Next generation cosmological analysis with nested sampling

Will Handley
<wh260@cam.ac.uk>

Royal Society University Research Fellow & Turing Fellow
Astrophysics Group, Cavendish Laboratory, University of Cambridge
Kavli Institute for Cosmology, Cambridge
Gonville & Caius College
github.com/williamjameshandley/talks
willhandley.co.uk

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The Alan Turing Institute

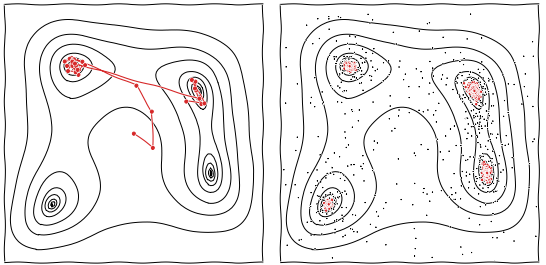
UNIVERSITY OF CAMBRIDGE

DiRAC

Overview

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

DiRAC



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

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

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

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

Tension quantification

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

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

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

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_*:

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

- 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

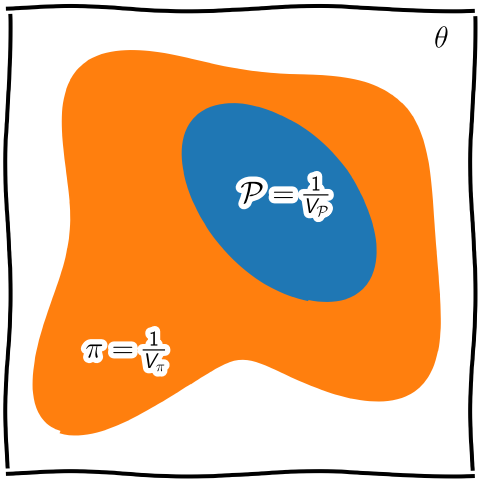
- The KL divergence between prior π and posterior $\mathcal{P}$ is is defined as:

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

- 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":

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

(this is exact for top-hat distributions).

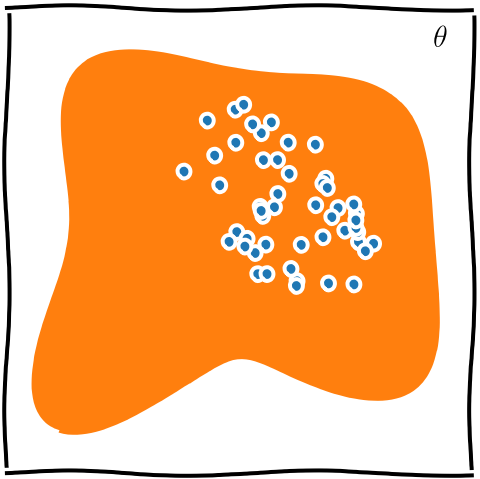


Why do sampling?

- 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

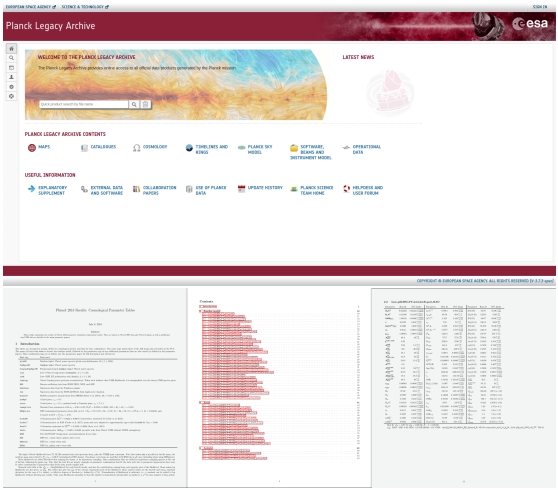
$$\boxed{f(\langle X \rangle) \neq \langle f(X) \rangle}$$

