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BAYESIAN INFERENCES ON NONLINEAR FUNCTIONS OF THE PARAMETERS IN LINEAR REGRESSION

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Abstract. A variety of statistical problems (e.g. the x-intercept in linear regression, the abscissa of the point of intersection of two simple linear regression lines or the point of extremum in quadratic regression) can be viewed as questions of inference on nonlinear functions of the parameters in the general linear regression model. In this paper inferences on the threshold temperatures and summation constants in crop development will be made. A Bayesian approach for the general formulation of this problem will be developed. By using numerical integration, credibility intervals for individual functions as well as for linear combinations of the functions of the parameters can be obtained. The implementation of an odds ratio procedure is facilitated by placing a proper prior on the ratio of the relevant parameters.

Key words and phrases: Bayesian inferences, threshold temperatures, summation constants, regression, intervals of highest posterior density, posterior odds ratio.

1. Introduction

Consider the general linear regression model $\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\phi} + \boldsymbol{\epsilon}$ where $\boldsymbol{y}$ is a $n \times 1$ vector of observable random variables, $\boldsymbol{X}$ a $n \times p$ matrix of known constants, $\boldsymbol{\phi}$ a $p \times 1$ vector of unknown parameters and $\boldsymbol{\epsilon}$ a $n \times 1$ vector of unobservable random variables, referred to as errors. It is assumed that $\boldsymbol{\epsilon}$ is normally distributed with mean $\mathbf{0}$ and covariance matrix $\sigma^2 \boldsymbol{I}_n$ where $\mathbf{0}$ is a $n \times 1$ vector of zeros and $\boldsymbol{I}_n$ the identity matrix of order n. Also $(\boldsymbol{X}'\boldsymbol{X})$ is assumed to be nonsingular.

Our interest is in nonlinear functions of the parameters $\boldsymbol{\phi}$. Examples where nonlinear functions of the parameters are of interest include:

(i) the x-intercept in linear regression,

(ii) the abscissa of the point of intersection of two simple linear regression lines,

(iii) the point of extremum in quadratic regression,

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(iv) relative potency in a slope ratio bio-assay and

(v) bio-equivalence of two treatments.

In this note, inferences on nonlinear functions in crop development models will be considered. The simplest crop development model assumes a linear relationship between temperature (x) and rate of development (y) (Holmes and Robertson (1959), Edey (1977), Robertson (1983)) and can be written as $y = \alpha + \beta x + \epsilon$. In crop development models, nonlinear functions of the parameters α and β have certain physical meanings. For example the x-intercept, $\gamma = -\alpha/\beta$, is the "apparent" threshold temperature at which development begins to take place while $k = 1/\beta$ is the value of the summation constant, the number of degree days, or the sum of the daily temperature remainder indices required for the crop to pass through the phenological phase in question.

The Department of Agricultural Meteorology at the University of the Orange Free State has studied the influence of temperature on the rate of wheat development. Five wheat varieties, namely Wilge, Betta, Karee, Scheepers 69 and SST 102, were used in the experiment and the research was conducted at a number of experimental stations throughout South Africa. The main reasons for doing this research were

(1) to obtain sample data for the construction of confidence intervals on the threshold temperatures and summation constants and

(2) to do tests of hypotheses.

An example of such a set of data and the regression analysis is given in van der Merwe *et al.* (1989). The data for the other wheat varieties is available on request.

The usual tests for normality, heteroscedasticity, outliers, serial correlation, influential observations, etc. show no violations of model assumptions. The only exception is that the error variances among the five varieties (according to Bartlett's test) seem to differ from each other, which makes pooling inappropriate and the estimation of a common σ^2 invalid.

In the next paragraphs a Bayesian approach for the general formulation of this problem will be developed. By assuming improper priors on the parameters α, β and σ, the posterior distributions for γ and k can be derived. By using numerical integration, credibility intervals for individual functions as well as for linear combinations of the functions of the parameters can be obtained easily. The implementation of the odds ratio procedure is facilitated by placing a proper prior on the ratio of relevant parameters.

