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THE FULLY BAYESIAN SIGNIFICANCE TEST FOR THE COVARIANCE STRUCTURE PROBLEM

Júlio Michael Stern

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Julio Michael Stern *

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Abstract

The Fully Bayesian Significance Test (FBST) for precise hypotheses is presented, with some relevant biological applications. 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 sub-manifold (of the parameter space) that defines the null hypothesis. We use the FBST in an application testing a covariance structure.

KEY WORDS: Covariance structure, Credibility, Evidence, Genetic expression, Global optimization; Linear pattern, Numerical integration; Quality control, Wishart distribution. AMS: 62A15; 62F15; 62H15.

1 Introduction

The Fully 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 "Fully" Bayesian and consists in the analysis of credible sets. By Fully 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.

*jstern@ime.usp.br , BIOINFO and IME-USP - University of Sao Paulo

The application presented in this paper is very similar in spirit. The implementation of FBST for the example 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), Geist (1994). The test presented takes only a few seconds to run on Pentium machines.

In the application presented in this paper, as well as in those in Pereira and Stern (1999b and 2000), it is desirable or necessary to use a test with the following characteristics:

- Be formulated directly in the original 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 parameterization of the (manifold representing the) null hypothesis being tested.
- 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 implemented 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. 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.

2 Normal-Wishart Distribution

The conjugate prior and posterior for multivariate normal distribution can be specified using the Wishart distribution, DeGroot (1970). Consider the matrix $X_{i,j}$, $i = 1 : n$, $j = 1 : m$, $m > n$ where each row contains a sample element from a n-multivariante normal distribution with known expected vector $\bar{x}$ and known covariance matrix S. Let W and V denote the random matrices:

$$W = \sum_{j=1}^{m} (X_{\bullet,j} - \bar{x}) (X_{\bullet,j} - \bar{x})' \quad , \quad V = \frac{1}{m} W \quad .$$

The random matrix W has Wishart distribution with m degrees of freedom and covariance matrix S. The Wishart pdf has the expression:

$$\begin{aligned} f(W \,|\, m, S) &= \kappa \, |W|^{(m-n-1)/2} \, e^{-\mathrm{tr}(S^{-1} W)/2} \\ 1/\kappa &= |S|^{m/2} \, 2^{mn/2} \, \pi^{n(n-1)/4} \prod_{j=1}^{n} \Gamma(\frac{m+1-j}{2}) \end{aligned}$$

Now consider the matrix X as above, with unknown covariance matrix. Taking as prior distribution for the precision matrix $R \equiv S^{-1}$ the wishart distribution with $a > n-1$ degrees of freedom and precision matrix $\breve{W}$, the posterior distribution for R has the form:

$$f(R \,|\, m, W) \propto |R|^{(a+m-n-1)/2} e^{-\mathrm{tr}((\breve{W}+W)\,R)/2}$$

i.e., the posterior distribution for R is a Wishart distribution with $a+m$ degrees of freedom and precision $\breve{W} + W$. All covariance and precision matrices are supposed to be positive definite.

Taking Jeffreys' improper prior, we make $a \to -1$, and $\breve{W} \to 0$, so the posterior pdf becomes a Wishart distribution with m degrees of freedom and precision W. Now we can write the posterior pdf, $f(\,)$ and log-posterior kernel, $fl(\,)$ for R, given m and W or V, as:

$$\begin{aligned} f(R \,|\, m, W) &\propto |R|^{(m-n-1)/2} \, e^{-\mathrm{tr}(W\,R)/2} \quad , \\ fl(R \,|\, m, W) &= \frac{m-n-1}{2} \log(|R|) - \frac{1}{2} \mathrm{tr}(W\,R) \quad , \\ fl(R \,|\, m, V) &= \frac{m-n-1}{2} \log(|R|) - \frac{m}{2} \mathrm{tr}(R\,V) \quad . \end{aligned}$$

Johnson (1980) describes a simple procedure to generate U, the cholesky factor of a Wishart variate W with m degrees of freedom and covariance parameter S, from the cholesky factor $S = C'\,C$:

$$T_{i,j} = N(0,1) \;,\; i < j \;;\quad T_{i,i} = \sqrt{\chi^2(m-i+1)} \;;\quad U = T\,C \quad .$$

3 The Linear Pattern Covariance Model

We want to test the linear structure covariance hypothesis. Our application involves testing levels of genetic expression measured by micro-arrays, but the same model is classic in psychology, biology, and pharmacology, as described in Jiang and Sarkar (1999, 2000a, 2000b).

