

# Introducing doubt in Bayesian model comparison

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There are things we know, things we know we don't know, and then there are things we don't know we don't know. In this paper we address the latter two issues in a Bayesian framework, introducing the notion of doubt to quantify the degree of (dis)belief in a model given observational data in the absence of explicit alternative models. We demonstrate how a properly calibrated doubt can lead to model discovery when the true model is unknown.

## I. INTRODUCTION

Given two or more competing models to describe observed data, Bayesian model comparison offers a way of determining the preferred model given the data and explicit assumptions about prior beliefs. The key feature of Bayesian model comparison is that it implements Occam's razor, by selecting the model that optimally balances quality-of-fit and high model predictivity. (See [1] for an introduction.) Given a set of known models, however, the Bayesian framework usually has little to say about the absolute quality-of-fit of the preferred model. This is because the underlying philosophy is that there is little virtue in rejecting a model if no better alternative is present.

In the frequentist approach, a popular (absolute) measure of the goodness-of-fit is given by the  $\chi^2$ -per-degree-of-freedom ( $\chi^2/\text{dof}$ ) rule-of-thumb, where  $\chi^2$  is (twice) the best-fit log-likelihood. For normally distributed data points,  $\chi^2/\text{dof}$  is distributed as a  $\chi^2$  distribution. Therefore, if the model is appropriate for the data, one expects that  $\chi^2/\text{dof} \approx 1$ . An unsatisfactory fit is signaled by  $\chi^2/\text{dof} \gg 1$ , while  $\chi^2/\text{dof} \ll 1$  usually implies overfitting, hence a model overspecification. Complementary to this, principle component analysis (PCA) can be used to determine the maximal number of parameters a given observational data set can reasonably constrain [2]. Diagonalizing the covariance matrix of the parameters and determining how many eigenvalues are below a given threshold gives an upper limit on the number of parameters that are well-constrained by observations, preventing the use of a too-general model. The Bayesian framework replaces this with the notion of model complexity, see [3].

In the Bayesian framework, the question of whether the preferred model describes the observations "well enough" can be phrased as follows: what is the degree of belief that there are no other "reason-

able" models that would better describe the observations? Historically, the need for fundamentally new physics has often been driven by a poor fit between data and existing models, at a point where an explicit alternative was not available. For example, the development of General Relativity was driven in part by the need to explain a single number – the anomalous perihelion precession rate of Mercury. The increasing complexity of data makes it harder to simply evaluate discrepancies between theory and experiment and decide on their significance. In light of the increasing usage of Bayesian statistical techniques, like Markov Chain Monte Carlo (MCMC) algorithms, it would be advantageous to develop a reliable measure of confidence in the best-fit model that can deal with today's large data sets and multi-dimensional parameter spaces. This is particularly true in the cosmological context, which faces unique difficulties – some observations are now so advanced as to be constrained by fundamental limitations on the quality of data (cosmic variance). Thus, cosmologists must take particular care to extract the maximum amount of information from available measurements.

Our confidence in the (absolute) adequacy of the best model can only be determined under general assumptions about any hypothetical better fitting model. In this paper, we propose a set of assumptions for such a model, define the notion of statistical doubt and illustrate its use by computing the doubt for a toy linear model. In a future work, we will apply this tool to evaluate the current concordance model of cosmology.

First, we give a short review of Bayesian model selection. We introduce the notion of doubt, then discuss a technique for the calibration of the level of false doubt and demonstrate the usefulness of doubt for model discovery in an application to a toy linear model. Finally, we present our conclusions.

## II. BAYESIAN MODEL SELECTION

In this section, we briefly review Bayesian model selection. For more details we refer the reader to [1]. From Bayes’ theorem, the posterior probability of model  $\mathcal{M}_j$  given the data  $d$ ,  $p(\mathcal{M}_j|d)$ , is related to the Bayesian evidence (or model likelihood)  $p(d|\mathcal{M}_j)$  by

$$p(\mathcal{M}_j|d) = \frac{p(d|\mathcal{M}_j)p(\mathcal{M}_j)}{p(d)}, \quad (1)$$

where  $p(\mathcal{M}_j)$  is the prior belief in model  $\mathcal{M}_j$ . Here and in the following, “model” denotes a choice of theory, with specification of its free parameters,  $\theta_j$ , and of their prior probability distribution,  $p(\theta_j|\mathcal{M}_j)$ . The specification of the prior might be somewhat ambiguous for models with continuous free parameters, especially when one is working with an effective parameterisation only loosely tied to the underlying physics. (For further discussion of these points, see [4] and, for a critical view, [5]). In Eq. (1),  $p(d) = \sum_i p(d|\mathcal{M}_i)p(\mathcal{M}_i)$  is a normalisation constant (where the sum runs over all available known models  $\mathcal{M}_i$ ,  $i = 1, \dots, N$ ) and

$$p(d|\mathcal{M}_j) = \int d\theta p(d|\theta_j, \mathcal{M}_j)p(\theta_j|\mathcal{M}_j) \quad (2)$$

is the Bayesian evidence, where  $p(d|\theta_j, \mathcal{M}_j)$  is the likelihood.

Given two competing models,  $\mathcal{M}_0$  and  $\mathcal{M}_1$ , the Bayes factor  $B_{01}$  is the ratio of the models’ evidences

$$B_{01} \equiv \frac{p(d|\mathcal{M}_0)}{p(d|\mathcal{M}_1)}, \quad (3)$$

where large values of  $B_{01}$  denote a preference for  $\mathcal{M}_0$ , and small values of  $B_{01}$  denote a preference for  $\mathcal{M}_1$ . The “Jeffreys’ scale” (Table I) gives an empirical prescription for translating the values of  $B_{01}$  into strengths of belief.