2. Posterior distribution for $\gamma = -\alpha/\beta$

2.1 *Improper priors on the parameters*

One possible prior on α, β and σ is

$$p(\alpha, \beta, \sigma) \propto \frac{1}{\sigma} \qquad -\infty < \alpha, \beta < \infty \tag{2.1}$$

which implies that α, β and $\log \sigma$ are locally uniform and independently distributed.

Then on combining (2.1) with the likelihood function

$$p(\boldsymbol{y} \mid \boldsymbol{X}, \alpha, \beta, \sigma) \propto \frac{1}{\sigma^n} \exp\left[\frac{-1}{2\sigma^2} \sum_{i=1}^{n} (y_i - \alpha - \beta x_i)^2\right]$$

and integrating with respect to σ it can easily be shown (Zellner ((1971), p. 61)) that the joint posterior distribution for the parameters α and β is given by

$$f(\alpha, \beta \mid \boldsymbol{y}, \boldsymbol{X}) \propto \{1 + (\alpha - \hat{\alpha}, \beta - \hat{\beta})(vS^2)^{-1}(\boldsymbol{X}'\boldsymbol{X})(\alpha - \hat{\alpha}, \beta - \hat{\beta})'\}^{-n/2} \tag{2.2}$$

which is a vector Student t distribution with

$$v = n - p, \quad \boldsymbol{\phi} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \quad \hat{\boldsymbol{\phi}} = \begin{pmatrix} \hat{\alpha} \\ \hat{\beta} \end{pmatrix} = (\boldsymbol{X}'\boldsymbol{X})^{-1}(\boldsymbol{X}'\boldsymbol{y}),$$

$$(vS^2)^{-1}(\boldsymbol{X}'\boldsymbol{X}) = (vS^2)^{-1} \begin{pmatrix} n & \sum_{i=1}^{n} x_i \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 \end{pmatrix} = \begin{pmatrix} S^{11} & S^{12} \\ S^{21} & S^{22} \end{pmatrix},$$

$S^2 = (\boldsymbol{y} - \boldsymbol{X}\hat{\boldsymbol{\phi}})'(\boldsymbol{y} - \boldsymbol{X}\hat{\boldsymbol{\phi}})/v$ and $p = 2$ in the case of simple regression. The posterior distribution serves as a basis for making inferences on $\gamma = -\alpha/\beta$ and $k = 1/\beta$.

By using (2.2) it can be shown (Press (1969), Zellner ((1971), p. 279) and Hunter and Lamboy (1981)) that the posterior distribution for the threshold temperature, γ, is given by

$$f(\gamma \mid \boldsymbol{y}, \boldsymbol{X}) \propto \frac{b_0^{-(v+1)/2}}{b_1^{1/2}} \left\{ b_2[1 - 2F(d)] - 2\left(\frac{b_0}{(v+1)b_1}\right)^{1/2} F_1(d) \right\} \tag{2.3}$$

where $F(d) = \int_{-\infty}^{d} p(t)dt$, $F_1(d) = \int_{-\infty}^{d} tp(t)dt$, $p(t)$ is the Student t p.d.f. with $(v+1)$ degrees of freedom,

$$d = -\{(v+1)b_1/b_0\}^{1/2} b_2, \quad b_1 = \gamma^2 S^{11} - 2\gamma S^{12} + S^{22},$$

$$b_2 = \frac{-\gamma\hat{\alpha}S^{11} + (\hat{\alpha} - \gamma\hat{\beta})S^{12} + \hat{\beta}S^{22}}{b_1} \quad \text{and}$$

$$b_0 = 1 + \hat{\alpha}^2 S^{11} + 2\hat{\alpha}\hat{\beta}S^{12} + \hat{\beta}^2 S^{22} - \frac{[-\gamma\hat{\alpha}S^{11} + (\hat{\alpha} - \gamma\hat{\beta})S^{12} + \hat{\beta}S^{22}]^2}{b_1}.$$

The Bayesian posterior density for γ is the posterior density for a ratio of bivariate t random variables and yields a distribution that has infinite moments. According to Hunter and Lamboy (1981) this fact is not disturbing because one can always plot the posterior density of γ and readily interpret it. One may choose, for example, to find its mode and the highest posterior density (HPD) interval. From a Bayesian point of view, the existence of a finite variance is unnecessary.

