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EXACT MULTIVARIATE BAYESIAN BOOTSTRAP DISTRIBUTIONS OF MOMENTS[1]

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The common unknown probability law P of a random sample $Y_1, \dots, Y_n$ is assigned a Dirichlet process prior with index α. It is shown that the posterior joint density of several moments of P converges, as $\alpha(\mathbb{R}) \to 0$, to a multivariate B-spline, which is, therefore, the Bayesian bootstrap joint density of the moments. The result provides the basis for possible default nonparametric Bayesian inference on unknown moments.

1. Introduction. The need for a default prior to represent vague initial information in nonparametric Bayesian statistics is generally recognized. For this purpose, in the presence of a random sample $Y_1, \dots, Y_n$, with unknown common probability law P, some researchers would consider using a Dirichlet prior on P [Ferguson (1973)] with a very small total mass $\alpha(\mathbb{R})$ of the index α, or a limit as $\alpha(\mathbb{R}) \to 0$. The reason is that, in such a limit case, the posterior law of the infinite dimensional parameter P is centered around the empirical measure. The results obtained are then comparable to standard frequentist results, as illustrated by the applications in Section 5 of Ferguson (1973) and much of the following literature on Dirichlet priors. This reconciliation between the frequentist and Bayesian approaches is appealing to the scientist who feels opposed to the use of prior information for philosophical reasons. It also provides a possible default choice for the compilation of Bayesian software.

Limiting results from Dirichlet priors of the above nature have been referred to as the Bayesian bootstrap (BB) by Rubin (1981) and Lo (1987), among others. Such a convention is followed in the present paper, where a few more applications of the BB are illustrated. The focus is on the posterior limiting distribution—the BB distribution—of the vector-valued functional of the parameter P composed of the first s moments: $\boldsymbol{\mu}'(P) = (\mu_1, \dots, \mu_s)(P)$, where $\mu_j(P) := \int y^j P(dy)$, $j = 1, \dots, s$ and the prime denotes transpose.

Cifarelli and Regazzini (1990) obtain the proper distribution of the mean $\mu_1(P)$ when P is chosen according to a Dirichlet process satisfying minimal conditions. In particular, their results, applied to the posterior process on P, provide the researcher with a bona fide nonparametric posterior distribution

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on $\mu_1(P)$. Letting $\alpha(\mathbb{R}) \to 0$, they obtain, as a by-product, an expression for the BB density of $\mu_1(P)$, namely,

$$M(\mu; y_{(1)}, \dots, y_{(n)}) = (n-1) \sum_{i=1}^{k} \frac{(\mu - y_{(i)})^{n-2}}{\prod_{j \neq i} (y_{(j)} - y_{(i)})} \quad \text{if } y_{(k)} \le \mu < y_{(k+1)}, \tag{1}$$

for $k = 1, \dots, n-1$ and 0 otherwise, where $y_{(1)} < y_{(2)} < \cdots < y_{(n)}$ are the order statistics, supposed distinct for the sake of simplicity. Although the interest of the authors is not on its applications to statistical practice, such a density turns out to be $n-3$ times continuously differentiable, bell-shaped, log concave, centered around $\overline{Y} = \Sigma Y_i/n$ and with variance $S^2/(n+1)$, where $S^2 = \Sigma(Y_i - \overline{Y})^2/n$ is the sample variance [cf. (7) and (8)]. These results are comparable to those derived by a classical sampling theoretical approach or by bootstrap-based inference on $\mu_1(P)$.

Generalizing the limit result of Cifarelli and Regazzini to more than one dimension is of some relevance because of the possibility of constructing, for example, joint BB regions for unknown moments. Multidimensional results of this sort may actually be obtained by referring to a conspicuous amount of work done in the field of numerical analysis. Density (1) is in fact a well known classical univariate B-spline, introduced first by Curry and Schoenberg (1966). Its natural extension to higher dimensions, the multivariate B-spline, is precisely the BB density of the functional $\boldsymbol{\mu}(P)$. Multivariate B-splines are nowadays well understood objects; see, for example, Dahmen and Micchelli (1983).

