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## Bayesian and Empirical Bayesian Bootstrapping

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ABSTRACT. Let  $X_1, \ldots, X_n$  be a random sample from an unknown probability distribution P on the sample space  $\mathcal{X}$ , and let  $\theta = \theta(P)$  be a parameter of interest. The present paper proposes a nonparametric 'Bayesian bootstrap' method of obtaining Bayes estimates and Bayesian confidence limits for  $\theta$ . It uses a simple simulation technique to numerically approximate the exact posterior distribution of  $\theta$  using a (non-degenerate) Dirichlet process prior for P. Asymptotic arguments are given which justify the use of the Bayesian bootstrap for any smooth functional  $\theta(P)$ . When the prior is fixed and the sample size grows five approaches become first-order equivalent: the exact Bayesian, the Bayesian bootstrap, Rubin's degenerate-prior bootstrap, Efron's bootstrap, and the classical one using delta methods. The Bayesian bootstrap method is also extended to the semiparametric regression case. A separate section treats similar ideas for censored data and for more general hazard rate models, where a connection is made to a 'weird bootstrap' proposed by Gill. Finally empirical Bayesian versions of the procedure are discussed, where suitable parameters of the Dirichlet process prior are inferred from data.

Our results lend Bayesian support to the classic Efron bootstrap. It is the Bayesian bootstrap under a noninformative reference prior; it is a limit of natural approximations to good Bayes solutions; it is an approximation to a natural empirical Bayesian strategy; and the formally incorrect reading of a bootstrap histogram as a posterior distribution for the parameter isn't so incorrect after all.

Key words and phrases: BAYESIAN BOOTSTRAP, BETA AND DIRICHLET PROCESSES, CONFIDENCE INTERVALS, EMPIRICAL BAYES, FIVE (AT LEAST) STATISTICIANS, SEMIPARAMETRIC BAYESIAN REGRESSION

1. Introduction and summary. Let  $X_1, \ldots, X_n$  be independent and identically distributed (i.i.d.) according to an unknown distribution P. For convenience take the sample space to be  $\mathcal{X} = \mathcal{R}$ , the real line, so that P can be identified with its distribution function (c.d.f.) F. Most of the methods and results in this report have natural extensions to  $\mathcal{R}^k$  and indeed to any complete, separable metric space  $\mathcal{X}$ .

Let  $\theta = \theta(F)$  be a parameter functional of interest, like the mean, or median, or the standard deviation, or  $\int |x - F^{-1}(\frac{1}{2})| dF(x)$ . We shall be concerned with nonparametric Bayesian estimates of and confidence statements about  $\theta$ , and need to start out with a prior distribution on the space of all c.d.f.'s. A natural class from which to choose is provided by Ferguson's (1973, 1974) Dirichlet processes; this class is rich, each member has large support, and at least posterior expectations (Bayes estimates under quadratic loss) can be calculated for a fair list of cases. Thus let

$$F \sim \operatorname{Dir}(aF_0),\tag{1.1}$$

i.e. F is a Dirichlet process with parameter  $aF_0$ . Here  $F_0(.) = E_B F(.)$  is the prior guess c.d.f. whereas a > 0 has interpretation as prior sample size, see Ferguson (op. cit.). Subscript B means that the operation in question is relative to the Bayesian framework.

The observed sample  $x_1, \ldots, x_n$  gives rise to and can be identified with the empirical c.d.f.  $F_n(t) = \frac{1}{n} \sum_{i=1}^n I\{x_i \leq t\}$ . The posterior distribution of F is

$$\mathcal{L}_B\{F|\text{data}\} = \mathcal{L}_B\{F|F_n\} = \text{Dir}(aF_0 + nF_n). \tag{1.2}$$

Thus the distribution function

$$G_n(t) = \Pr_B\{\theta(F) \le t | \text{data}\} = \Pr_B\{\theta(F) \le t | F_n\}$$
(1.3)

is in principle known to the statistician. In addition to the Bayesian point estimate  $\theta_B = E_B\{\theta(F)|\text{data}\} = \int t \, dG_n(t)$  we wish to calculate Bayesian confidence limits  $\theta_L$  and  $\theta_U$  from the data, obeying  $\Pr_B\{\theta_L \leq \theta(F) \leq \theta_U|\text{data}\} \doteq 1 - 2\alpha$ , say. Thus

$$\theta_L = G_n^{-1}(\alpha), \qquad \theta_U = G_n^{-1}(1 - \alpha)$$
 (1.4)

are the natural choices, where  $G_n^{-1}(p) = \inf\{t: G_n(t) \ge p\}$ .

