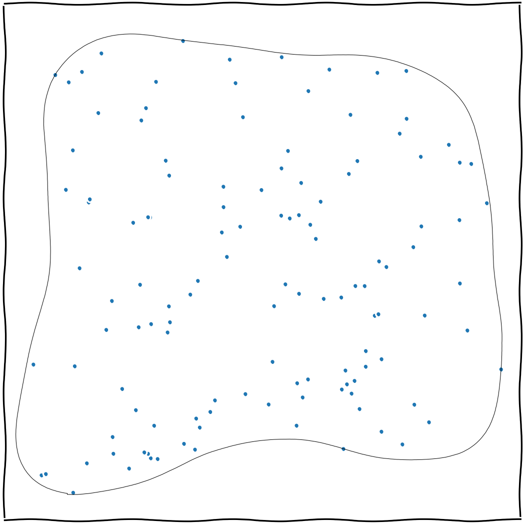

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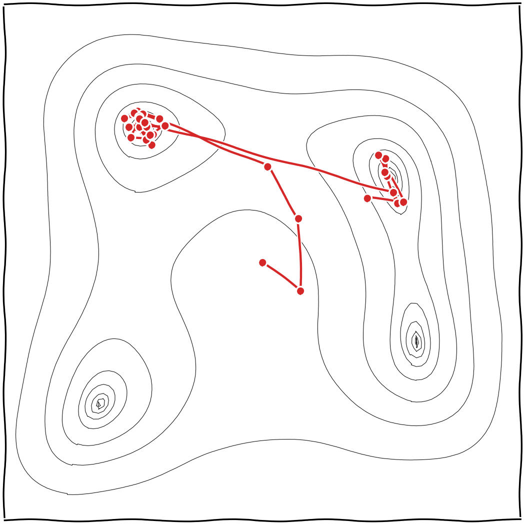

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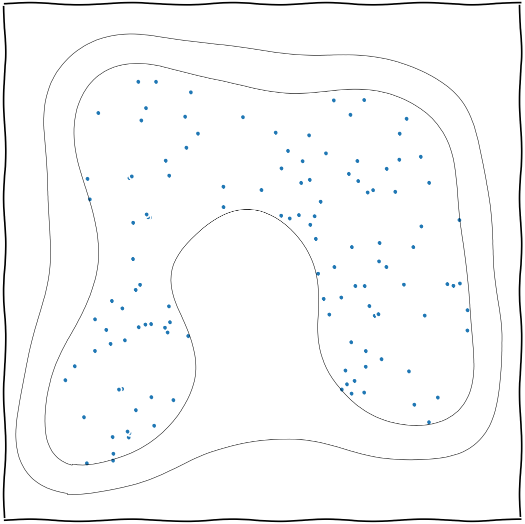

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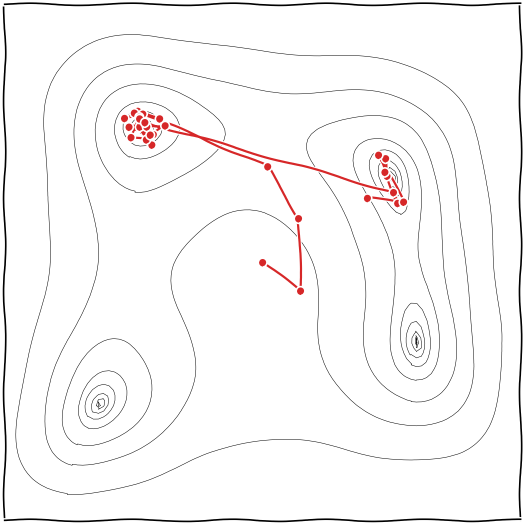

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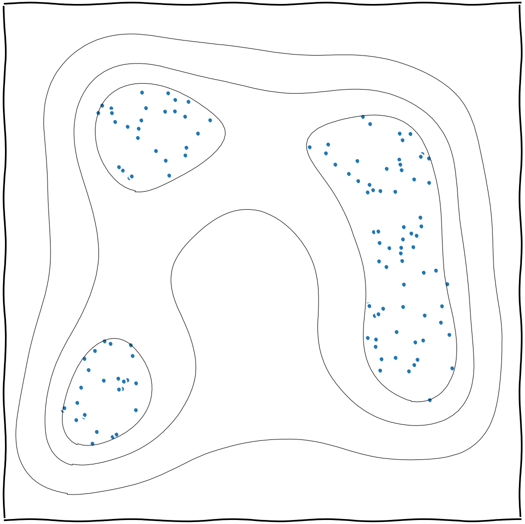