Sections 2 and 3 contain a summary of the relevant definitions and results about Dirichlet priors and multivariate B-splines. Section 4 is an application of these results to the Bayesian nonparametric problem. Section 5 contains asymptotic results.

2. The Bayesian bootstrap as a limit of Dirichlet posterior processes. Let P, the unknown probability measure of real observations $Y_1, Y_2, \dots,$ be distributed a priori as a Dirichlet process with index α, as in Ferguson (1973). Write $P \sim \mathscr{D}(\alpha)$. A fundamental property of Dirichlet process priors is that they are conjugate to random sampling, in the sense expressed by the following theorem.

THEOREM 1 [Ferguson (1973)]. *If $P \sim \mathscr{D}(\alpha)$ and if, given P, $Y_1, \dots, Y_n$ are i.i.d. P, then the posterior law of P is again Dirichlet, namely,*

$$P | Y_1 = y_1, \dots, Y_n = y_n \sim \mathscr{D}\left(\alpha + \sum_{i=1}^{n} \delta_{y_i}\right), \tag{2}$$

where δ_x represents the unit mass measure of x.

The Bayesian bootstrap describes the limit of the posterior law of P as $\alpha(\mathbb{R}) \to 0$. More formally, the Bayesian bootstrap may be understood in terms of weak convergence of probability laws if P is viewed as a random element taking values on the space $\mathscr{P}$ of all probability measures on the real numbers, endowed with the topology of weak convergence. We then have the following theorem.

THEOREM 2. *Under the same conditions of Theorem* 1, $\mathscr{D}(\alpha + \sum_{i=1}^{n} \delta_{y_i})$, *the posterior law of* P, *converges weakly to* $\mathscr{D}(\sum_{i=1}^{n} \delta_{y_i})$, *as* $\alpha(\mathbb{R}) \to 0$.

PROOF. This is a corollary of Theorem 3.2 in Sethuraman and Tiwari (1982). □

$\mathscr{D}(\sum_{i=1}^{n} \delta_{y_i})$ may be called the BB law of P. The result is equivalent to stating that P is, in the limit, a random distribution with finite support $\{y_1, \dots, y_n\}$ and masses $(\Pi_1, \dots, \Pi_n)$ distributed according to a Dirichlet distribution with parameter $(1, \dots, 1)$, as defined, for example, in Wilks (1962).

The BB behavior of the random vector $\boldsymbol{\mu}(P)$ may also be related to Dirichlet posterior processes in terms of weak convergence, as in the following theorem.

THEOREM 3. *Under the same conditions of Theorem* 1, *if* $\alpha = \alpha(\mathbb{R})Q$ *and* Q *is a probability measure such that* $\int y^{2s} Q(dy) < \infty$, *then, as* $\alpha(\mathbb{R}) \to 0$, $\boldsymbol{\mu}(P)$ *converges in distribution to* $\boldsymbol{\mu} := (\sum y_i \Pi_i, \sum y_i^2 \Pi_i, \dots, \sum y_i^s \Pi_i)'$, *where* $(\Pi_1, \dots, \Pi_n)$ *is a random vector having a Dirichlet distribution with parameter* $(1, \dots, 1)$.

PROOF. By application of the so-called Cramér–Wold device, consider a linear combination of the components of $\boldsymbol{\mu}(P)$, say $C = \int \sum a_j y^j P(dy)$. Then C satisfies the conditions of Corollary 2.7 of Hannum, Hollander and Langberg (1981) and converges in distribution to the corresponding linear combination of the components of $\boldsymbol{\mu}$. □

A direct analysis of the convergence of the multivariate densities, possibly leading to stronger results than Theorem 3, would require consideration of coalescent knots of the corresponding B-spline and is avoided here, for the sake of simplicity. Also, notice that $\boldsymbol{\mu}(P)$ is not an a.s. weakly continuous functional, so its weak convergence is not a direct corollary of Theorem 2.