The fact that  $G_n$  above is only very rarely explicitly available, however, necessitates devising computational approximations. There are a couple of rather laborious ways to simulate variables from a close approximation to  $G_n$ . That is, a sequence  $Y_1, Y_2, \ldots$  being i.i.d. with a distribution very close to  $G_n$  can be generated, thus enabling one to obtain a close approximation to  $G_n$  and to the sought-after  $\theta_B$ ,  $\theta_L$ ,  $\theta_U$ ; see 2A and 9B below. It turns out that the following rather simpler alternative simulation strategy gives a good approximation to the posterior distribution  $G_n$ : Generate a 'Bayesian bootstrap (BB) sample'  $X_1^*, \ldots, X_{n+a}^*$  of size n+a from the mixture distribution

$$F_{n,B}(t) = E_B\{F(t)|\text{data}\} = \frac{a}{a+n}F_0(t) + \frac{n}{a+n}F_n(t), \tag{1.5}$$

the natural Bayes estimate of the underlying c.d.f. F, and compute a 'BB parameter value'

$$\theta_{BB}^* = \theta(F_{BB}^*) = \theta\left(\frac{1}{n+a} \sum_{i=1}^{n+a} I\{X_i^* \le .\}\right) = \theta(X_1^*, \dots, X_{n+a}^*)$$
 (1.6)

on the basis of the empirical c.d.f.  $F_{BB}^*$  of these values. The proposed approximation to  $G_n$  is

$$\widehat{G}_n(t) = \Pr_* \{ \theta_{BB}^* \le t \}, \tag{1.7}$$

where subscript '\*,' is used to indicate operations relative to the (data-conditional) BB framework. In practice  $\widehat{G}_n(.)$  is evaluated via simulations as

$$\widehat{G}_n(t) \doteq \widehat{G}_{n,\text{boot}}(t) = \frac{1}{\text{boot}} \sum_{b=1}^{\text{boot}} I\{\theta_{BB}^{*b} \leq t\}$$

for a large number boot of independent  $\theta_{BB}^{*b}$  of the type described. This idea, inserting  $\widehat{G}_n$  for  $G_n$ , leads to using

$$\widehat{\theta}_B = \int t \, d\widehat{G}_n(t) \doteq \frac{1}{\text{boot}} \sum_{b=1}^{\text{boot}} \theta_{BB}^{*b}, \tag{1.8}$$

the BB-based Bayes estimate of  $\theta(F)$ , and to the BB percentile interval

$$\widehat{\theta}_{L} = \widehat{G}_{n}^{-1}(\alpha) \doteq \widehat{G}_{n,\text{boot}}(\alpha) \leq \theta(F) \leq \widehat{\theta}_{U} = \widehat{G}_{n}^{-1}(1-\alpha) \doteq \widehat{G}_{n,\text{boot}}(1-\alpha). \tag{1.9}$$

Other Bayesian posterior calculations can be carried out with the same relative ease, like computing Bayes estimates with non-quadratic loss functions.

The motivation for the BB method lies in the fact that the two conditional distributions  $\mathcal{L}_B\{F|\text{data}\}$  and  $\mathcal{L}_*\{F_{BB}^*|\text{data}\}$  are reasonably close. This is explained in Section 2. When the prior sample size parameter a goes to zero (corresponding in a certain sense to the case of a 'noninformative nonparametric prior' for F) the BB becomes Efron's classic bootstrap. In particular the BB percentile interval becomes Efron's (uncorrected) percentile interval. One may therefore think of the BB as an 'informative extension' of the usual bootstrap method, capable of incorporating prior information on F. This also lends some Bayesian credit to Efron's bootstrap, and shows that the incorrect interpretation of the traditional bootstrap distribution as a posterior distribution for the parameter isn't so incorrect after all. Note that the BB smooths also outside the data points, unlike the classic bootstrap. In the a close to zero case the BB is also an approximation to Rubin's (1981) 'degenerate prior Bayesian bootstrap', as indicated in Section 2. A large-sample justification for the BB is given in Section 3. Under frequentist circumstances it is shown that five different approaches tend to agree, asymptotically; the exact Bayesian, the bootstrap Bayesian, the Rubin bootstrap, the ordinary nonparametric large-sample method, and the classic bootstrap.

Section 4 gives two Bayesian bias correction methods for the BB. In Section 5 the BB method is shown at work for a couple of parameters. Some suggestions on how to select parameters in the prior Dirichlet process is briefly discussed in Section 6, thus opening for empirical Bayes versions of the bootstrap. In particular the Rubin method, for which the Efron method is the BB approximation, can be seen as a natural empirical Bayes strategy. Section 7 presents the BB for semiparametric regression, where the residual distribution is given a Dirichlet prior. This leads in particular to an interesting frequentist bootstrap scheme suggestion. In Section 8 we deviate a bit from the main story and report on a brief investigation into bootstrapping schemes for censored data and hazard rate models. Finally several supplementing remarks are made in Section 9.