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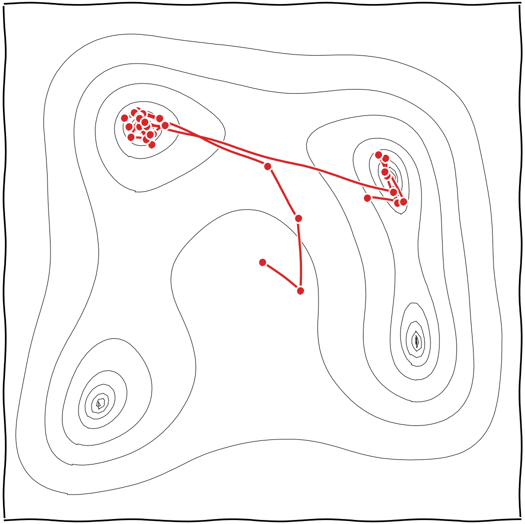

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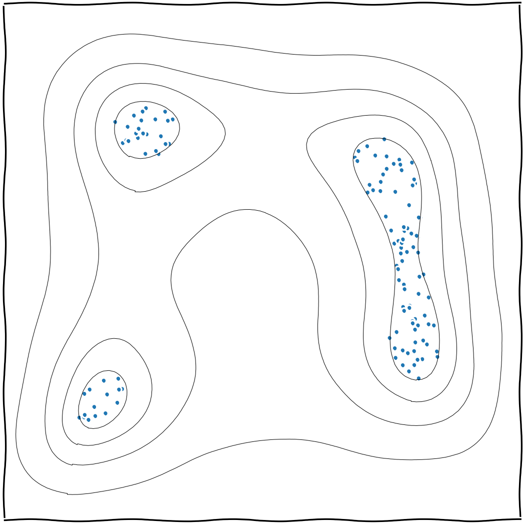

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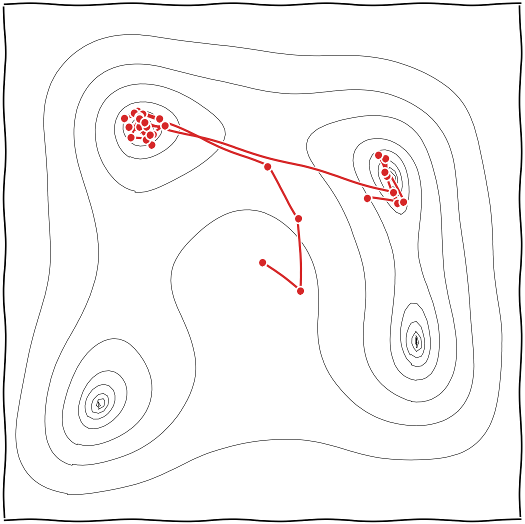

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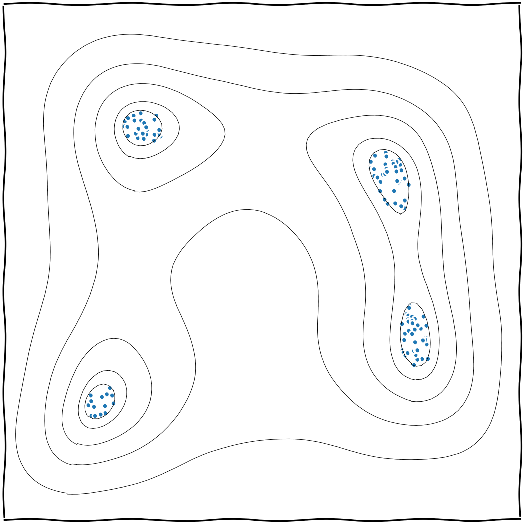

