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A NESTED SAMPLING ALGORITHM FOR COSMOLOGICAL MODEL SELECTION

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ABSTRACT

The abundance of new cosmological data becoming available means that a wider range of cosmological models are testable than ever before. However, an important distinction must be made between *parameter fitting* and *model selection*. While parameter fitting simply determines how well a model fits the data, model selection statistics, such as the Bayesian Evidence, are now necessary to choose between these different models, and in particular to assess the need for new parameters. We implement a new evidence algorithm known as *nested sampling*, which combines accuracy, generality of application and computational feasibility, and apply it to some cosmological datasets and models. We find that a five-parameter model with Harrison–Zel’dovich initial spectrum is currently preferred.

Subject headings: cosmology: theory

1. INTRODUCTION

The higher-level inference problem of allowing the data to decide the set of parameters to be used in fitting is known as *model selection*. In the Bayesian framework, the key model selection statistic is the *Bayesian evidence* (Jeffreys 1961; MacKay 2003), being the average likelihood of a model over its prior parameter space. The evidence can be used to assign probabilities to models and to robustly establish whether the data require additional parameters.

While the use of Bayesian methods is common practice in cosmological parameter estimation, its natural extension to model selection has lagged behind. Work in this area has been hampered by difficulties in calculating the evidence to high enough accuracy to distinguish between the models of interest. The issue of model selection has been raised in some recent papers (Marshall, Hobson & Slosar 2003; Niarchou, Jaffe & Pogosian 2004; Saini, Weller & Bridle 2004; Bassett, Corasaniti & Kunz 2004), and information criterion based approximate methods introduced in Liddle (2004). Semi-analytic approximations such as the Laplace approximation, which works well only for gaussian likelihoods, and the Savage–Dickey density ratio which works for more general likelihood functions but requires the models being compared to be nested, are methods that were recently exploited by Trotta (2005). A more general and accurate numerical method is thermodynamic integration, but Beltrán et al. (2005) found that in realistic applications around 10^7 likelihood evaluations were needed per model to obtain good accuracy, making it a supercomputer-class problem in cosmology where likelihood evaluations are computationally costly.

In this paper we present a new algorithm which, for the first time, combines accuracy, general applicability, and computational feasibility. It is based on the method of *nested sampling*, proposed by Skilling (2004), in which the multi-dimensional integral of the likelihood of the data over parameter space is performed using Monte Carlo sampling, working through the prior volume to the regions of high likelihood.

2. BAYESIAN INFERENCE

Using Bayes’ theorem, the probability that a model (hypothesis: H) is true in light of observed data (D) is given by

$$P(H|D) = \frac{P(D|H)P(H)}{P(D)}. \quad (1)$$

It shows how our prior knowledge $P(H)$ is modified in the presence of data.

The posterior probability of the parameters (θ) of a model in light of data is given by

$$P(\theta|D, H) = \frac{P(D|\theta, H)P(\theta|H)}{P(D|H)}, \quad (2)$$

where $P(D|\theta, H)$ is the likelihood of the data given the model and its parameters, and $P(\theta|H)$ is the prior on the parameters. This is the relevant quantity for parameter estimation within a model, for which the denominator $P(D|H)$ is of no consequence. $P(D|H)$ is however the *evidence* for the model H , the key quantity of interest for the purpose of model selection (Jeffreys 1961; MacKay 2003; Gregory 2005). Normalizing the posterior $P(\theta|D, H)$ marginalized over θ to unity, it is given by

$$E = P(D|H) = \int d\theta P(D|\theta, H)P(\theta|H), \quad (3)$$

the prior also being normalized to unity.

The evidence for a given model is thus the normalizing constant that sets the area under the posterior $P(\theta|D, H)$ to unity. In the now-standard Markov Chain Monte Carlo method for tracing the posterior (Gilks et al. 1996; Lewis & Bridle 2002), the posterior is reflected in the binned number density of accumulated samples. The evidence found in this way would not generally be accurate as the algorithm would sample the peaks of the probability distribution well, but would under-sample the tails which might occupy a large volume of the prior.