Given two or more models, specified in terms of their parameterisation and priors on the parame-

$ \ln B_{01} $	Odds	Strength of evidence
$< 1.0$	$\lesssim 3 : 1$	Inconclusive
$1.0$	$\sim 3 : 1$	Weak evidence
$2.5$	$\sim 12 : 1$	Moderate evidence
$5.0$	$\sim 150 : 1$	Strong evidence

TABLE I: Empirical scale for evaluating the strength of evidence when comparing two models,  $\mathcal{M}_0$  versus  $\mathcal{M}_1$  (so-called “Jeffreys’ scale”, here slightly modified following the prescriptions given in [1, 6]). The right-most column gives our convention for denoting the different levels of evidence above these thresholds.

ters, it is straightforward (although sometimes computationally challenging) to compute the Bayes factor. Depending on the problem at hand, semi-analytical [7, 8] and numerical [9, 10, 11] techniques are available. In the usual case where the prior of the models is taken to be non-committal (i.e.,  $p(\mathcal{M}_j) = 1/N$ ), the model with the largest Bayes factor ought to be preferred. Thus the computation of  $B_{01}$  allows to select one (or a few) promising model(s) from a set of known models. However, it contains no information about whether the selected model is actually a good explanation for the data. This information is contained in  $p(\mathcal{M}_j|d)$ . From Eq. (1), it is clear that a correct computation of  $p(\mathcal{M}_j|d)$  requires the denominator  $p(d)$  to be computed from a reasonably complete sum of models.

We now turn to the question of how to evaluate our absolute degree of belief in the adequacy of a set of known models.

## III. BAYESIAN DOUBT

### A. Introducing doubt

In light of the observations in the previous section, we seek to capitalise on the information in  $p(\mathcal{M}_j|d)$ . We introduce the concept of *doubt*  $\mathcal{D}$  to describe in a quantitative way our degree of (dis)belief in the ability of any known model in a list  $\mathcal{M}_i$  ( $i = 1, \dots, N$ ) to describe the data. We begin by expanding our space of models to include an as-yet unknown model  $\mathcal{X}$ , which represents the possibility that the collection of models presently under consideration is incomplete and that there might be a “better” (in a Bayesian sense) model that we have not yet identified. We then define the doubt  $\mathcal{D} = \mathcal{D}(\{\mathcal{M}_i\}|d)$  as the posterior probability of the unknown model,  $p(\mathcal{X}|d)$ , which from Bayes’ theorem is given by

$$\begin{aligned} \mathcal{D} \equiv p(\mathcal{X}|d) &= \frac{p(d|\mathcal{X})p(\mathcal{X})}{p(d)} \\ &= \frac{1}{1 + \sum_i \frac{p(d|\mathcal{M}_i)p(\mathcal{M}_i)}{p(d|\mathcal{X})p(\mathcal{X})}}, \end{aligned} \quad (4)$$

where the sum runs over the known models,  $i = 1, \dots, N$ . The prior for the unknown model is

$$p(\mathcal{X}) = 1 - \sum_{i=1}^N p(\mathcal{M}_i). \quad (5)$$

Given some openness about the possibility that our list of known models is incomplete, and given an estimate of the Bayesian evidence  $p(d|\mathcal{X})$  for  $\mathcal{X}$ , the doubt expresses the posterior probability that the list of models  $\mathcal{M}_i$  is missing a model that is a better description of the available data. If  $p(\mathcal{X}) > 0$ ,

then “sufficiently poor evidence” for the known models  $\mathcal{M}_i$  (i.e.,  $p(d|\mathcal{M}_i) \ll p(d|\mathcal{X})$ ) will instill enough doubt to question the appropriateness of  $\mathcal{M}_i$ . Obviously, assuming *a priori* that the known models exhaust the model space, i.e.  $p(\mathcal{X}) = 0$ , would leave no room for doubt:  $\mathcal{D} = 0$  independent of the evidence  $p(d|\mathcal{X})$ .

The crucial step in evaluating the doubt is estimating the evidence for the unknown model,  $p(d|\mathcal{X})$ . Clearly this quantity cannot be computed using Eq. (2), as this would require the unknown model to be fully specified in terms of its parameters and priors. If this was possible, then  $\mathcal{X}$  could be included in the list of  $\mathcal{M}_i$  and would not be unknown in the first place.

Fortunately, even without an explicitly specified mode, but given the data  $d$ , we can produce an informed guess as to what the evidence for a “good” model should be. If the evidences of the models on the table,  $\mathcal{M}_i$ , are poor compared to this value, then the Bayes factors in favour of the unknown model

$$B_{xi} \equiv \frac{p(d|\mathcal{X})}{p(d|\mathcal{M}_i)} \gg 1, \quad (6)$$

and as consequently (see Eq. (4)) the posterior probability of doubt will increase.

What we are suggesting is in fact a *calibration of the absolute value of the evidence*. Bayesian model comparison focuses on the Bayes factor, which indicates the change of our *relative* confidence in the models in light of the observed data. Since the Bayes factor is the ratio of the models’ evidences, the absolute value of the evidence itself is usually deemed irrelevant. (This is only actually strictly true for nested models, where the normalisation of the evidence drops out of the ratio.) A shortcoming of ignoring the absolute value of the evidence is that the model comparison will always return a preferred model, even in cases when all of the available models fit the data poorly. The notion of doubt is designed to remedy this obviously unsatisfactory situation, by introducing a Bayesian way of dealing with the concept of absolute quality of fit. This is a familiar concept from the usual frequentist goodness-of-fit tests, which have the advantage of flagging strong discrepancies between the model and the observed data. Intuitively, it is sensible that we should start doubting the adequacy of our model(s) whenever the observed data are in poor agreement with their predictions. An appropriately calibrated absolute value of the evidence can be employed within a Bayesian-style reasoning to substantiate our intuition that “something fishy” must be going on whenever the data are a poor fit to the best model available.