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

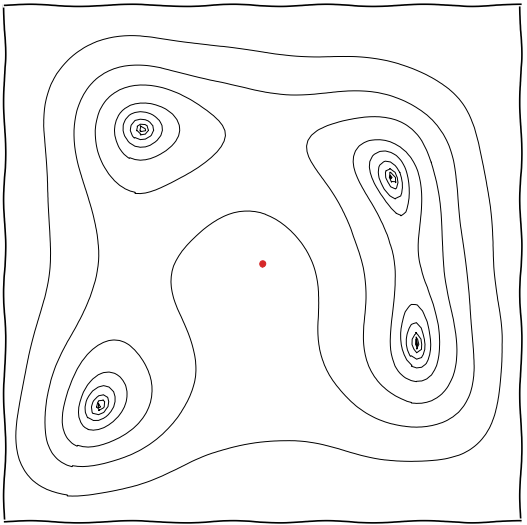


The Planck legacy archive

- *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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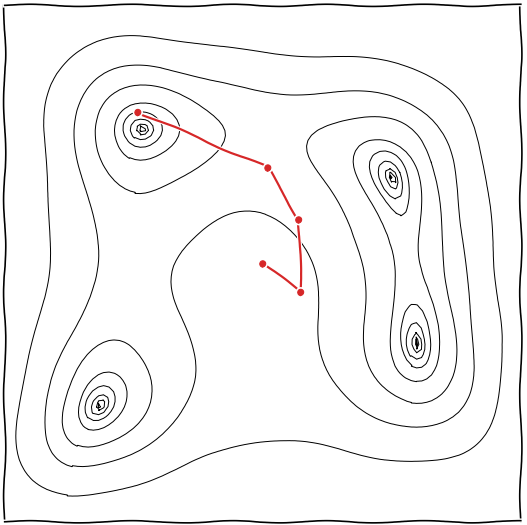

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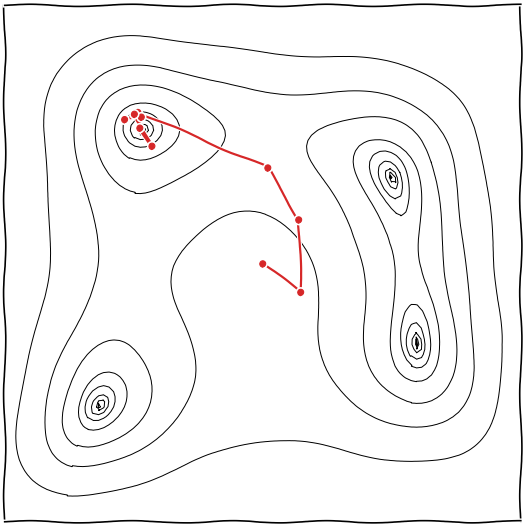

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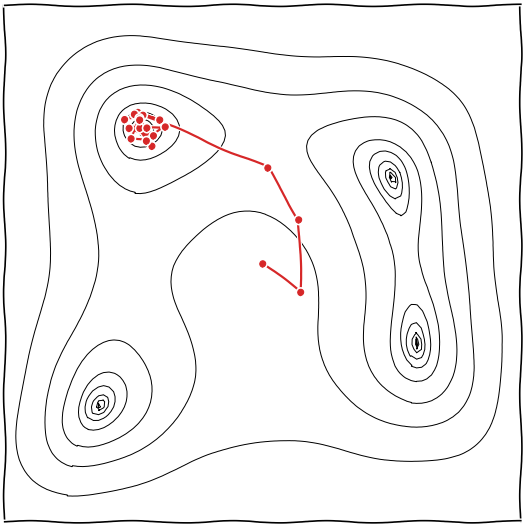

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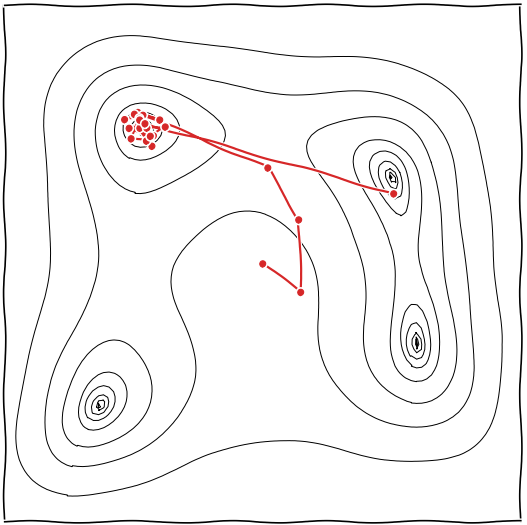

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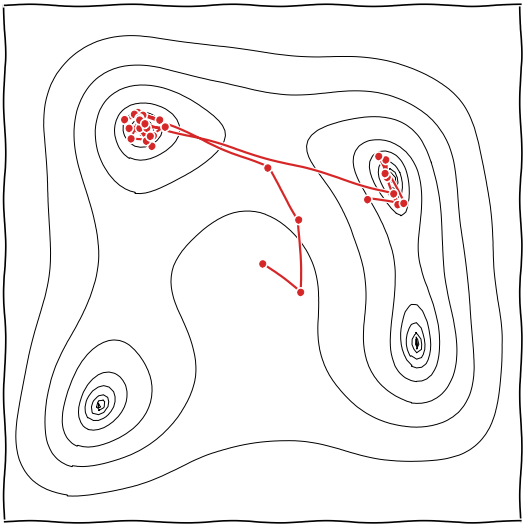