We will use the following notation: A family of matrices numbered $1, 2 \ldots$ is writen $M^1, M^2 \ldots$. The i-th row, the j-th column, and the i,j-th element of matrix M^t are, $M^t_{i,\bullet}$, $M^t_{\bullet,j}$ and $M^t_{i,j}$. The Hadamard or pointwise product, $\odot$, is defined by, respectively, $M = A \odot B \Leftrightarrow M_{i,j} = A_{i,j} B_{i,j}$.

The linear structure covariance model can be tested using the FBST, with parameter space:

$$\Theta = \{S(\gamma) = \sum_{t=1}^{10} \gamma_t G^t \ , \ \gamma \,|\, S > 0\} \ , \ \Theta_0 = \{\gamma \in \Theta \,|\, h(\gamma) = 0\}.$$

The $n \times n$, $n = 4$, symmetric matrices have the basis $G^1, \ldots G^{10}$, given by:

$$G^1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad G^2 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$G^3 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad G^4 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$G^5 = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad G^6 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

$$G^7 = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad G^8 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

$$G^9 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad G^{10} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

The hypothesis H is given by the 3-dimentional constraint

$$h(\gamma) = \begin{bmatrix} \gamma_1 - \gamma_3 \\ \gamma_2 - \gamma_4 \\ \gamma_5 - \gamma_6 \end{bmatrix} = 0$$

At the optimization step we minimize the reduced log-posterior multiplied by a factor $(-2/m)$, plus a centralization term,

$$\begin{aligned} f(S\,|\,m,V) &= \mathrm{tr}(RV) - \frac{m-n-1}{m}\log(|R|) + c\,\mathrm{frob2}(S-V) \\ \mathrm{frob2}(M) &= \sum_{i,j=1}^{n}(M_{i,j})^2 \end{aligned}$$

The function $f(\,)$ has the following properties:

1. A large enough centralization factor, c, times the squared frobenius norm of $S - V$, makes the first points of the optimization sequence remain in the neighborhood of V. As the optimization proceeds, we relax the centralization factor, i.e. make $c \to 0$, and maximize the pure likelihood function. In practice this strategy let us avoid handling explicitly the difficult constraint $S > 0$.

2. $f(\,)$ is written in terms of V, not W, and the factor $(2/m)$ cancels the almost linear scaling in m. Therefore, $\frac{\partial f}{\partial m} \to 0$ as $m \to \infty$. This allows efficient "hot" reoptimizations, for a sequence of different values of m.

3. Using the identities, Anderson (1969), McDonald (1974), Rogers (1980),

$$\begin{aligned} \frac{\partial S}{\partial \gamma_t} &= G^t\,, \qquad \frac{\partial R}{\partial \gamma_t} = -RG^tR\,, \\ \frac{\partial \log(|S|)}{\partial \gamma_t} &= \sum_{i,j=1}^{n}\frac{\partial \log(|S|)}{\partial S_{i,j}}\frac{\partial S_{i,j}}{\partial \gamma_t} = \sum_{i,j=1}^{n}\frac{\mathrm{cof}(S_{i,j})}{|S|}G^t_{i,j} = \mathrm{tr}(RG^t) \end{aligned}$$

the Jacobian and Hessian matrices of $f(\,)$ and $h(\,)$, have simple analytical expressions, given in the sequel. Notice that the expressions could be somewhat simplified for the this particular basis, but we prefer to present them in general form.

$$\begin{aligned} \frac{\partial f}{\partial \gamma_t} &= \frac{m-n-1}{m}\mathrm{tr}(RG^t) - \mathrm{tr}(RG^tRV) + 2p\sum_{i,j=1}^{n}(S-V)\odot G^t \\ \frac{\partial h}{\partial \gamma_t} &= \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \end{bmatrix} \end{aligned}$$

$$\frac{\partial^2 f}{\partial \gamma_s \partial \gamma_t} = \mathrm{tr}(R(G^s R G^t + G^t R G^s) R V) - \frac{m-n-1}{m} \mathrm{tr}(R G^s R G^t) + 2p \sum_{i,j=1}^{n} G^s \odot G^t$$

For the optimization step in FBST, the characteristics of $f(\,)$ allow us to implement very efficient and robust algorithms. Since we are interested in studying more general (non-linear) mean-covariance and mean-correlation structures, we handle the constraints by penalization and sequential unconstrained programming. Trust Region algorithms, working with explicit analytical derivatives, proved to be very stable, in contrast with the often unpredictable behavior of some methods found in most statistical software, like Newton-Raphson or "Scoring". Optimization problems of small dimension, like above, allow us to use dense matrix representation, without significant loss.

