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FULL BAYESIAN SIGNIFICANCE TEST: THE BEHRENS-FISHER AND COEFFICIENTS OF VARIATION PROBLEMS

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Full Bayesian Significance Test: the Behrens-Fisher and Coefficients of Variation Problems

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Abstract

The Full Bayesian Significance Test (FBST) for precise hypotheses is presented, with some applications relevant to Biology. The FBST is an alternative to significance tests or, equivalently, to *p-values*. In the FBST we compute the evidence of the precise hypothesis. This evidence is the probability of the complement of a credible set "tangent" to the submanifold (of the parameter space) that defines the null hypothesis. We use the FBST in applications arising in population dynamics, genetics and biology, like testing the Behrens-Fisher problem, coefficients of variation and Hardy-Weinberg equilibrium.

KEY WORDS: Behrens-Fisher; Coefficient of Variation; Evidence, Global optimization; Numerical integration; p-value; Posterior density; Hardy-Weinberg equilibrium. AMS: 62A15; 62F15; 62H15.

1 Introduction

The Full Bayesian Significance Test (FBST) is presented in Pereira and Stern (1999b) as a coherent Bayesian significance test. The FBST is intuitive and has a geometric characterization. It can be easily implemented using modern numerical optimization and integration techniques. The method is "Full" Bayesian and consists in the analysis of credible sets. By Full we mean that we need only the knowledge of the parameter space represented by its posterior distribution.

The FBST needs no additional assumption, like a positive probability for the precise hypothesis, that generates the Lindley's paradox effect. The FBST regards likelihoods as the proper means for representing statistical information, a principle stated by Royall (1997) to simplify and unify statistical analysis. Another important aspect of the FBST is its consistency with the "benefit of the doubt" juridical principle. These remarks will be understood in the sequel.

Significance tests are regarded as procedures for measuring the consistency of data with a null hypothesis, Cox (1977) and Kempthorne and Folks (1971). *p-values* are a tail area under the null hypothesis, calculated in the sample space, not in the parameter space where the hypothesis is formulated.

Previously defined Bayesian significance tests, like Bayes Factor or the posterior probability of the null hypothesis, consider the *p-value* as a measure of evidence of the null hypothesis and present alternative Bayesian measures of evidence, Aitkin (1991), Berger and Delampady (1987), Berger *et al.* (1997), Irony and Pereira (1986 and 1995), Pereira and Wechsler (1993), Sellke *et al.* (1999). As pointed out in Cox (1977), the first difficulty to define the *p-value* is the way the sample space is ordered under the null hypothesis. Pereira and Wechsler (1993) suggests a *p-value* that always regards the alternative hypothesis. To each of these measures of evidence one could find a great number of counter arguments. The most important argument against Bayesian tests for precise hypothesis is presented by Lindley (1957). Arguments against the classical *p-value* are full in the literature. The book by Royall (1997) and its review by Vieland *et al.* (1998) present interesting and relevant arguments for statisticians to start thing about new methods of measuring evidence. In a more philosophical terms, Carnap (1962), de Finetti (1989), Good (1983) and Popper (1989) discuss, in a great detail, the concept of evidence.

2 Motivation

In order to better illustrate the FBST we discus a well known problem. Given a sample from a normal distribution with unknown parameters, we want to test if the mean is equal to a constant. The hypothesis $\mu = c$ is a straight line. We have a precise hypothesis since it is defined by a manifold (surface) of dimension (one) strictly smaller than the dimension of the parameter space (two).