## B. Calibration of the evidence

The absolute upper bound on the value of the evidence for the unknown model is achieved for a model  $\mathcal{S}$  which predicts exactly the data that have been observed (and which has a prior that goes to zero for any other observation). Such a model can be dubbed a “sure-thing model”, because it is totally deterministic. However, in most situations of interest, such a model is unrealistic, because it does not allow for the statistical nature of the measurement process, which is subject to noise, neither does it accommodate a possible statistical connection between the observables and the underlying physical model, which introduces sample variance in certain contexts (e.g. cosmic variance in cosmology). Furthermore (as discussed in [12] for the conceptually simple case of coin tossing), such models are usually thrown out from the beginning, simply because there is a large number of them: e.g. for any outcome of  $N$  coin flips, there are  $2^N$  different sure-thing models  $\mathcal{S}_i$  “predicting” exactly the data that might have been observed. Because of their large number, each of the  $\mathcal{S}_i$  should be penalised by a prior probability  $p(\mathcal{S}_i) \sim 2^{-N}$ , which goes quickly to 0 for even moderate values of  $N$ . For all those reasons, calibrating off the absolute maximum value of the evidence is undesirable. A more realistic calibration is required.

We suggest to calibrate the evidence using the properties of the likelihood and a default (weak) reference prior. The first step is to approximate the evidence for the unknown model,  $p(d|\mathcal{X})$ , via the Bayesian Information Criterion (BIC) [1, 13, 14, 15, 16], the derivation of which we sketch below (see e.g. [14] for further details).

Let us denote the likelihood of the unknown model by  $\mathcal{L}(\theta) \equiv p(d|\theta, \mathcal{X})$  and the prior by  $p(\theta|\mathcal{X})$ . We begin by Taylor expanding  $g(\theta) = \ln[\mathcal{L}(\theta)p(\theta|\mathcal{X})]$  around the maximum likelihood value,  $\theta_{\max}$ . To second order,

$$g(\theta) \approx g(\theta_{\max}) - \frac{1}{2}(\theta - \theta_{\max})^t H(\theta - \theta_{\max}), \quad (7)$$

where  $H$  is minus the Hessian matrix evaluated at the maximum likelihood point,

$$H_{ab} \equiv - \left. \frac{\partial^2 g(\theta)}{\partial \theta_a \partial \theta_b} \right|_{\theta=\theta_{\max}}. \quad (8)$$

Using this approximation in the calculation of the evidence, Eq. (2), we obtain

$$\begin{aligned} \ln p(d|\mathcal{X}) &= \ln \mathcal{L}_{\max} + \ln p(\theta_{\max}|\mathcal{X}) + \frac{k}{2} \ln(2\pi) \quad (9) \\ &\quad - \frac{1}{2} \ln |H| + \mathcal{O}(n^{-1}), \end{aligned}$$

where  $k$  is the number of parameters in the unknown model. For large samples, we can approximate  $H \approx nI$  (to order  $\mathcal{O}(n^{-1/2})$ ), where  $I$  is the expected Fisher matrix from a single observation. We now assume that the (unknown) prior  $p(\theta|\mathcal{X})$  is a multivariate Gaussian approximately centred at  $\theta_{\max}$  with Fisher matrix  $I$ . This means that the assumed prior distribution contains about the same (weak) information as would an average single observation. Then

$$\ln p(\theta_{\max}|\mathcal{X}) = -\frac{k}{2} \ln(2\pi) + \frac{1}{2} \ln |I|. \quad (10)$$

Plugging this reference prior into (9) and with the above approximation for  $H$ , terms of order  $\mathcal{O}(1)$  cancel and we obtain

$$\ln p(d|\mathcal{X}) = \ln \mathcal{L}_{\max} - \frac{k}{2} \ln n + \mathcal{O}(n^{-1/2}). \quad (11)$$

This is the standard expression for the BIC, which we will employ to estimate the evidence for the unknown model. It requires an estimate of the best-fit likelihood  $\mathcal{L}_{\max}$  and of the number of free parameters,  $k$ , for the unknown model  $\mathcal{X}$ . Notice that the likelihood, when normalised over the data space, is a dimensionful quantity, with dimensions  $[\text{data}]^{-n}$ . In the following we will always drop such a prefactor (and the associated factors of  $2\pi$ ) as it always cancels when considering evidence ratios (for the same data), therefore  $\mathcal{L}_{\max}$  has to be regarded as dimensionless.

In order to compute the evidence for the unknown model from Eq. (11), we need to specify an estimator  $\widehat{\mathcal{L}}_{\max} \equiv -2 \ln \widehat{\mathcal{L}}_{\max}$  for (minus twice) the best-fit log-likelihood,  $-2 \ln \mathcal{L}_{\max}$ , of the unknown model  $\mathcal{X}$ . This can be obtained from the requirement of ‘‘typicality’’ of the observed realization under  $\mathcal{X}$ . Assuming that the data are normally distributed,  $-2 \ln \mathcal{L}_{\max}$  follows an approximate  $\chi^2$ -distribution with  $m = (n - k)$  degrees of freedom. Then the expectation value of  $\mathcal{L}_{\max}$  (as taken over different realizations of the data, represented by  $\langle \cdot \rangle$ ) follows from

$$\langle -2 \ln \mathcal{L}_{\max} \rangle = m. \quad (12)$$

Employing  $\langle -2 \ln \mathcal{L}_{\max} \rangle$  as an estimator for  $-2 \ln \mathcal{L}_{\max}$  would be equivalent to assuming that the unknown model has  $\chi^2/\text{dof} = 1$ , in agreement with the rule-of-thumb for goodness-of-fit tests. This however is too harsh a requirement on the performance of the known models  $\mathcal{M}_i$ . Even if one of the known models is indeed the correct one, the realized maximum likelihood value for that model will be smaller than the estimator (i.e.  $-2 \ln \mathcal{L}_{\max}^{\text{obs}} < \langle -2 \ln \mathcal{L}_{\max} \rangle$ ) in about 50% of realizations of the data (for the median and the mean of the chi-square distribution are very close). This would lead in many

cases to unjustified doubt of the correct model as a consequence of harmless statistical fluctuations in the observed data realization.