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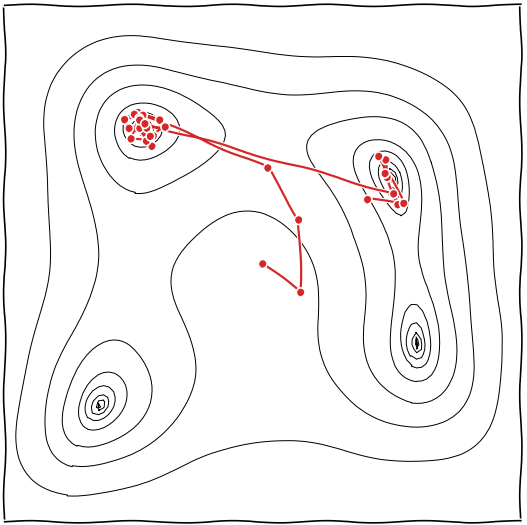
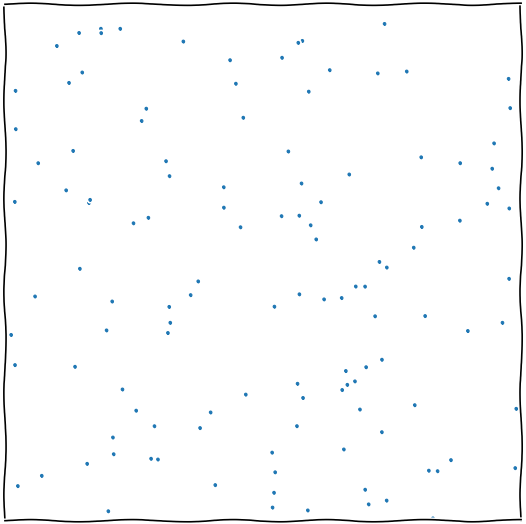


Nested sampling



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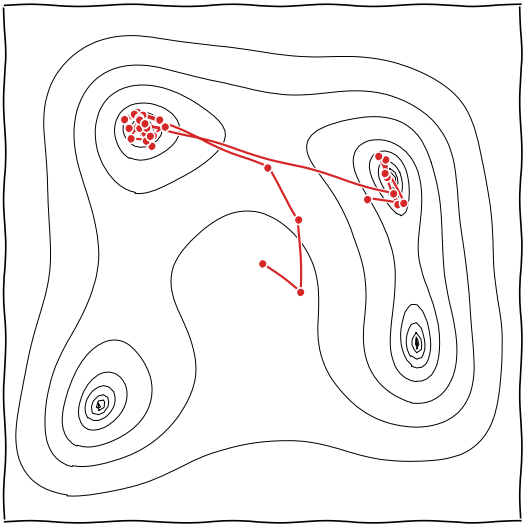

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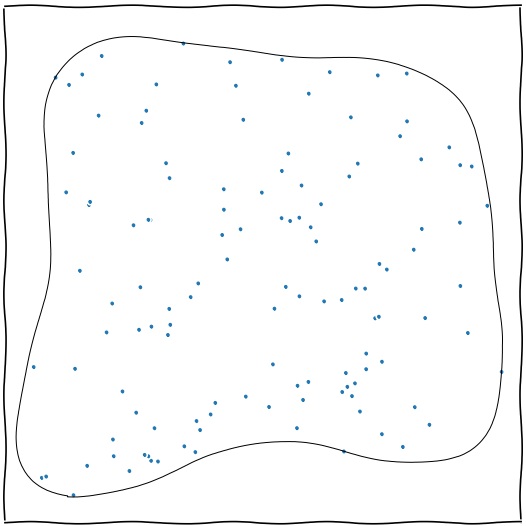

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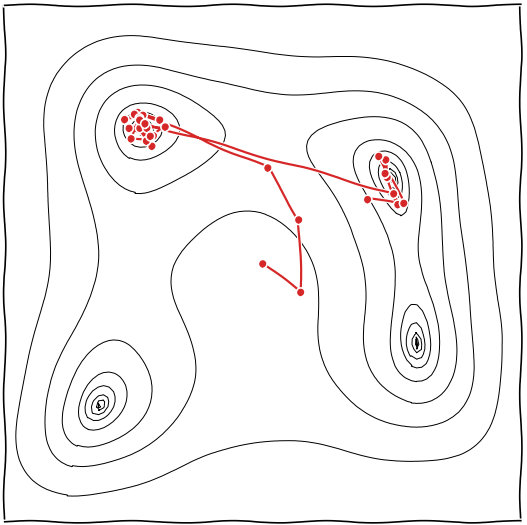