Theoretically, if one's model is adequate, all the relevant information is contained in the appropriate posterior distribution. Furthermore, it is easy and natural for practitioners to use posterior distributions in making inferences.

The classical frequency approach for making inferences on γ is to estimate it by $\hat{\gamma} = -\hat{\alpha}/\hat{\beta}$ (the maximum likelihood estimate) and apply Fieller's theorem (Fieller (1932, 1954)) for the construction of confidence intervals or tests. It is, however, well-known that the Fieller region can be empty, the whole line, or the complement of a finite interval and that this tends to occur when the F statistic for testing $\beta = 0$ is sufficiently small. Since this cannot occur with a proper posterior distribution (such as (2.3)), the Bayesian approach is preferred.

On the other hand, it is true that Fieller's theorem will sometimes provide adequate approximations for the desired Bayesian results. Hunter and Lamboy (1981) conjectured that Fieller's method will provide approximate $(1-\alpha)100\%$ intervals differing by not more than $2\,\Pr(t_v \geq |\hat{\beta}|/S^{22})$ from the probability actually contained in the $(1-\alpha)100\%$ HPD intervals. The posterior density function $f(\gamma \mid \boldsymbol{y}, \boldsymbol{X})$ for variety Wilge is given in Fig. 1.

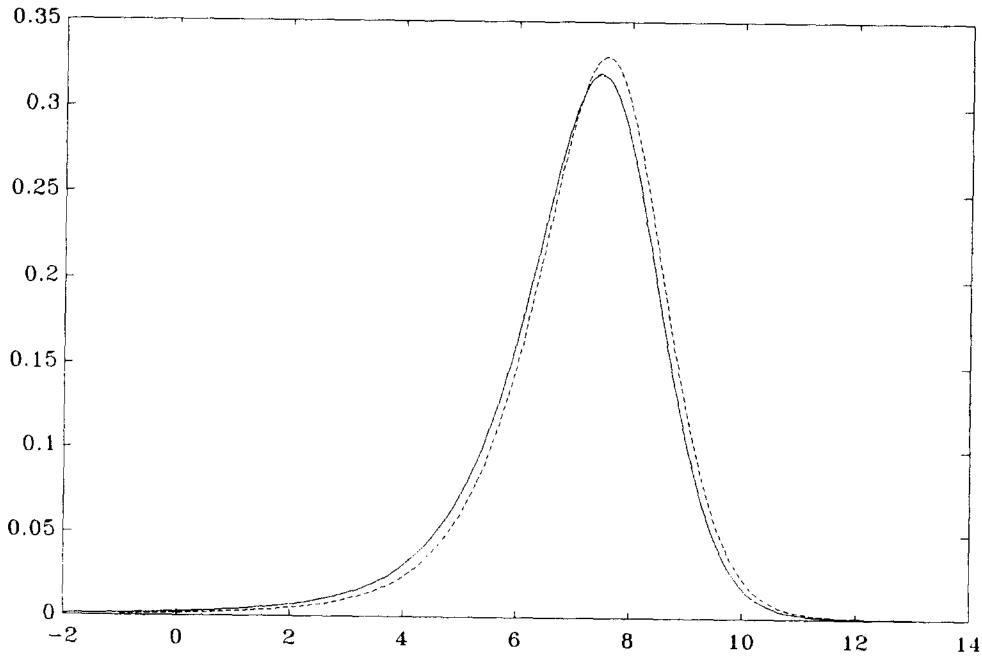

Fig. 1. Density functions $f(\cdot \mid \boldsymbol{X}, \boldsymbol{y})$ ("- -") and $\tilde{f}(\cdot \mid \boldsymbol{X}, \boldsymbol{y})$ ("—")—for variety Wilge.