Therefore, instead of using the expectation value, the value of  $\mathcal{L}_{\max}$  should be more conservatively estimated so that for example,  $-2 \ln \mathcal{L}_{\max}^{\text{obs}} < \widehat{\mathcal{L}}_{\max}$  only in  $100\alpha\%$  of the data realizations, where we are free to choose the value of  $\alpha$ . This can be achieved by taking  $\widehat{\mathcal{L}}_{\max}$  to be the  $\alpha$  quantile  $\chi_{m,(\alpha)}^2$  of the chi-square distribution with  $m$  dof,  $P_{\chi_m^2}$ ,  $\widehat{\mathcal{L}}_{\max} = \chi_{m,(\alpha)}^2$ , defined through

$$\int_{\chi_{m,(\alpha)}^2}^{\infty} P_{\chi_m^2}(x) dx = 1 - \alpha. \quad (13)$$

As  $\chi_{m,(\alpha)}^2$  increases monotonically with  $\alpha$ , larger values of  $\alpha$  lead to smaller (and hence more conservative) values for the evidence  $p(d|\mathcal{X}) \propto \exp(-\chi_{m,(\alpha)}^2/2)$  via Eq. (11). In principle, one is free to choose the value of  $\alpha$ , and we calibrate it by demanding the wrongful rejection rate of correct models to be smaller than a given value  $\gamma$  (see Tables II and III below).

In summary, we suggest to use as an estimator of the unknown model’s evidence,

$$\ln p(d|\mathcal{X}, k, \alpha) = -\frac{\chi_{m,(\alpha)}^2}{2} - \frac{k}{2} \ln n, \quad (14)$$

where on the left-hand side we have conditioned explicitly on the number of parameters  $k$  of  $\mathcal{X}$ , and on the quantile value  $\alpha$ .

In a Bayesian spirit, one could treat  $k$  and  $\alpha$  as hyperparameters, by specifying a prior and marginalising over them in the evidence. Here, we investigate the behaviour of doubt in a Gaussian linear toy model, where  $k$  is fixed at a plausible value and  $\alpha$  is chosen by calibrating its value on the fraction of cases where doubt wrongfully grows.

### C. Change in the amount of doubt: independence of prior doubt

The final quantity that needs to be specified in order to compute the posterior doubt is the prior doubt,  $p(\mathcal{X})$ . It seems to us that values  $10^{-5} \lesssim p(\mathcal{X}) \lesssim 10^{-1}$  might be plausible in many cases of interest, but higher or lower values are certainly possible. The interesting question is in fact whether doubt increases or decreases in the light of the observed data. We assume that the prior probability of the known models is equally split among them, i.e.

$$p(\mathcal{M}_1) = p(\mathcal{M}_2) = \dots = p(\mathcal{M}_N) = \frac{1 - p(\mathcal{X})}{N}. \quad (15)$$

(This simplifying assumption can easily be relaxed.) This leads to the following expression for the relative change between the prior and posterior doubt:

$$\mathcal{R} \equiv \frac{\mathcal{D}}{p(\mathcal{X})} = \frac{p(\mathcal{X}|d, k, \alpha)}{p(\mathcal{X})} \quad (16)$$

$$= \left[ p(\mathcal{X}) + (1 - p(\mathcal{X})) \frac{\bar{\Sigma}}{e^{-\chi_{m,(\alpha)}^2/2} n^{-k/2}} \right]^{-1},$$

where we have defined the average known models' evidence

$$\bar{\Sigma} \equiv \frac{1}{N} \sum_{i=1}^N p(d|\mathcal{M}_i). \quad (17)$$

The doubt grows if  $\mathcal{R} > 1$ , i.e. for

$$\frac{\bar{\Sigma}}{e^{-\chi_{m,(\alpha)}^2/2} n^{-k/2}} < 1, \quad (18)$$

independently of the prior probability for doubt (as long as this is strictly greater than zero).

Let us consider the asymptotic behaviour of the criterion given by Eq. (18) for a large number of data points, both under the assumption that the true model is present in and the assumption that it is absent from the list of known models.

If the true model  $\mathcal{M}_T$  is within the list  $\mathcal{M}_i$ , then by construction of the BIC

$$\lim_{n \rightarrow \infty} p(d|\mathcal{M}_T) = e^{-\text{BIC}/2} = e^{-\chi_{m,(0.5)}^2/2} n^{-k/2}, \quad (19)$$

hence to leading order

$$\frac{\bar{\Sigma}}{e^{-\chi_{m,(\alpha)}^2/2} n^{-k/2}} \rightarrow \frac{1}{N} \exp(\Delta_\alpha/2). \quad (20)$$

Here  $\Delta_\alpha \equiv \chi_{m,(\alpha)}^2 - \chi_{m,(0.5)}^2$ , with  $\chi_{m,(\alpha)}^2$  the inverse of the  $\chi^2$  cumulative distribution function (CDF) with  $m$  degrees of freedom. Clearly,  $\Delta_\alpha > 0$  for  $\alpha > 0.5$ . In the limit of many data points,  $n \rightarrow \infty$  (or equivalently  $m \rightarrow \infty$ ),  $\chi_{m,(\alpha)}^2$  can be approximated by the inverse of the CDF of the normal distribution with mean  $m$  and variance  $2m$ ,  $\mathcal{N}(m, 2m)$ , so that

$$\lim_{n \rightarrow \infty} \Delta_\alpha = m \times \left( 2\sqrt{2} \text{InverseErf}(2\alpha - 1) \right), \quad (21)$$

where  $\text{InverseErf}(x)$  is the inverse of the Error Function. It follows that  $\Delta_\alpha \gg 1$  and therefore from (20) and (16) for many data points  $n$  (or degrees of freedom  $m$ ),  $\mathcal{R} \rightarrow 0$ , and hence  $\mathcal{D} \rightarrow 0$ . In other words: if the true model is in the list of known models, the doubt goes to zero as expected. Notice that in Eq. (20) the extra factor  $1/N$  of penalising for the true model comes from the fact that its predictivity has been spread among a set of  $N$  possibilities. More

precisely, the  $1/N$  factor assumes that the evidences for the other known models are negligible in the sum. However, if there are  $M < N$  other models which are unnecessarily more complicated than the true model with parameters that are unconstrained by the data, one would expect that the evidence for each of those models is of the same order as for the true model (because the evidence does not penalise unconstrained parameters). Therefore the  $1/N$  factor would be replaced by a factor  $\sim (M + 1)/N$ .