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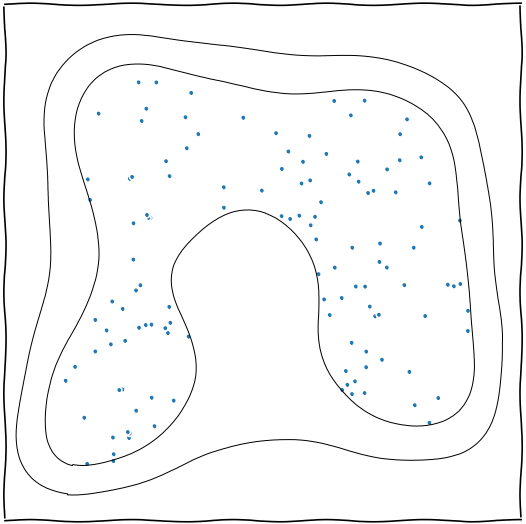

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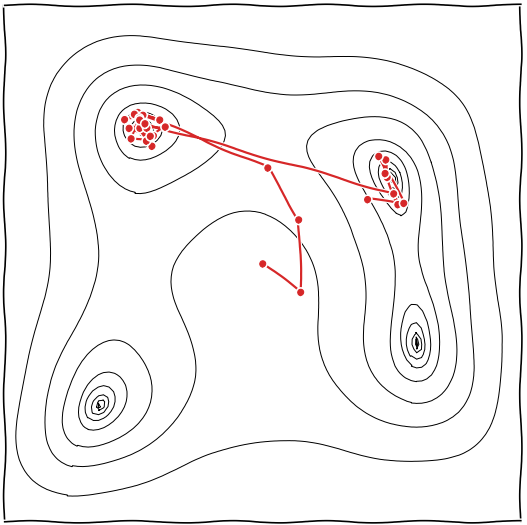

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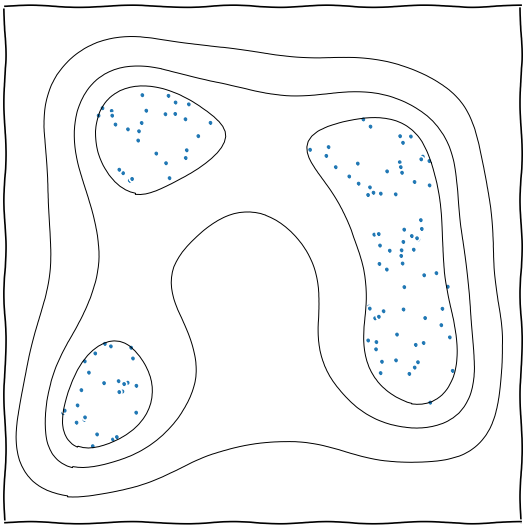

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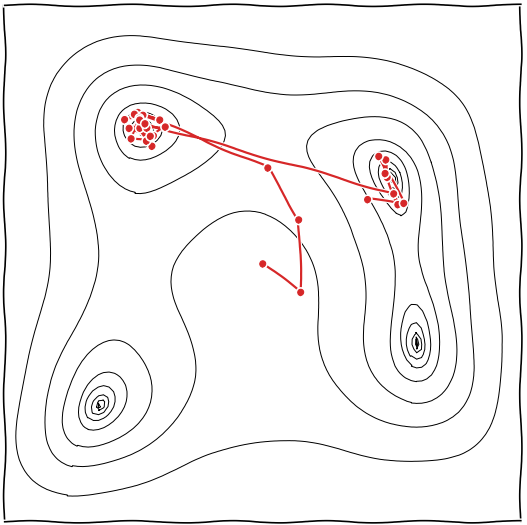

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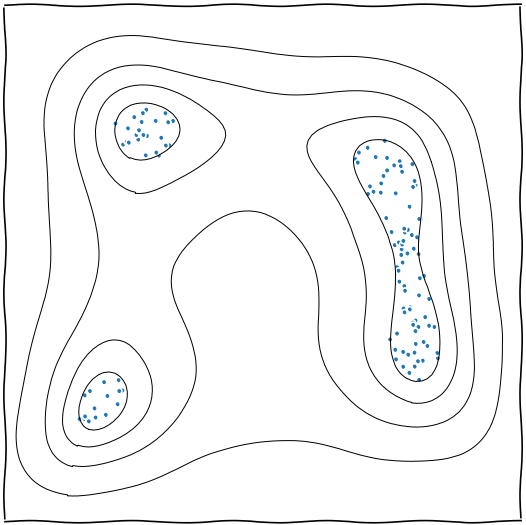

