Robust sampling for weak lensing and clustering analyses with the Dark Energy Survey

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ABSTRACT

Recent cosmological analyses rely on the ability to accurately sample from high-dimensional posterior distributions. A variety of algorithms have been applied in the field, but justification of the particular sampler choice and settings is often lacking. Here we investigate three such samplers to motivate and validate the algorithm and settings used for the Dark Energy Survey (DES) analyses of the first 3 years (Y3) of data from combined measurements of weak lensing and galaxy clustering. We employ the full DES Year 1 likelihood alongside a much faster approximate likelihood, which enables us to assess the outcomes from each sampler and demonstrate the robustness of our full results. We find that the elliptipodal nested sampling algorithm MultiNest reports inconsistent estimates of the Bayesian evidence and somewhat narrower parameter credible intervals than the sliced nested sampling implemented in PolyChord. We compare the findings from MultiNest and PolyChord with parameter inference from the Metropolis–Hastings algorithm, finding good agreement. We determine that PolyChord provides a good balance of speed and robustness for posterior and evidence estimation, and recommend different settings for testing purposes and final chains for analyses with DES Y3 data. Our methodology can readily be reproduced to obtain suitable sampler settings for future surveys.

Key words: cosmology: cosmological parameters – cosmology: observations – cosmology: large-scale structure of the Universe – methods: statistical

1 INTRODUCTION

The sampling of a posterior distribution is one of the central elements in current cosmological analyses. With the increasing complexity of cosmological surveys and the large amount of data available, it is a complicated challenge to extract cosmological parameters because of the high dimensionality and complex shapes of the

1 In this work, we use the term parameters to refer to the parameters characterizing a model, both nuisance and cosmological, for which we want to generate samples. We use the term hyperparameters to refer to the parameters specific to sampler settings, which affect their performance, such as the number of samples we want to obtain, the stopping criteria, etc. This terminology is common in the machine learning literature. Note that the term hyperparameters can refer to different concepts, even in the field of
distributions. Nuisance parameters (accounting for various calibra-
tion and systematic effects) complicate the analysis by increasing the
number of parameters well beyond the six of the standard ΛCDM
model of cosmology.

Bayesian techniques give a principled framework for prob-
abilistic inference, for instance characterising information about
complex, usually non-Gaussian, posterior distributions for which
the mean and standard deviation alone are insufficient to fully de-
scribe the shape of the distribution. Markov Chain Monte Carlo
methods have traditionally been used for this purpose (Metropolis
et al. 1953; Neal 1997), and have a long history of applications in
cosmology (e.g. Christensen et al. 2001; Knox et al. 2001; Lewis
& Bridle 2002; Verde et al. 2003; Tegmark et al. 2004; Dunkley
et al. 2005; Shaw et al. 2007). However, for some applications (such
as model comparison and the comparison of different datasets) it
is necessary to calculate not only the shape of the posterior distri-
bution but also the Bayesian evidence. Nested Sampling (Skilling
2006) is the method most commonly used for this purpose, because
of its speed and its ability to obtain both the Bayesian evidence and
the posterior distribution in the same calculation.

Because of their wide applicability, many tools have been
developed to implement these sampling algorithms given a user-
defined likelihood, and the choice to use one over another may
be more driven by accessibility and ease of implementation than
rigorous testing for the specific analysis at hand.

As the constraining power of cosmological datasets has grown,
different analyses have begun to diverge in their inferred parameter
posteriors. Perhaps most famous is the discrepancy in the mea-
surement of the Hubble parameter H_0 by the Planck collaboration (Planck Collaboration 2020) versus that obtained via distance
ladder measurements (Riess et al. 2021), but there exists also tension
between measurements of S_8 ≡ σ_8(Ω_m/0.3)^0.5 from large-scale structure probes and that inferred by Planck under ΛCDM (see
Di Valentino et al. 2021a; Shah et al. 2021, for reviews on these tensions). As these discrepancies could be indicators of new physics, it is vital that the inferences upon which they are based are robust to analysis choices such as the specific sampler and settings used.

Most samplers include hyperparameters that allow one to tune
the algorithm and, in the limit of infinite computing time and re-
sources, allow one to obtain arbitrarily precise constraints. In prac-
tice, we require a balance of speed and accuracy, where it is feasible
to run a large number of chains but the error introduced by the
sampler is a negligible (or at least quantifiable) contribution to the
analysis’ error budget. This is particularly true for the Dark En-
ergy Survey (DES, The Dark Energy Survey Collaboration 2005)
combined weak lensing and galaxy clustering cosmology analysis
(henceforth, 3x2pt), where the complexity of the data and analysis
pipeline results in the need to run a large number of chains for
validation purposes.

In this work, we perform a careful investigation of several
leading sampling algorithms available within the CosmoSIS analy-
sis framework. We focus on PolyChord and MultiNeat because
of their ability to estimate the Bayesian evidence, and calculation
of model comparison and dataset tension statistics are of particu-
lar interest for the DES Y3 analysis. We investigate how hyper-
parameters impact performance and focus particularly on avoiding
biases in the parameter constraints and evidence, which could lead
to mistaken interpretation of the core analysis results. We make rec-
ommendations for the sampler and settings for three different use
cases of the DES Y3 data, which strike different balances of speed
and accuracy.

There have been previous attempts at characterizing sampler
performance. For example, Allison & Dunkley (2014) compared
MCMC and Nested Sampling methods, and Higson et al. (2019)
developed diagnostic methods to assess errors from Nested Sam-
pling chains, including the use of bootstrapping individual chain
samples to assess uncertainty. We use some of these tools, but as-
sess uncertainty using full independent chain realizations run over a
wide range of parameter settings, and using high-resolution chains
as benchmarks. We combine tests on the first year of DES data
(DES Y1) and on the results of a fast, approximate version of the
likelihood that allows us to generate a large number of sampling
runs under the same hyperparameter settings.

The paper is structured as follows: In Sec. 2 we introduce
the methodology and notation of Bayesian parameter estimation, as
well as the summary statistics that we will use throughout this work.
In Sec. 3 we present the methodology and data used in this work.
Our results are shown in Sec. 4, and we present our conclusions
in Sec. 5. All the data produced from this work is available upon
request.

2 SAMPLERS

This section describes the formalism of parameter estimation in
a Bayesian framework, as well as the three different sampling al-
gorithms employed in this work. Detailed descriptions of the for-
malism can be found for example in MacKay (2002) and Sivia &
Skilling (2006).