By performing numerical integration on $f(\gamma \mid \boldsymbol{y}, \boldsymbol{X})$, the modal values and 95% highest posterior density (HPD) intervals for the five varieties were calculated and are given in Table 1.

Table 1. The modal values and 95% highest posterior density (HPD) intervals of the threshold temperatures for the five varieties.

Varieties	Modal values	95% HPD intervals	
		Lower limits	Upper limits
Wilge	7.60	4.13	9.91
Betta	8.51	3.30	11.45
Karee	8.45	0.63	11.81
Scheepers 69	9.51	5.58	11.62
SST 102	6.65	−0.18	9.98

2.2 *Proper prior on* γ

Another approach for obtaining the posterior distribution of γ is to put a prior on γ itself, independent of the locally uniform priors on β and $\log \sigma$, so that

$$p(\gamma, \beta, \sigma) \propto g(\gamma)\sigma^{-1}. \tag{2.4}$$

This is similar to an approach used by Buonaccorsi and Gatsonis (1988). The likelihood function is then written as

$$f(\boldsymbol{y} \mid \boldsymbol{X}, \gamma, \beta, \sigma) \propto \frac{1}{\sigma^n} \exp\left[-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i + \beta(\gamma - x_i))^2\right].$$

The posterior distribution of γ is given by

$$\tilde{f}(\gamma \mid \boldsymbol{X}, \boldsymbol{y}) \propto g(\gamma) G(\gamma \mid \boldsymbol{X}, \boldsymbol{y}) \tag{2.5}$$

where

$$\begin{aligned} G(\gamma \mid \boldsymbol{X}, \boldsymbol{y}) = {} & [S_{xx} + n(\gamma - \bar{x})^2]^{n/2-1} \\ & \cdot [nS_{yy}(\gamma - b')^2 + S_{xx}(1 - r^2)(S_{yy} + n\bar{y}^2)]^{-(n-1)/2} \end{aligned} \tag{2.6}$$

and

$$S_{xx} = \sum_{i=1}^{n}(x_i - \bar{x})^2, \quad S_{yy} = \sum_{i=1}^{n}(y_i - \bar{y})^2, \quad S_{xy} = \sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}),$$
$$b' = \bar{x} - \frac{S_{xy}}{S_{yy}}\bar{y}, \quad r^2 = \frac{S_{xy}^2}{S_{xx}S_{yy}}.$$

Note that G is not integrable on $(-\infty, \infty)$ and thus an improper prior on γ will lead to an improper posterior for γ and should not be used. However, any proper prior on γ will lead to a proper distribution, since G is a bounded function. If a uniform prior is used on the interval $[L, U]$, then

$$\tilde{f}(\gamma \mid \boldsymbol{X}, \boldsymbol{y}) \propto G(\gamma \mid \boldsymbol{X}, \boldsymbol{y}), \qquad L < \gamma < U. \tag{2.7}$$

The posterior is quite robust to the actual values of L and U, as long as the integrated likelihood G is effectively covered by the interval $[L, U]$.

In Fig. 1 the posterior distributions (2.3) and (2.7) for variety Wilge are given and it can be seen that they are fairly close together. Similar patterns of agreement were observed for the other wheat varieties.

The range of integration for obtaining $\tilde{f}(\cdot \mid \boldsymbol{X}, \boldsymbol{y})$ as shown in Fig. 1 was quite large, from -10 to 15. This approach (i.e. the procedure leading to (2.7)) will be used in the next section for the posterior odds ratio, mainly because of less complicated numerical calculations than in the case of (2.3).

3. Comparing threshold temperatures

3.1 *Credibility intervals*

As mentioned in the introductory paragraph one of the main reasons for conducting this experiment was to determine whether the threshold temperatures of the five varieties differ from each other, i.e. to test the hypothesis

$$H_0 : \gamma_1 = \gamma_2 = \gamma_3 = \gamma_4 = \gamma_5 (= \gamma_0), \tag{3.1}$$

where 1 stands for Wilge, 2 for Betta, etc. in the same order as given in Table 1. The classical frequency approach is to obtain the likelihood ratio statistic, which is extremely difficult to derive. Even if this was done, the result would be complicated and not of much practical use.

