# Nested sampling cross-checks using order statistics

Andrew Fowlie, Will Handley, and Liangliang Su (June 2020). In: arXiv: 2006.03371 [stat.CO]

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# Table of contents

1. Model selection

2. Nested sampling

3. A new cross-check

# Model selection

# Model selection

Throughout science, we have the following problem:

*I have data and some models. What is the status of my models in light of the data?*

# Bayesian updates

Compute the change in plausibility of a model in light of data relative to another model or set of models.

We just apply probability theory to the problem. All models treated equally.

Simple in theory; in practice there are difficulties.

# Bayes factors

Let's pursue the Bayesian approach (Jeffreys 1939).

*The Bayes factor (Kass and Raftery 1995) relates the relative plausibility of two models after data to their relative plausibility before data;*

$$\textit{Posterior odds} = \textit{Bayes factor} \times \textit{Prior odds}$$

*where*

$$\textit{Bayes factor} = \frac{p\left(\textit{Observed data} \,|\, \textit{Model a}\right)}{p\left(\textit{Observed data} \,|\, \textit{Model b}\right)}$$

A nice result — by applying laws of probability, we see that models should be compared by nothing other than their ability to predict the observed data.

# Bayesian evidence

The factors in the ratio are Bayesian evidences

$$\mathcal{Z} \equiv p\left(D \,\middle|\, M\right) = \int_{\Omega_{\boldsymbol{\Theta}}} \mathcal{L}(\boldsymbol{\Theta})\, \pi(\boldsymbol{\Theta})\, \mathrm{d}\boldsymbol{\Theta},$$

where $D$ is the observed data, $\mathcal{L}(\boldsymbol{\Theta}) = p\left(D \,\middle|\, \boldsymbol{\Theta}, M\right)$ is the likelihood and $\pi(\boldsymbol{\Theta}) = P\left(\boldsymbol{\Theta} \,\middle|\, M\right)$ is our prior, and $\boldsymbol{\Theta}$ are the model's parameters.

# Bayesian evidence

> *The evidence is often the single most important number in the problem and I think every effort should be devoted to calculating it*
>
> Mackay (2003)

The single most important number in inference? Let's think about how to compute it!

# It's a difficult integral

**Multi-dimensional:** Our models of physics might have many parameters. Even simple models contain $\mathcal{O}(10)$ parameters

**Multi-modal:** We don't live in Gaussian land. In physics, the likelihoods can feature degeneracies and multiple modes

**Fat-tailed:** Large variance if you try Monte Carlo integration

# Nested sampling

# Algorithm

Skilling's idea (Skilling 2004; Skilling 2006). We can write

$$\mathcal{Z} = \int \mathcal{L}(X)\,\mathrm{d}X$$

where the volume variable

$$\begin{aligned} X(\mathcal{L}^\star) &= \text{Fraction of prior volume with } \mathcal{L}(\boldsymbol{\Theta}) \geq \mathcal{L}^\star \\ &= \int_{\mathcal{L}(\boldsymbol{\Theta}) \geq \mathcal{L}^\star} \pi(\boldsymbol{\Theta})\,\mathrm{d}\boldsymbol{\Theta} \end{aligned}$$

and $\mathcal{L}(X(\lambda)) = \lambda$. This is a one-dimensional integral. We can approximate it by a Riemann sum

$$\mathcal{Z} \approx \sum \mathcal{L}(X)\Delta X$$

# Compression

*We haven't achieved much yet. The trick is how to estimate X?*

# Compression

0. Draw $n_{\text{live}}$ samples from the prior — the live points

So we evolve a set of $n_{\text{live}}$ live points to higher and higher likelihoods, replacing one live point at a time.