2.1 The Bayesian framework

In parameter estimation we have obtained some data D, we have
assumed a theoretical model M, and we seek an estimate of the
parameters θ of the model. This is accomplished by applying Bayes’
theorem

\[ P(\theta|D, M) = \frac{P(D|\theta, M) \times P(\theta|M)}{P(D|M)} \]  

(1)

The quantities in this equation are usually labelled as

\[ \mathcal{P} = \mathcal{L} \times \Pi \frac{d\theta}{Z} \]  

(2)

where \( \mathcal{P} \) is the posterior, \( \mathcal{L} \) the likelihood, \( \Pi \) the prior, and \( Z \) the marginal likelihood or Bayesian evidence. The latter can be expressed as

\[ Z = \int \mathcal{L} \times \Pi \, d\theta. \]  

(3)

This is typically a complicated and high-dimensional integral. Be-
cause \( Z \) acts as a normalising factor that does not depend on the
parameters, it often plays no role for parameter estimation. There
are, however, other applications where the Bayesian evidence is
fundamental; one such case is Bayesian model comparison. Here we
have two competing theoretical models \( M_A \) and \( M_B \) and we want
to know which of these models is preferred given some measured
data D. For this we calculate the ratio

\[ \frac{P(M_A|D)}{P(M_B|D)} = \frac{P(D|M_A)}{P(D|M_B)} \times \frac{P(M_A)}{P(M_B)}. \]  

(4)
where the equality follows from Bayes’ theorem. The second factor on the right-hand side is the ratio of the prior beliefs in the two models. If there is no prior reason to prefer one model over the other, then this term is unity and hence disappears. The first factor on the right-hand side is the ratio of the Bayesian evidences for the two models. Therefore, under the assumption of equal prior beliefs in the two models, we can find which model is preferred by the data by calculating the ratio

\[ R = \frac{Z_A}{Z_B} \]

This quantity is called the Bayes factor. Bayesian evidences are also used to quantify tension between different datasets (Marshall et al. 2006).

In addition to the Bayesian evidence of Eq. (3), we will compute two more summary statistics from our chains, which contain important information about our problem. The first one is the Kullback–Leibler divergence (Kullback & Leibler 1951), given by

\[ D_{KL} = \int P(\theta) \log \frac{P(\theta)}{\pi(\theta)} \, d\theta. \]

The Kullback-Leibler divergence measures the information gain when going from the prior to the posterior distribution, measured in natural bits, or nats. The Kullback–Leibler divergence can be used amongst other things to calculate the information between two data sets, which in turn can be used to calculate the Suspiciousness (Handley & Lemos 2019b), and quantify the concordance between the data sets in a way that does not depend on prior volumes.

Our last summary statistic is the Bayesian Model Dimensionality (henceforth BMD), which provides an estimate of how many Gaussian dimensions are constrained by our data

\[ d = 2 \int P(\theta) \left( \log \frac{P(\theta)}{\pi(\theta)} - D_{KL} \right)^2 \, d\theta. \]

Handley & Lemos (2019a) discuss the advantages of characterizing dimensionality via the BMD as opposed to other commonly-used measures like the Bayesian Model Complexity (Spiegelhalter et al. 2002), such as not relying on a single point estimator. Another advantage of the BMD is that it can be computed directly from both nested sampling and Markov Chain Monte Carlo chains as

\[ \bar{D} = \frac{1}{N} \sum_i \left( \langle \log L \rangle_i - \langle \log L \rangle_p \right)^2, \]

where \( \langle \cdot \rangle_p \) indicates an average over the posterior distribution.

### 2.2 Metropolis–Hastings

Markov Chain Monte Carlo (MCMC) is one of the most widely used methods for sampling probability distributions. It consists of using chains in which each element depends only on the previous one, known as Markov Chains, to obtain samples from the target distribution. The Metropolis–Hastings algorithm (Hastings 1970) (denoted MH in the following) is a common MCMC method, widely used in various fields such as statistical mechanics or as here, Bayesian inference. Here we use MH in order to generate samples from the posterior distribution of the cosmological and nuisance parameters. Below we describe the fundamental aspects of MCMC algorithms in general, and MH in particular, as well as details of its implementation within this work.

Note that we include the MH sampler primarily as a benchmark against which we can compare the parameter estimation results of the nested samplers that are the main focus of this work. We have not made a significant effort to optimize the MH sampler’s speed and performance, so a fair assessment of its computational cost compared to PolyChord and MultiNest is beyond the scope of this paper.

#### 2.2.1 The Metropolis–Hastings algorithm

The goal of MCMC algorithms is to return samples from a distribution that converges towards a unique stationary distribution \( \pi(\theta) \) (where \( \theta \) are the cosmological and nuisance parameters) of the target distribution, in this case the posterior \( P(\theta) \). Given the transition matrix \( p_{ij} \) of a Markov chain, which corresponds to the probability of moving from state \( i \) at time \( t \) to state \( j \) at time \( t+1 \), we thus have

\[ \pi_j = \sum_i p_{ij} \pi_i. \]

We now need to construct such a transition matrix.

The MH algorithm proposed in Hastings (1970) does so by requiring \( p_{ij} \) and \( \pi \) to satisfy the so-called detailed balance

\[ \pi_i p_{ij} = \pi_j p_{ji}. \]

In MH, the transition matrix is then defined as

\[ p_{ij} = q_{ij} \alpha_{ij} \]

where \( q_{ij} \) is the proposal distribution (corresponding to a proposed ‘jump’ in parameter space) and \( \alpha_{ij} \) the acceptance distribution (corresponding to accepting this ‘jump’ or not), defined as

\[ \alpha_{ij} = \min \left[ 1, \frac{\pi_j q_{ji}}{\pi_i q_{ij}} \right]. \]

If a chain of samples is selected using this algorithm for a large number of steps, the density of their resulting distribution will follow the target distribution, \( \pi \), i.e. the posterior \( P(\theta) \).

Depending on the initial point in parameter space and the provided proposal, some samples drawn at the beginning of this process should be discarded as they are not representative of the posterior distribution. This period is called burn-in, where the accepted points may be far from the peak of the posterior, and can be minimized if starting at a point in parameter space closer to the best-fit value (see Hogg & Foreman-Mackey (2018) for a discussion on choices to limit the burn-in period). It can be explored by plotting the posterior or parameter values as a function of step number (or over-plotting these values from chains that started at different points), where the burn-in corresponds to samples before these values converge around the typical set.

One potential way of speeding up MH algorithms often used in cosmology is to take advantage of the fact that some parameters, known as ‘fast’, do not affect the slowest parts of the likelihood calculation, which in the case of cosmology often involve the transfer function or line-of-sight integration. These parameters can be decorrelated and sampled separately, making sampling nearly as fast as if it would for the ‘slow’ parameters alone (Lewis 2013). When fast and slow parameters cannot be fully decorrelated in principle, they can be sampled using ‘dragging’ (Neal 2005), which consists of ‘dragging’ the fast parameters while keeping the slow ones fixed, leading to fast likelihood evaluations. Both of these methods are implemented in the Cobaya package (Torrado & Lewis 2021).
towards the target distribution. Several criteria for testing the convergence have been proposed (An et al. 1998; Sinharay 2003). It is also useful to study the autocorrelation of the MH chains to verify that the samples are independent on scales much smaller than the chain length. In the following, we will mainly use the Gelman–Rubin diagnostic which is derived from the method proposed in Gelman & Rubin (1992) to monitor the convergence of MH chains. This diagnostic works by comparing parameter estimates from a number of independent chains. Specifically, adopting the standard notation, it estimates the potential scale reduction factor $\hat{R}$ for a given parameter $\theta$, defined as

$$\hat{R} = \frac{\hat{V}}{W},$$

(13)

where $\hat{V}$ is the estimator of the variance of the parameter and $W$ is the average of the variance of $\theta$ within a chain (in the above expression, the impact of degrees of freedom defined in Gelman & Rubin (1992) is neglected). $\hat{R} \approx 1$ implies that the distribution of the sampled parameter is close to stationary; while this does not guarantee that the chain has converged, it is a good indication of convergence for unimodal posteriors when $\hat{R}$ is nearing 1 for all parameters. A typical convergence criterion is to stop when $\hat{R} - 1 < 0.1$. When considering $M$ independent chains, the variance estimator $\hat{V}$ is defined as

$$\hat{V} = \frac{N - 1}{N} W + \frac{M + 1}{MN} B,$$

(14)

where $N$ is the length of the chains and $B/N$ is an estimate of the variance of the parameter mean $\bar{\theta}$ across chains i.e.