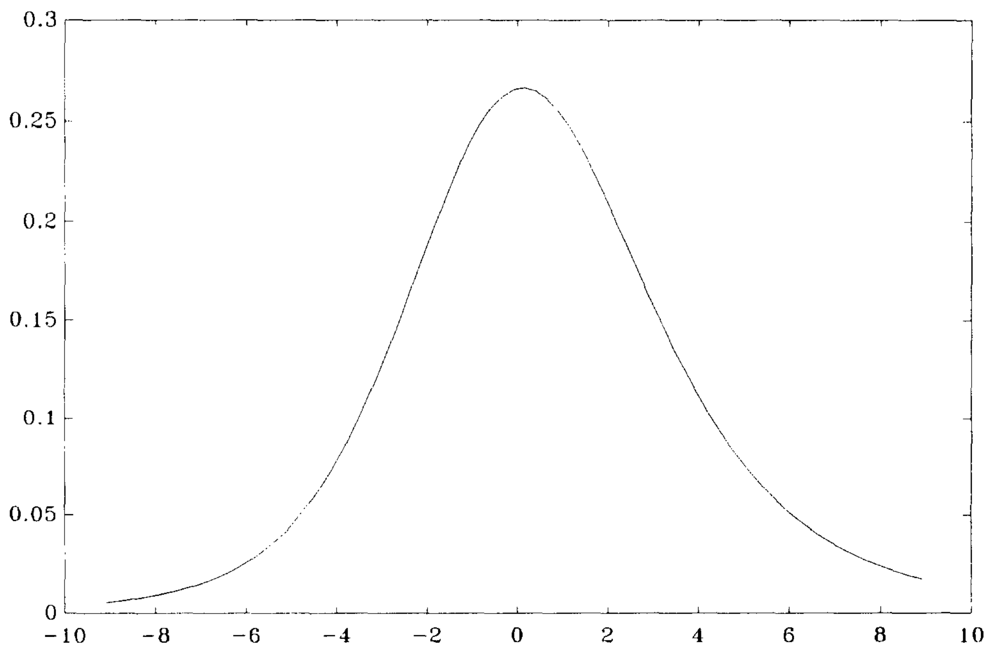

Fig. 2. The posterior distribution of the difference in threshold temperatures between Betta and Karee.

In the Bayesian case, the posterior distribution contains all the available information about a parameter. Therefore, one approach to determine if the threshold temperatures of the five wheat varieties differ from each other is to calculate the 95% credibility intervals of the differences between parameter values for all possible pairs. If these intervals contain zero, the conclusion will be made that the hypothesis (3.1) is true.

Using the approach that leads to (2.3) it follows that the posterior distribution of $\Pi_{i,j} = \gamma_i - \gamma_j$ $(i = 1, \ldots, 5,\ j = 1, \ldots, 5)$ is given by

$$f_{\Pi_{i,j}}(\Pi) = \int_{-\infty}^{\infty} f(\Pi + \gamma_i) f(\gamma_j) d\gamma_j.$$

By using numerical integration the posterior distribution of $\Pi_{2,3} = \gamma_2 - \gamma_3$ (i.e. the posterior distribution of the difference in threshold temperatures between Betta and Karee) was calculated and is shown in Fig. 2, while in Table 2 the 95% credibility intervals of the differences between threshold temperatures for all possible pairs are given.

From Table 2 it is clear that all these intervals contain zero, which is a good indication of no real differences among the threshold temperatures of the five varieties. We must, however, warn that indiscriminate use of this procedure may be dangerous, for if we have say r varieties, where r is large, then the probability is high that at least one of the $r(r-1)/2$ differences will, due to chance alone, be judged significantly different. In other words, this method will tend to give too many significantly different cases. Having obtained none in this case means that we can be confident that there are no real differences among the threshold temperatures.