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0. Draw $n_{\text{live}}$ samples from the prior — the live points
1. Denote the smallest likelihood amongst the live points by $\mathcal{L}^\star$
2. Replace that live point by one drawn from the constrained prior

$$\pi^\star(\boldsymbol{\Theta}) \propto \begin{cases} \pi(\boldsymbol{\Theta}) & \mathcal{L}(\boldsymbol{\Theta}) \geq \mathcal{L}^\star \\ 0 & \text{otherwise} \end{cases}$$

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4. Increment estimate of evidence, $\mathcal{Z} \rightarrow \mathcal{Z} + \mathcal{L}^\star \Delta X$

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3. Make a statistical estimate of $X(\mathcal{L}^\star)$ from this procedure
4. Increment estimate of evidence, $\mathcal{Z} \to \mathcal{Z} + \mathcal{L}^\star \Delta X$
5. If we have completed evidence sum to given tolerance, stop. Otherwise go to 1.

So we evolve a set of $n_{\text{live}}$ live points to higher and higher likelihoods, replacing one live point at a time.

# Compression

*We know that $X_0 = 1$. How much do we expect $X$ to contract when we replace the worst point?*

Drawing from the constrained prior means live points are distributed uniformly in $X$ from 0 to $X(\mathcal{L}^\star)$.

In other words, the

$$f_i = \frac{X(\mathcal{L}_i)}{X(\mathcal{L}^\star)}$$

are uniformly distributed from 0 to 1.

# Compression

*We know that $X_0 = 1$. How much do we expect $X$ to contract when we replace the worst point?*

The largest one, $t \equiv \max f_i$, gives us the compression. We can write

$$p(t) = \binom{n_{\text{live}}}{1} \cdot t^{n_{\text{live}}-1} \cdot 1 = n_{\text{live}} t^{n_{\text{live}}-1}$$

where the factors are combinatorial, the probability of $n_{\text{live}} - 1$ samples less than $t$, and lastly the probability density of a point at $t$.

# Compression

*We know that $X_0 = 1$. How much do we expect $X$ to contract when we replace the worst point?*

We find the expected compression:

$$\langle \log t \rangle = n_{\text{live}} \int_0^1 t^{n_{\text{live}}-1} \log t \, \mathrm{d}t = -\frac{1}{n_{\text{live}}}$$

*Thus we may estimate that at iteration i*

$$X_i \equiv X(\mathcal{L}_i^\star) \approx e^{-i/n_{live}}$$

# Exploration

*How can we find an independent sample from the constrained prior?*

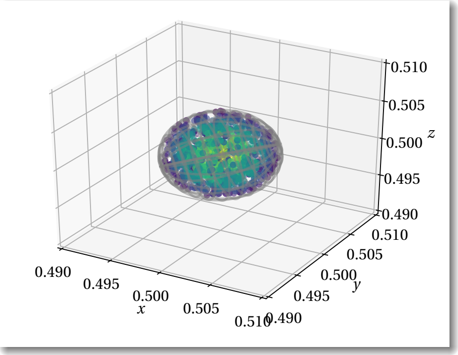
This step in nested sampling was needed for our estimates of the volume, $X$.

Failure to correctly sample from the constrained prior leads to faulty estimates of the evidence.

This requires an exploration strategy.

# Exploration

MultiNest (Feroz and Hobson 2008; Feroz, Hobson, and Bridges 2009; Feroz et al. 2013) — bound live points by ellipsoids. Use them to approximate iso-likelihood contour. Sample from the ellipsoids.



Two-dimensional Gaussian.

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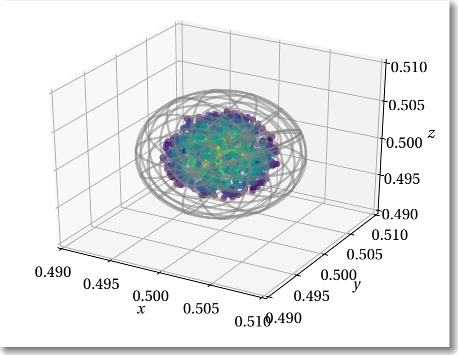
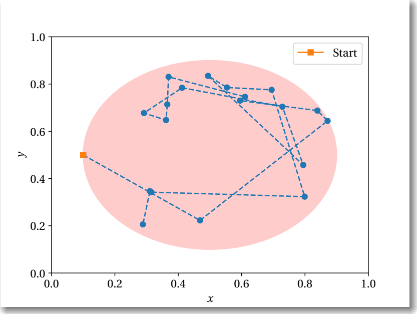


Expand to be safe — at expense of sampling efficiency.