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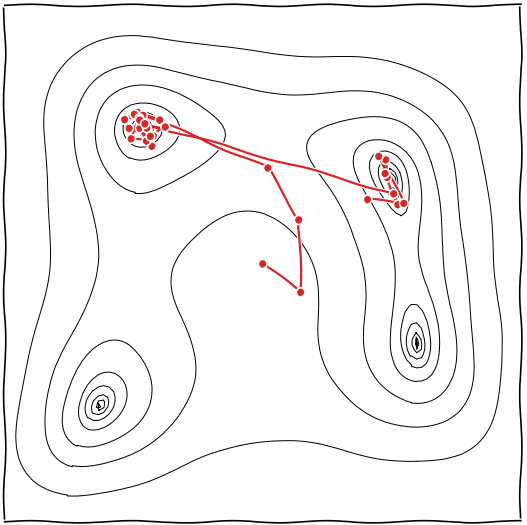

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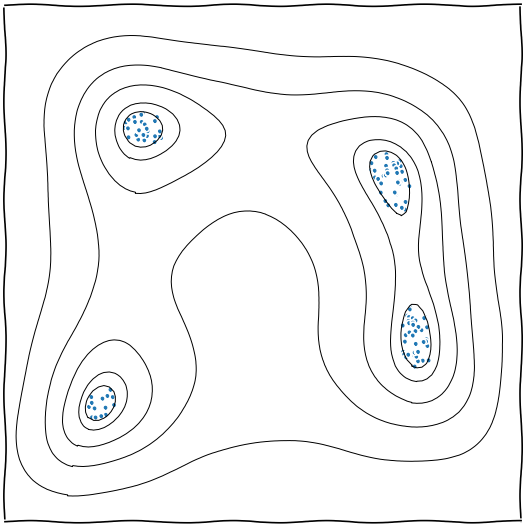

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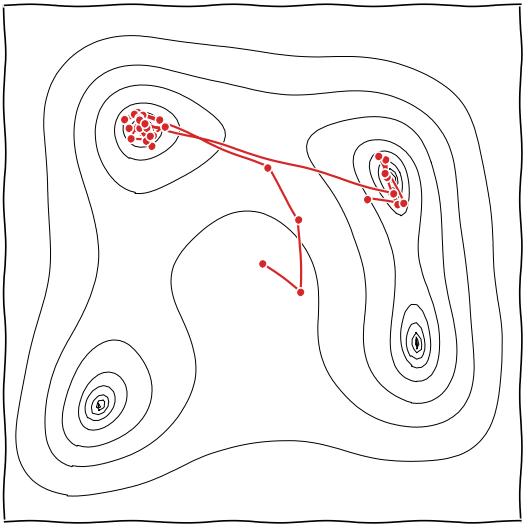

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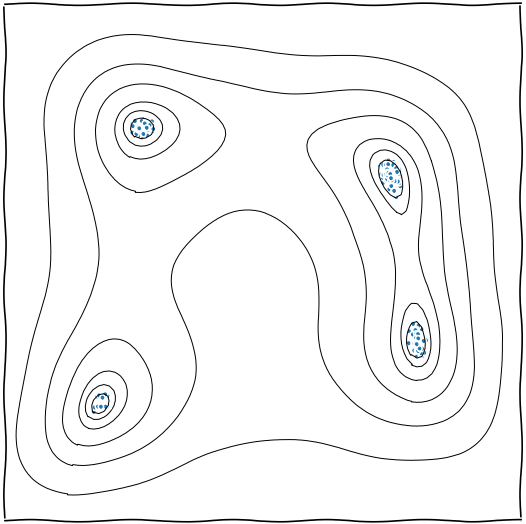

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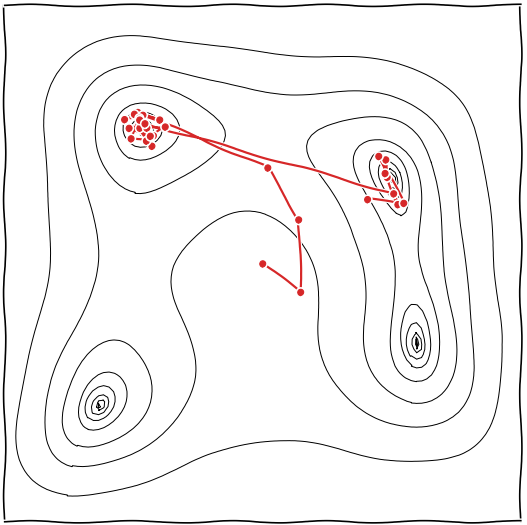

