Bayesian model checking: A comparison of tests

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ABSTRACT

Two procedures for checking Bayesian models are compared using a simple test problem based on the local Hubble expansion. Over four orders of magnitude, p -values derived from a global goodness-of-fit criterion for posterior probability density functions agree closely with posterior predictive p -values. The former can therefore serve as an effective proxy for the difficult-to-calculate posterior predictive p -values.

Key words. methods: statistical – binaries: general

1. Introduction

In a recent paper (Lucy 2018; L18), straightforward procedures are proposed for Bayesian model checking.

Because all Bayesian inferences derive from the posterior probability density function $\Lambda(\alpha|D)$, where α is the parameter vector and D is the data, these tests check the global goodness-of-fit (GOF) to D provided by Λ . The proposed checks take the form of p -values closely analogous to those familiar in frequentist analyses. The first test derives from the χ^2_B statistic (L18, Appendix C) for uncorrelated measurement errors. The second test derives from the ψ^2_B statistic (L18, Appendix C.1) for correlated measurement errors.

The need for readily-applied Bayesian model checking procedures has recently been persuasively pointed out by Ford – see Sect. 4.1 in Fischer et al. (2016). Ford attributes the frequent neglect of model checking by Bayesians to the absence of a “neat and tidy” test criterion for Bayesian analyses, in contrast to the χ^2 criterion for frequentist analyses. For Bayesian model checking, Ford recommends the book by Gelman et al. (2013), which advocates posterior predictive checks.

In Sect. 6.4 of L18, a numerical experiment is briefly reported in which p -values from posterior predictive checking are compared to those derived from the same data with the χ^2_B statistic. Given the importance of establishing the merits of the simpler approach provided by the χ^2_B statistic, this short paper presents the numerical experiment in some detail.

2. Bayesian p -values

In this section, the basics of the p -values to be compared are stated.

2.1. Posterior predictive p -value

On the assumption that χ^2 is an appropriate test quantity – other possibilities are discussed in Gelman et al. (2013), the steps required to obtain the posterior predictive p -value are as follows:

* With profound sadness we note that Prof. Leon Lucy passed away after the final stages of acceptance of this article.

- 1) Compute the posterior probability density function, given by

$$\Lambda(\alpha|D) = \pi(\alpha)\mathcal{L}(\alpha|D) \bigg/ \int \pi(\alpha)\mathcal{L}(\alpha|D)dV_\alpha \quad (1)$$

where π is the prior, and $\mathcal{L}$, the likelihood, is given by

$$\mathcal{L}(\alpha|D) = \text{Pr}(D|\alpha) \propto \exp\left[-\frac{1}{2}\chi^2(\alpha|D)\right]. \quad (2)$$

- 2) Randomly select a point α' from the posterior density $\Lambda(\alpha|D)$.
- 3) Compute a simulated data set D' at α' by randomly sampling $\text{Pr}(D|\alpha')$.
- 4) Compute and record the values of $\chi^2(\alpha'|D')$ and $\chi^2(\alpha'|D)$.
- 5) Repeat steps 2) to 5) N_{tot} times.

The resulting Bayesian p -value is then

$$p_B = N(\chi^2(\alpha'|D') > \chi^2(\alpha'|D)) / N_{\text{tot}}. \quad (3)$$

2.2. p -value from the χ^2_B statistic

Following earlier work (Lucy 2016; L16) on the statistical properties of the posterior mean of χ^2 , the general form of the χ^2_B statistic is (Appendix C in L18)

$$\chi^2_B(D) = \langle \chi^2 \rangle_\pi - k \quad (4)$$

where k is the number of parameters and

$$\langle \chi^2 \rangle_\pi = \int \chi^2(\alpha)\Lambda(\alpha|D)dV_\alpha. \quad (5)$$

The p -value corresponding to the χ^2_B statistic is derived from the χ^2 distribution with $\nu = n - k$ degrees of freedom, where n is the number of measurements. Specifically,

$$p(\chi^2_B) = \text{Pr}(\chi^2_{n-k} > \chi^2_B). \quad (6)$$

The theoretical basis of this p -value is as follows: in the majority of astronomical applications of Bayesian methods, the priors are weak and non-informative. Typically, $\pi(\alpha)$ defines a

box in α -space representing a search volume that the investigator is confident includes all points α with significant likelihood. In consequence, a weak prior has negligible effect on the posterior density Λ and therefore also on any resulting inferences.

In the weak prior limit, Eq. (1) simplifies to

$$\Lambda(\alpha|D) = \mathcal{L}(\alpha|D) \int \mathcal{L}(\alpha|D) dV_\alpha \quad (7)$$

and the resulting posterior mean of χ^2 is written as $\langle \chi^2 \rangle_u$.

Now, in Appendix A of L16, it is proved that, for linearity in α and normally-distributed measurement errors,

$$\langle \chi^2 \rangle_u - k = \chi_0^2 \quad (8)$$

where χ_0^2 is the minimum value of $\chi^2(\alpha|D)$. Since, under the stated assumptions, the minimum- χ^2 solution χ_0^2 has a χ_ν^2 distribution with $\nu = n - k$ degrees of freedom, it follows that, with the extra assumption of a weak prior, the statistic χ_B^2 defined in Eq. (4) is distributed as χ_{n-k}^2 . This is the theoretical basis of the p -value given in Eq. (6).

