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Bayesian comparison of models with inequality and equality constraints

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ABSTRACT

A Bayesian model selection procedure for comparing models subject to inequality and/or equality constraints is proposed. An encompassing prior approach is used, and a general form of the Bayes factor of a constrained model against the encompassing model is derived. A simple estimation method is proposed which can estimate the Bayes factors for all candidate models *simultaneously* by using one set of samples from the *encompassing* model. A simulation study and a real data analysis demonstrate performance of the method.

1. Introduction

Consider the one-way ANOVA model

$$y_{ij} = \mu_i + \varepsilon_{ij}, \quad j = 1, \ldots, n_i, \; i = 1, \ldots, k, \tag{1}$$

where y_{ij} is the response from the j-th subject under the i-th treatment, μ_i is the mean of the i-th treatment, and ε_{ij}'s are error terms which are independent $N(0, \sigma^2)$ random variables.

A main interest in the ANOVA is comparing the treatment means μ_i's. In particular, in many practical situations interest lies in comparing models with inequality and/or equality constraints on the treatment means. For example, in a dose–response study with 4 dose levels, interesting models may be

$$\begin{aligned} &M_f : \text{no constraint}, && M_3 : \mu_1 < \mu_2 < \mu_3 < \mu_4, \\ &M_1 : \mu_1 < \mu_2, && M_4 : \mu_1 < \mu_2 < \mu_3 = \mu_4, \\ &M_2 : \mu_1 < \mu_2, \mu_1 < \mu_3, \mu_1 < \mu_4, && M_5 : \mu_1 = \mu_2 = \mu_3 = \mu_4. \end{aligned} \tag{2}$$

See Klugkist et al. (2005) for illustrative examples.

Inference on inequality/equality constrained models has received a lot of attention in the frequentist literature. See, for example, Barlow et al. (1972), Robertson et al. (1988), Silvapulle and Sen (2004), Dykstra et al. (2002), and Shyamal et al. (2005). However, in frequentist methods for testing the hypotheses subject to inequality constraints on the parameters, statistical distributions of test statistics are often hard to find or are complicated. Also, the frequentist methods may have problems when non-nested models are compared (Marden, 2000; Klugkist et al., 2005).

Simple model selection criteria such as AIC (Akaike, 1987) and BIC (Shwartz, 1978), which incorporate model complexity in terms of the number of parameters in the model, are inappropriate for comparing models subject to inequality constraints.

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For instance, the model M_1 in (2) has the same number of parameters as the model M_f and hence the penalty terms in AIC and BIC would be the same for the two models. To get around this, Anraku (1999) and Kuiper et al. (2011, 2012) proposed information criteria which incorporate the model complexity from inequality constraints. However, it is often difficult to calculate the penalty terms of the criteria especially when the number of means is large.

Recently, Bayesian model selection methods in the context of testing hypotheses subject to inequality constraints on parameters have attracted many practitioners and researchers, since it implicitly account for model complexity induced by the number of parameters as well as the restricted parameter space of models. See Moreno (2005), Klugkist et al. (2005), Hoijtink et al. (2008) and Hoijtink (2012).

In practice, interesting models often contain both inequality and equality constraints on parameters, such as the models M_4 and M_5 in (2). Inequality constraints are easy to handle since the Bayes factor of a model with only inequality constraints against the unrestricted, encompassing model is the ratio of posterior and prior probabilities of the restricted region, under the encompassing model (Klugkist and Hoijtink, 2007). The probabilities can be easily estimated by the proportions of samples satisfying the restriction. On the other hand, equality constraints cannot be handled in the same way because the probability of a equality constrained region is zero under a continuous distribution. To get around this, Laudy and Hoijtink (2007) and Klugkist and Hoijtink (2007) converted equality constraints such as $\mu_1 = \mu_2$ to about equality constraints $|\mu_1 - \mu_2| < \varepsilon$, and apply the method for models with inequality constraints. This procedure is repeated for a decreasing sequence of ε, $\varepsilon_1 > \varepsilon_2 > \cdots$, until there is no significant change in the Bayes factors for two consecutive ε_i's. Wetzels et al. (2010) showed that the Bayes factor obtained from this iterative procedure converges to the Savage–Dickey density ratio (Dickey, 1971) when the model is subject to only equality constraints. The iterative procedure has been used to handle equality constraints in models with both inequality and equality constraints in Mulder et al. (2010), Klugkist et al. (2010), and Van Wesel et al. (2011). However, the iterative method is only an approximation and it may be time consuming.