It can be shown that the conjugate family for the Normal Distribution is a family of bivariate distributions, where the conditional distribution of the mean, μ, for a fixed precision, $\rho = 1/\sigma^2$, is normal, and the marginal distribution of the precision, ρ, is gamma, DeGroot (1970), Lindley (1978). We use the standard improper priors, uniform on $]-\infty, +\infty[$ for μ, and $1/\rho$ on $]0, +\infty[$ for ρ, in

order to get a fair comparison with p-values, DeGroot (1970). Hence we have the parameter space, hypothesis and posterior joint distribution:

$$\Theta = \{(\mu, \rho) \in R \times R_+\} \ , \ \Theta_0 = \{(\mu, \rho) \in \Theta \,|\, \mu = c\}$$

$$f(\mu, \rho \,|\, x) \propto \sqrt{\rho}\, exp(-n\rho(\mu - u)^2/2) exp(-b\rho)\rho^{a-1}$$

$$x = [x_1 \ldots x_n] \ , \ a = \frac{n-1}{2} \ , \ u = \frac{1}{n}\sum_{i=1}^{n} x_i \ , \ b = \frac{n}{2}\sum_{i=1}^{n}(x_i - u)^2$$

In Figure 1 we plot some level curves of the posterior density function, including the level curve tangent to the hypothesis manifold. At the tangency point, θ^*, the posterior density attains its maximum, f^*, on the hypothesis. The interior of the tangent level curve, T^*, includes all points with posterior density greater than f^*, i.e. it is the highest probability density set tangent to the hypothesis.

The posterior probability of T^*, κ^*, gives an indication of inconsistency between the posterior and the hypothesis: Small values of κ^* indicate that the hypothesis traverses high density regions, favoring the hypothesis. Therefore we define $Ev(H) = 1 - \kappa^*$ as the measure of evidence (for the precise hypothesis).

In Figure 1 we test $c = 10$ with $n = 16$ observations of mean $m = 11$ and standard deviation $s = 1$, 2 and 3. We give the FBST evidence, Ev, and the standard t-test, tt.

Of course this example is a mere illustration: there is no need of new methods to test the mean of a normal distribution. However, efficient numerical optimization and integration computer programs, make it straightforward to extend the FBST to more complex structures. In sections 5 and 6 we present two important tests involving the normal distribution: Behrens-Fisher and Coefficient of variation comparison of two populations. These problems appear in several biological and pharmacological applications, and the tests in the literature are somewhat controversial. In section 7 we present the Hardy-Weinberg equilibrium problem, of extreme relevance in contemporary applied genetics, Weir (1996). Again, the tests in the literature are either asymptotic or exact but conditional. The FBST is exact and, more important, it performs well independently of sample size and low frequencies. For the sake of comparison with the standard tests, we present the simple case of two alleles.

The FBSF is also motivated by the authors' activities in the role of audit, control or certification agents, whose activities had to be consistent with the benefit of the doubt juridical principle, or safe harbor liability rule. This kind of principle establishes that there is no liability as long as there is a reasonable basis for belief, effectively placing the burden of proof on the plaintiff, who, in a

lawsuit, must prove false a defendant's misstatement. Such a rule also prevents the plaintiff of making any assumption not explicitly stated by the defendant, or tacitly implied by existing law or regulation. The use of an a priori point mass on the null hypothesis, as on standard Bayesian tests, can be regarded as such an ad hoc assumption. In the next section we give a more formal definition of the FBST.

3 The Evidence Calculus

Consider the random variable D that, when observed, produces the data d. The statistical space is represented by the triplet (Ξ, Δ, Θ) where Ξ is the sample space, the set of possible values of d, Δ is the family of measurable subsets of Ξ and Θ is the parameter space. We define now a prior model (Θ, B, π_d), which is a probability space defined over Θ. Note that in this model $Pr\{A \mid \theta\}$ has to be Θ measurable. As usual, after observing data d, we obtain the posterior probability model (Θ, B, π_d), where π_d is the conditional probability measure on B given the observed sample point, d. In this paper we restrict ourselves to the case where the functions π_d has a probability density function f.

To define our procedure we should concentrate only on the posterior probability space (Θ, B, π_d). First, we define T_φ as the subset of the parameter space where the posterior density is greater than φ.

$$T_\varphi = \{\theta \in \Theta \mid f(\theta) \geq \varphi\}$$

The credibility of T_φ is its posterior probability,

$$\kappa = \pi_d(T_\varphi) = \int_{T_\varphi} f(\theta \mid d)d\theta = \int_\Theta f_\varphi(\theta \mid d)d\theta$$

where $f_\varphi(x) = f(x)$ if $f(x) \geq \varphi$ and zero otherwise.