If, instead, the true model (or another model that is about as good as the true model in explaining the data) is not within the list of known models, then the numerator in Eq. (18) will drop very quickly to zero, hence

$$\lim_{n \rightarrow \infty} \mathcal{R} = \frac{1}{p(\mathcal{X})}. \quad (22)$$

Therefore the doubt goes to unity,  $\mathcal{D} \rightarrow 1$ , which leads to questioning the completeness of our list of known models.

Further modelling requires the explicit specification of the known models and computation of  $\bar{\Sigma}$  from the observed data. We therefore proceed with an illustration based on linear models.

#### IV. ILLUSTRATION: LINEAR TOY MODEL

It is instructive to look at an example for the usage of doubt in a simple toy model. Consider the case of a *Gaussian linear model*:

$$y = A\theta + \epsilon, \quad (23)$$

where the dependent variable  $y$  is a  $n$ -dimensional vector of observations,  $\theta$  is a vector of dimension  $c$  of unknown regression coefficients and  $A$  is a  $n \times c$  matrix of known constants which specify the relation between the input variables  $\theta$  and the dependent variables  $y$ . Furthermore,  $\epsilon$  is a  $n$ -dimensional vector of random variables with zero mean (the *noise*). We assume that the observations are independent identically distributed (i.i.d.), hence  $\epsilon$  follows a multivariate Gaussian distribution with unit covariance and the likelihood is given by

$$\mathcal{L}(\theta) = \exp \left[ -\frac{1}{2} \sum_{i=1}^n \left( \frac{y_i - y_i^{\text{th}}}{\sigma} \right)^2 \right], \quad (24)$$

where  $y_i(y_i^{\text{th}})$  are the values of the observed (predicted) observables, and  $\sigma = 1$ .

For the purpose of our example, let us assume that we have  $n$  data points, and that two models are available:

- $\mathcal{M}_0 : y = \theta$ , i.e.  $c = 1$  and  $A = (1, \dots, 1)^t$  and

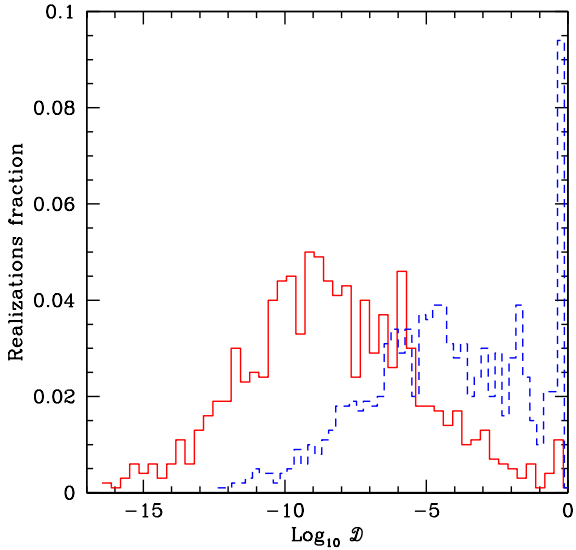


FIG. 1: Distribution of doubt values when the correct model is used to fit the data, for 1000 realizations of 100 data points, for prior doubt  $p(\mathcal{X}) = 10^{-1}$  (blue, dashed) and  $p(\mathcal{X}) = 10^{-5}$  (red, solid), and  $\alpha = 0.95$ .

- $\mathcal{M}_1 : y = \theta x$ , i.e.  $c = 1$  and  $A = (x_1, \dots, x_n)^t$ .

In both cases there is one free parameter,  $\theta$ , and we will assume that a prior is available of the form  $p(\theta|\mathcal{M}_0) = p(\theta|\mathcal{M}_1) = 1/4$  for  $\theta \in [-2, 2]$  (and vanishes outside that range). We will assume that there is one free parameter in the unknown model, i.e.  $k = 1$ . (The number of effective free parameters can be investigated further by the mean of the Bayesian complexity, see [3].)

We are interested in investigating the behaviour of the ratio of the posterior to the prior doubt  $\mathcal{R}$ . We expect  $\mathcal{R} < 1$  (decreasing doubt) when the known model is the correct underlying distribution, and  $\mathcal{R} > 1$  when an incorrect known model is used. For definiteness, we will take the true model to be  $\mathcal{M}_1$ , with  $\theta_{\text{true}} = 0.1$ .

#### A. Doubt when fitting data with the correct model: false doubt

Let us assume that our list of known models contains only  $\mathcal{M}_1$  (i.e.  $N = 1$  and  $\mathcal{M}_0$  is not on the list). We first fit the dataset (generated from  $\mathcal{M}_1$ ) with the correct model  $\mathcal{M}_1$  and we compute the posterior  $p(\mathcal{M}_1|d)$  and the doubt  $p(\mathcal{X}|d)$  from Eq. (4), using  $\alpha = 0.95$ . In this case, there should be no reason for doubt as we expect  $\mathcal{M}_1$  to be an adequate description of the data. We show the ensuing distribution of posterior doubt in Fig. 1 (from 1000 data realizations

with  $n = 100$  data points each), for two different choices of prior doubt,  $p(\mathcal{X}) = 10^{-5}$  (red/solid histogram) and  $p(\mathcal{X}) = 10^{-1}$  (blue/dashed histogram). The posterior doubt of the vast majority of the realizations is smaller than the prior doubt, consistent with expectations. Clearly, the absolute value of the posterior doubt depends on the choice of prior doubt, and quite reasonably so. If *a priori* one is quite certain that the model is correct, then small deviations from a perfect fit will not shake one’s belief in the model. However, if the prior doubt is relatively large,  $p(\mathcal{X}) = 10^{-1}$  (i.e., if *a priori* one is quite uncertain that the model being used is correct) then already small fluctuations in the data will lead to relatively strong posterior doubt. The less confident one is to begin with, the more easily one’s belief in a model is shaken by statistical fluctuations. In any case, larger amounts of data will lessen the effect of fluctuations, leading to little doubt about the correct model, with the amount of data required for persuasion dependent on the prior doubt. For both values of prior doubt in Fig. 1, about 14% of the realizations lead to a posterior doubt that is larger than the prior doubt. This number is independent of the prior doubt as can be seen from Eq. (16) and decreases with increasing number of data points  $n$  and as  $\alpha$  approaches unity. We call realizations that incorrectly give an increase of doubt (although the model being used is the correct one) cases of “false doubt”.