$$B/N = \frac{1}{M - 1} \sum_{i=1}^M (\bar{\theta}_i - \bar{\theta})^2.$$

(15)

### 2.2.2 Implementation

For this study we use a simple version of the MH sampler implemented within CosmoSIS. In the configuration used here the MH sampler uses a fast–slow scheme in which each parameter subspace uses a separate multivariate Gaussian proposal, with a 1/3 chance of each proposed jump length being drawn instead from an exponential distribution, to better explore parameter tails. We oversampled the fast subspace by a factor of 5 and have 9 fast parameters. In typical distribution, to better explore parameter tails. We oversampled the each proposed jump length being drawn instead from an exponential to other parameters is small, which causes the proposal covariance just over a longer period of time.

### 2.3 MultiNest

MultiNest is an example of a nested sampling algorithm (Skilling 2006) which, in contrast to MCMC samplers like MH, can be used to calculate the Bayesian evidence in addition to estimating the posterior. Instead of selecting individual samples sequentially, nested sampling starts with a large number of points (called ‘live’ points), and then repeatedly selects the live point with the smallest value of the posterior density, eliminates it (turning it into a ‘dead point’), and then finds a new replacement live point with a posterior value larger than that of the point that was eliminated. The collection of all points (live and dead) can then be used to calculate the evidence while also serving as a (weighted) sample of the posterior. The most difficult part of Nested Sampling is finding new live points. It is extremely inefficient simply to randomly generate points until one with a higher posterior value is found (especially when most live points are close to the maximum of the posterior and when the problem has high dimensionality). This is the challenge that specific algorithms like MultiNest are designed to address.

MultiNest is a publicly available code for Nested Sampling (Feroz et al. 2009; Feroz et al. 2019). It has been extensively used for cosmology analyses, including that of the first year (Y1) of DES data (Abbott et al. 2018). MultiNest uses a technique called ellipsoidal sampling (Mukherjee et al. 2006), where it calculates a D-dimensional ellipsoid from current set of live points, and finds the next point within that ellipsoid, expanded by a certain factor. MultiNest also includes a clustering algorithm to identify multiple peaks in the posterior distribution, allowing it to sample multimodal posteriors. This was its main improvement over the ellipsoidal nested sampling code CosmoNest (Mukherjee et al. 2006b; Mukherjee et al. 2006a; Parkinson et al. 2006; Pahud et al. 2006). There are other examples of ellipsoidal Nested Sampling algorithms, such as nestle and dynesty (Speagle 2020), which uses dynamic sampling whilst still relying on ellipsoidal nested sampling.

As described in Skilling (2006), the standard Nested Sampling approach calculates the evidences using the accepted samples, and using an approximation for the distribution of sampling weights. In addition to this calculation, MultiNest produces an alternative calculation of the Bayesian evidence using Importance Nested Sampling (henceforth INS). INS, first introduced in the context of Nested Sampling in Cameron & Pettitt (2014), uses all likelihood evaluations to estimate the evidence, instead of using only the accepted points in the MultiNest run (which in some cases has acceptance rates as low as ~ 1%). In an ideal case, both estimates of the evidence should agree. In this work, when we refer to the MultiNest evidence, we are referencing the ‘default’ evidence calculation, and we will explicitly make reference to the INS evidence when that is not the case.

While ellipsoidal nested sampling leads to fast sampling, it can also lead to biases in both the posterior and the evidence estimation, as discussed later in the paper. This is illustrated by Fig. 1: If the ellipsoid is not expanded enough, the calculation of the evidence will ‘miss’ parts of the distribution. These issues are discussed using MultiNest as an example, but apply to any implementation of ellipsoidal nested sampling.

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2 https://github.com/farhanferoz/MultiNest
3 http://kylebarbary.com/nestle/index.html
4 https://dynesty.readthedocs.io/en/latest/
2.4 PolyChord

An alternative code for Nested Sampling is PolyChord (Handley et al. 2015a,b). The difference between this algorithm and MultiNest is in the approach to generating new live points. Instead of the ellipsoidal sampling, it uses so-called slice sampling (Aitken & Akman 2013), where new live points are generated by taking a random slice through the parameter space that includes the current live point, and randomly generating new points until one with higher likelihood is found. The process is then repeated with the new point and a slice in a new random direction, for a user-defined number of repetitions (n_repeats) until the candidate live point is sufficiently uncorrelated with the initial live point. In practice, the sample covariance of existing points is used to decorrelate and whiten the parameter space, such that slices are performed on an affine transformation of parameter space where the relevant likelihood width is $O(1)$ in each direction. This both simplifies and accelerates the generation of new samples.

Like MultiNest, PolyChord has a clustering algorithm which allows it to sample multimodal posterior distributions. In addition, PolyChord is compatible with the fast-slow parameter implementation used by the code CosmoMC (Lewis & Bridle 2002; Lewis 2013), which provides a significant increase in speed for cosmological likelihoods. While it is slower than MultiNest in obtaining posterior distributions and Bayesian evidences for the models studied here, we will show that it more reliably gives unbiased results.

Figure 1. An example of MultiNest’s ellipsoidal sampling, and how it can lead to biases. When trying to sample a certain distribution (top left), MultiNest randomly generates some points (top right). It then uses the covariance matrix obtained from those points point to calculate an ellipsoid enclosing all existing live points (bottom left, dashed line). That ellipsoid is expanded in volume by a factor inversely proportional to the efficiency, and samples are drawn from that ellipsoid (bottom right, dot-dashed line). As the latter plot shows in the light blue regions, if the magnification factor is not big enough (i.e. the efficiency is too high), this can lead to a bias in the estimation of the evidence.

2.5 Other samplers

In this work, we focus on three sampling algorithms commonly used in cosmology (Metropolis–Hastings, ellipsoidal nested sampling and slice nested sampling). One common sampler that we do not implement is Emcee, which is an affine-invariant MCMC sampler that uses an ensemble of walkers to traverse the posterior and update the proposal distribution before applying standard Metropolis–Hastings acceptance criteria (Foreman-Mackey et al. 2013). We found that in the large-dimensional parameter spaces tested here, the samples generated by Emcee had high enough levels of correlation so as to require intractable runtimes. Coupled with the inability to apply convergence criteria like the Gelman–Rubin statistic to correlated walkers and the large amount of samples that need to be discarded as burn-in, we decided not to include it in this study.

There exist other algorithms that, while perhaps not yet as widely used in cosmology, could become more common in the future. Zeus (Karamanis et al. 2021) is an implementation of ensemble slice sampling (Karamanis & Beutler 2021) for MCMC, and has the advantage of not requiring tuning of any hyperparameters, thus providing a promising alternative to traditional MCMC algorithms. We provide a more detailed discussion of Zeus, and compare it to Emcee, MultiNest and PolyChord in Appendix A. Other algorithms such as Hamiltonian Monte Carlo (Betancourt 2017) or the No-U-Turn Sampler algorithm (Hoffman & Gelman 2014) have existed for some time, but require accurate derivatives, which can-

5 https://github.com/PolyChord/PolyChordLite
6 https://zeus-mcmc.readthedocs.io/en/latest/
not be accessed easily in current cosmological theory codes such as CAMB.