3. Multivariate B-splines. Let the random vector $\boldsymbol{\Pi} = (\Pi_1, \dots, \Pi_n)$ have a Dirichlet distribution with parameter $(1, \dots, 1)$. This is equivalent to saying that $(\Pi_1, \dots, \Pi_{n-1})$ has constant Lebesgue density—equal to $(n-1)!$ —over the simplex $\{(\pi_1, \dots, \pi_{n-1});\ \pi_j \geq 0,\ \sum_1^{n-1} \pi_j \leq 1\}$ and 0 otherwise. The mean vector of $\boldsymbol{\Pi}$ is $E(\boldsymbol{\Pi}) = n^{-1}(1, \dots, 1)$ and its variance–covariance matrix is $V(\boldsymbol{\Pi}) = n^{-2}(n+1)^{-1}\mathbf{A}$, where the matrix $\mathbf{A}$ has diagonal elements equal to $(n-1)$ and off-diagonal elements equal to -1.

Let $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^s$ be distinct and not restricted to a hyperplane.

DEFINITION 1. The density of the random vector

$$\boldsymbol{\mu} := \Pi_1 \mathbf{x}_1 + \cdots + \Pi_n \mathbf{x}_n \tag{3}$$

is called the s-variate B-spline, or simplex spline, with knots $\mathbf{x}_1, \dots, \mathbf{x}_n$ and is denoted by $M(\boldsymbol{\mu}; \mathbf{x}_1, \dots, \mathbf{x}_n)$.

Such fundamental objects like densities of linear combinations of uniform variates made various appearances in the statistical literature [see, e.g., Watson (1956) and related works] and were called multivariate B-splines in de Boor (1976), where a geometrical interpretation, equivalent to the definition above, is given. This geometrical interpretation is a multivariate extension of the work by Curry and Schoenberg (1966), where an explicit formula for the univariate B-spline is derived through a Peano representation of the divided differences and a classical formula due to Hermite and Genocchi. For $s = 1$,

$$M(\mu; x_1, \dots, x_n) = (n-1) \sum_{i=1}^{n} \frac{(x_i - \mu)_+^{n-2}}{\prod_{j \neq i}(x_i - x_j)}, \tag{4}$$

where $(\cdot)_+$ denotes positive part.

In the multivariate case, for a small to moderate n, recursive formulae due to Dahmen and Micchelli [see the bibliography in Dahmen and Micchelli (1983)], together with the computing power attained in recent years, provide viable alternatives to cumbersome explicit formulae and approximations of the earlier statistical literature. For an account of these formulae and for other applications of multivariate B-splines in statistics and probability, see Dahmen and Micchelli (1986) and Karlin, Micchelli and Rinott (1986). For the present purposes, the following result is sufficient:

THEOREM 4 [Micchelli (1980)]. *For any* $\boldsymbol{\mu} \in \mathbb{R}^S$ *and* $\lambda_i \in \mathbb{R}$ *such that* $\sum_{i=1}^n \lambda_i = 1$ *and* $\boldsymbol{\mu} = \sum_{i=1}^n \lambda_i \mathbf{x}_i$, *we have for* $n > s + 1$,

$$M(\boldsymbol{\mu}; \mathbf{x}_1, \dots, \mathbf{x}_n) = \frac{n-1}{n-1-s} \sum_{i=1}^{n} \lambda_i M(\boldsymbol{\mu}; \mathbf{x}_1, \dots, \mathbf{x}_{i-1}, \mathbf{x}_{i+1}, \dots, \mathbf{x}_n). \tag{5}$$

From a practical point of view, in order to calculate a multivariate B-spline at a specific point $\boldsymbol{\mu}$, the recursion in (5) above is iterated down to $n = s + 1$, for which

$$M(\boldsymbol{\mu}; \mathbf{x}_1, \dots, \mathbf{x}_{s+1}) = \frac{s!}{\left|\det\begin{bmatrix} 1 & \cdots & 1 \\ \mathbf{x}_1 & \cdots & \mathbf{x}_{s+1} \end{bmatrix}\right|} \tag{6}$$

for $\boldsymbol{\mu}$ in the interior of the convex hull of $\mathbf{x}_1, \dots, \mathbf{x}_{s+1}$ and 0 otherwise. See Micchelli (1979) and Grandine (1988) for further discussion on evaluation problems.