# Exploration

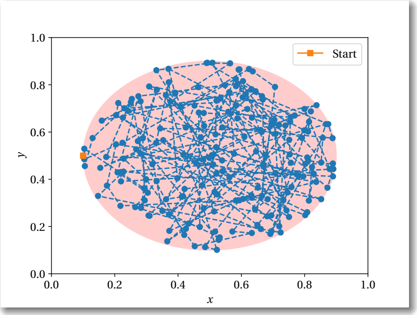
PolyChord (Handley, Hobson, and Lasenby 2015a; Handley, Hobson, and Lasenby 2015b) — slice sampling walk, starting from a randomly chosen live point.



Two-dimensional Gaussian. 20 steps.

# Exploration

PolyChord (Handley, Hobson, and Lasenby 2015a; Handley, Hobson, and Lasenby 2015b) — slice sampling walk, starting from a randomly chosen live point.



200 steps. More steps to reduce correlation — at expense of sampling efficiency.

# Things can go wrong…

- What if I don’t expand the ellipsoids enough?
- What if I don’t use enough steps?
- What if my exploration strategy isn’t actually drawing independent samples from the constrained prior?

It would violate assumption and lead to faulty estimate of evidence.

But how would I know?

# A new cross-check

# What if we new the $X$ of every sample?

Suppose we knew the $X$ of every sample, $X(\mathcal{L}_i)$. We could look at

$$f_i = \frac{X(\mathcal{L}_i)}{X(\mathcal{L}^\star)}$$

it should be uniformly distributed from 0 to 1 as each new $X(\mathcal{L}_i)$ should be uniformly distributed from 0 to $X(\mathcal{L}^\star)$.

*You could test whether the $f$ indeed followed a uniform distribution (Buchner 2016).*

# What do we know?

We don't know that. We do know the likelihood of every new sample, $\mathcal{L}_i$, and that $X(\mathcal{L})$ is a monotonic function.

So we can rank the $n_{\text{live}}$ points by $X(\mathcal{L}_i)$ by ranking them by $\mathcal{L}_i$.

*The rank of every new sample, r, should be uniformly distributed from 1 to $n_{live}$.*

It's just as likely to be the worst, second worst, …, second best, best likelihood.

*We can test whether the r indeed follow a discrete uniform distribution.*

# KS test

To compare the samples with the uniform distribution, we compute a $p$-value form a Kolmogorov-Smirnoff test.

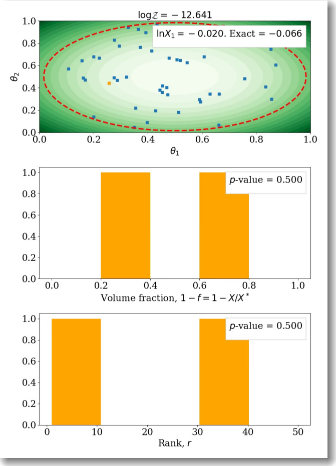
*Sorry to sully a Bayesian algorithm with a p-value.*

We use all the iterations and we test chunks of $n_{\text{live}}$ iterations.

The latter stops biased periods in long runs being diluted by lots of unbiased iterations.

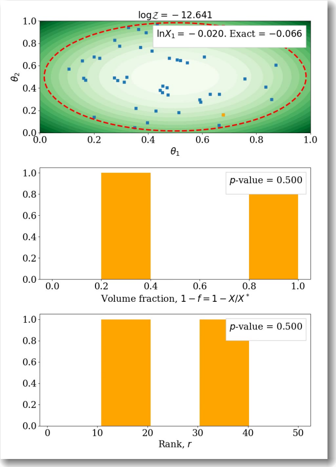
# Histogram of ranks $r$

Let's run a two-dimensional Gaussian nested sampling run. We will monitor the fractions and the insertion ranks, $r$.