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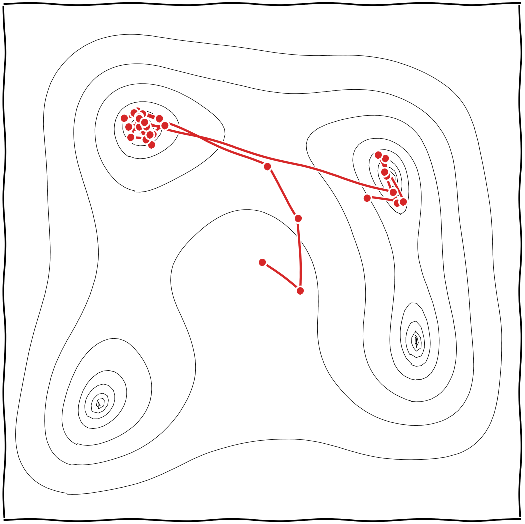

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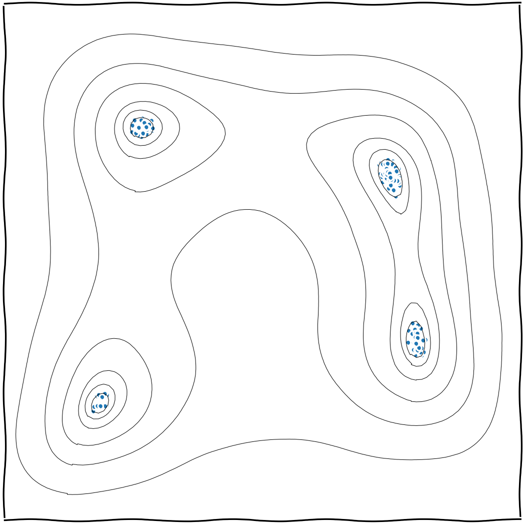

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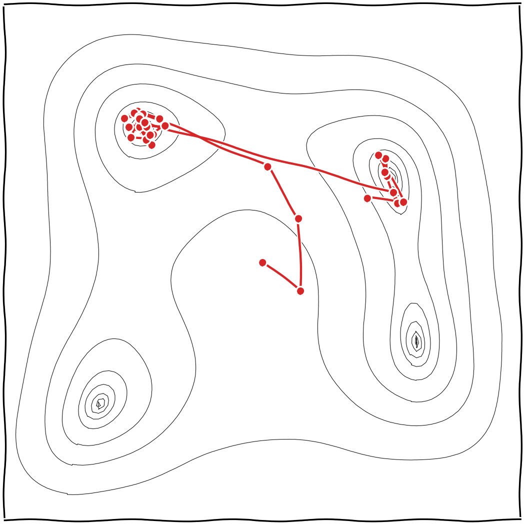

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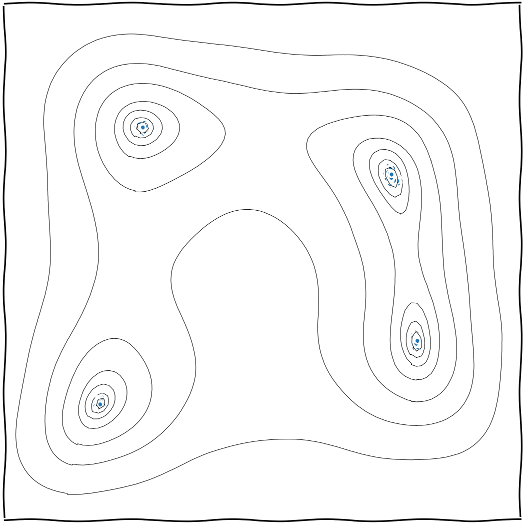

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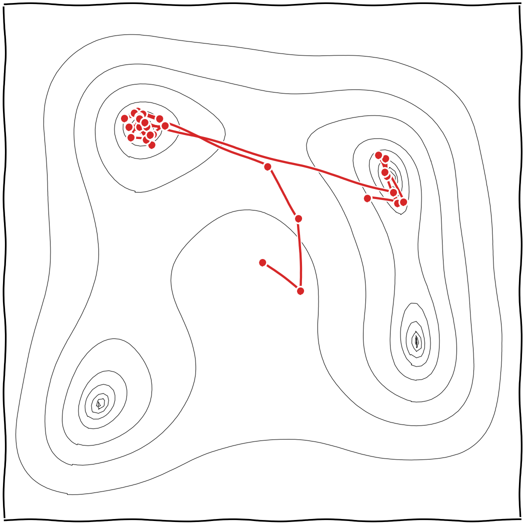