We now turn to investigate the relative change in doubt,  $\mathcal{R}$ , which is plotted in Fig. 2, for two choices of the number of data points  $n$  and of the calibration parameter  $\alpha$ . Recall that  $\log \mathcal{R} > 0$  ( $< 0$ ) corresponds to an increase (decrease) in doubt in light of the observed data. In fact,  $\mathcal{R}$  can be regarded as a sort of “Bayes factor” for doubt change — it gives the relative change in our “state of doubt” after we have seen the data. While the actual value of  $\mathcal{R}$  is dependent on the prior doubt, the threshold separating increasing doubt from decreasing doubt (i.e.,  $\log \mathcal{R} = 0$ ) is independent of  $p(\mathcal{X})$ . As expected, a larger number of data points leads to a decrease in the fraction of realizations for which doubt wrongfully grows (values  $\log \mathcal{R} > 0$ ). The same is true if one increases  $\alpha$ . As explained above, this is because a larger value of  $\alpha$  leads to a less harsh penalty for odd features in the realized data.

By construction of the doubt, there is a strong correlation between the value of  $\log \mathcal{R}$  and the chi-square per dof of the best fit. This is depicted in Fig. 3. First, it is obvious that for a given choice of  $\alpha$ , data realizations leading to a wrongful increase in doubt ( $\log \mathcal{R} > 0$ ) are the ones that present “unlucky” features, i.e. the ones with a large value of  $\chi^2/\text{dof}$ . In other words, cases of false doubt would be suspicious even using a more traditional measure of the quality of fit. However, the second, crucial

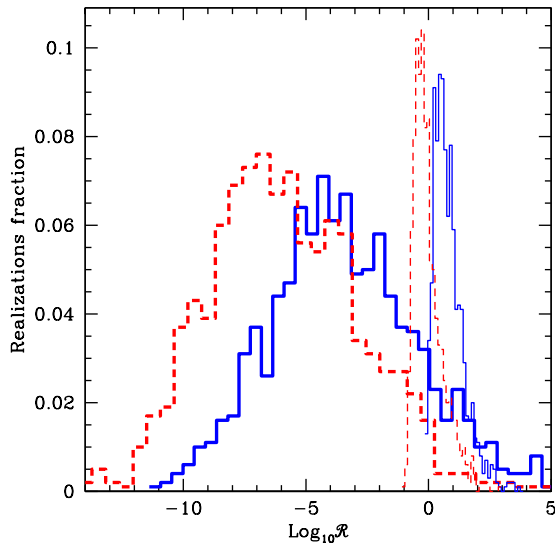


FIG. 2: Distribution of the change in doubt  $\log \mathcal{R}$  when fitting data with the correct model, from 1000 data realizations for  $n = 5, \alpha = 0.95$  (blue/solid, thin),  $n = 5, \alpha = 0.99$  (red/dashed, thin),  $n = 100, \alpha = 0.95$  (blue/solid, thick) and  $n = 100, \alpha = 0.99$  (red/dashed, thick). Values  $\log \mathcal{R} < 0$  correspond to a decrease in the amount of doubt. A larger value of  $\alpha$  and a larger number of data points  $n$  lead to a reduction of the number of cases where the doubt wrongly grows (values  $\log \mathcal{R} > 0$ ).

point is that the parameter  $\alpha$  can be calibrated in order to achieve a pre-determined fraction of false doubt from a known model. By increasing  $\alpha$ , the locus of the realizations shifts to the left of the plot. Therefore one can choose  $\alpha$  in such a way that the probability of false doubt is below a given threshold. This is discussed in the next section.

### B. Calibration of the level of false doubt

As shown above, some fraction of data realizations will always lead to false doubt. This fraction depends on the value of  $\alpha$  and on the number of data points,  $n$ , but not on the level of prior doubt. (There is a further, if subdominant, dependence on  $k$ .)

For a given number of data points, it is desirable to tune the value of  $\alpha$  such that the fraction of false doubt  $\gamma$  is (on average) below a predetermined threshold. This is achieved as follows. Starting from the model distribution (here,  $\mathcal{M}_1$ ), we employ current data to derive constraints on its free parameters, as usual in the inference step. We then select an estimator  $\hat{\theta}$  for the value of the parameters (here,  $\theta$ ), which will usually be either the best-fit point or the posterior mean. We simulate  $10^4$  realizations of the

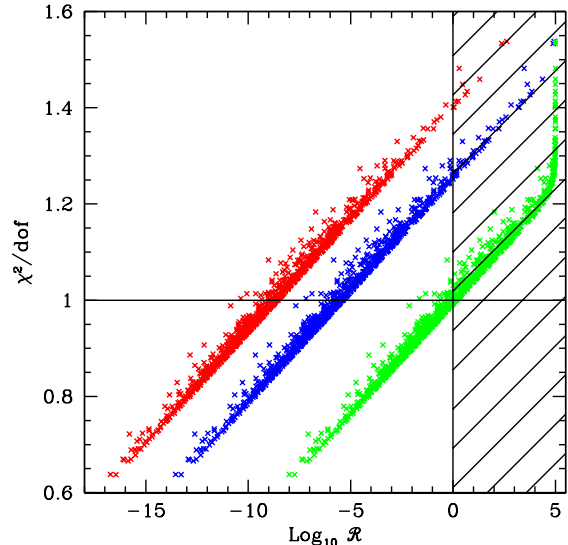


FIG. 3: Correlation between the “chi-square-per-dof” rule and the change in doubt,  $\log \mathcal{R}$ , for different values of the calibration parameter  $\alpha$ , increasing from right to left (for 1000 data realizations). The parameter  $\alpha$  can be chosen so that only a pre-determined fraction  $\gamma$  of data realizations lie in the “false doubt” zone (shaded,  $\log \mathcal{R} > 0$ ). Here,  $\alpha$  has been chosen in such a way that (from right to left)  $\gamma = 0.50, 0.05, 0.01$ .