When comparing two different models using Bayes Theorem, the ratio of posterior probabilities of the two models would be the ratio of their evidences (called the Bayes Factor) multiplied by the ratio of any prior probabilities that we may wish to assign to these models (Eq. 1). It can be seen from Eq. (3) that while more

complex models will generally result in better fits to the data, the evidence, being proportional to the volume occupied by the posterior relative to that occupied by the prior, automatically implements Occam’s razor. It favours simpler models with greater predictive power provided they give a good fit the data, quantifying the tension between model simplicity and the ability to fit to the data in the Bayesian sense. Jeffreys (1961) provides a useful guide to what constitutes a significant difference between two models: $1 < \Delta \ln E < 2.5$ is substantial, $2.5 < \Delta \ln E < 5$ is strong, and $\Delta \ln E > 5$ is decisive. For reference, a $\Delta \ln E$ of 2.5 corresponds to odds of about 1 in 13.

While for parameter fitting the priors become irrelevant once the data are good enough, for model selection some dependence on the prior ranges always remains however good the data. The dependence on prior parameter ranges is a part of Bayesian reasoning, and priors should be chosen to reflect our state of knowledge about the parameters before the data came along. The Bayesian evidence is unbiased, as opposed to approximations such as the information criteria.

Perhaps the most important application of model selection is in assessing the need for a new parameter, describing some new physical effect proposed to influence the data. Frequentist-style approaches are commonplace, where one accepts the parameter on the basis of a better fit, corresponding to an improvement in $\Delta(\ln L)$ by some chosen threshold (leading to phrases such as ‘two-sigma detection’). Such approaches are non-Bayesian: the evidence shows that the size of the threshold depends both on the properties of the dataset and on the priors, and in fact the more powerful the dataset the higher the threshold that must be set (Trotta 2005). Further, as the Bayesian evidence provides a rank-ordered list of models, the need to choose a threshold is avoided (though one must still decide how large a difference in evidence is needed for a robust conclusion).

The main purpose of this paper is to present an algorithm for evidence computation with widespread applications. However as a specific application we examine the need for extra parameters against the simplest viable cosmological model, a Λ CDM model with Harrison–Zel’dovich initial spectrum, whose five parameters are the baryon density $\Omega_b h^2$, cold dark matter density $\Omega_{\text{cdm}} h^2$, the Hubble parameter $H_0 = 100 h \text{kms}^{-1} \text{Mpc}^{-1}$ (or the ratio Θ of the approximate sound horizon at decoupling to its angular diameter distance), the optical depth τ , and the amplitude A_s of primordial perturbations. We study the case for two additional parameters, the scalar spectral index and the dark energy equation of state (assumed constant).

3. NESTED SAMPLING

3.1. Basic Method

Nested sampling (Skilling 2004) is a scheme to trace the variation of the likelihood function with prior mass, with the effects of topology, dimensionality and everything else implicitly built into it. It breaks up the prior volume into a large number of ‘equal mass’ points and orders them by likelihood. Rewriting Eq. (3) in the notation of Skilling (2004), with X as the fraction of total prior mass such that $dX = P(\theta|H)d\theta$ and the likelihood

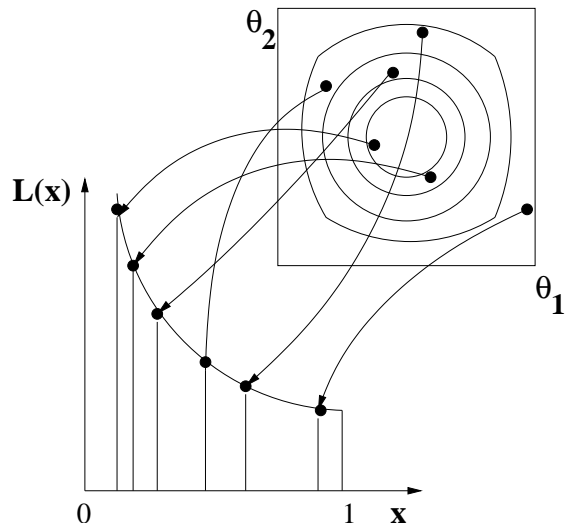


FIG. 1.— The nested sampling algorithm integrates the likelihood over the prior volume by peeling away thin iso-surfaces of equal likelihood.