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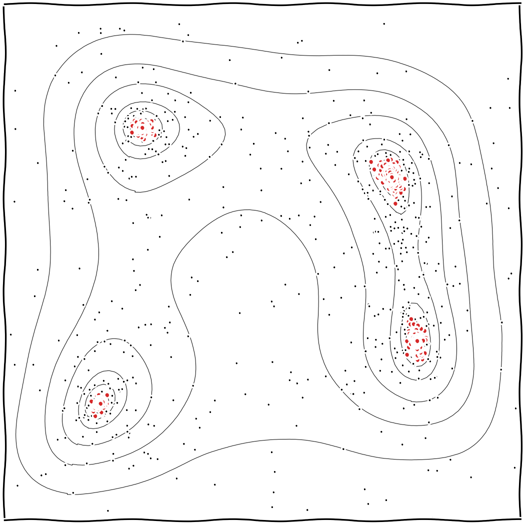
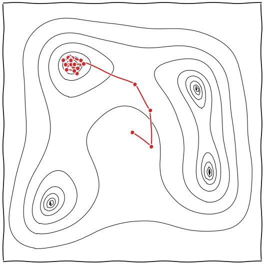


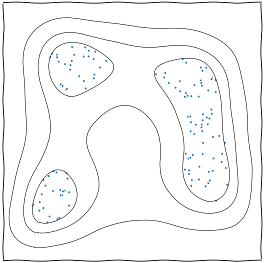
MCMC

- 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 grid (so far)

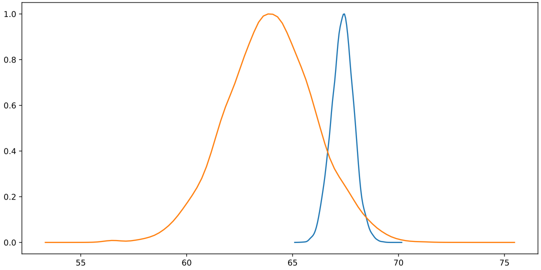
- Models: $[\Lambda\text{CDM}, \Omega_K, \nu, r, w, w(a)]$
- Data: [`plik`, `camspec`, `DESY1`, `bicep+keck`, `BAO(DR16)`, `pantheon`]
- Pairwise combinations of datasets
- Breakdown of Planck & BAO data
- Samplers: [Metropolis Hastings MCMC, Nested Sampling]
- These exhaust what is currently available by default in `cobaya`
- Wide priors to allow for importance readjustment as desired
- roughly halfway through computational allocation.
- Feedback desirable as to what extensions to the grid would be of community interest (email wh260@cam.ac.uk) (`Pantheon+`, SH_0ES, `NPIPE`, `DESY3`,...).
- Further checking needed before first release by end of this year.

unimpeded

Universal Model comparison and Parameter Estimation Distributed over Every Dataset

- Python tool for seamlessly downloading, uploading and cacheing of chains
- Data stored on zenodo
- hdf5 storage for fast & reliable storage
- anesthetic compatible for processing of chains [1905.04768]
- α-testers wanted! (email wh260@cam.ac.uk)
- End goal – community library which everyone contributes to so expensive inference products are reusable and reused.

```python
from unimpeded import Unimpeded
store = Unimpeded(cache='data.hdf5')
samps = store('planck')
samps.H0.plot.kde_1d()
samps = store('planck', model='klcdm')
samps.H0.plot.kde_1d()
```



$\boxed{\mathcal{L}(\theta, \alpha)}$

Harry Bevins
[2205.12841]
[2207.11457]

- Can use machine learning to dramatically speed up inference
- Emulate the marginal posterior and prior with masked autoregressive flows (`margarine`)
- Use nested sampling evidences to compute nuisance marginalised likelihood $\mathcal{L}(\theta) = \mathcal{P}(\theta)\mathcal{Z}/\pi(\theta)$

- Library of trained bijectors to be used as priors/emulators/nuisance marginalised likelihoods
- e.g. easy to apply a *Planck* prior/likelihood to your existing MCMC chains without using the whole cosmology machinery.