For the integration step in FBST, we use a Monte-Carlo algorithm. At the integration step it is important to perform all matrix computations directly from the cholesky factors, Jones (1985). The computation of a single FBST evidence and empirical power takes only a few seconds on Pentium machines.

4 Numerical Results

Table 1 displays the evidence in favor of the hypothesis for some sample matrices. V^1 to V^{11} are variations of standard test matrices, and V^{12} is an application example, all from Jiang (2000a). The test as performed is not directly comparable to Jiang(2000a) and others, because we used a very conservative non-informative prior. More aggresive versions of the test, its power, and other aspects are going to be analyzed in subsequent work.

$$V^1 = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.2 & 0.0 \\ 0.0 & 0.0 & 0.0 & 1.0 \end{bmatrix} \quad V^2 = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.2 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.8 \end{bmatrix}$$

$$V^3 = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & 0.2 \\ 0.0 & 0.0 & 0.2 & 1.0 \end{bmatrix} \quad V^4 = \begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 1.0 & -0.2 \\ 0.0 & 0.0 & -0.2 & 1.0 \end{bmatrix}$$

$$V^5 = \begin{bmatrix} 1.0 & 0.1 & 0.2 & 0.3 \\ 0.1 & 1.0 & 0.3 & 0.5 \\ 0.2 & 0.3 & 1.0 & 0.6 \\ 0.3 & 0.5 & 0.6 & 1.0 \end{bmatrix} \quad V^6 = \begin{bmatrix} 1.0 & 0.1 & 0.2 & 0.3 \\ 0.1 & 1.0 & 0.3 & 0.5 \\ 0.2 & 0.3 & 1.0 & 0.6 \\ 0.3 & 0.5 & 0.6 & 3.0 \end{bmatrix}$$

$$V^7 = \begin{bmatrix} 1.0 & 0.1 & 0.2 & 0.3 \\ 0.1 & 2.0 & 0.3 & 0.5 \\ 0.2 & 0.3 & 3.0 & 0.6 \\ 0.3 & 0.5 & 0.6 & 4.0 \end{bmatrix} \quad V^8 = \begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 2 & 0 & 0 \\ 0 & 0 & 3 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix}$$

$$V^9 = \begin{bmatrix} 1.0 & 0.1 & 0.2 & 0.3 \\ 0.1 & 1.0 & 0.4 & 0.5 \\ 0.2 & 0.4 & 1.0 & 0.6 \\ 0.3 & 0.5 & 0.6 & 1.0 \end{bmatrix} \quad V^{10} = \begin{bmatrix} 1.0 & 0.1 & 0.2 & 0.3 \\ 0.1 & 1.0 & 0.4 & 0.5 \\ 0.2 & 0.4 & 1.0 & 0.6 \\ 0.3 & 0.5 & 0.6 & 3.0 \end{bmatrix}$$

$$V^{11} = \begin{bmatrix} 1.0 & 0.1 & 0.2 & 0.3 \\ 0.1 & 2.0 & 0.4 & 0.5 \\ 0.2 & 0.4 & 3.0 & 0.6 \\ 0.3 & 0.5 & 0.6 & 4.0 \end{bmatrix} \quad V^{12} = 0.2 * \begin{bmatrix} 6.577 & 1.602 & 6.006 & -0.265 \\ 1.602 & 5.349 & 0.841 & 1.250 \\ 6.006 & 0.841 & 7.291 & -0.063 \\ -0.265 & 1.250 & -0.063 & 4.600 \end{bmatrix}$$

	Covar. Matrix	– Samples –						
	250	200	150	100	75	50	25	20
1	0.97	0.98	0.99	1.00	1.00	1.00	1.00	1.00
2	0.87	0.90	0.95	0.97	0.98	0.99	1.00	1.00
3	0.86	0.91	0.94	0.97	0.98	0.99	1.00	1.00
4	0.87	0.91	0.94	0.97	0.98	0.99	1.00	1.00
5	0.02	0.04	0.13	0.32	0.47	0.70	0.90	0.94
6	0.00	0.00	0.02	0.10	0.22	0.43	0.78	0.86
7	0.00	0.00	0.01	0.04	0.12	0.31	0.70	0.80
8	0.00	0.00	0.00	0.00	0.00	0.00	0.10	0.20
9	0.01	0.04	0.12	0.30	0.47	0.67	0.90	0.94
10	0.00	0.00	0.02	0.10	0.21	0.43	0.79	0.86
11	0.00	0.00	0.01	0.04	0.12	0.31	0.70	0.80
12	0.28	0.40	0.55	0.73	0.83	0.92	0.98	0.99

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