For a large n instead, normal approximations hold under usual moment conditions and are discussed in Section 5.

4. Exact Bayesian bootstrap densities of moments. The results described in Sections 2 and 3 can now be combined by considering $\mathbf{x}_i = (y_i, y_i^2, \dots, y_i^s)'$, for $i = 1, \dots, n$, where y_i's are distinct observed values. We conclude that the BB density of $\boldsymbol{\mu}(P)$, is a multivariate B-spline with knots $\mathbf{x}_1, \dots, \mathbf{x}_n$. (The theory could be extended to the case of coincident observations by defining B-splines with coalescent knots appropriately, but this is not done here, for the sake of simplicity.)

For example, for $s = 1$, it is easy to secure the equivalence of formulae (4) and (1), with $x_i = y_{(i)}$—the order of the x_i's does not matter—by noticing that their difference can be written as

$$(n-1) \sum_{i=1}^{n} \frac{(x_i - \mu)^{n-2}}{\prod_{j \neq i}(x_i - x_j)},$$

which is the divided difference of the polynomial $(n-1)(\cdot - \mu)^{n-2}$ at $x_1, \dots, x_n$ and therefore equals 0 [see, for example, Theorem 2.1.3.10 in Stoer and Bulirsch (1993)].

The multivariate BB density of $\boldsymbol{\mu}(P)$ is log concave and of global continuity class $\mathscr{C}^{n-s-2}$ if every $s+1$ knot spans a convex hull of positive volume in $\mathbb{R}^s$ (see references in Section 3). Multivariate B-splines are therefore very smooth, even for a small sample size. This is particularly relevant, since critics of the use of Dirichlet priors have often emphasized their essentially discrete character (and consequently their inappropriateness) for the analysis of continuous data.

Let $m_j := \sum_{i=1}^{m} y_i^j / n$ be the jth sample moment, $j = 1, \dots, s$. Then, since $\boldsymbol{\mu} = [\mathbf{x}_1, \dots, \mathbf{x}_n]\boldsymbol{\Pi}'$, its mean is

$$E(\boldsymbol{\mu}) = [\mathbf{x}_1, \dots, \mathbf{x}_n]E(\boldsymbol{\Pi}') = (m_1, \dots, m_s)' =: \mathbf{m} \tag{7}$$

and its variance–covariance matrix is

$$V(\boldsymbol{\mu}) = [\mathbf{x}_1, \dots, \mathbf{x}_n]V(\boldsymbol{\Pi})[\mathbf{x}_1, \dots, \mathbf{x}_n]' = \frac{1}{n+1}[m_{j+k} - m_j m_k]_{s \times s}. \tag{8}$$

Figure 1 contains contour and perspective plots of BB joint densities of first and second moments $(\mu_1, \mu_2)'(P)$ for two samples of size $n = 5$ and $n = 10$ simulated from a Normal(0, 1) distribution. The convex hull of points $(y_i, y_i^2)'$, $i = 1, \dots, n$, supports the BB density and is drawn on the contour plots. Edge effects are attenuated as the sample size increases and the posterior density approaches normality, as described in the next section.

It is clear how to use computations of this sort to obtain, numerically, high posterior density regions and decision theoretical quantities for unknown moments and smooth transformations of them, like the variance $\mu_2 - \mu_1^2$.

The methodology illustrated here extends to the joint posterior density of functionals of the form $\int \psi_i(y)P(dy)$, for smooth real measurable functions ψ_i, $i = 1, \dots, s$, as in Corollary 1 of Cifarelli and Regazzini (1990).