# Detecting faults

This time, let's make the sampling biased by sampling from the wrong iso-likelihood contour — we find the correct one then contract it by a (random) factor $0.8 \pm 0.1$.



# Detecting faults

We see a tiny $p$-value and a biased overestimate of $\mathcal{Z}$ — overestimated because the likelihoods that we draw are greater than they should be.

# Correlations

The ranks $r$ are not, however, independent — the distribution of the live points only changes by one point every iteration.

If live points a are clustered together in $X$, insertion indexes in that region are unlikely.

We ignore this complication. However, if anything, correlations make the insertion ranks repel each other,

# Toy problems

# Toy problems

In our paper, we introduce 4 toy problems. Here we discuss only one of them.

We compute the evidence using MultiNest and PolyChord, and *p*-values from our test.

We do 100 repeats. And good efr $\ll 1$ and bad efr $\gg 1$ exploration settings.

# Gaussian

Multi-dimensional Gaussian likelihood

$$\mathcal{L}(\mathbf{\Theta}) \propto e^{-\frac{\sum(\mathbf{\Theta}-\mu)^2}{2\sigma^2}}$$

We pick a uniform prior from 0 to 1 for each dimension.

The analytic evidence is always $\log \mathcal{Z} = 0$ since the likelihood is a pdf in $\mathbf{\Theta}$, modulo small errors as the infinite domain is truncated by the prior.

We pick $\mu = 0.5$ and a diagonal covariance matrix with $\sigma = 0.001$ for each dimension.

# MultiNest. Gaussian, $\log \mathcal{Z} = 0$

Tiny $p$-values and biased results shown in red.

Smaller efr ⇔ stricter run

| efr | $d$ | $\log \mathcal{Z}$ | Inaccuracy | Bias | $p$-value | Rolling |
|---|---|---|---|---|---|---|
| 0.10 | 2 | $-0.00 \pm 0.10$ | $-0.04$ | $-0.47$ | 0.50 | 0.49 |
| 0.10 | 10 | $0.01 \pm 0.23$ | 0.04 | 0.48 | 0.59 | 0.60 |
| 0.10 | 30 | $0.38 \pm 0.41$ | 0.93 | 10.56 | 0.52 | $2.7 \cdot 10^{-4}$ |
| 0.10 | 50 | $2.08 \pm 0.52$ | 3.98 | 41.25 | 0.38 | $4.5 \cdot 10^{-24}$ |
| 1 | 2 | $-0.00 \pm 0.10$ | $-0.04$ | $-0.46$ | 0.52 | 0.49 |
| 1 | 10 | $0.57 \pm 0.23$ | 2.43 | 26.07 | 0.21 | $1.2 \cdot 10^{-4}$ |
| 1 | 30 | $2.35 \pm 0.40$ | 5.83 | 63.82 | 0.23 | $2.2 \cdot 10^{-23}$ |
| 1 | 50 | $4.06 \pm 0.52$ | 7.81 | 92.99 | 0.30 | $1.3 \cdot 10^{-34}$ |
| 10 | 2 | $-64.75 \pm 0.11$ | $-532.44$ | $-6.95$ | $7.7 \cdot 10^{-3}$ | 0.06 |
| 10 | 10 | $2.81 \pm 0.23$ | 12.30 | 150.55 | $2.1 \cdot 10^{-6}$ | $1.7 \cdot 10^{-19}$ |
| 10 | 30 | $4.30 \pm 0.40$ | 10.75 | 174.47 | 0.02 | $3.1 \cdot 10^{-68}$ |
| 10 | 50 | $6.04 \pm 0.52$ | 11.66 | 197.79 | 0.08 | $1.1 \cdot 10^{-93}$ |

# PolyChord. Gaussian, $\log \mathcal{Z} = 0$

Tiny $p$-values and biased results shown in red.