3 METHODOLOGY

The goal of this paper is to compare the performance of the previously introduced methods for cosmological analysis. In cosmology, we usually perform inference with about six to eight cosmological parameters, and a number of nuisance parameters used to model systematic uncertainties. The nuisance parameters are usually marginalised over for cosmological constraints, though they may also be interesting in their own right (e.g. constraining galaxy bias or the amplitude of intrinsic alignment of galaxies). Here we ally marginalised over for cosmological constraints, though they model systematic uncertainties. The nuisance parameters are usually introduced methods for cosmological analysis. In cosmological theory codes such as CAMB not be accessed easily in current cosmological theory codes such as CAMB.

3.1 Fast Likelihood Analysis

The sampling methods described in this work can be slow, and in some cases we can only understand the effects of tuning different hyperparameters by repeating the sampling a large number of times. For that purpose, we generated a fast likelihood, which produces posterior distributions that are similar to those of the DES Y1 pipeline, but uses multiple approximations to significantly reduce the run time. The resulting likelihood is an approximation to the true likelihood that allows for a large number of chains to be run and thus for the variance of samplers to be characterized. It can be considered a toy model that is substantially more applicable to our use case than the analytic models (e.g. Gaussian mixture models) that are often employed to characterize sampler behaviour.

The primary changes in the fast likelihood are:

(i) Using the fitting function presented in Eisenstein & Hu (1998) for the transfer function when computing the linear matter power spectrum;
(ii) Acceleration of the calculation of the Halofit nonlinear scale (Equation A4 in Takahashi et al. 2012) using a non-iterative interpolation-based root-finding algorithm and trapezoidal integration;
(iii) Calculation of the lensing efficiencies and Limber angular correlation functions (Equations IV.3-IV.6 in Abbott et al. 2018) using a simplified trapezoidal integration scheme.

3.2 Application to DES Y1 data

We apply all the samplers described above to the DES 3x2pt analysis, running MultiNest and PolyChord with a large number of different hyperparameter settings. Because the bulk of the work presented in this paper was performed while the analysis pipeline for the recently-released Y3 analysis (Abbott et al. 2022) was being developed, these tests are run using the DES Y1 data (Abbott et al. 2018) and the Y1 version of the DES modelling pipeline. These data consist of a combination of three two-point correlation function measurements: Cosmic shear, galaxy–galaxy lensing, and galaxy clustering.

There are mainly two purposes to this paper: to find sampler settings that yield unbiased results for the DES analysis whilst minimizing the running time, and to generally understand the causes of bias in the parameter estimation or evidence calculation. The results presented in this work depend heavily on the dimensionality of the likelihood, as well as the form of the likelihood, and so cannot be generalized to all sampling problems. However, as most cosmological sampling problems have similar dimensionality and characteristics, these results should still be useful in guiding sampler choices in future cosmological analyses.

4 RESULTS

In this work, we have explored different sampling settings, to compare their performance and run time. Unless stated otherwise, all runs use the same likelihood, priors, and data, and are run using the same computing platform (the Cori system at NERSC) and with the same number of nodes.

4.1 Posterior validation with Metropolis–Hastings

MCMC methods are expected to produce more reliable posteriors than Nested Sampling, because their convergence criterion is based on the posterior, not on the Bayesian evidence (which is difficult to estimate well from standard MCMC chains). Given this, before looking in detail at the effects of hyperparameters, we compare constraint contours from MH and PolyChord in order to benchmark the accuracy of the nested sampling posterior estimates.

We run 8 MH chains in parallel using 4 processors per chain, spread across 2 nodes. We stopped the chains once $R - 1 < 0.02$ for all parameters (see Sec. 2.2 for a description of the Gelman–Rubin statistic $R$), amounting to 762,000 samples. We burn the first 20% of the chains, as described in Sec. 2.2. Figure 2 shows the posterior estimated with these two sets of chains on the cosmological parameters $w, \Omega_m$ and $\sigma_8$ along with the posterior estimated from a high quality PolyChord chain.

We note that our MH run was slower than most nested sampling runs, using around 4,600 CPU-hours (6 days of walltime). Nested sampling is known to scale better with dimensionality, so this is on some level expected. However, we emphasize that this is not necessarily a fair comparison because, as was discussed in Sec. 2.2, our MH runs did not employ a number of speed-up techniques which would likely be used in practice if MH were being used as the main sampler in an analysis. This is fine for our purposes, because as noted above we are using the MH chains to compare posterior distributions, not runtime.

We interpret the good agreement observed in Fig. 2 between MH and the high quality PolyChord chain as confirmation that with good enough settings, Nested sampling can accurately sample the posterior. We then explore what these settings need to be for both MultiNest and PolyChord.

4.2 Multinest

MultiNest has several hyperparameters that can be tuned. These changes can increase accuracy in computing different quantities,
Table 1. Comparison of time required and output values for MultiNest with different settings. All runs use the DES Y1 3x2pt likelihood and a wCDM cosmology, with 128 cores. The settings `OMP=threads` = 1 corresponds to 128 MPI threads, while `OMP=threads` = 4 corresponds to 32 MPI threads. CE refers to 'Constant efficiency'. L Eval refers to the number of Likelihood evaluations. INS refers to the Importance Nested Sampling reported by MultiNest, $D_{KL}$ is the Kullback-Leibler divergence, and BMD is the Bayesian Model Dimensionality. Reported uncertainties are via bootstrap resampling as computed by Anesthetic (Handley 2019).