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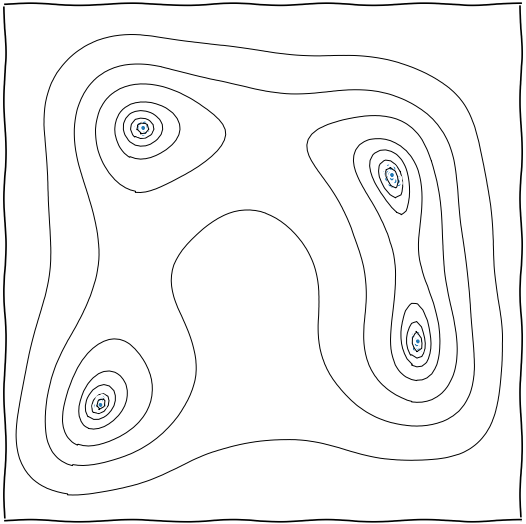

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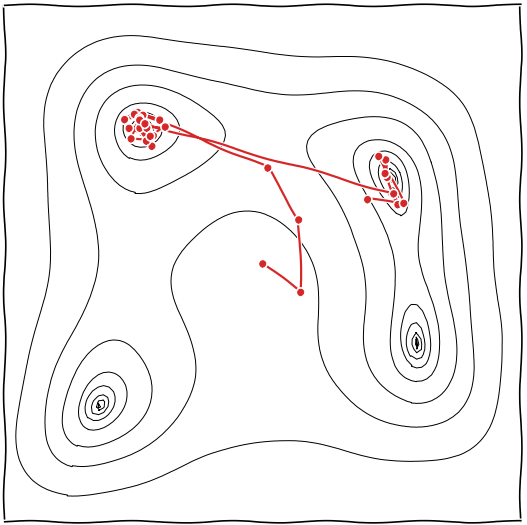

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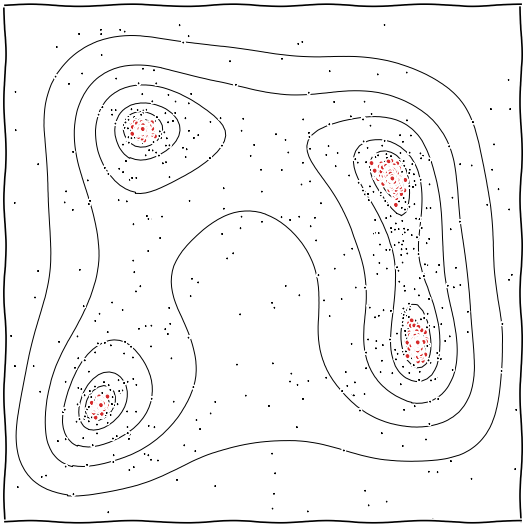
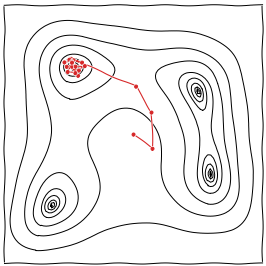


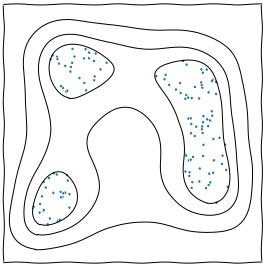
MCMC

- 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



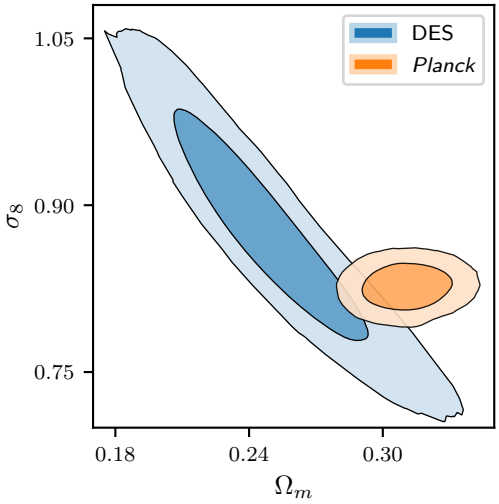
The grid (so far)

- 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
- 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 gred would be of community interest.
- Further checking needed before first release by end of this year.

- Python tool for seamlessly downloading and cacheing chains
- Data stored on `zenodo`
- hdf5 storage for fast & reliable download & storage
- Library of trained bijectors to be used as priors/emulators [2102.12478]/nuisance marginalised likelihoods [2207.11457]
- `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 runs reusable.