- 2. The Bayesian bootstrap. This section motivates the Bayesian bootstrap method (1.5)–(1.9) and explains why it can be expected to work. Then connections to Efron's (1979, 1982) traditional bootstrap and to Rubin's (1981) degenerate-prior Bayesian bootstrap are commented on.
- 2A. Approximating the posterior distribution. Before discussing our Bayesian bootstrap method further, let us mention that the posterior distribution  $G_n$  of (1.3) can be

evaluated exactly for a few parameter functionals. Section 5 provides calculations for  $\theta = F\{A\}$ , A a set of interest, and  $\theta = F^{-1}(p)$ , the p-quantile. For other parameters it may be possible to carry out almost-exact simulation of  $\mathcal{L}_B\{\theta|\text{data}\}$ , as hinted at before (1.5).

For such an example, let  $\theta = \int x \, dF(x)$  be the mean of F. The exact distribution of  $\theta$  given data can be obtained, but the resulting expressions are complicated and make exact simulation difficult. See Hannum, Hollander, and Langberg (1981), Yamato (1984), and Cifarelli and Regazzini (1990). However, the posterior distribution can be approximated with that of  $\theta' = \sum_{i=1}^n x_i F\{x_i\} + \sum_{j=1}^m y_j F\{A_j\}$ , say, where  $A_1, \ldots, A_m$  is a fine partition of  $\mathcal{R} - \{x_1, \ldots, x_n\}$ , and  $y_j \in A_j$ . This  $\theta'$  can then be simulated, since  $(F\{x_1\}, \ldots, F\{x_n\}, F(A_1), \ldots, F(A_m))$  has a (finite-dimensional) Dirichlet distribution. Hjort (1976) showed that  $\beta_m \to_d \beta$  in  $\mathcal{X}$  implies  $\mathrm{Dir}(\beta_m) \to_d \mathrm{Dir}(\beta)$  in the space of probability masures on  $\mathcal{X}$ , w.r.t. various metrics, and  $\int x \, dF_m(x) \to_d \int x \, dF(x)$  under a mild extra condition on  $\{\beta_m\}$ . This result justifies  $\mathcal{L}(\theta) \approx \mathcal{L}(\theta')$  above, and can be used to approximate  $G_n$  also in more general cases, using a simpler variable that involves only finite-dimensional Dirichlet distributions. Another almost-exact simulation strategy is described in Section 9B.

This example illustrates that (1.3) in general will be difficult to obtain via exact or almost-exact simulation from  $G_n$ . The Bayesian bootstrap method described in (1.5)–(1.9) is clearly much simpler. Note that  $X_i^*$  is from  $F_0$  with probability a/(a+n) and is equal to  $x_j$  with probability 1/(a+n), for  $j=1,\ldots,n$ . The description in (1.6)–(1.7) assumed a to be an integer. If  $a=m+\beta$ , say, with m an integer and  $0<\beta<1$ , generate n+m+1  $X_i^*$ 's from  $F_{n,B}$  instead, and use  $F_{BB}^*(t)=\left[\sum_{i=1}^{n+m}I\{X_i^*\leq t\}+\beta I\{X_{n+m+1}^*\leq t\}\right]/(n+m+\beta)$ .

To explain why the BB method can be expected to work, consider the two dataconditional distributions  $\mathcal{L}_B\{F|\text{data}\}$  and  $\mathcal{L}_*\{F_{BB}^*|\text{data}\}$ . Judicious calculations give

$$E_{B}\{F(t)|\text{data}\} = F_{n,B}(t),$$

$$E_{*}\{F_{BB}^{*}(t)|\text{data}\} = F_{n,B}(t),$$

$$\text{cov}_{B}[\{F(s), F(t)\}|\text{data}] = \frac{1}{n+a+1}F_{n,B}(s)\{1 - F_{n,B}(t)\},$$

$$\text{cov}_{*}[\{F_{BB}^{*}(s), F_{BB}^{*}(t)\}|\text{data}] = \frac{1}{n+a}F_{n,B}(s)\{1 - F_{n,B}(t)\},$$

$$(2.1)$$

for all  $s \leq t$ . Accordingly, for well-behaved functionals  $\theta = \theta(F)$  we would expect

$$\mathcal{L}_B\{\theta(F)|\text{data}\} \approx \mathcal{L}_*\{\theta(F_{BB}^*)|\text{data}\}, \text{ that is } G_n \doteq \widehat{G}_n.$$
 (2.2)