| $n_{\text{live}}$ | Eff | Tol | OMP | CE | Time (hrs) | Acceptance | L Eval | $\log Z$ | INS $\log Z$ | $D_{KL}$ | BMD |
|-------------------|-----|-----|-----|----|-----------|------------|--------|--------|------------|---------|-----|
| 675               | 1   | 0.3 | 1   | F  | 11.2      | 0.067      | 265314 | $-277.71 \pm 0.17$ | $-285.14 \pm 0.05$ | 18.54 $\pm 0.16$ | 13.0 $\pm 0.3$ |
| 675               | 1   | 0.1 | 1   | F  | 13.8      | 0.056      | 340783 | $-277.68 \pm 0.17$ | $-284.93 \pm 0.22$ | 18.61 $\pm 0.15$ | 13.5 $\pm 0.4$ |
| 675               | 1   | 0.01| 1   | F  | 20.3      | 0.042      | 510583 | $-277.63 \pm 0.17$ | $-284.94 \pm 0.14$ | 18.42 $\pm 0.15$ | 13.0 $\pm 0.4$ |
| 675               | 1   | 0.4 | 4   | F  | 46.3      | 0.053      | 356248 | $-277.53 \pm 0.17$ | $-285.09 \pm 0.06$ | 18.33 $\pm 0.16$ | 12.8 $\pm 0.4$ |
| 675               | 1   | 0.1 | 1   | T  | 3.8       | 0.228      | 78561 | $-275.41 \pm 0.16$ | $-286.36 \pm 0.19$ | 17.59 $\pm 0.15$ | 12.3 $\pm 0.3$ |
| 250               | 0.3 | 0.1 | 1   | F  | 4.3       | 0.053      | 134554 | $-278.68 \pm 0.28$ | $-285.46 \pm 0.27$ | 19.32 $\pm 0.28$ | 13.3 $\pm 0.6$ |
| 675               | 0.3 | 0.3 | 1   | F  | 14.6      | 0.054      | 346242 | $-278.52 \pm 0.17$ | $-285.01 \pm 0.14$ | 19.16 $\pm 0.16$ | 13.5 $\pm 0.4$ |
| 675               | 0.3 | 0.1 | 1   | F  | 16.2      | 0.048      | 396284 | $-278.37 \pm 0.17$ | $-285.13 \pm 0.10$ | 19.14 $\pm 0.17$ | 12.6 $\pm 0.4$ |
| 675               | 0.3 | 0.1 | 1   | F  | 21.4      | 0.040      | 531284 | $-278.53 \pm 0.17$ | $-284.63 \pm 0.28$ | 19.18 $\pm 0.16$ | 13.5 $\pm 0.4$ |
| 675               | 0.3 | 0.1 | 4   | F  | 50.3      | 0.050      | 383602 | $-278.45 \pm 0.17$ | $-285.13 \pm 0.04$ | 19.21 $\pm 0.16$ | 13.0 $\pm 0.3$ |
| 675               | 0.3 | 0.1 | 1   | T  | 4.6       | 0.199      | 94746  | $-276.56 \pm 0.17$ | $-285.78 \pm 0.24$ | 18.64 $\pm 0.16$ | 12.3 $\pm 0.4$ |
| 250               | 0.1 | 0.1 | 1   | F  | 5.9       | 0.041      | 178614 | $-279.09 \pm 0.28$ | $-285.69 \pm 0.04$ | 19.98 $\pm 0.26$ | 13.4 $\pm 0.7$ |
| 675               | 0.1 | 0.1 | 1   | T  | 23.7      | 0.035      | 562784 | $-278.88 \pm 0.17$ | $-283.16 \pm 0.10$ | 19.44 $\pm 0.17$ | 12.9 $\pm 0.4$ |
| 675               | 0.1 | 0.1 | 1   | T  | 6.9       | 0.106      | 189995 | $-285.27 \pm 0.06$ | $-285.67 \pm 0.02$ | 20.79 $\pm 0.30$ | 14.4 $\pm 0.7$ |
| 250               | 0.01| 0.1 | 1   | F  | 11.7      | 0.026      | 294202 | $-280.78 \pm 0.29$ | $-285.67 \pm 0.02$ | 20.14 $\pm 0.17$ | 13.6 $\pm 0.4$ |
| 675               | 0.01| 0.1 | 1   | F  | 39.3      | 0.025      | 825487 | $-280.62 \pm 0.18$ | $-285.38 \pm 0.02$ | 21.84 $\pm 0.17$ | 13.6 $\pm 0.4$ |
| 675               | 0.01| 0.1 | 1   | T  | 28.1      | 0.027      | 754351 | $-280.76 \pm 0.18$ | $-285.23 \pm 0.02$ | 20.96 $\pm 0.16$ | 14.0 $\pm 0.4$ |
| 250               | 0.001| 0.1 | 1   | F  | 39.0      | 0.010      | 823090 | $-281.78 \pm 0.30$ | $-285.93 \pm 0.01$ | 21.62 $\pm 0.28$ | 14.6 $\pm 0.7$ |
| 675               | 0.001| 0.1 | 1   | F  | 109.5     | 0.010      | 2116032| $-282.01 \pm 0.18$ | $-285.29 \pm 0.02$ | 21.99 $\pm 0.17$ | 14.9 $\pm 0.4$ |
| 675               | 0.001| 0.1 | 1   | T  | 126.3     | 0.008      | 2756262| $-280.92 \pm 0.19$ | $-285.52 \pm 0.09$ | 20.77 $\pm 0.17$ | 15.2 $\pm 0.4$ |

Figure 2. Posterior distribution for a high quality Nested Sampling run (red) and a Metropolis-Hastings run (yellow) which uses a full proposal covariance.

at the expense of computing time. Tab. 1 shows timing and summary statistic results of running MultiNest chains with the DES likelihood using a variety of different choices for the sampler’s hyperparameters. We briefly describe these MultiNest hyperparameters, for more details see Feroz et al. (2009); Feroz et al. (2019).

The efficiency of is thus a rough estimate of the acceptance rate, the probability that a point sampled from the expanded ellipsoid will have a higher likelihood than the point needing replacement. However the algorithm’s acceptance scales better than this due to the ellipsoid hitting the prior boundaries in some of the parameter directions, as indicated by the fact that the BMD is less than the number of sampled parameters.

7 Reported uncertainties are via bootstrap resampling as computed by the Anesthetic software package Handley (2019).
PolyChord getsmorereliableevidenceestimates,motivatingusto
in Fig.5. Comparisons to this Gaussian toy model also show that
posterior distribution, which has a known true evidence, as shown
the best
a lack of convergence in summary statistics and disagreement with
systematically wrong. Even for efficiencies as low as
is too high, all the summary statistics calculated in this work are
intheresultsshowninTab.1,Fig.3,andFig.4.Whentheefficiency
confidence level of the best
INS evidence estimates in orange, and the grey band shows the 68%
Nest
and therefore gets narrower contours.

Figure 3. Marginalised one- and two-dimensional posterior distributions for
two extreme values of the efficiency on MultiNest. In red, a low value,
which is therefore more likely to have fully sampled the tails of the distribu-
tion, and in the yellow dotted contours, a high value. We can see how the
high efficiency does not fully sample the tails of the posterior distributions,
and therefore gets narrower contours.

Figure 4. MultiNest calculations of the evidence for different values of the
efficiency. The MultiNest values are plotted as red points, the Multi-
Nest INS evidence estimates in orange, and the grey band shows the 68%
confidence level of the best PolyChord estimate.

in the results shown in Tab. 1, Fig. 3, and Fig. 4. When the efficiency
is too high, all the summary statistics calculated in this work are
systematically wrong. Even for efficiencies as low as $10^{-3}$, we find
a lack of convergence in summary statistics and disagreement with
the best PolyChord values.

This bias can be reproduced using a 27-dimensional Gaussian
posterior distribution, which has a known true evidence, as shown
in Fig. 5. Comparisons to this Gaussian toy model also show that
PolyChord gets more reliable evidence estimates, motivating us to
adopt the best PolyChord run on the DES likelihood as a benchmark
‘correct value’.

We also see in Tab. 1 that there is an approximately power-law re-
lationship between runtime and efficiency. Therefore, it can become ex-
tremely computationally expensive to achieve a low enough value of
efficiency to obtain unbiased evidence estimates with MultiNest.
The importance of the efficiency hyperparameter for MultiNest
presents another challenge in that there is no principled way of
knowing what value of the efficiency should be used, or if the value
used was low enough, without running the algorithm multiple times.

Note that biases from high efficiencies have a less severe im-
 pact on marginalized posteriors than on estimates of the Bayesian
evidence. We can see this in Fig. 3. While higher efficiency does
cause the sampler to miss the tails of the distribution, even for very
high values those missing tails are unlikely to significantly affect
interpretation of the contours. Thus, if we are only interested in the
posterior distributions, we do not need to use efficiencies as low as
would be needed if we wanted to compute the Bayesian evidence.