$P(D|\theta, H) = L(X)$, the equation for the evidence becomes

$$E = \int_0^1 L dX. \quad (4)$$

Thus the problem of calculating the evidence has become a one-dimensional integral, in which the integrand is positive and decreasing. Suppose we can evaluate the likelihood as $L_j = L(X_j)$, where the X_j are a sequence of decreasing values, such that

$$0 < X_m < \dots < X_2 < X_1 < 1, \quad (5)$$

as shown schematically in Figure 1. Then the evidence can be estimated by any numerical method, for example the trapezoid rule

$$E = \sum_{j=1}^m E_j, \quad E_j = \frac{L_j}{2}(X_{j-1} - X_{j+1}). \quad (6)$$

The nested sampling algorithm achieves the above summation in the following way:

1. Sample N points randomly from within the prior, and evaluate their likelihoods. Initially we will have the full prior range available, i.e. $(0, X_0 = 1)$.
2. Select the point with the lowest likelihood (L_j). The prior volume corresponding to this point, X_j , can be estimated probabilistically. The average volume decrease is given as $X_j/X_{j-1} = t$ where t is the expectation value of the largest of N random numbers from uniform(0,1), which is $N/(N+1)$.
3. Increment the evidence by $E_j = L_j(X_{j-1} - X_{j+1})/2$.
4. Discard the lowest likelihood point and replace it with a new point, which is uniformly distributed within the remaining prior volume $(0, X_j)$. The new point must satisfy the hard constraint on likelihood of $L > L_j$.
5. Repeat steps 2–4, until the evidence has been estimated to some desired accuracy.

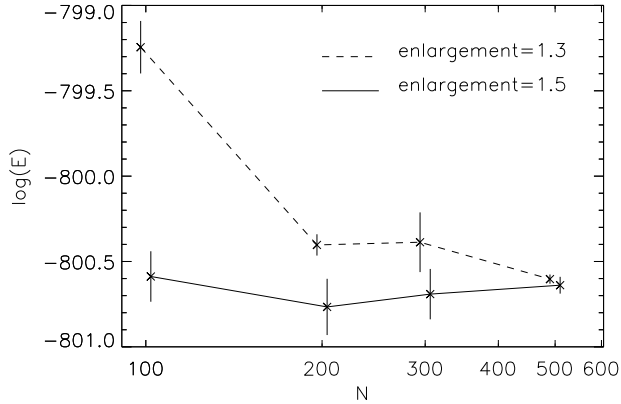


FIG. 2.— Evidence against the number of sample points N for a 6D Gaussian likelihood function as a test case. The horizontal lines show the actual analytical value. Points are displaced slightly horizontally for visual clarity.

The method thus works its way up the likelihood surface, through nested surfaces of equal likelihood. After j steps the prior mass remaining shrinks to $X_j \sim (N/(N+1))^j$. The process is terminated when some stopping criterion is satisfied, and a final amount of $\langle L \rangle \times X_j$ due to the $N - 1$ remaining sample points is added to the thus far accumulated evidence.

Thus a multi-dimensional integral is performed using Monte Carlo sampling, imposing a hard constraint in likelihood on samples that are uniformly distributed in the prior, implying a regularized probabilistic progression through the prior volume. Besides implementing and testing this scheme in the cosmological context, our main contribution lies in developing a general strategy to sample new points efficiently.

3.2. Details

The prior space to sample from reduces by a constant factor of $N/(N+1)$ every time the lowest likelihood point is discarded. The most challenging task in implementing the algorithm is to sample uniformly from the remaining prior volume, without creating too large an overhead in likelihood evaluations even when the remaining volume of prior space may be very small. The new point must be uncorrelated to the existing points, but we can still use the set of existing points as a guide. We find the covariance of the live points, rotate our coordinates to the principal axes, and create an ellipsoid which just touches the maximum coordinate values of the existing points. To allow for the iso-likelihood contours not being exactly elliptical, these limits are expanded by a constant enlargement factor, aiming to include the full volume with likelihood exceeding the current limit (if this is not done new points will be biased towards the centre, thus overestimating the evidence). New points are then selected uniformly within the expanded ellipse until one has a likelihood exceeding the old minimum, which then replaces the discarded lowest-likelihood point.