2.3. p -value from the ψ_B^2 statistic

The χ_B^2 statistic of Sect. 2.2 is appropriate when the measurement errors are uncorrelated. When errors are correlated, $\chi^2(\alpha|D)$ is replaced by (see Appendix C.1 in L18)

$$\psi^2(\alpha|D) = \mathbf{v}' \mathbf{C}^{-1} \mathbf{v} \quad (9)$$

where $\mathbf{C}$ is the covariance matrix and $\mathbf{v}$ is the vector of residuals. The statistic ψ^2 reduces to χ^2 when the off-diagonal elements of $\mathbf{C}^{-1}$ are zero – i.e., no correlations.

By analogy with the statistic $\chi_B^2(D)$, a statistic $\psi_B^2(D)$ is derived from the posterior mean of ψ^2 . Specifically,

$$\psi_B^2(D) = \langle \psi^2 \rangle_\pi - k \quad (10)$$

with corresponding p -value

$$p(\psi_B^2) = \Pr(\chi_{n-k}^2 > \psi_B^2). \quad (11)$$

The theoretical basis for this p -value is essentially identical to that for the p -value derived from χ_B^2 . If we have linearity in α and normally-distributed errors, then in the weak prior limit

$$\langle \psi^2 \rangle_u - k = \psi_0^2 \quad (12)$$

and ψ_0^2 is distributed as χ_ν^2 with $\nu = n - k$ degrees of freedom.

Note that posterior predictive p -values (Sect. 2.1) can similarly be generalized to treat correlated measurement errors. The quantity ψ^2 replaces χ^2 , and the random sampling to create simulated data sets can be accomplished with a Cholesky decomposition of the covariance matrix (e.g., Gentle 2009).

3. Test model

A simple 1-D test model is now defined. This allows numerous simulated data sets to be created so that the p -values computed according to Sects. 2.1 and 2.2 can be compared and any differences established with high statistical confidence.

3.1. Hubble expansion

The null hypothesis is that the local Universe is undergoing an isotropic, cold Hubble expansion with Hubble parameter $h_0 = 70 \text{ km s}^{-1} \text{ Mpc}^{-1}$. Moreover throughout the local Universe there exists a population of perfect standard candles of absolute bolometric magnitude $M = -19.0$. Finally, we suppose that the redshifts z of these standard candles are measured exactly, but that their apparent bolometric magnitudes m have normally-distributed measurement errors with $\sigma_m = 0.3 \text{ mag}$.

3.2. Ideal samples

In order to test p -values when the null hypothesis is correct, we need data sets consistent with the above description of the Hubble flow.

We define the local Universe as extending to $z_{\max} = 0.2$, so that to a good approximation the geometry is Euclidean. If we suppose the standard candles to be uniformly distributed in space, a sample $\{z_i\}$ is created with the formula

$$z_i = z_{\max} x_i^{1/3} \text{ for } i = 1, 2, \dots, n \quad (13)$$

where the x_i are independent random numbers $\in (0, 1)$. The distances of these n standard candles are

$$d_i = cz_i/h_0 \text{ Mpc} \quad (14)$$

and their measured apparent bolometric magnitudes are

$$\tilde{m}_i = M + 5 \log d_i + 25 + \sigma_m z_{G_i} \quad (15)$$

where the z_{G_i} are independent gaussian variates from $\mathcal{N}(0, 1)$.

The n pairs $(\tilde{m}_i, z_i)$ comprise a data set D from which the posterior probability density $\Lambda(h|D)$ of the Hubble parameter h can be inferred. Moreover, the global GOF between $\Lambda(h|D)$ and D can be tested with the p -values of Sects. 2.1 and 2.2.

3.3. Imperfect samples

In order to test p -values when the null hypothesis is false, we need to modify either the model or the data. If we continue to make inferences based on the Hubble flow defined in Sect. 3.1, we can introduce a violation of the null hypothesis by contaminating the data sample with an unrecognized second class of standard candles with a different absolute bolometric magnitude. Thus the data set D now comprises n_1 pairs $(\tilde{m}_i, z_i)$ with $\tilde{m}_i$ given by Eq. (15) and n_2 pairs $(\tilde{m}_i, z_i)$ with $\tilde{m}_i$ given by

$$\tilde{m}_i = M - \Delta M + 5 \log d_i + 25 + \sigma_m z_{G_i} \quad (16)$$

and where $n = n_1 + n_2$. Thus, the sample is now contaminated with a second population of standard candles that are brighter by ΔM magnitudes. The investigator is unaware of this, and so carries out a Bayesian analysis assuming an ideal sample.

4. Comparison of p -values

The Bayesian p -values defined in Sect. 2 are now computed for simulated data samples derived as described in Sect. 3.

Fig. 1. Comparison of p -values. For $J = 200$ ideal samples D_j , $\log p(\chi^2_B)$ is plotted against $\log p_B$.