- Tolerance: the stopping criterion. Both MultiNest and Poly-
Chord can estimate how much the existing live points will contribute
to the estimate of the evidence. When that contribution is smaller
than the chosen value of the tolerance, the algorithm terminates.
One can check whether the tolerance is low enough by plotting the
progression of the weights of the chain, as shown in Fig. 6. If the
tolerance is low enough, this plot will show a peak that reaches
unity, and will then decay back toward zero. A spike at the end
shows that the contribution to the evidence from the final set of live
points is too high, and the tolerance should be decreased.

Tab. 1 shows that tolerance does not have a significant impact
on either run-time nor on summary statistics. Because of this, and
because a chain initially run with higher tolerance can be resumed
to reach a lower tolerance, the choice of this parameter is not con-
sidered a challenge: we simply recommend a tolerance that ensures
that weights look similar to those on the right panel of Fig. 6.

- OpenMP threads: MultiNest in CosmoSIS uses a double paral-
lelization scheme: The Boltzmann solver CAMB (Lewis et al. 2000;
Howlett et al. 2012) is parallelized using OpenMP, and the Multi-
Nest sampling algorithm uses MPI parallelization. We tested two
settings, both using the same number of nodes, but changing the
number of cores used on each type of parallelization. We find that
not using the OpenMP parallelization greatly improves the sampling
speed. We expected this, as MultiNest will be faster when all cores
are used by MPI parallelization, up to the number of live points. As
expected, changing this setting does not affect the results in any way
apart from the run time.

- Constant Efficiency: MultiNest can use a different sampling
method, called ‘constant efficiency’ mode. In this setting, we aban-
don the strategy of increasing the volume of the ellipse by a factor of
1/efficiency. Instead, the increase in the size of the ellipses changes at
every step to match the input ’constant efficiency’ value in the sampling
efficiency (i.e. the ratio of points accepted to points sampled). F13 describe how:

"Despite the increased chances of the fitted ellipsoids encroach-
ing within the constrained likelihood volume (i.e. missing regions
of parameter space for which $\mathcal{L} > L_0$), past experience has shown
(e.g. F08) this constant efficiency mode may nevertheless produce
reasonably accurate posterior distributions for parameter estima-
tion purposes."

Our results agree with these statements in F13, with some caveats.
Indeed, for efficiencies set to values of 0.3 and 0.1, constant effi-
ciency mode produces significantly quicker runtimes and worse
Figure 5. MultiNest and PolyChord estimations of the evidence for different values of the efficiency and $n_{\text{repeats}}$ parameters, for a Gaussian posterior distribution with known truth (dashed line). In both cases, we use $n_{\text{live}} = 250$ and $\text{tolerance} = 0.1$. For each setting, we show 10 different sampling runs, which we displace along the x axis for visualization purposes. The figure shows how distribution with known truth (dashed line). In both cases, we use a toy model of Fig. 5, in which the convergence to the ‘truth’, this is believed by results from the Gaussian settings. Fig. 4 shows this graphically, with the INS estimates of the evidence in orange. They are significantly and consistently lower than the best estimate from PolyChord. While this might suggest convergence to the ‘truth’, this is belied by results from the Gaussian model of Fig. 5, in which the MultiNest INS evidence estimates are also systematically biased low. Our results thus appear to contradict the findings of Fré, which showed that in some toy models INS was more accurate than the baseline evidence estimate of MultiNest. Note that in addition to being lower than the truth, the INS evidence reported also significantly underestimates its sampling error, i.e., the uncertainty caused by imperfect sampling.

4.3 PolyChord

Like MultiNest, PolyChord has a number of hyperparameters which can be adjusted to balance running time and the accuracy of estimates for posterior distributions and summary statistics. The result of varying them is shown in Tab. 2.

- $n_{\text{live}}$, the number of live points. As with MultiNest, more live points leads to an increase in the accuracy of the posterior distribution, and a decrease in the error estimate for the evidence. Also, as was the case for MultiNest, PolyChord run-times scale linearly with the number of live points.
- $\text{tolerance}$, the stopping criterion. It is defined in the same way for Sec. 4.2, and the same conclusions apply: a lower tolerance does not have a significant impact on either runtime nor summary statistic accuracy. In fact, the tolerance seems to have even less of an impact on runtime for PolyChord than for MultiNest. As before, we recommend using the weight-vs-step-number convergence diagnostic illustrated in the right panel of Fig. 6 to select a reasonable tolerance for a chain, and note that a PolyChord chain can be resumed to reach a lower tolerance.
- $n_{\text{repeats}}$, the number of repeats. This hyperparameter is specific to PolyChord’s slice-sampling algorithm described in Sec. 2.4. Recall that at every step, PolyChord repeats the process of creating a slice through parameter space in a random direction, in which it finds a new potential live point. The value of $n_{\text{repeats}}$ dictates how many times this process is repeated for each sample selection. If this number is too low, the new live point will be correlated with the previous sample in the chain. Such correlations between live points could bias the posterior distribution and summary statistics. In this sense, a higher value of $n_{\text{repeats}}$ is somewhat akin to increasing the degree of ‘thinning’ of a standard MCMC chain, with the result that more likelihood evaluations are performed but then discarded, in the interest of reducing systematic uncertainty.

The official PolyChord paper (Handley et al. 2015b) recommends using at least $n_{\text{repeats}} \sim 2D$, where $D$ is the number of dimensions being sampled. In this work, we tested values that are approximately $\{0.5, 1, 2, 4\}$ times the number of dimensions. Fig. 7 shows the corresponding values of the summary statistics. We see that a value $n_{\text{repeats}} = 15$ obtains biased estimates of the evi-
4.4 Fast-likelihood tests of sampler variance

While the studies above give us an indication of how changing the values of PolyChord and MultiNest hyperparameters affect runtime and the accuracy of summary statistic estimates, they do not tell us much about noise in those relations due to the particular realization of random points sampled in a given chain run. In order to assess this sampler variance, we run a large number of independent chains, which long runtimes make infeasible with the full DES likelihood studied above. Thus, to more robustly assess convergence properties and characterize how sampler variance changes across settings, we use the approximate fast likelihood to generate multiple chain realizations at each set of sampler hyperparameters.