Now, we define f^* as the maximum of the posterior density over the null hypothesis, attained at the argument θ^*,

$$\theta^* \in arg\max_{\theta \in \Theta_0} f(\theta)\ , \quad f^* = f(\theta^*)$$

and define $T^* = T_{f^*}$ as the set "tangent" to the null hypothesis, H, whose credibility is κ^*.

The measure of evidence we propose in this article is the complement of the probability of the set T^*. That is, the evidence of the null hypothesis is

$$Ev(H) = 1 - \kappa^* \ \text{ or } \ 1 - \pi_d(T^*)$$

If the probability of the set T^* is "large", it means that the null set is in a region of low probability and the evidence in the data is against the null hypothesis. On the other hand, if the probability of T^* is "small", then the null hypothesis is in a region of high probability and the evidence in the data is in its favor. In the next section we give an operational construction of the FBST.

4 Numerical Optimization and Integration

We restrict the parameter space, Θ, to be always a subset of R^n, and the hypothesis is defined as a further restricted subset $\Theta_0 \subset \Theta \subseteq R^n$. Usually, Θ_0 is defined by vector valued inequality and equality constraints:

$$\Theta_0 = \{\theta \in \Theta \,|\, g(\theta) \leq 0 \wedge h(\theta) = 0\}.$$

Since we are working with precise hypotheses, we have at least one equality constraint, hence $dim(\Theta_0) < dim(\Theta)$. Let $f(\theta)$ be the posterior probability density function, as defined in the last section.

The computation of the evidence measure defined in the last section is performed in two steps, a numerical optimization step, and a numerical integration step. The numerical optimization step consists of finding an argument θ^* that maximizes the posterior density $f(\theta)$ under the null hypothesis. The numerical integration step consists of integrating the posterior density over the region where it is greater than $f(\theta^*)$. That is,

- Numerical Optimization step:

$$\theta^* \in arg\max_{\theta \in \Theta_0} f(\theta) \;, \quad \varphi = f^* = f(\theta^*)$$

- Numerical Integration step:

$$\kappa^* = \int_{\Theta} f_\varphi(\theta \,|\, d) d\theta$$

  where $f_\varphi(x) = f(x)$ if $f(x) \geq \varphi$ and zero otherwise.

Efficient computational algorithms are available, for local and global optimization as well as for numerical integration, Bazaraa *et al.* (1993), Horst *et al.* (1995), Luenberger (1984), Nocedal and Wright (1999), Pinter (1996), Krommer and Ueberhuber (1998), and Sloan and Joe (1994). Computer codes for several such algorithms can be found at software libraries as ACM, GSL and NAG, or at internet sites as *www.ornl.gov* and *www-rocq.inria.fr*.

We notice that the method used to obtain T^* and to calculate κ^* can be used under general conditions. Our purpose, however, is to discuss precise hypothesis testing, i.e. $dim(\Theta_0) < dim(\Theta)$, under absolute continuity of the posterior probability model, the case for which most solutions presented in the literature are controversial.

5 Behrens-Fisher

At the Behrens-Fisher problem we want to test the hypothesis that two normal random variables, with unknown means, μ_1 and μ_2, and unknown variances, σ_1^2 and σ_2^2, have the same mean:

$$\Theta = \{[\mu_1, \rho_1, \mu_2, \rho_2] \in (R \times R_+)^2\}$$

$$\Theta_0 = \{[\mu_1, \rho_1, \mu_2, \rho_2] \in \Theta \,|\, \mu_1 = \mu_2\}$$

At the optimization step it is better, for numerical stability, to maximize the log-likelihood. Given two samples, of size n_1 and n_2,

$$\begin{aligned} fl(\mu_1, \rho_1, \mu_2, \rho_2 \,|\, n_1, u_1, b_1, n_2, u_2, b_2) = \\ (n_1/2 - 1)log(\rho_1) - b_1\rho_1 - (n_1\rho_1/2)(\mu_1 - u_1)^2 \\ +(n_2/2 - 1)log(\rho_2) - b_2\rho_2 - (n_2\rho_2/2)(\mu_2 - u_2)^2 \end{aligned}$$