As a point of further comparison it may be considered a bit annoying that the skewness of F|data is about twice that of  $F_{BB}^*|\text{data}$ , but they are both small for moderate to large n:

$$E_{B}\{F(t) - F_{n,B}(t)\}^{3} | \text{data} = \frac{2F_{n,B}(t)\{1 - F_{n,B}(t)\}\{1 - 2F_{n,B}(t)\}}{(n+a+1)(n+a+2)},$$

$$E_{*}\{F_{BB}^{*}(t) - F_{n,B}(t)\}^{3} | \text{data} = \frac{F_{n,B}(t)\{1 - F_{n,B}(t)\}\{1 - 2F_{n,B}(t)\}}{(n+a)^{2}}.$$
(2.3)

One might therefore expect the (uncorrected) BB and the exact Bayes methods to be first order but not second order equivalent; see Section 3.

We could have made the second order moments agree completely and not only approximatively in (2.1) by drawing n+a+1 BB-data, instead of n+a, to form  $F_{BB}^*$ . The difference is tiny and disappears for moderate to large samples. We have chosen BB-sample size n+a to better reflect the Bayesian balancing of prior information and data and to better highlight the generalisation from the usual Efron bootstrap.

2B. Connections to other bootstraps. Consider the non-informative case a close to zero (or, rather, a/n close to zero). Then the BB procedure advocates taking bootstrap samples of size n from the usual  $F_n$ , and basing analysis on simulating  $\theta^* = \theta(X_1^*, \ldots, X_n^*)$ . But this is the familiar nonparametric Efron bootstrap! In particular the BB percentile interval becomes Efron's (uncorrected) percentile interval. Thus the BB method is a proper Bayesian generalisation of the classic bootstrap. And since the BB really works, by Section 3, this also lends Bayesian credit to the classic bootstrap; it is the 'vague prior' version of a natural nonparametric Bayesian strategy. The incorrect interpretation of the bootstrap distribution (say in the form of a histogram of 1000 bootstrap values) as a posterior distribution for the parameter isn't that incorrect after all; it is an approximation to the true posterior distribution if the starting point is a Dirichlet with a small a.

There are better confidence interval methods than the percentile method for the classic bootstrap, but the more sophisticated versions, incorporating bias and acceleration corrections, are still first-order large-sample equivalent to the simple one. Corrections to the BB percentile interval appear in Section 4 below. It should also be remarked that the classic bootstrap has several other uses than the making of confidence intervals, like estimating variances of complicated estimators. The BB scheme is general enough to handle such problems too, but would in general need an inside bootstrap loop as well.

Rubin (1981) and Efron (1982, Ch. 10) discuss a simple Bayesian bootstrap different from the one proposed here. The Rubin bootstrap, although somewhat differently presented in his paper, can be seen to be the limiting Bayes method obtained by using  $F \sim \text{Dir}(aF_0)$  as prior and then letting  $a \to 0$ , i.e. using  $\mathcal{L}_B\{\text{data}\} = \text{Dir}(nF_n)$ , see (1.2). (Actually, Rubin and Efron consider only finite sample spaces, but the extension to the present generality is not difficult using the available theory of Dirichlet processes.) In this limiting case F|data is concentrated on the observed data values,  $F = \sum_{i=1}^{n} d_i \delta(x_i)$ , with weights  $(d_1, \ldots, d_n)$  following a Dirichlet  $(1, \ldots, 1)$  distribution (uniform on the simplex of nonnegative weights summing to one). In particular values of  $\theta(F)$  can be simulated from the exact  $G_n$  of (1.3). The  $d_i$ 's may be simulated as  $e_i/(e_1+\cdots+e_n)$ , where the  $e_i$ 's are unit exponential. If  $\theta(F) = \int x \, dF(x)$  is the mean, for example, then a large number of realisations of  $\theta(F) = \sum_{i=1}^n d_i x_i = \sum_{i=1}^n e_i x_i / \sum_{i=1}^n e_i$  can be generated, the distribution of these values will approximate  $G_n$ , enabling one to get good numerical approximations to  $\theta_B$  and to the interval (1.4). Rubin (1981) notes that this approach, though different in interpretation, agrees well, operationally and inferentially, with the ordinary bootstrap procedure.

The Rubin bootstrap does not come out of letting  $a \to 0$  in the BB method proposed here. Results of Section 3 show that these are large-sample equivalent to the first order,

in particular the Bayesian using a Dirichlet prior with a small a (Rubin) may view the Efron bootstrap (which is our BB with small a) as a numerical simulation device giving approximately the same results. Rubin's method smooths the weights, but rigidly sticks to the observed data poins (as does the ordinary bootstrap), whereas the more generally applicable BB method proposed here smooths also outside the data points, using  $F_{n,B}$ . One might call this paper's BB the informative Bayesian bootstrap and Rubin's BB the degenerate-prior bootstrap. (And with due fairness Rubin didn't advocate its general use, but concentrated on connections to and comparisons with Efron's method.) The results and remarks above suggest that the present informative BB comes much closer to being a proper Bayesian generalisation of Efron's bootstrap, both in operation and in spirit.