- **OMP threads.** As with MultiNest, we obtain the best results when we use all our cores for MPI parallelization, up to the number of cores matching the number of live points.

| $n_{\text{live}}$ | Tol | $n_{\text{repeats}}$ | OMP | Time (hrs) | Acceptance | L Evals | $\log Z$ | $D_{R,L}$ | BMD |
|------------------|-----|----------------------|-----|-----------|------------|---------|---------|---------|------|
| 50               | 0.1 | 60                   | 1   | 21.3      | 0.003      | 473705  | $-282.22 \pm 0.63$ | 22.26 $\pm 0.64$ | 12.1 $\pm 1.3$ |
| 250              | 0.3 | 60                   | 1   | 51.7      | 0.006      | 1171509 | $-282.04 \pm 0.29$ | 21.85 $\pm 0.27$ | 14.3 $\pm 0.7$  |
| 250              | 0.1 | 15                   | 1   | 11.9      | 0.022      | 342878  | $-281.47 \pm 0.32$ | 21.51 $\pm 0.30$ | 14.3 $\pm 0.7$  |
| 250              | 0.1 | 30                   | 1   | 23.7      | 0.011      | 675895  | $-282.64 \pm 0.29$ | 22.35 $\pm 0.27$ | 15.6 $\pm 0.7$  |
| 250              | 0.1 | 60                   | 1   | 46.2      | 0.006      | 1319862 | $-282.91 \pm 0.30$ | 22.34 $\pm 0.26$ | 15.2 $\pm 0.7$  |
| 250              | 0.1 | 60                   | 4   | 75.5      | 0.007      | 1016058 | $-282.48 \pm 0.29$ | 22.26 $\pm 0.29$ | 14.3 $\pm 0.7$  |
| 250              | 0.1 | 120                  | 1   | 87.4      | 0.003      | 2597251 | $-282.87 \pm 0.30$ | 22.30 $\pm 0.32$ | 14.9 $\pm 0.8$  |
| 250              | 0.03| 60                   | 1   | 60.9      | 0.006      | 1379582 | $-282.46 \pm 0.30$ | 22.21 $\pm 0.30$ | 14.4 $\pm 0.7$  |
| 250              | 0.01| 60                   | 1   | 62.4      | 0.006      | 1504234 | $-282.72 \pm 0.30$ | 22.72 $\pm 0.34$ | 13.5 $\pm 0.6$  |
| 250              | 0.001| 60                | 1   | 68.3      | 0.005     | 167076  | $-282.09 \pm 0.30$ | 22.12 $\pm 0.29$ | 14.2 $\pm 0.6$  |
| 675              | 0.1 | 15                   | 1   | 22.5      | 0.020     | 733506  | $-281.54 \pm 0.18$ | 21.38 $\pm 0.18$ | 14.1 $\pm 0.4$  |
| 675              | 0.1 | 30                   | 1   | 47.5      | 0.014     | 1458873 | $-282.52 \pm 0.19$ | 22.32 $\pm 0.19$ | 14.6 $\pm 0.4$  |
| 675              | 0.1 | 60                   | 1   | 117.9     | 0.007     | 2863702 | $-282.09 \pm 0.19$ | 21.95 $\pm 0.17$ | 14.4 $\pm 0.5$  |
| 675              | 0.01| 60                   | 1   | 131.2     | 0.007     | 3289309 | $-282.14 \pm 0.18$ | 21.79 $\pm 0.17$ | 14.5 $\pm 0.4$  |
| 675              | 0.1 | 120                  | 1   | 194.4     | 0.003     | 5795180 | $-282.34 \pm 0.18$ | 22.32 $\pm 0.17$ | 14.3 $\pm 0.4$  |
As we increase with the sampler variance uncertainty reported from each evidence, the sample variance in evidence estimates between different evidences differs significantly between different evidence estimators. In contrast, the reported statistical uncertainty in MultiNest evidences is much greater than the observed scatter across chain realizations.

The uncertainty in log Z given by PolyChord is more solidly grounded than that of MultiNest, having been derived analytically by Keeton (2011), whereas the MultiNest evidence estimates use the relative entropy and are based on information theoretic arguments. Our numerical results affirm the greater reliability of evidence errors from PolyChord.

Despite MultiNest overestimating the statistical uncertainty in log Z, the reported evidences are still inconsistent across hyperparameter settings, due to even greater systematic shifts as n_live is increased. However, none of the MultiNest settings tested resulted in evidence values approaching the stable PolyChord estimates.

We can also use this ensemble of chains to estimate and limit the contribution of sampler bias to the systematic error budget of the DES Y3 analysis. The DES Y3 analysis requires that unmodeled systematic shifts the maximum posterior point of key cosmological parameters by no more than 0.3σ in the 2D plane of Ω_0 and S_8 (c.f. Krause et al. 2021). Here we adopt a somewhat simplified but nonetheless strict criterion that the typical variation of parameter means across chain realizations is far below their statistical uncertainty. We thus require

\[ \sigma_{\theta} = \frac{\sigma_{(\theta|\mathcal{D})}}{(\theta_0 - \theta_c)} c, \]  

(17)

where the left-hand side is the standard deviation of the parameter mean across chain realizations and the right-hand side is a threshold, set equal to a fraction of the average of the standard deviations of the parameter computed from the individual chains. Note that this requirement is closely related to requiring the Gelman–Rubin statistic defined in Sec. 2.2 to be below a given threshold.

We are primarily interested in shifts on Ω_0 and S_8, and so require that any recommended sampler settings satisfy Eq. (17) for those parameters. Fig. 11 confirms this requirement is fulfilled for n_live > 200 with the fiducial values of the other hyperparameters.

5 CONCLUSIONS

In this paper we have studied the performance of two commonly-used tools used to sample posteriors for cosmological analysis, MultiNest and PolyChord, as a function of their hyperparameter settings. Our analysis had two parts: testing multiple sampler settings on the DES Y1 3x2pt analysis to calibrate the time needed to get unbiased posterior distributions in the Y3 analysis, and also using a faster approximate version of the likelihood to characterize the amount of sampler variance and further validate those findings.

We found that these Nested Sampling algorithms require careful tuning of their hyperparameters, especially n_live and MultiNest’s ellipsoidal sampling efficiency. Particularly for MultiNest, the wrong settings can lead to a poor sampling of the tails of the posterior distribution, and to a biased evidence estimation. Furthermore, the superior speed of the MultiNest algorithm compared...
Figure 8. Left: 1D marginalized mean and 68% credible intervals of $\Omega_m$ for both MultiNest (red) and PolyChord (blue) run using the fast likelihood at different values of $n_{\text{live}}$ ((100, 250, 675)), while other hyperparameters are held constant at the default values listed in Sec. 4.4. 20 chains are run at each setting of $n_{\text{live}}$, corresponding to the clusters of jittered points. The mean and standard error of chains at each setting are indicated by stars at the center of each cluster. Horizontal lines correspond to the average mean and 1σ credible intervals of three high quality PolyChord runs ($n_{\text{live}}=1000, n_{\text{repeats}}=120$, tolerance=10^{-3}). There is good agreement between PolyChord and MultiNest on the mean and small discrepancies between the credible intervals. MultiNest credible intervals are consistently smaller than those reported by PolyChord. Fig. 9 shows this in greater detail for $S_8$. Right: Estimates of the Bayesian evidence (and its sampler-reported uncertainty) for the same chains as the left-hand plot. The shaded band shows 1σ uncertainty on the mean evidence of the three high quality PolyChord chains. The PolyChord values are consistent at all settings, including at the lowest settings, with each individual run consistent with the high-resolution ‘truth’ within its reported uncertainty. In contrast, MultiNest evidence estimates display a systematic bias that is greater for small $n_{\text{live}}$, and the reported uncertainty for individual chains is insufficient to make runs consistent across different values of $n_{\text{live}}$. The reported uncertainties in log Z for each individual chain (given by the error bars) is consistent with the sampling variance across chain means for PolyChord, but is greatly overestimated for MultiNest where the means across chains are much more tightly clustered. This is shown more directly in Fig. 10.