data from the model, assuming a fiducial value  $\hat{\theta}$  for its parameters. We then compute the doubt for each realization, and calibrate the value of  $\alpha$  by requiring that the fraction of realizations with  $\log \mathcal{R} > 0$  be below a value  $\gamma$  [18]. To further reduce the scatter in  $\alpha$ , we average over the resulting  $\alpha$  values from 1000 such procedures. Table II shows such values of  $\alpha(\gamma, n, \mathcal{M}_1)$  for a few representative choices of  $\gamma$  and  $n$ . One striking feature of the calibration table is that the value of  $\alpha$  required for a false doubt rate  $\gamma$  is systematically much larger than  $1 - \gamma$ . This is another reflection of the well known fact that how likely the data are given the hypothesis does not by itself determine how probable the hypothesis is given the data. Inferring the latter requires the use of Bayes theorem. (For an in-depth discussion of this point, see [6]).

Because the calibrated value of  $\alpha$  decreases monotonically with increasing  $n$ , the above calibration procedure, once carried out for a certain number of data points, is expected to be conservative when the amount of data increases. This is shown in Fig. 4, where we plot the fraction of realizations leading to false doubt after  $\alpha$  has been calibrated at  $n = 100$ . We can see that for  $n > 100$  the fraction of false doubt remains below the calibrated level, and that

$n$	$\gamma = 0.01$	$\gamma = 0.05$	$\gamma = 0.50$
10	0.99969(3)	0.9980(1)	0.9550(8)
100	0.9980(2)	0.9869(7)	0.747(4)
200	0.9968(3)	0.9810(9)	0.684(4)
1000	0.9942(6)	0.968(1)	0.586(5)

TABLE II: Values of  $\alpha(\gamma, n, \mathcal{M}_1)$ , as a function of the number of data points,  $n$ , ensuring an average fraction of false doubt of  $\gamma = 1\%$ ,  $5\%$ ,  $50\%$  and for model distribution  $\mathcal{M}_1$ . The number in brackets denotes the uncertainty in the last digit.

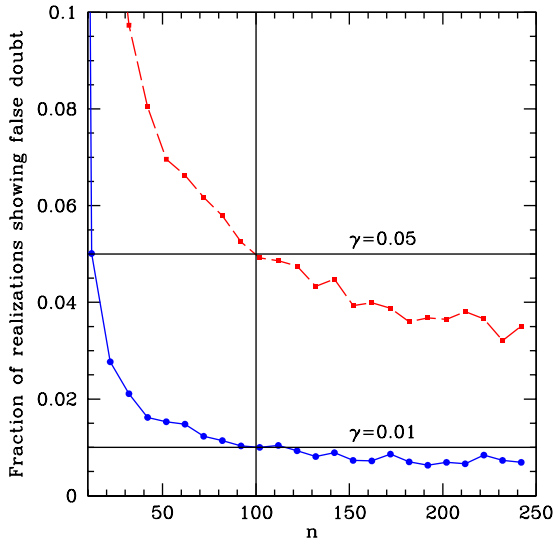


FIG. 4: Fraction of cases of false doubt,  $\log \mathcal{R} > 0$  as a function of the number of data points,  $n$ , employing a doubt calibration parameter  $\alpha$  corresponding to a false doubt probability of  $\gamma = 5\%$  (dashed red) and  $\gamma = 1\%$  (solid blue) for  $n = 100$ . For a number of data points  $n > 100$  there is a residual (if mild)  $n$  dependence in the fraction of false doubt, which however is always below the calibration level. The calibration is independent of the prior doubt.

the residual  $n$  dependency is fairly mild.

### C. Doubt when fitting data with an incorrect model: model discovery

We now pretend that the true model where the data come from,  $\mathcal{M}_1$ , is unknown to us. We take  $\mathcal{M}_0$  to be the only known model, and consequently fit the data with it. We repeat the calibration procedure for  $\alpha$  for the known model  $\mathcal{M}_0$ . The corresponding calibrated values of  $\alpha(\gamma, n, \mathcal{M}_0)$  are given in Table III.

Using the calibrated values of  $\alpha$  we then compute

$n$	$\gamma = 0.01$	$\gamma = 0.05$	$\gamma = 0.50$
2	0.9944(5)	0.973(1)	0.781(2)
3	0.9938(6)	0.969(1)	0.692(3)
4	0.9935(6)	0.967(2)	0.654(4)
5	0.9933(7)	0.966(2)	0.633(4)
6	0.9932(7)	0.965(2)	0.618(4)
7	0.9931(7)	0.965(2)	0.607(4)
8	0.9929(7)	0.964(2)	0.600(4)
9	0.9928(7)	0.963(2)	0.593(4)
10	0.9928(7)	0.963(2)	0.588(5)

TABLE III: Values of  $\alpha(\gamma, n, \mathcal{M}_0)$ , as a function of the number of data points,  $n$ , ensuring an average fraction of false doubt of  $\gamma = 1\%$ ,  $5\%$ ,  $50\%$  and for the known model  $\mathcal{M}_0$ . The number in brackets denotes the uncertainty in the last digit.

the posterior doubt on  $\mathcal{M}_0$ . The result is shown in Fig. 5 (again averaged over 1000 realizations). We can see that doubt increases immediately from its prior value  $p(\mathcal{X}) = 10^{-5}$ , and tends very quickly to 1. This clearly signals the inadequacy of the known model to fit the data. We should therefore question the correctness of the known model and suspect the existence of a better model. Therefore our procedure leads to model discovery in the absence of an explicit specification of the alternative, true model.

### D. Generalisation to multi-models cases and discussion

In the example considered so far, we have only dealt with doubt (or its absence) for one model at a time. The situation is qualitatively similar when several alternative known models are available (i.e. for  $N > 1$ ).