In a recent paper Newton and Raftery (1991) have developed a Bayesian-inspired weighted likelihood bootstrap. In its nonparametric form it generalises Rubin's method in a way different from our BB. Their method does not smooth outside the data points, whereas our does, in presence of a prior guess  $F_0$ . See further discussion in their Section 8. There are finally indirect connections to some of the bootstrapping schemes we discuss for hazard rate models in Section 8 below.

- 3. Large-sample justification: Five statisticians agree. In this section it is proved that the two conditional distributions  $\mathcal{L}_B\{\theta(F)|\text{data}\}$  and  $\mathcal{L}_*\{\theta(F)|\text{data}\}$  are asymptotically equivalent to the first order. We also show that five different approaches tend to give the same inference for large samples; the classical using delta methods, the classic bootstrap, the accurate Bayesian using Dirichlet priors, Rubin's non-informative prior bootstrap, and the BB. Then some supplementing remarks are made.
- 3A. Finite sample space. Assume first, and mostly for illustrational purposes, that the sample space is finite, say  $\mathcal{X} = \{1, \dots, L\}$ . Let

$$f_{\text{true}}(l) = \Pr_{F}\{X_i = l\}, \quad f_n(l) = \frac{1}{n} \sum_{i=1}^n I\{x_i = l\}, \quad \text{and } f_{n,B}(l) = \frac{af_0(l) + nf_n(l)}{a+n}.$$

Efron (1982, Ch. 5.6) observed that

$$\mathcal{L}\{\sqrt{n}(f_n - f_{\text{true}})\} \to N_L\{0, \Sigma(f_{\text{true}})\},$$
 (3.1)

$$\mathcal{L}_*\{\sqrt{n}(f_n^* - f_n)|\mathrm{data}\} \approx N_L\{0, \Sigma(f_n)\} \rightarrow N_L\{0, \Sigma(f_{\mathrm{true}})\} \text{ a.s.},$$
 (3.2)

where  $f_n^*(l) = (1/n) \sum_{i=1}^n I\{\tilde{x}_i = l\}$  stems from the ordinary bootstrap, and where  $\Sigma(f)$  has elements  $f(l)\delta_{l,m} - f(l)f(m)$ . Efron discussed why (3.1)-(3.2) may be taken as an asymptotic justification for a class of inferential procedures based on the bootstrap. Note that the (3.1)-(3.2) results rely only on asymptotic theory for the multinomial distribution, and that the 'almost surely' statement refers to the set  $\Omega_0$  of probability 1 under which each  $f_n(l)$  goes to  $f_{\text{true}}(l)$ .

These can now be accompanied by results for the exact and the BB approximated posterior distributions  $\mathcal{L}_B\{f|\text{data}\}$ ,  $\mathcal{L}_*\{f_{BB}^*|\text{data}\}$ . The framework is the frequentist one, where the  $X_i$ 's are truly i.i.d. from  $f_{\text{true}}$ . One can prove

$$\mathcal{L}_B\{(n+a+1)^{1/2}(f-f_{n,B})|\text{data}\} \approx N_L\{0,\Sigma(f_{n,B})\} \to N_L\{0,\Sigma(f_{\text{true}})\} \text{ a.s.,}$$
 (3.3)

$$\mathcal{L}_*ig\{(n+a)^{1/2}(f_{BB}^*-f_{n,B})|{
m data}ig\} pprox N_L\{0,\Sigma(f_{n,B})\} o N_L\{0,\Sigma(f_{
m true})\} \ {
m a.s.} \ \ (3.4)$$

The first follows from asymptotic properties of the Dirichlet distribution, while the second is essentially the multidimensional central limit theorem. Note that exactly the same a.s. set  $\Omega_0$  is at work in (3.1)-(3.4). The parameter a is supposed to be fixed in (3.3)-(3.4), so that  $f_{n,B} \to f_{\text{true}}$  on  $\Omega_0$ , but arguments underlying the indicated approximations show that the two distributions are approximately equal even if a goes to infinity with n. [Certain minimax procedures correspond to using a proportional to  $\sqrt{n}$ , for example; see Hjort (1976).] Efron's discussion of the consequences of (3.1) and (3.2) (1979, p. 23; 1982, Ch. 5.6) can now be applied to (3.3) and (3.4) as well, and provides the asymptotic justification for the BB procedure for the case of a finite sample space.