the hypothesis being represented by the constraint

$$g(\mu_1, \rho_1, \mu_2, \rho_2) = \mu_1 - \mu_2 = 0$$

The gradients of $fl(\,)$ and $g(\,)$ have easy analytical expressions, that can be given to the optimizer:

$$\begin{aligned} dfl &= [\, -n_1\rho_1(\mu_1 - u_1)\,,\ (n_1/2 - 1)/\rho_1 - b_1 - (n_1/2)(\mu_1 - u_1)^2\,, \\ &\quad -n_2\rho_2(\mu_2 - u_2)\,,\ (n_2/2 - 1)/\rho_2 - b_2 - (n_2/2)(\mu_2 - u_2)^2\,] \\ dg &= [1, 0, 1, 0] \end{aligned}$$

Table 1 presents results for some illustrative examples, comparing the FBST with the p-values of the Welsh approximated t-test, Lehmann (1986 pp. 208-209). While the FBST is a probability in the parameter space, the p-value is a probability in the sample space. Therefore we can only check if they agree in tendency, but there would be no meaning in a direct comparison of the figures. We are comparing the mean of a first sample, of size, mean, and standard deviation $n_1 = 16$, $m_1 = 100$ and $s_1 = 3$, with a second sample, of size and standard deviation $n_2 = 20$ and $s_2 = 3$. The mean of the second sample, m_2, is at the table.

Table 1: Tests for Behrens-Fisher

m_2	$FBST$	tt
100	1.00	1.00
101	0.93	0.34
102	0.50	0.06
103	0.13	0.01
104	0.02	0.00
105	0.00	0.00
$n_1 = 16$ $n_2 = 20$		
$m_1 = 100$ $s_1 = s_2 = 3$		

6 Coefficient of Variation Applications

The Coefficient of Variation (CV) of a random variable X is defined as the ratio $CV(X) = Std(X)/E(X)$, i.e. the ratio of its standard deviation by its mean. We want to test the hypothesis that two normal random variables, with unknown mean and variance, have the same CV. Using the same notation of the last section,

$$\Theta_0 = \{[\mu_1, \rho_1, \mu_2, \rho_2] \in \Theta \mid \mu_1^2\rho_1 = \mu_2^2\rho_2\}$$

The hypothesis is represented by the constraint

$$g(\mu_1, \rho_1, \mu_2, \rho_2) = \mu_1^2\rho_1 - \mu_2^2\rho_2 = 0$$

whose gradient can be given to the optimizer:

$$dg = [2\mu_1\rho_1 \ , \ \mu_1^2 \ , \ -2\mu_2\rho_2 \ , \ -\mu_2^2]$$

Table 2 presents results for some illustrative examples. Some simpler hypothesis on the CV are analyzed in Lehmann (1986). However we are not aware of exact p-values to compare with the FBST. We are comparing the coefficient of variation of a first sample, of size, mean, and standard deviation $n_1 = 16$, $m_1 = 100$ and $s_1 = 2$, with a second sample of size and mean $n_2 = 20$ and $m_2 = 200$. The standard deviation of the second sample, s_2, is at the table.

7 Hardy-Weinberg Equilibrium

In this biological application there is a sample of n individuals, where x_1 and x_3 are the two homozygote sample counts and $x_2 = n - x_1 - x_3$ is hetherozygote

Table 2: Tests for Coefficients of Variation

s_2	CV_1/CV_2	$FBST$
1	4.00	0.00
2	2.00	0.10
3	1.33	0.83
4	1.00	1.00
5	0.80	0.95
6	0.67	0.68
8	0.50	0.17
10	0.40	0.03
12	0.33	0.00

$n_1 = 16$ $n_2 = 20$ $s_1 = 2$
$m_1 = 100$ $m_2 = 200$

sample count. $\theta = [\theta_1, \theta_2, \theta_3]$ is the parameter vector. Here we consider only the uniform prior, for easier comparison with frequentist procedures. However other priors can be used, in particular, Dirichlet priors render a posterior with the same functional form. We present the simple biallelic case, but the FBST can be extended to multi-allelic problems, as required in studies of DNA databases.