In this article, we propose a Bayesian model selection approach for comparing models subject to both inequality and equality constraints. We adopt the encompassing prior approach proposed by Klugkist et al. (2005) and Hoijtink et al. (2008) and derive the Bayes factor for a model with a combination of inequality and equality constraints, which is a generalization of the Bayes factor for a model with only inequality (equality) constraints. We then propose a method which estimates the Bayes factors for all inequality/equality constrained models under consideration *simultaneously* by using a set of samples from the *encompassing* model. Note that the method requires samples only from the encompassing model even for equality constrained models, unlike other methods which need to fit reduced dimensional models to handle equality constraints.

The paper is organized as follows. Section 2 introduces priors and derives posteriors of the means under the encompassing model. In Section 3, the Bayes factors of models with inequality and equality constraints are derived and a simple estimation method is proposed. Section 4 provides the results of a simple simulation study, which demonstrate performance of the proposed method. Section 5 analyzes a real example. Section 6 concludes with a summary and discussion.

2. Prior and posterior

Following the suggestions from Klugkist et al. (2005), we assume that μ_i's have a common prior distribution, independently of each other. As the common prior distribution of μ_i's we choose a normal distribution with a variance proportional to the sample variance σ^2, and as a prior of σ^2 we choose an inverse gamma distribution. Thus, the priors are given as

$$\mu_i|\sigma^2 \sim N\left(\mu_0, \frac{1}{k_0}\sigma^2\right), \quad \sigma^2 \sim IG(a, b), \tag{3}$$

where $N(\mu_0, \frac{1}{k_0}\sigma^2)$ denotes the normal distribution with mean μ_0 and variance $\frac{1}{k_0}\sigma^2$, and $IG(a, b)$ denotes the inverse gamma distribution with mode b/a.

Given the likelihood from (1) and the prior (3), it can be shown that the posterior distribution of σ^2 and the conditional posterior distribution of μ_i given σ^2 are given as

$$\sigma^2|\mathbf{y} \sim IG\left(a + \frac{1}{2}\sum_i n_i,\ b + \frac{1}{2}\sum_i\sum_j (y_{ij} - \bar{y}_i)^2 + \frac{1}{2}\sum_i \frac{n_i k_0}{n_i + k_0}(\bar{y}_i - \mu_0)^2\right),$$

$$\mu_i|\sigma^2, \mathbf{y} \sim N\left(\frac{n_i\bar{y}_i + k_0\mu_0}{n_i + k_0}, \frac{\sigma^2}{n_i + k_0}\right), \quad i = 1, \ldots, k.$$

Thus, independent samples of $(\boldsymbol{\mu}, \sigma^2)$, $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_k)$, can be generated easily from the posterior distributions.

For models with equality constraints on μ_i's, $\mu_1 = \mu_2 = \mu_3$, for instance, we will need the marginal densities of $(\mu_2 - \mu_1, \mu_3 - \mu_2)$ to compute Bayes factors in the next section. Thus, we apply linear transformations on μ_i's for ease of exposition. For instance, if we let $\theta_1 = \mu_1$, $\theta_2 = \mu_2 - \mu_1$, $\theta_3 = \mu_3 - \mu_2$, and $\theta_4 = \mu_4 - \mu_3$, the restrictions of the model M_4 in (2) becomes $\theta_2 > 0$, $\theta_3 > 0$, $\theta_4 = 0$ so that the inequality (equality) constraints on μ_i's are equivalent to positivity (zero) constraints on θ_i's. We will use both $\boldsymbol{\theta}$ and $\boldsymbol{\mu}$ interchangeably since one can be retrieved easily from the other. Obviously, the conditional prior and posterior distributions of $\boldsymbol{\theta}$ given σ^2 are also multivariate normals and samples of $\boldsymbol{\theta}$ can be obtained