It is interesting to note that if only  $a/\sqrt{n} \to 0$  as n grows, then  $\sqrt{n}\{f(l) - f_n(l)\} - \sqrt{n}\{f(l) - f_{n,B}(l)\}$  goes to zero, which implies

$$\mathcal{L}_B\{\sqrt{n}(f-f_n)|\mathrm{data}\} \to N_L\{0,\Sigma(f_{\mathrm{true}})\} \text{ a.s.},$$
 (3.5)

$$\mathcal{L}_*\{\sqrt{n}(f_{BB}^* - f_n)|\text{data}\} \to N_L\{0, \Sigma(f_{\text{true}})\} \text{ a.s.}$$
 (3.6)

Accordingly, looking back at (3.1)–(3.2), four different approaches will lead to the same inferential statements, up to first order asymptotics: the classical based on  $f_n$ ; the ordinary Efron bootstrap; the proper posterior Bayes; and the BB. This holds for each fixed a, also for  $a \to 0$ , which means that Rubin's degenerate-prior bootstrap (see Section 2) also is large-sample equivalent to the other four.

3B. The real line. Now consider extension of the preceding results and conclusions to  $\mathcal{X} = \mathcal{R}$ . The degree to which (3.1) and (3.2) and its consequences have analogues for  $\mathcal{X} = \mathcal{R}$  was investigated in Bickel and Freedman (1981) and Singh (1981), and later on in the form of extensions and refinements by other authors. The canonical parallel to (3.1) is

$$\mathcal{L}\left[\sqrt{n}\left\{F_n(.) - F(.)\right\}\right] \to W_0(F(.)) \quad \text{in } D[-\infty, \infty], \tag{3.7}$$

where  $W_0$  is a Brownian bridge and convergence takes place in the space  $D[-\infty, \infty]$  of all right continuous functions y(.) on the line with left hand limits and obeying  $y(-\infty) = y(\infty) = 0$ , see for example Billingsley (1968). Bickel and Freedman (1981) proved the bootstrap companion

$$\mathcal{L}_*\big[\sqrt{n}\{F_n^*(.) - F_n(.)\}| \text{data}\big] \to W_0(F(.)) \quad \text{in } D[-\infty, \infty] \text{ a.s.}, \tag{3.8}$$

and concluded that the bootstrap works for well-behaved functionals  $\theta = \theta(F)$ .

These results can be parallelled in the present Bayesian posterior context. Again, we look at limiting properties in an ordinary framework in which  $F_n$  according to the Glivenko-Cantelli theorem converges uniformly to  $F = F_{\text{true}}$  on a set  $\Omega_0$  of probability one.

THEOREM. Let a vary with n in such a way that  $F_{n,B} = (aF_0 + nF_n)/(a+n)$  goes to some  $F_{\infty}$  on  $\Omega_0$ ;  $F_{\infty}$  is just  $F_{\text{true}}$  if only a/n goes to zero. Then

$$\mathcal{L}_{B}[(n+a+1)^{1/2}\{F(.)-F_{n,B}(.)\}|\text{data}] \to W_{0}(F_{\infty}(.)),$$
 (3.9)

$$\mathcal{L}_*[(n+a)^{1/2}\{F_{BB}^* - F_{n,B}(.)\}|\text{data}] \to W_0(F_{\infty}(.)),$$
 (3.10)

along every sequence in  $\Omega_0$ .

PROOF: The second statement is within reach of the (triangular version of) the classical Donsker invariance theorem for i.i.d. random variables. The first statement involves proving finite-dimensional convergence and tightness. Finite-dimensional convergence follows upon studying asymptotic properties of (finite-dimensional) Dirichlet distributions. To prove tightness (with probability 1), calculate first  $E(k+1)^2(U-\alpha)^2(V-\beta)^2$  where (U,V,W) is Dirichlet  $(k\alpha,k\beta,k\gamma)$  and  $\alpha+\beta+\gamma=1$ . The resulting expression can be bounded by  $3\alpha\beta$ , regardless of k. Hence

$$(n+a+1)^2 E_B[F(s,t] - F_{n,B}(s,t]]^2 \{F(t,u] - F_{n,B}(t,u]\}^2 |\text{data}]$$
  
  $\leq 3F_{n,B}(s,t)F_{n,B}(t,u)$ 

for  $s \leq t \leq u$ . Taking limsup gives the bound  $3F_{\infty}(s,t]F_{\infty}(t,u]$  on the right hand side, for sequences in  $\Omega_0$ . This implies tightness by the proof of Billingsley's (1968) Theorem 15.6 (but not quite by the theorem itself).  $\square$ 