4.1. Null hypothesis correct

In order to compare p -values in this case, J independent ideal samples D_j are created as described in Sect. 3.2, and then p -values for each D_j computed as described in Sects. 2.1 and 2.2.

With a constant prior $\pi(h)$ in the interval (h_1, h_2) with $h_1 = 64$ and $h_2 = 76$ km s⁻¹ Mpc⁻¹, the posterior density $\Lambda(h|D_j)$ is obtained from Eq. (1) with the scalar h replacing the vector α .

The posterior predictive p -value for D_j is computed as described in Sect. 2.1. First, a value h' is derived by randomly sampling $\Lambda(h, D_j)$. This is achieved by solving the equation

$$\int_{h_1}^{h'} \Lambda(h, D_j) dh = x_\ell \quad (17)$$

where x_ℓ is a random number $\in (0, 1)$. Second, an ideal sample D' for Hubble parameter h' is computed according to Sect. 3.2. Third, the GOF values $\chi^2(h'|D')$ and $\chi^2(h'|D_j)$ are computed, where

$$\chi^2(h, D) = \sum_{i=1}^n (\bar{m}_i - m_i)^2 / \sigma_m^2 \quad (18)$$

where the predicted apparent bolometric magnitude is

$$m_i = M + 5 \log cz_i / h + 25. \quad (19)$$

These steps are repeated N_{tot} times with independent random numbers x_ℓ in Eq. (17). The posterior predictive p -value for the ideal sample D_j is then given by Eq. (3).

The corresponding p -value for D_j from the χ^2_B statistic is given by Eq. (4), where

$$\langle \chi^2 \rangle_\pi = \int \chi^2(h, D_j) \Lambda(h|D_j) dh \quad (20)$$

with $\chi^2(h, D)$ from Eq. (18).

The calculations described in Sects. 4.1 and 4.2 are carried out for $J = 200$ ideal samples D_j , with D_j comprising $n = 200$

Fig. 2. Comparison of p -values for imperfect samples. Each imperfect sample contains 180 standard candles of magnitude M and 20 of magnitude $M - \Delta M$ with $\Delta M = 0.5$.

Fig. 3. p -values for imperfect samples. Each imperfect sample contains 180 standard candles of magnitude M and 20 of magnitude $M - \Delta M$. For each ΔM , the p values are computed for 200 independent samples.

pairs $(z_i, \bar{m}_i)$. In calculating posterior predictive p -values, we take $N_{tot} = 10^5$ randomly selected Hubble parameters h' for each D_j in order to achieve high precision for p_B .

The results are plotted in Fig. 1. This reveals superb agreement between the two p -values with no outliers. The mean value of $|\Delta \log p| = 2.3 \times 10^{-3}$ confirms that there is almost exact agreement. Accordingly, this experiment indicates that the readily-calculated $p(\chi^2_B)$ is an almost exact proxy for the posterior predictive p -value p_B , the calculation of which is undoubtedly cumbersome.

4.2. Null hypothesis false

In order to compare p -values when $p \lesssim 0.001$, $J = 200$ independent imperfect samples D_j are created as described in Sect. 3.3.

Again $N_{tot} = 10^5$ and $n = 200$, but now $n = n_1 + n_2$, with $n_1 = 180$ perfect standard candles and $n_2 = 20$ belonging to a second population brighter by $\Delta M = 0.5$ mag. With these changes, the calculations described above are repeated.

The results are plotted in Fig. 2. Because the null hypothesis is false, p -values < 0.01 occur frequently, so that the comparison provided by Fig. 1 now extends to $p \lesssim 10^{-4}$. However, at these small p -values, the values of p_B are subject to noticeable Poisson noise even with $N_{tot} = 10^5$. Because of this, $|\Delta \log p| = 3.2 \times 10^{-2}$, somewhat larger than in Sect. 4.1 but nevertheless again confirming the excellent agreement between the two p -values.

In Fig. 3, the behavior of the p -values derived from the χ_B^2 statistic as a function of ΔM is plotted. With increasing ΔM , the points shift to smaller p -values, increasing the likelihood that the investigator will conclude that the Bayesian model is suspect.

5. Conclusion

The aim of this paper is to investigate the performance of a recently proposed global GOF criterion χ_B^2 for posterior probability densities functions. To do this, a toy model of the local

Hubble expansion is defined (Sect. 3) for which both ideal (Sect. 3.2) and flawed (Sect. 3.3) data samples can be created. The p -values derived for such samples from χ_B^2 are then compared to the p -values obtained with the well-established procedure of posterior predictive checking. The two p -values are found to be in close agreement (Figs. 1 and 2) throughout the interval (0.0001, 1.0), thus covering the range of p -values expected when a Bayesian model is supported ($p \gtrsim 0.01$) to those when the model is suspect ($p \lesssim 0.01$).

Because carrying out a posterior predictive check is cumbersome or even infeasible, the p -value derived from χ_B^2 can serve as an effective proxy for posterior predictive checking. Of course, this recommendation derives from just one statistical experiment. Other investigators may wish to devise experiments relevant to different areas of astronomy.

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