The posterior density for this trinomial model is

$$f(\theta \mid x) \propto \theta_1^{x_1}\theta_2^{x_2}\theta_3^{x_3}$$

The parameter space and the null hypothesis set are:

$$\Theta = \{\theta \in R_+^3 \mid \theta_1 + \theta_2 + \theta_3 = 1\}$$

$$\Theta_0 = \{\theta \in \Theta \mid \theta_3 = (1 - \sqrt{\theta_1})^2\}$$

The log-likelihood to be optimized, the constraints, and all the gradients are:

$$\begin{aligned}
fl(\theta \mid x) &= x_1 \log(\theta_1) + x_2 \log(\theta_2) + x_3 \log(\theta_3) \\
dfl &= [x_1/\theta_1 \ , \ x_2/\theta_2 \ , \ x_2/\theta_2] \\
g_1 &= \theta_1 + \theta_2 + \theta_3 - 1 = 0 \\
g_2 &= (1 - \sqrt{\theta_1})^2 - \theta_3 = 0 \\
dg_1 &= [1 \ , \ 1 \ , \ 1] \\
dg_2 &= [-(1 - \sqrt{\theta_1})/\sqrt{\theta_1} \ , \ 0 \ , \ -1]
\end{aligned}$$

Table 3 presents figures, for $n = 20$, to compare $Ev(H)$ with the p-value with Yates continuity correction and the p-value for the Fisher exact test. Figure 2 presents Θ_0 and T^* for $x_1 = 5$, $x_2 = 5$ and $x_3 = 10$.

Table 3: Tests of Hardy-Weinberg equilibrium, $n = 20$

x_1	x_3	Ev	pV	Fisher	x_1	x_3	Ev	pV	Fisher
1	2	0.01	0.01	1.00	5	1	0.09	0.09	1.00
1	3	0.01	0.02	1.00	5	2	0.29	0.26	0.97
1	4	0.04	0.04	1.00	5	3	0.61	0.54	0.90
1	5	0.09	0.09	1.00	5	4	0.89	0.87	0.79
1	6	0.18	0.17	0.99	5	5	1.00	1.00	0.63
1	7	0.31	0.29	0.97	5	6	0.90	0.88	0.46
1	8	0.48	0.46	0.95	5	7	0.66	0.60	0.30
1	9	0.66	0.65	0.91	5	8	0.40	0.35	0.17
1	10	0.83	0.85	0.85	5	9	0.21	0.18	0.09
1	11	0.95	0.81	0.78	5	10	0.09	0.08	0.04
1	12	1.00	0.59	0.69	9	0	0.21	0.21	1.00
1	13	0.96	0.73	0.58	9	1	0.66	0.65	0.91
1	14	0.84	0.85	0.47	9	2	0.99	0.76	0.69
1	15	0.66	0.78	0.35	9	3	0.86	0.84	0.43
1	16	0.47	0.59	0.25	9	4	0.49	0.44	0.22
1	17	0.27	0.37	0.15	9	5	0.21	0.18	0.09
1	18	0.13	0.16	0.08	9	6	0.06	0.07	0.03
5	0	0.02	0.02	1.00	9	7	0.01	0.02	0.01

8 Final Remarks

The theory presented in this paper, grew out of the necessity of testing precise hypotheses made on the behavior of software controlled machines, Pereira and Stern (1999a). The authors had the responsibility of certifying whether those machines were working according to some legal requirements and the manufacturer's specifications. The real machine software was not available, but a emulator could be used for limited input-output black-box simulation. Compliance with those requirements and specifications was the precise hypotheses being tested, formulated as equality constraints on contingency tables. In Pereira and Stern (1999b) we describe several applications based on contingency tables,

comparing the use of FBST with standard Bayesian and Classical tests. The applications presented in this paper are very similar in spirit. The implementation of FBST for all examples presented here is immediate, as long as good numerical optimization and integration programs are available in a user friendly, interactive and extensible environment, like Matlab, or the open source software Scilab, Gomez (1999). Any one of the tests presented takes only a few seconds to run on a Pentium-PC.