Thus the conditional distributions  $\theta(F)|\text{data}$  and  $\theta(F_{BB}^*)|\text{data}$  will be close to each other for well-behaved functionals, justifying the BB method. Particular examples can be worked through, as in Bickel and Freedman (1981). Their tentative description of well-behavedness (p. 1209) can also be subscribed to here. Sufficient conditions for

$$\mathcal{L}_Big[(n+a+1)^{1/2}\{ heta(F)- heta(F_{n,B})\}| ext{data}ig] o N\{0,\sigma^2(F_\infty)\} ext{ a.s.},$$
  $\mathcal{L}_*ig[(n+a)^{1/2}\{ heta(F_{BB}^*)- heta(F_{n,B})\}| ext{data}ig] o N\{0,\sigma^2(F_\infty)\} ext{ a.s.}$ 

to hold, for appropriate variance  $\sigma^2(F_{\infty})$ , can be written down using von Mises or influence function methods. See for example Boos and Serfling (1980) and Parr (1985), who use Frechét differentiability, or Shao (1989) who uses Lipschitz differentiability, or Gill (1989) with Hadamard or compact differentiability. The limit results obtainable using such machinery imply

$$\widehat{G}_n^{-1}(p) \doteq G_n^{-1}(p) \doteq \theta(F_{n,B}) + z_p \, \sigma(F_{\infty}) / \sqrt{n+a},$$

where  $z_p$  is the p-quantile of the standard normal.

If a is fixed, or only  $a/\sqrt{n} \to 0$ , then

$$\mathcal{L}_{B}ig[\sqrt{n}\{F(.)-F_{n}(.)\}| ext{data}ig]
ightarrow W_{0}(F_{ ext{true}}(.)) ext{ a.s.,}$$

$$\mathcal{L}_*ig[\sqrt{n}\{F_{BB}^*(.)-F_n(.)\}|\mathrm{data}ig] o W_0(F_{\mathrm{true}}(.))$$
 a.s.

A conclusion concerning the approximate agreement among the five statisticians referred to after (3.5)–(3.6) is therefore reached also for  $\mathcal{X} = \mathcal{R}$  (and for more general spaces). Each of them reaches confidence intervals that are first-order equivalent to

$$\theta(F_n) - z_{1-\alpha} \, \sigma(F_n) / \sqrt{n} \le \theta(F) \le \theta(F_n) + z_{1-\alpha} \, \sigma(F_n) / \sqrt{n}, \tag{3.11}$$

albeit from different perspectives and with partly different interpretations. This holds for each  $Dir(aF_0)$  prior, and, regarding the classic bootstrap, holds for both the simple

percentile interval and for the somewhat better reflected bootstrap interval  $[2\theta(F_n) - G_n^{*-1}(1-\alpha), 2\theta(F_n) - G_n^{*-1}(\alpha)]$ , where  $G_n^*$  is the bootstrap distribution.

It is perhaps surprising that a simple method like the BB, constructed merely to make the mean function and covariance function of the exact and approximate distributions of F(.) agree, can work well for the vast majority of parameter functionals. As indicated in (3.9)–(3.10) this is at least partly the work and the magic of the functional central limit theorem. This also points to the possibility of using 'small-sample asymptotics' machinery to arrive at other approximations to the posterior distribution  $G_n$ , for example Edgeworth–Cramér expansions combined with Taylor expansions. Such an approach would be functional-dependent, however; a primary virtue of the BB is that it is both simple and versatile. A similar remark applies to the classic bootstrap, of course.

The results in this section are taken from the technical report Hjort (1985). Results resembling (3.9) and (3.10) have also been found by Lo (1987), who also worked with rates of convergence.

4. A Bayesian bias correction to the BB percentile interval. The ordinary frequentist bootstrap percentile intervals can be corrected for bias and acceleration, see Efron (1987). The BB percentile interval (1.9) cannot be corrected in the same way, cf. Hjort (1985, Section 4). There is another possibility of detecting and repairing a bias, however. For each in a respectable catalogue of examples there is a known transformation h, perhaps the identity, such that the posterior expected value of  $h(\theta(F))$  is explicitly calulable by some published formula, i.e.  $\nu_0 = E_B\{h(\theta(F))|\text{data}\}$  is known. The BB procedure uses

$$\widehat{H}_n(t) = \Pr_*\{h(\theta(F_{BB}^*)) \le t | \text{data}\} = \widehat{G}_n(h^{-1}(t))$$

to estimate  $H_n$ , the c.d.f. of  $h(\theta(F))$  given data, and approximates  $\nu_0$  with

$$\widehat{\nu}_0 = \int t \, d\widehat{H}_n(t) \doteq \frac{1}{\text{boot}} \sum_{i=1}^{\text{boot}} h(\theta(F_{BB}^{*b})) = \nu_0 + \varepsilon, \tag{4.1}$$