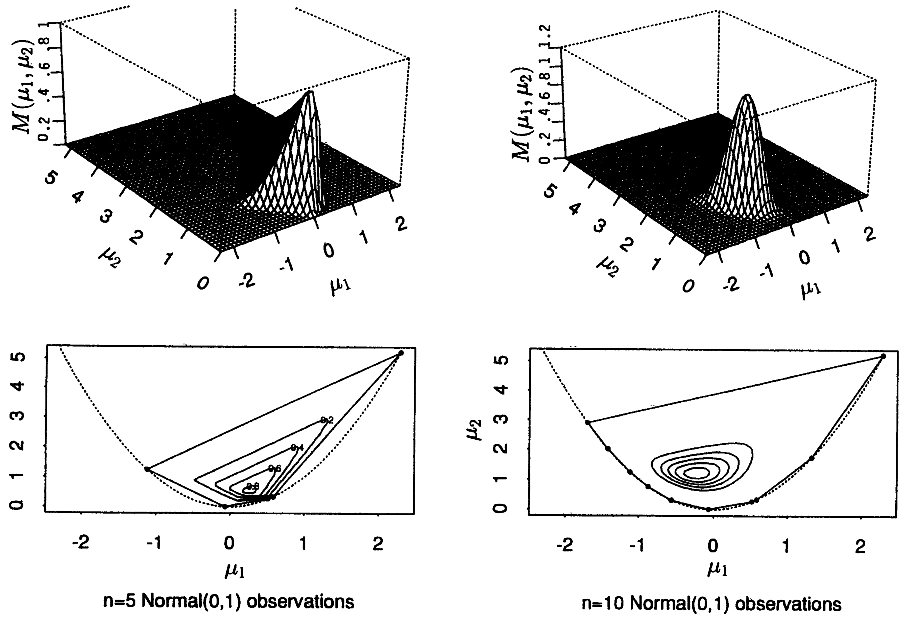

FIG. 1.

5. Asymptotic Bayesian bootstrap densities of moments. A frequentist asymptotic analysis of the results obtained in the previous sections may be carried out by supposing $Y_1, \ldots, Y_n$ are independent and identically distributed random variables with unknown "true" distribution F_0, unknown "true" mean $\mu_{0,1}$ and so forth. From this point of view, the BB density of several moments is to be viewed as a *random* multivariate B-spline, since its knots are random.

THEOREM 5. *If F_0 possesses finite moments $\mu_{0,1}, \ldots, \mu_{0,2s}$, then*

$$\boldsymbol{\mu}^* := \sqrt{n}\,(\boldsymbol{\mu} - \mathbf{m})$$

converges weakly, a.s.-$F_0 \times F_0 \times \cdots$, to an s-variate normal with mean $(0, \ldots, 0)'$ and variance–covariance matrix $[\,\mu_{0,j+k} - \mu_{0,j}\mu_{0,k}]_{s \times s}$.

PROOF. The standardized vector $\boldsymbol{\mu}^*$ has a multivariate B-spline density, since it can be written as $\boldsymbol{\mu}^* = \sum \Pi_i \mathbf{x}^*_{i,n}$, with $\mathbf{x}^*_{i,n} := \sqrt{n}(\mathbf{x}_i - \mathbf{m})$. It suffices to show that conditions of Corollary 4 of Dahmen and Micchelli (1981) hold almost surely.

Condition (a) holds a.s. since $\mu_{0,2s} < \infty$ implies

$$\left(\frac{1}{n} \max_{1 \le i \le n} \|\mathbf{x}^*_{i,n}\|\right)^2 = \frac{1}{n} \max_{1 \le i \le n} \|\mathbf{x}_i - \mathbf{m}\|^2 \to 0 \quad \text{a.s.}$$

by the strong law of large numbers.

Condition (b) holds a.s., trivially, with (using Dahmen and Micchelli's notation) $y = (0, \ldots, 0)'$.

Condition (c) holds a.s. with A (using Dahmen and Micchelli's notation) equal to half of the variance–covariance matrix in the statement of the theorem, since $\mu_{0,2s} < \infty$, by the strong law of large numbers. □

Theorem 5, parallel to standard normal asymptotic theory [see, e.g., Serfling (1980), page 68], is also a generalization of Theorem 4.1 of Lo (1987).

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