In the applications presented in this paper, as well as in those in Pereira and Stern (1999b), it is desirable or necessary to use a test with the following characteristics:

- Be formulated directly in the parameter space.
- Take into account the full geometry of the null hypothesis as a manifold (surface) imbedded in the whole parameter space.
- Have an intrinsically geometric definition, independent of any non-geometric aspect, like the particular parametrization of the (manifold representing the) null hypothesis being used.
- Be consistent with the benefit of the doubt juridical principle (or safe harbor liability rule), i.e. consider in the "most favorable way" the claim stated by the hypothesis.
- Considering only the observed sample, allowing no ad hoc artifice (that could lead to judicial contention), like a positive prior probability distribution on the precise hypothesis.
- Consider the alternative hypothesis in equal standing with the null hypothesis, in the sense that increasing sample size should make the test converge to the right (accept/reject) decision.
- Give an intuitive and simple measure of significance for the null hypothesis, ideally, a probability in the parameter space.

FBST has all these theoretical characteristics and can be efficiently implementated with the appropriate computational tools. Moreover, as shown in Madruga *et al.* (2000), the FBST is also in perfect harmony with Bayesian decision theory of Rubin (1987), in the sense that there are specific loss functions which render the FBST. In case an alternative parametrization in the likelihood function is adopted, an invariance correction like in Evans (1997) should be used. Finally, we notice that statements like "increase sample size to reject (accept) the hypothesis" made by many users of frequentist (standard Bayesian) tests, do not hold for the FBST.

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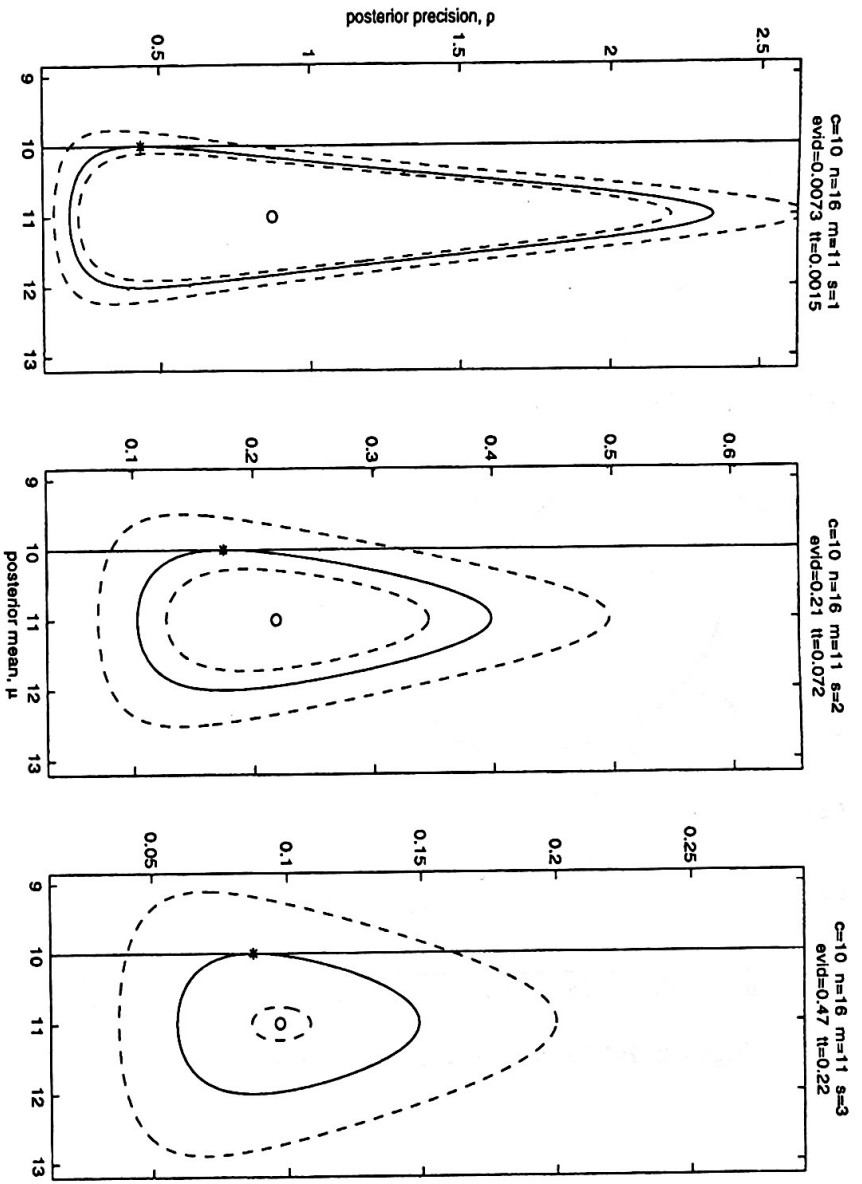