The two algorithm parameters to be chosen are the number of points N and the enlargement factor of the ellipsoid. Figure 2 shows evidence versus N , for a flat Harrison–Zel’dovich model with a cosmological constant. The mean evidence values and standard deviations obtained from 4 repetitions are shown. These are shown

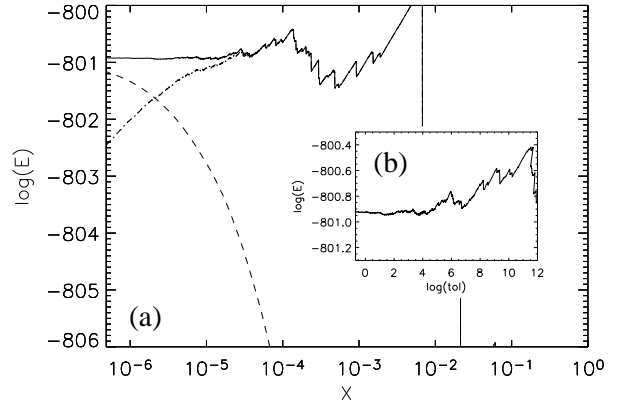


FIG. 3.— (a) The accumulated evidence (dashed curve), the evidence contributed by the remaining points at each stage (dot-dashed curve), and their sum (solid curve), shown against prior volume remaining for a 6D Gaussian likelihood function. (b) A later part of the solid curve shown against the $\log(\text{tol})$ (see text).

for two different values of the enlargement factor. When the enlargement factor is large enough (here 1.5) the evidence obtained with 100 sample points agrees with that obtained with 500, while when the enlargement factor is not large enough, the evidences obtained with small N are systematically biased high. Similar tests done on multi-dimensional Gaussian likelihood functions, for which the expected evidence can be found analytically, indicated the same. Based on such tests we choose to work with N of 300, and enlargement factors of 1.5 for the 5D model (this corresponds to a 50% increase in the range of each parameter), 1.7 for 6D and 1.8 for 7D models. These choices are conservative (smaller values would reduce the computing time), and were made in order to ensure evidences that are accurate and free of systematics. In our cosmological applications we have also computed evidences with larger enlargement factors and found that they remained unchanged. The typical acceptance rate in finding a new point during the course of the algorithm was found to be roughly constant at $\sim 20 - 25\%$ for an enlargement factor of 1.5, and lower for larger enlargement factors, after an initial period of almost 100% acceptance, as expected.

Figure 3a shows the accumulated evidence, the evidence contributed by the remaining points at each stage, and their sum, against prior volume remaining, again for a flat Harrison–Zel’dovich model with a cosmological constant. The X at which the calculation can be terminated will depend on the details of the problem (e.g. dimensionality, priors etc.). We define a parameter tol as the maximum possible fractional amount that the remaining points could increase the evidence by: $\text{tol} \equiv (L_{\max})_j X_j / E$ where L_{\max} is the maximum likelihood of the current set of sample points. Figure 3b zooms into a late part of the solid curve, now plotting it against the value of the parameter tol . The calculation need only be carried out until the standard error on the mean evidence, computed for a certain number of repetitions, drops below the desired accuracy. An uncertainty in $\ln E$ of 0.1 would be the highest conceivable accuracy one might wish, and with 8 repetitions this happens when $\ln(\text{tol}) \sim$ a few. This takes us to quite small X , of order $10^{-6} - 10^{-7}$ in our actual cosmological simulations.

TABLE 1
PARAMETER RANGES AND EVIDENCES FOR VARIOUS COSMOLOGICAL MODELS. OTHER PARAMETER RANGES ARE GIVEN IN TEXT.