Table 2. 95% credibility intervals of the differences between the threshold temperatures.

Pair (i,j)	95% credibility intervals of $\Pi_{i,j} = \gamma_i - \gamma_j$	
	Lower limit	Upper limit
(1,2)	−3.95	5.98
(1,3)	−5.49	8.66
(1,4)	−7.66	7.29
(1,5)	−3.24	8.00
(2,3)	−7.67	9.06
(2,4)	−11.00	7.30
(2,5)	−5.10	8.36
(3,4)	−9.13	6.34
(3,5)	−7.99	10.05
(4,5)	−3.98	8.92

3.2 *Bayes factor*

Another method to determine if the threshold temperatures differ from each other is to examine the posterior odds ratio or Bayes factor in favour of the null hypothesis (3.1). Using the approach described in Subsection 2.2, it follows that the likelihood function of all the data under H_0 is given by

$$(3.2)\qquad \prod_{j=1}^{5} p(\boldsymbol{y}_j \mid \boldsymbol{X}, \beta_j, \sigma_j, \gamma_0) = (2\pi)^{\sum n_j/2} \prod_{j=1}^{5} \sigma_j^{n_j} \exp\left[-\sum_{j=1}^{5} \frac{1}{2\sigma_j^2} \sum_{i=1}^{n_j} (y_{ij} + \beta_j(\gamma_0 - x_{ij}))^2\right]$$

and by $\prod_{j=1}^{5} p(\boldsymbol{y}_j \mid \boldsymbol{X}, \beta_j, \sigma_j, \gamma_j)$ under a composite alternative.

The Bayes factor is then defined by $bf = f_0/f_1$ where

$$(3.3)\qquad f_0 = \int \cdots \int \prod_{j=1}^{5} p(\boldsymbol{y}_j \mid \boldsymbol{X}, \beta_j, \sigma_j, \gamma_0) p_0(\gamma_0, \boldsymbol{\beta}, \boldsymbol{\sigma}) d\gamma_0 d\beta_j d\sigma_j,$$

$$(3.4)\qquad f_1 = \int \cdots \int \prod_{j=1}^{5} p(\boldsymbol{y}_j \mid \boldsymbol{X}, \beta_j, \sigma_j, \gamma_j) p_1(\boldsymbol{\gamma}, \boldsymbol{\beta}, \boldsymbol{\sigma}) d\gamma_j d\beta_j d\sigma_j.$$

The prior distributions under the null and alternative hypotheses are

$$(3.5)\qquad p_0(\gamma_0, \boldsymbol{\beta}, \boldsymbol{\sigma}) \propto g_0(\gamma_0) \prod_{j=1}^{5} \frac{1}{\sigma_j}$$

and

$$(3.6)\qquad p_1(\boldsymbol{\gamma}, \boldsymbol{\beta}, \boldsymbol{\sigma}) \propto g_1(\boldsymbol{\gamma}) \prod_{j=1}^{5} \frac{1}{\sigma_j}$$

respectively, where $\boldsymbol{\beta}, \boldsymbol{\gamma} \in R^5$, $\gamma_0 \in R^1$ and $0 < \sigma_i < \infty$.

The density functions $g_0(\cdot)$ and $g_1(\cdot)$ should be proper, since they are of different dimensionalities and the Bayes factor can then be extremely sensitive to an improper prior used under the alternative. The same does not apply to the other parameters $\boldsymbol{\beta}$ and $\boldsymbol{\sigma}$. Since we assume identical distributions for these parameters under both hypotheses, the Bayes factor is quite robust with respect to these priors. For a discussion of improper priors for hypothesis testing, see Shafer (1982) and Groenewald and de Waal (1989). Equations (3.3) and (3.4) reduce to

$$(3.7)\qquad f_0 = \int g_0(\gamma_0) \prod_{j=1}^{5} [T_{0j}^{n_j/2-1} R_{0j}^{-(n_j-1)/2}] d\gamma_0$$