`margarine`: machine learning-enhanced Bayesian inference

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$$\begin{tikzcd} \boxed{\mathcal{L}(\theta, \alpha)} \arrow[dr] & & \boxed{\pi(\theta, \alpha)} \arrow[dl] \\ & \boxed{\text{Nested Sampling}} & \end{tikzcd}$$

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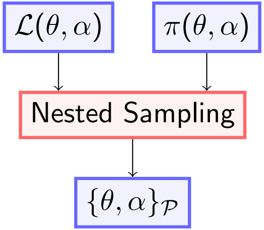

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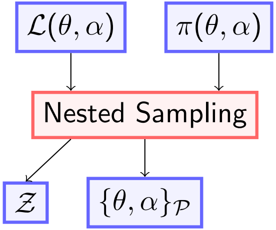

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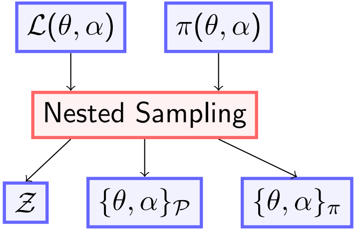

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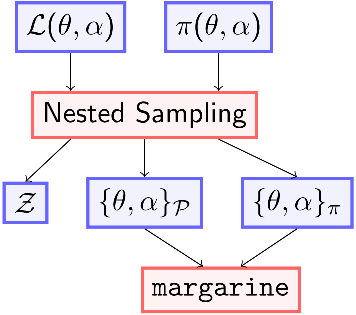

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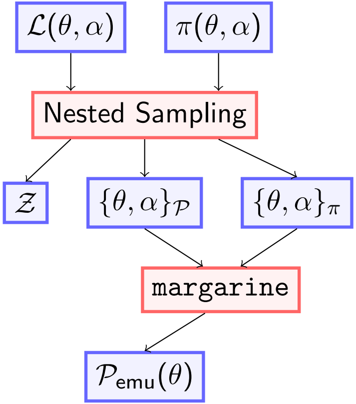

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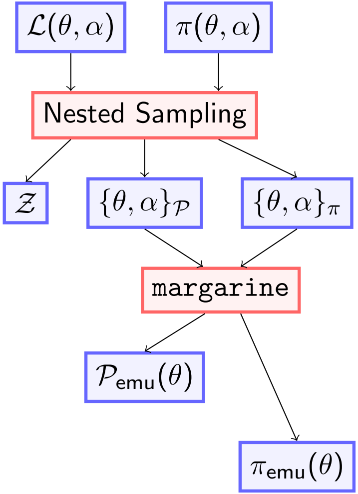

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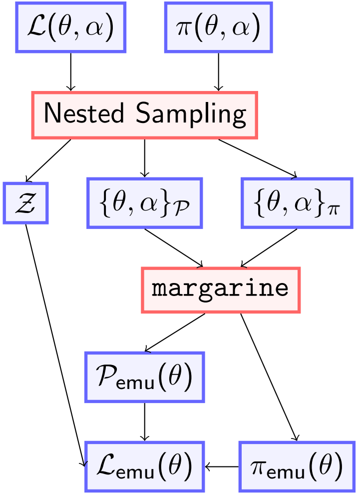

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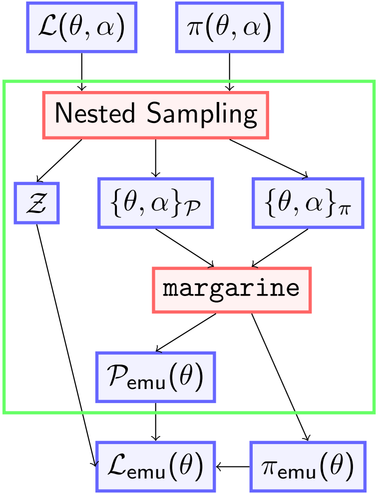

Conclusions

- DiRAC RAC allocation for building a legacy grid of
  - MCMC & Nested sampling chains
  - gridded over (pairwise) up-to-date datasets
  - gridded over extensions to ΛCDM
  - Bijectors & emulators for fast re-use
  - Importance sampling toolkit via `anesthetic` for (re)processing
  - Long-term goal: community repository of chains to share model comparison compute resource
- Looking for:
  - α-testers for `unimpeded`
  - Suggestions for more datasets (and their incorporation into `cobaya`)