Model	Λ CDM+HZ	Λ CDM+ n_s	Λ CDM+ n_s (wide prior)	HZ+ w	$w + n_s$
n_s	1	0.8 – 1.2	0.6 – 1.4	1	0.8 – 1.2
w	-1	-1	-1	$-\frac{1}{3} - -1$	$-\frac{1}{3} - -1$
e.f	1.5	1.7	1.7	1.7	1.8
$N_{\text{like}} (\times 10^4)$	8.4	17.4	16.7	10.6	18.0
$\log E$	0.00 ± 0.08	-0.58 ± 0.09	-1.16 ± 0.08	-0.45 ± 0.08	-1.52 ± 0.08

4. RESULTS

We have calculated the evidences of four different cosmological models: 1) a flat, Harrison–Zel’dovich model with a cosmological constant (Λ CDM+HZ), 2) the same as 1, except allowing the tilt of the primordial perturbation spectrum n_s to vary (Λ CDM+ n_s), 3) the same as 1, except allowing the equation of state of the dark energy to take alternative values to $w = -1$ (w +HZ), and finally 4) allowing both n_s and w to vary ($w + n_s$). The prior ranges for the other parameters were fixed at $0.018 \leq \Omega_b h^2 \leq 0.032$, $0.04 \leq \Omega_{\text{cdm}} h^2 \leq 0.16$, $0.98 \leq \Theta \leq 1.1$, $0 \leq \tau \leq 0.5$, and $2.6 \leq \ln(A_s \times 10^{10}) \leq 4.2$.

The data sets we use are CMB TT and TE anisotropy power spectrum data from the WMAP experiment (Bennett et al. 2003; Spergel et al. 2003; Kogut et al. 2003), together with higher l CMB temperature power spectrum data from VSA (Dickinson et al. 2004), CBI (Pearson et al. 2003) and ACBAR (Kuo et al. 2004), matter power spectrum data from SDSS (Tegmark et al. 2004) and 2dFGRS (Percival et al. 2001), and supernovae apparent magnitude–redshift data from Riess et al. (2004).

Results are shown in Table 1. For the spectral tilt, evidences have been found for two different prior ranges, as an additional test of the method. For a prior range twice the size of the original in n_s the evidence is expected to change by $-\ln 2$ at most and that difference is recovered. The first 2 rows show the priors on the additional parameters of the model, or their constant values if they were fixed. The 3rd row shows the enlargement factor (e.f) we used for the model. The 4th row shows the total number of likelihood evaluations needed to compute the mean ln evidence to an accuracy ~ 0.1 , and the 5th row shows the mean $\ln E$ and the standard error in that mean computed from 8 repetitions of the calculation, normalized to the Λ CDM+HZ evidence.

The Λ CDM+HZ model has the highest evidence, and as such is the preferred fit to the data. Hence we do not find any indication of a need to introduce parameters be-

yond the base set of 5, in agreement with the conclusions of Liddle (2004) and Trotta (2005). However, the difference between the $\ln E$ of the higher-dimensional models and the base model is not large enough to significantly exclude any of those models at present.

5. CONCLUSIONS

We introduce the nested sampling algorithm for the computation of Bayesian evidences for cosmological model selection. We find that this new algorithm uniquely combines accuracy, general applicability and computational feasibility. It is able to attain an accuracy (standard error in the mean ln evidence) of 0.1 in $O(10^5)$ likelihood evaluations. It is therefore much more efficient than thermodynamic integration, which is the only other method that shares the general applicability of nested sampling. Nested sampling also leads to a good estimate of the posterior probability density of the parameters of the model for free, which we will discuss in a forthcoming paper. We also plan to make a public release of the code in the near future.

Using nested sampling we have computed the evidence for the simplest cosmological model, with a base set of 5 parameters, which provides a good fit to current cosmological data. We have computed the evidence of models with additional parameters — the scalar spectral tilt, a constant dark energy equation of state parameter, and both of these together. We find that current data offer no indication of a need to add extra parameters to the base model, which has the highest evidence amongst the models considered.

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