and

$$(3.8)\qquad f_1 = \int \cdots \int g_1(\boldsymbol{\gamma}) \prod_{j=1}^{5} [T_{1j}^{n_j/2-1} R_{1j}^{-(n_j-1)/2} d\gamma_j],$$

where

$$T_{0j} = S_{xxj} + n_j(\gamma_0 - \bar{x}_j)^2, \tag{3.9}$$

$$R_{0j} = n_j S_{yyj}(\gamma_0 - b'_j)^2 + S_{xxj}(1 - r_j^2)(S_{yyj} + n_j\bar{y}_j^2), \tag{3.10}$$

and the quantities in the equations are defined as in Subsection 2.2, but for the j-th sample. T_{1j} and R_{1j} are as (3.9) and (3.10) with γ_0 replaced by γ_j.

To obtain a reasonable prior distribution for γ for the application to threshold temperatures, experts at the Department of Meteorology were consulted. Consensus was reached on a range of about 15, from -2 to 13, approximately symmetrical and with values near the end points highly unlikely. So we assume identical normal prior distributions under the null and alternative hypotheses, all with standard deviations of $\tau = 2.5$.

The Bayes factor is then a convex function of the prior mean with minimum $bf^* = 2.71$ at a prior mean $\mu = 7.35$. This indicates that the data supports the null hypothesis.

This lower bound on the Bayes factor is of course sensitive to the dispersion of the prior and will move from zero to infinity as τ moves from zero to infinity. For example, if $\tau = 2$, then $bf^* = 1.84$ at $\mu = 7.46$, and $bf^* < 1$ when $\tau < 1.2$.

The minimum Bayes factor for a uniform prior was also examined and gave similar results. For a uniform prior over an interval of length 8 (2.9 to 10.9), it was found that $bf^* = 2.63$ and bf^* drops below 1 only when the length of the interval is reduced to about 4.

The conclusion is that the null hypothesis should be accepted unless the prior opinion about the value of γ is very strong, i.e. a small prior variance. Clearly the prior opinion in this application is not strong enough to reduce the Bayes factor to a critical level.

4. Credibility intervals for the summation constant $k = 1/\beta$

It is well-known that the $(1-\alpha)100\%$ credibility (confidence) limits for β are given by the interval

$$[\hat{\beta} - t_{v;\alpha/2}[\hat{V}(\hat{\beta})]^{1/2}; \hat{\beta} + t_{v;\alpha/2}[\hat{V}(\hat{\beta})]^{1/2}] \tag{4.1}$$

where $[\hat{V}(\hat{\beta})] = S^2C$ and $S^2 = (\boldsymbol{y} - \boldsymbol{X}\hat{\phi})'(\boldsymbol{y} - \boldsymbol{X}\hat{\phi})/v$ and C is obtained from $(\boldsymbol{X}'\boldsymbol{X})^{-1} = \begin{pmatrix} A & B \\ B & C \end{pmatrix}$. Once again $t_{v;\alpha/2}$ is the $(1-\alpha/2)$ percentile of the Student t distribution with v degrees of freedom.

From (4.1) it can be seen that a $(1-\alpha)100\%$ credibility interval for $k = 1/\beta$ is given by

$$\left[\frac{1}{\hat{\beta} + t_{v;\alpha/2}[\hat{V}(\hat{\beta})]^{1/2}}; \frac{1}{\hat{\beta} - t_{v;\alpha/2}[\hat{V}(\hat{\beta})]^{1/2}}\right]. \tag{4.2}$$

Contrary to (4.1), the interval (4.2) is not a symmetrical interval nor is it the shortest possible interval. The reason for this is that the transformation $k = 1/\beta$ is not linear which means that the posterior density for k, i.e.

$$(4.3)\quad f(k \mid \boldsymbol{X}, \boldsymbol{y}) = \frac{\Gamma\left(\frac{v+1}{2}\right)(vS^2)^{v/2}\sqrt{\sum_{i=1}^{n}(x_i-\bar{x})^2}}{\Gamma\left(\frac{v}{2}\right)\sqrt{\pi}k^2\left[vS^2+\sum_{i=1}^{n}(x_i-\bar{x})^2\left(\frac{1}{k}-\hat{\beta}\right)^2\right]^{(v+1)/2}}$$

$$-\infty < k < \infty$$

can be non-symmetrical. This can be seen from Fig. 3 where the posterior density $f(k \mid \boldsymbol{X}, \boldsymbol{y})$ for variety Betta is given.