Smaller efr ⇔ stricter run

| efr | $d$ | $\log \mathcal{Z}$ | Inaccuracy | Bias | $p$-value | Rolling |
|---|---|---|---|---|---|---|
| 0.50 | 2 | $0.01 \pm 0.11$ | 0.11 | 1.03 | 0.54 | 0.60 |
| 0.50 | 10 | $-0.00 \pm 0.23$ | $-0.01$ | $-0.10$ | 0.48 | 0.52 |
| 0.50 | 30 | $-0.06 \pm 0.41$ | $-0.15$ | $-1.61$ | 0.54 | 0.57 |
| 0.50 | 50 | $-0.05 \pm 0.52$ | $-0.10$ | $-0.85$ | 0.58 | 0.51 |
| 1 | 2 | $-0.02 \pm 0.11$ | $-0.19$ | $-1.96$ | 0.42 | 0.48 |
| 1 | 10 | $-0.04 \pm 0.23$ | $-0.17$ | $-2.20$ | 0.55 | 0.59 |
| 1 | 30 | $-0.83 \pm 0.41$ | $-2.06$ | $-20.73$ | 0.61 | 0.46 |
| 1 | 50 | $-2.48 \pm 0.52$ | $-4.73$ | $-54.22$ | 0.49 | 0.59 |
| 2 | 2 | $-0.01 \pm 0.11$ | $-0.12$ | $-0.89$ | 0.47 | 0.53 |
| 10 | 10 | $2.20 \pm 0.23$ | 9.50 | 30.29 | 0.13 | 0.22 |
| 30 | 30 | $48.37 \pm 0.64$ | 112.25 | 70.58 | $8.2 \cdot 10^{-10}$ | 0.02 |
| 50 | 50 | $69.74 \pm 3.05$ | 23.31 | 106.51 | $8.0 \cdot 10^{-86}$ | $1.4 \cdot 10^{-6}$ |

# Summary of toy problem

A lot of numbers…

- Less strict exploration settings or high number of dimensions
- … leads to a biased estimate of evidece
- … often detected by tiny *p*-value by our test

# Example from cosmology

# Cosmology

Handley considered Bayesian evidence for a spatially closed Universe (Handley 2019a). Evidences from combinations of four datasets were computed using PolyChord for a spatially flat Universe and a curved Universe.

The Bayes factors showed that a closed Universe was favoured by odds of about 50/1 for a particular set of data.

There were 22 NS computations in total (Handley 2019b).

# Cosmology

We ran our cross-check on each of the 22 NS runs finding *p*-values in the range 4% to 98%.

THis does not suggest problems with the NS runs. The *p*-value of 4% is not particularly alarming, especially considering we conducted 22 tests.

| | Flat | | Curved | |
|---|---|---|---|---|
| Data | *p*-value | Rolling *p*-value | *p*-value | Rolling *p*-value |
| BAO | 0.89 | 0.82 | 0.07 | 0.05 |
| lensing+BAO | 0.72 | 0.54 | 0.19 | 0.43 |
| lensing | 0.26 | 0.14 | 0.04 | 0.64 |
| lensing+$SH_0$ES | 0.08 | 0.08 | 0.78 | 0.04 |
| Planck+BAO | 0.39 | 0.56 | 0.14 | 0.43 |
| Planck+lensing+BAO | 0.68 | 0.69 | 0.70 | 0.27 |
| Planck+lensing | 0.94 | 0.49 | 0.89 | 0.72 |
| Planck+lensing+$SH_0$ES | 0.92 | 0.92 | 0.33 | 0.82 |
| Planck | 0.81 | 0.69 | 0.84 | 0.88 |
| Planck+$SH_0$ES | 0.20 | 0.48 | 0.92 | 0.97 |
| $SH_0$ES | 0.59 | 0.59 | 0.98 | 0.98 |

# Summary

- Nested sampling is a popular algorithm for computing Bayesian evidence
- We developed the first test of single nested sampling runs
- Appears to work nicely on toy and realistic problems
- Could become an important part of nested sampling analysis
- Could become a best practice to apply the check whenever using nested sampling

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