The importance of global measures of tension

- Hubble tension [1907.10625]
  - *Planck*: $H_0 = 67.4 \pm 0.5$
  - SH_0ES: $H_0 = 74.0 \pm 1.4$
- In other situations the discrepancy doesn't exist in a single interpretable parameter
- For example: DES+*Planck* [1902.04029]
- Are these two datasets in tension?
- There are a lot more parameters – are we sure that tensions aren't hiding? Are we sure we've chosen the best ones to reveal the tension?
- Should use "Suspiciousness" statistic $\mathcal{S}$, or Bayes ratio $\mathcal{R}$ to determine global tension.



The importance of global measures of tension

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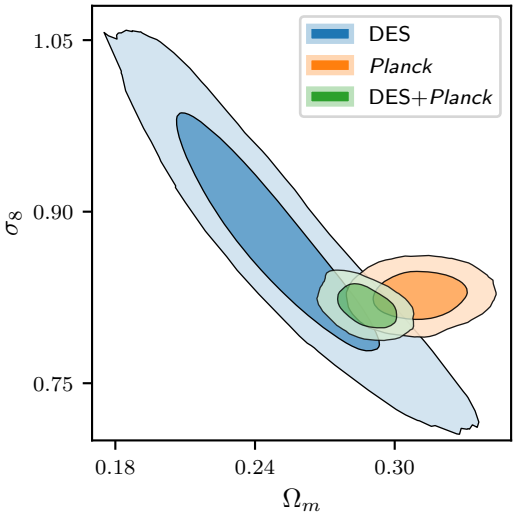


The DES evidence ratio R

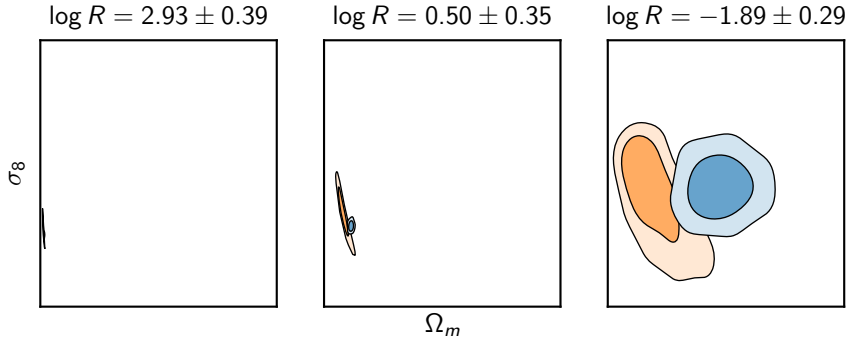
- The Dark Energy Survey [1708.01530] quantifies tension between two datasets A and B using the Bayes ratio:

$$R = \frac{\mathcal{Z}_{AB}}{\mathcal{Z}_A \mathcal{Z}_B} = \frac{P(A \cap B)}{P(A)P(B)} = \frac{P(A|B)}{P(A)} = \frac{P(B|A)}{P(B)}$$

  where $\mathcal{Z}$ is the Bayesian evidence.

- Many attractive properties:
  - Symmetry
  - Parameterisation independence
  - Dimensional consistency
  - Use of well-defined Bayesian quantities
- R gives the relative change in our confidence in data A in light of having seen B (and vice-versa).
- $R > 1$ implies we have more confidence in A having received B.
- Like evidences, it is prior-dependent from $\mathcal{D}$ in $\log \mathcal{Z} = \langle \log \mathcal{L} \rangle_{\mathcal{P}} - \mathcal{D}$
- Increasing prior widths $\Rightarrow$ decreasing evidence.
- Increasing prior widths $\Rightarrow$ increasing confidence.

The DES evidence ratio R: Prior dependency



- What does it mean if increasing prior widths $\Rightarrow$ increasing confidence?
- Wide priors mean *a-priori* the parameters could land anywhere.
- We should be proportionally more reassured when they land close to one another if the priors are wide

How do we deal with the prior dependency in R?

Option 1 Take the Bayesian route, accept the prior dependency, and spend time trying to justify why a given set of priors are "physical".

Option 2 Try to find a principled way of removing this prior dependency

- Decompose ratio using Occam's Razor equation $\log \mathcal{Z} = \langle \log \mathcal{L} \rangle_{\mathcal{P}} - \mathcal{D}$

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

  where we have defined the suspiciousness S, which is prior independent, and the information $\mathcal{I}$, which depends on the parameter compression of the shared space
- Focussing on the prior-independent portion $\mathcal{S}$ gives R for the "Narrowest reasonable priors" which do not impinge on the posterior
- One of the critical observations is that one can only hide tension by widening priors. Narrowing them will only ever show tension if it is present.