Figure 9. Histogram of the half-width of 68% credible intervals for $S_8$ for many chains using the fast likelihood for both PolyChord (top) and MultiNest (bottom). MultiNest systematically reports smaller credible intervals than PolyChord for the range of settings tested, here shown with colors indicating different numbers of live points. Red lines indicate the credible intervals for the three high quality PolyChord chains.

Figure 10. Histogram of reported log Z for many PolyChord (top) and MultiNest (bottom) chains run with different numbers of live points. Solid curves are Gaussian fits to the distribution in reported log Z across different chain realizations. Dashed Gaussian curves show the expected distribution based on the mean log Z and mean claimed uncertainty across chains. The relatively close agreement between solid and dashed curves indicates that the reported uncertainty in PolyChord chains is fairly representative of the true sampling error. MultiNest reports uncertainties considerably larger than the observed sampling variance.
with PolyChord’s slice sampling method is not present when sufficiently accurate sampling hyperparameters are used. PolyChord produces unbiased evidence estimates with reasonable settings, as well as contours that are in good agreement with those we find using Metropolis–Hastings. Therefore, our findings lead us to prefer PolyChord over MultiNest.

The studies described in this paper were used to guide recommendations for sampler settings used for the DES Y3 cosmology analysis (Krause et al. 2021) as well as some Y1 follow-up papers (Chen et al. 2021; Muir et al. 2021). These recommendations are summarized in Table 3 for three use-cases. We recommend that MultiNest only be used for preliminary testing and pipeline debugging. While it is relatively fast, we found the (fairly standard) settings described in Case III of Table 3 to produce marginalized posterior widths underestimated by about 10% and unreliable evidences. For most pre-publication testing, we recommend using the fast PolyChord settings described in Case II. Those settings will produce unbiased posteriors and evidence values, though the resulting contours for marginalized posteriors will be somewhat noisy. Case I in Table 3 presents our recommendation for publication-quality results, with an increased number of live points extending the run-time but resulting in reduced noise in both posterior contours and evidence estimates.

While this study was performed specifically for DES Y3, our findings should be useful as a guide for cosmological analyses of similar dimensionality. Though our results were broadly consistent across three different likelihoods: the full DES Y1 likelihood, a fast approximate DES Y1 likelihood, and a 27D Gaussian toy model, the exact settings of Tab. 3 will likely need to be adjusted for problems where the number of dimensions or the shape of the posterior distribution change significantly. We found that good posterior and evidence estimates can be obtained with relatively low settings of \( n_{\text{repeats}} \approx D \) with PolyChord, but that MultiNest evidences were systematically biased except at extreme values of efficiency, and

**Table 3.** Recommended sampler settings based on this work, used for the DES Y3 cosmology analysis. Approximate wall-time estimates are given for a wCDM DES Y1 3x2 chain run on 128 cores.

| Case I: Publication quality (one-time runs) | | |
| Sampler | PolyChord | | |
| \( n_{\text{live}} \) | 500 | | |
| Tol | 0.01 | | |
| \( n_{\text{repeats}} \) | 60 | | |
| fast\_fraction | 0.01 | | |
| Time to run: | ~ 4 days | | |

| Case II: Testing (noisy contours) | | |
| Sampler | PolyChord | | |
| \( n_{\text{live}} \) | 250 | | |
| Efficiency | 0.3 | | |
| Tol | 0.1 | | |
| constant\_efficiency | F | | |
| Time to run: | ~ 1 day | | |

| Case III: Very preliminary results only (unreliable evidences, \( \Omega_m \) & \( \sigma_8 \) posterior widths underestimated by ~ 10%) | | |
| Sampler | MultiNest | | |
| \( n_{\text{live}} \) | 250 | | |
| Efficiency | 0.3 | | |
| Tol | 0.1 | | |
| constant\_efficiency | F | | |
| Time to run: | ~ 6 hours | | |

**Figure 11.** Standard deviation of parameter means across chains relative to the average within-chain parameter standard deviation. We require that the contribution to mean parameter shifts from sampler variance is small for settings used to run chains testing the impact of unmodeled systematics. The PolyChord publication settings can be found in Tab. 3.

**DATA AVAILABILITY STATEMENT**

The data underlying this article are available in the Dark Energy Survey Data Management platform, at https://des.ncsa.illinois.edu

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et al. 2001), NumPy (Oliphant 2006), Matplotlib (Hunter 2007), CAMB (Lewis et al. 2000; Howlett et al. 2012), GetDist (Lewis 2019), MultiNest (Feroz & Hobson 2008; Feroz et al. 2009; Feroz et al. 2019), Polychord (Handley et al. 2015a,b), anesthetic (Handley 2019), and CosmoSIS (Zuntz et al. 2015). Elements of the DES modeling pipeline additionally use CosmLike (Krause & Eifler 2017), HaloFF (Takahashi et al. 2012; Bird et al. 2012), FastPT (McEwen et al. 2016), and NiCaea (Kilbinger et al. 2009).

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In this section, we briefly compare two nested samplers used in this paper, MultiNest and PolyChord with two other available sampling codes: emcee and Zeus. As already noted, emcee showed very poor convergence with the full DES likelihood and Zeus was not integrated into the CosmoSIS framework at the time of testing, a requirement for its use in the fiducial DES analysis. Furthermore, neither of these samplers provide an estimate of the Bayesian Evidence, a key summary statistic of interest for the DES Y3 analysis. We therefore use the toy model described in Sec. 4.2, a 27-dimensional Gaussian likelihood distribution, and compare the stability of posterior estimates.

For each sampler, we run ten chains with the same settings, and then plot the standard deviation of each parameter mean across chains divided by the average parameter standard deviation within each chain. Defining similar settings across different samplers can be challenging; we use the Case II settings showed in Tab. 3 for PolyChord, and tune the settings in the other samplers to obtain similar numbers of likelihood evaluations, and therefore expected to take similar amounts of time in realistic cases, where likelihood evaluations are the slowest part of the calculation. Likelihood evaluations and acceptance are averaged over each of the ten chains. The last column is averaged over each of the 27 parameters.

### Table A1. Comparison between PolyChord, emcee and Zeus

| Sampler   | (LEvals) | (Acceptance) | σc [σp]/(σp)ec |
|-----------|----------|--------------|-----------------|
| PolyChord | 1749508  | 0.0074       | 0.06            |
| emcee     | 1500000  | 0.26         | 0.06            |
| Zeus      | 1666525  | 0.18         | 0.01            |

This shows how poorly the required efficiency scales with an increase in dimensionality. In the case of DES, the required efficiency is $e \cong 10^{-5}$, which is consistent with the findings of Fig. 4, showing that an efficiency of $10^{-3}$ is not enough to reach the correct evidence values.

As a side note, we can also estimate the acceptance of MultiNest as

$$acc = eff^{BMD/N_d},$$

where BMD is the Bayesian Model Dimensionality.

### APPENDIX B: EFFICIENCY RULE OF THUMB

From the results of this paper, as well as our understanding of ellipsoidal nested sampling, we can set up an approximately guideline to correctly choose an efficiency that will not lead to biased sampling.

We estimate the enlargement of the ellipse in each direction from the efficiency and the number of dimensions $N_d$, as

$$enlargement = eff^{-1/N_d}$$

From Mukherjee et al. (2006a) and our work, we estimate that we need an enlargement of approximately $\geq 1.5$. Therefore, the required efficiency is approximately

$$eff \sim 1.5^{-N_d}.$$