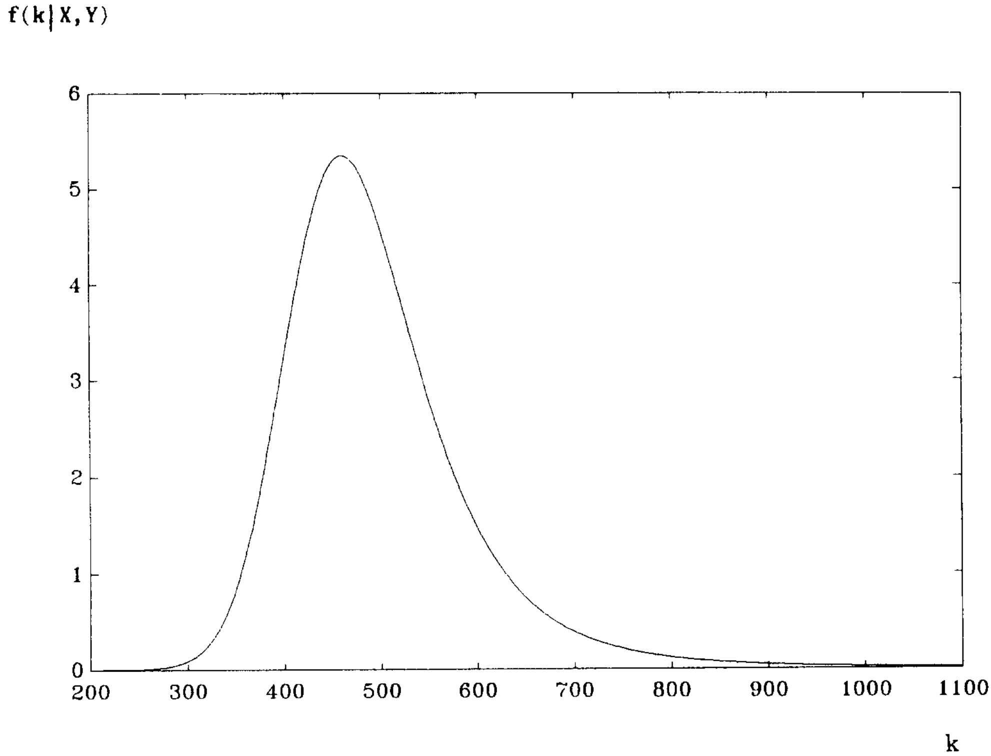

Fig. 3. The posterior density $f(k \mid \boldsymbol{X}, \boldsymbol{y})$ for variety Betta.

The shortest possible HPD interval (symmetrical round the modal value) can be obtained by numerically integrating $f(k)$ or by interpolating in tables of the Student t distribution. The lower and upper boundaries of these intervals are given in Table 3.

Table 3. The 95% inverse intervals (equation (4.2)) as well as the HPD intervals for the 5 varieties.

Varieties	Modal values	95% credibility intervals	
		Inverse interval	HPD interval
Wilge	462.5	376.9–627.8	374.9–621.6
Betta	460.0	356.1–738.5	302.9–675.2
Karee	394.1	292.6–792.9	252.6–697.4
Scheepers	350.7	273.9–556.0	256.5–520.7
SST 102	526.5	402.5–919.1	384.8–863.1

The average lengths of the inverse and HPD intervals are 386.46 and 361.25 respectively. The largest improvement in interval length is for variety Karee where the difference between the inverse and HPD interval is 55.5, an improvement of 11.1%.

The construction of credibility intervals and hypothesis testing can be done in the same way as for the threshold temperatures.

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