When several known models exist, the calibration procedure should be carried out on the model that is currently the best among them, i.e. on the model with the largest Bayes factor. This ensures that the probability of false doubt is under control for the currently favoured model (which has the largest evidence). If one of the known models is clearly preferred, then the situation is qualitatively similar to the case of  $N = 1$  (since the evidence from the other, poorer models contributes very little to the sum in the definition of doubt). If instead several models have a similar value of the evidence under present data, then it is expected that the outcome of the calibration should be quite similar for any of them. Also, as discussed above in the presence of  $M$  models with approximately the same evidence there is an extra “volume factor”  $M/N$  to take into account in



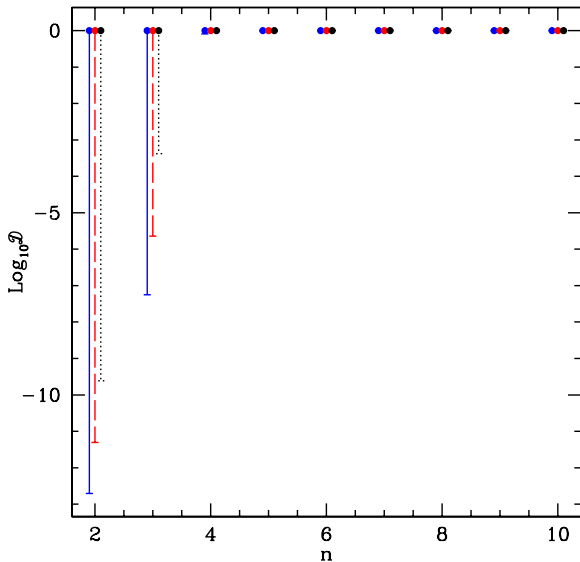


FIG. 5: Model discovery: posterior doubt on the (wrong) model  $\mathcal{M}_0$  as a function of the number of data points,  $n$ , here for prior doubt  $p(\mathcal{X}) = 10^{-5}$  using the value of  $\alpha$  calibrated to a fraction of false doubt  $\gamma = 1\%$  (solid blue line),  $\gamma = 5\%$  (dashed red line),  $\gamma = 50\%$  (dotted black line). The points give the mean doubt over 1000 data realizations and the vertical bars indicate the range of values enclosing 95% of the realizations. The posterior doubt goes very quickly to 1 (in fact, for  $n \geq 5$ , all realizations have a posterior doubt of unity), therefore leading to doubt the correctness of the model.

the rate of false doubt.

The false doubt calibration procedure introduced here insures against unjustified doubt of the known models at a given threshold (set by  $\gamma$ ). Because unknown models belong to the world of unknown unknowns, it is more difficult to calibrate the performance of doubt for model discovery, *i.e.* for justifiably doubting false models. Whether or not the doubt does increase when the true model is genuinely unknown depends on how different that unknown true model is from the known models. Here, “different” must be interpreted in terms of a “distance” in the space of models, as measured by the Bayesian evidence. In this sense, the notion of doubt introduces an absolute metric in model space, to complement the relative metric represented by the Bayes factor. In any case, if the true model is not very different in its observational consequences from one of the known models (in which case doubt will not increase), then one might conclude that the known model is a phenomenologically accurate description of the presently available data. If doubt does increase, though, this is a signal that the best available model is an inadequate description of the observations and that new

theoretical input is required.

In general, we remark that the existence of known models that are unnecessarily complex (*i.e.*, with more free parameters than the true model) is not directly addressed by doubt. In this case, an analysis of doubt (properly calibrated) will return a null result, *i.e.* no reason for doubting the adequacy of the overly complex model. One has to keep in mind that doubt is a tool for *model discovery*, whose primary goal is to point towards the need to enlarge (or change completely) the space of the known models. The shedding of unnecessary levels of complexity is instead a task best accomplished by simultaneously analysing the evidence and Bayesian complexity. (See [3] for an application.)

Finally, the usual caveats apply about the dependence on the volume in parameter space enclosed by the parameters’ prior  $p(\theta_j|\mathcal{M}_j)$ , as is always the case for calculations involving the Bayesian evidence. (See [1, 17] for a discussion.) However, the calibration procedure for  $\alpha$  automatically accounts for the volume enclosed by the chosen prior under  $\mathcal{M}_j$ , as compared with the reference prior employed for the unknown model. If one were to change the prior on the parameters of the known model, then this would amount effectively to a change of model. (As mentioned, we consider a model specification to consist of both the model parameters *and* their prior.) Therefore the calibration ought to be performed again on the new model.

## V. CONCLUSIONS

Checking the appropriateness of a given set of models to describe observations is not a usual task in a Bayesian framework. We have suggested an intuitive approach to doubt in a Bayesian context that shares some philosophy with the frequentist approach: after all, the estimator for  $\mathcal{L}_{\max}$  is based on a  $\chi^2/\text{dof}$  argument and strictly speaking, Bayesians should show little interest in the hypothetical outcome of different realizations of reality. Nevertheless, as we demonstrated with the example of a simple linear model, the concept of doubt is more powerful than traditional goodness-of-fit tests provided the parameter  $\alpha$  controlling the rate of false doubt is correctly calibrated.

As mentioned in the introduction, the concept of doubt is ideally suited for applications in cosmology. Huge data sets and multi-dimensional parameter spaces do not lend themselves very well to visual inspection. Computing the doubt  $\mathcal{D}$  – a single number – gives an indication of the trustworthiness of the model(s) under consideration in a Bayesian context. Applications range from questions about the very early inflationary phase of the universe (in par-

ticular about the shape of the primordial power spectrum generated during inflation) to the future evolution of the Universe which appears to be dominated by dark energy (in particular whether the equation of state during late-time acceleration is constant). Given the need to calibrate the doubt, such work requires a large amount of computational power even given recent advances in numerical techniques for the evaluation of the evidence, and it will be addressed in a future paper.

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  - [18] Strictly speaking, this procedure underestimates the uncertainty in the spread of values for the doubt, in that it ignores the current posterior uncertainty about  $\hat{\theta}$ . Such an approximation will be valid whenever the scale of the posterior width is much smaller than the width of the prior on the model's parameters (i.e., for informative data). A fuller calculation accounting for this extra layer of complexity will be presented elsewhere.