Suspiciousness S

- For a Gaussian set of posteriors:

$$\log \mathcal{S} = \frac{d}{2} - \frac{1}{2}(\mu_A - \mu_B)(\Sigma_A + \Sigma_B)^{-1}(\mu_A - \mu_B).$$

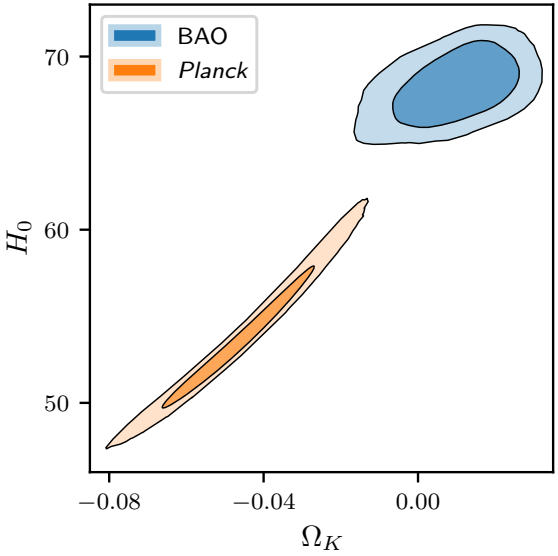
- The Malhanobis term is suggestive, so we can use this to calibrate a "sigma" level of tension using a χ^2 distribution for $\chi^2_d = d - 2\log\mathcal{S}$, or a tension probability.
- S is composed of evidences $\mathcal{Z}$ and KL divergences $\mathcal{D}$, which are Gaussian-independent concepts, so the only thing to determine is d, the "number of shared parameters".
- Can do this with Gaussian dimensionality $\frac{d}{2} = \mathrm{var}_{\mathcal{P}}(\log\mathcal{L})$ [1903.06682]

Planck vs BAO :	$p = 42 \pm 4\%$
Planck vs DESY1 :	$p = 3.2 \pm 1.0\%$
Planck vs SH_0ES :	$p = 0.25 \pm 0.17\%$

- Under this metric, SH_0ES is unambiguously inconsistent, although not quite as brutal as $> 4\sigma$. BAO is consistent, and DESY1 is inconsistent, but only just. This is pleasingly similar to ones intuition.

Curvature tension? [1908.09139]

- If you allow $\Omega_K \neq 0$, *Planck* (`plikTTTEEE`) has a moderate preference for closed universes (50:1 betting odds on), $\Omega_K = -4.5 \pm 1.5\%$ [1911.02087]
- *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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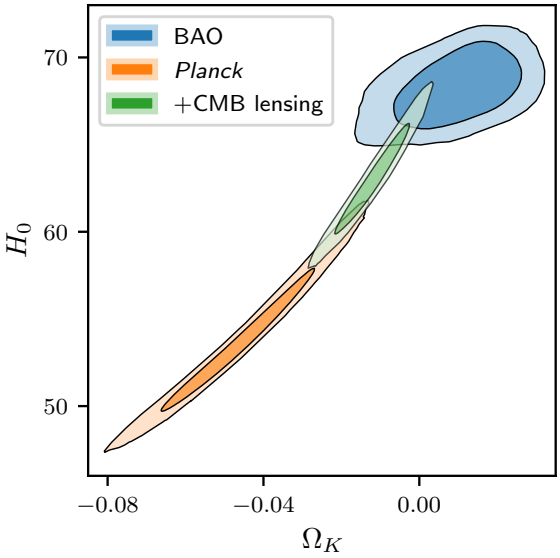

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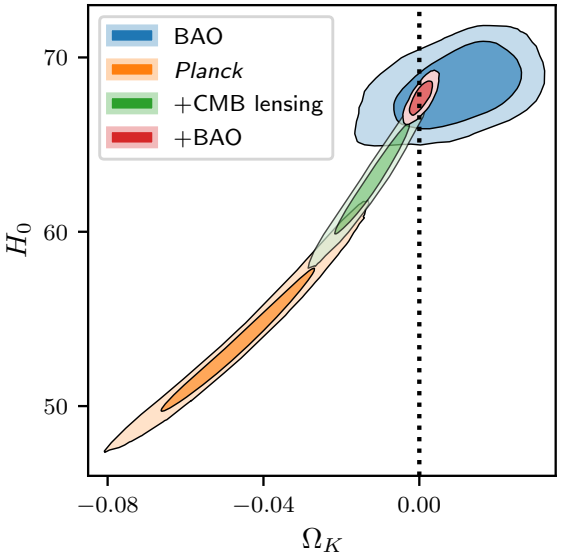

Conclusions

- 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`)