Figure 1: Tangent and other Highest Probability Density Sets

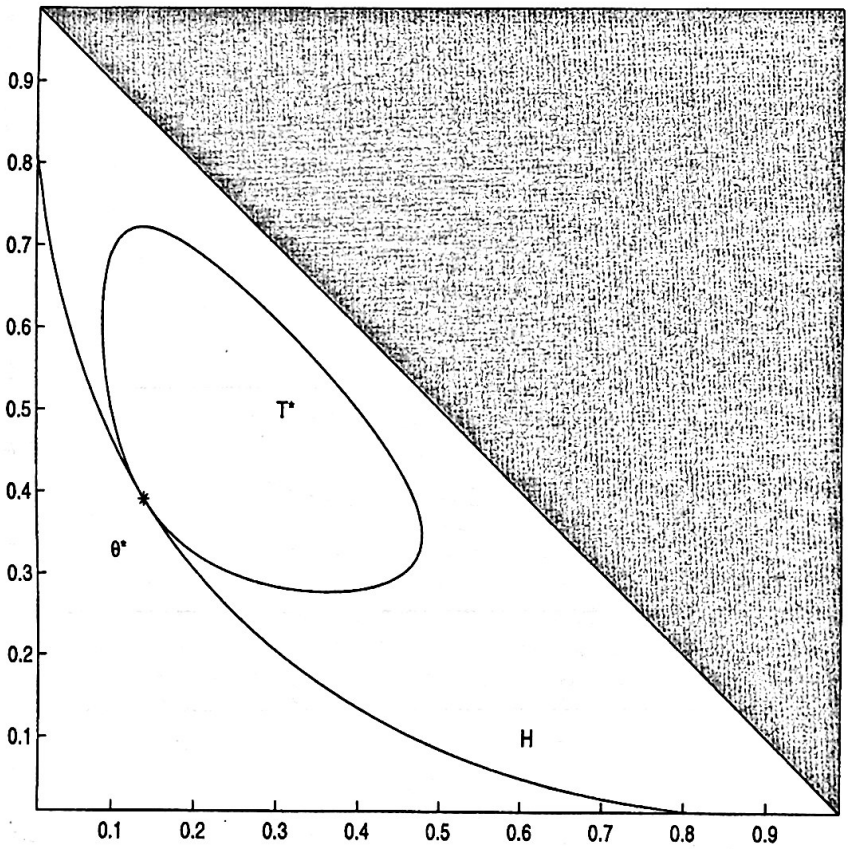

Figure 2: H-W $\theta_1 \times \theta_3$; $x_1 = x_2 = 5$, $x_3 = 10$; $evid = 0.09$

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Carlos Eduardo Ferreira, C. C. de Souza e Yoshiko Wakabayashi
REARRANGEMENT OF DNA FRAGMENTS: A BRANCH-AND-CUT ALGORITHM
RT-MAC-9701, janeiro de 1997, 24 pp.

Marcelo Finger
NOTES ON THE LOGICAL RECONSTRUCTION OF TEMPORAL DATABASES
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Flávio S. Corrêa da Silva, Wamberto W. Vasconcelos e David Robertson
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