say. Accordingly, if  $\varepsilon \neq 0$ , then  $\widehat{H}_n$  is not a perfect estimate of  $H_n$ . The repaired estimate  $\widehat{H}_{\varepsilon}(t) = \widehat{H}(t+\varepsilon)$  gets the mean right, however. Hence

$$\widehat{H}_{\epsilon}^{-1}(\alpha) = \widehat{H}^{-1}(\alpha) - \varepsilon \le h(\theta(F)) \le \widehat{H}^{-1}(1-\alpha) - \varepsilon = \widehat{H}_{\epsilon}(1-\alpha)$$

would be a natural corrected confidence interval for  $h(\theta(F))$ . Transforming back we obtain

$$h^{-1}\left[h(\widehat{G}_n^{-1}(\alpha)) - \varepsilon\right] \le \theta(F) \le h^{-1}\left[h(\widehat{G}_n^{-1}(1-\alpha)) - \varepsilon\right] \tag{4.2}$$

as the bias-corrected BB percentile interval for  $\theta(F)$ . Of course this interval is just (1.9) if  $\varepsilon = 0$ . We emphasise that the bias correction is not concerned with frequentist coverage probabilities, but is a simple way of repairing the BB estimate  $\widehat{G}_n$  of  $G_n$  so as to get the mean of  $h(\theta(F))$  straight.

As an example, suppose an interval is needed for  $\sigma(F)$ , the standard deviation. One may prove, using methods of Ferguson (1973) and Hjort (1976), that

$$E_{B}\{\sigma^{2}(F)|\text{data}\} = \frac{n+a}{n+a+1} \left[ \frac{a}{n+a} \sigma^{2}(F_{0}) + \frac{n}{n+a} \sigma^{2}(F_{n}) + \frac{a}{n+a} \frac{n}{n+a} \{\theta(F_{n}) - \theta(F_{0})\}^{2} \right]. \tag{4.3}$$

The bias corrected confidence interval for  $\sigma(F)$  is therefore

$$\{\widehat{G}_n^{-1}(\alpha)^2 - \varepsilon\}^{1/2} \le \sigma(F) \le \{\widehat{G}_n^{-1}(1-\alpha)^2 - \varepsilon\}^{1/2},$$

where  $\varepsilon$  is the difference between the average value of the observed  $(\sigma_{BB}^*)^2$  and  $E_B\{\sigma^2(F)|\text{data}\}$ .

One can also write down a slightly more general bias and variance corrected BB percentile interval which also takes into account the value of  $\tau_0^2 = \text{Var}\{h(\theta(F))|\text{data}\}$  if it is available. Assume that, in addition to (4.1),

$$\widehat{ au}_{0}^{2} = \int (t - \widehat{
u}_{0})^{2} d\widehat{H}_{n}(t) \doteq \frac{1}{\mathrm{boot}} \sum_{b=1}^{\mathrm{boot}} \{h(\theta_{BB}^{*b} - \widehat{
u}_{0})^{2} = \tau_{0}^{2} (1 + \delta)^{2}.$$

A perhaps better estimate of  $G_n(h^{-1}(t))$  is then  $\widehat{H}_{n,\varepsilon,\delta}(t) = \widehat{H}_n((1+\delta)t + \varepsilon - \nu_0\delta)$ , since it manages to get both the mean and the variance right. Using  $\widehat{H}_{n,\varepsilon,\delta}^{-1}(p) = \{\widehat{H}_n^{-1}(p) + \nu_0\delta - \varepsilon\}/(1+\delta)$  one ends up with

$$h^{-1}\left[\frac{h(\widehat{G}_n^{-1}(\alpha)) + \nu_0 \delta - \varepsilon}{1 + \delta}\right] \le \theta(F) \le h^{-1}\left[\frac{h(\widehat{G}_n^{-1}(1 - \alpha)) + \nu_0 \delta - \varepsilon}{1 + \delta}\right]. \tag{4.4}$$

For an example, consider the mean parameter  $\theta(F) = \int x \, dF(x)$ , for which the posterior expectation is  $\nu_0 = \frac{a}{a+n}\theta(F_0) + \frac{n}{a+n}\bar{X}_n$  and the posterior variance is

$$\tau_0^2 = \frac{1}{n+a+1} \left[ \frac{a}{n+a} \sigma^2(F_0) + \frac{n}{n+a} \sigma^2(F_n) + \frac{a}{n+a} \frac{n}{n+a} \{\theta(F_n) - \theta(F_0)\}^2 \right].$$

The last formula is proved using methods of Ferguson (1973) and Hjort (1976) again, cf. (4.3). The bias and variance corrected interval for  $\theta(F)$  is

$$\frac{\widehat{G}_n^{-1}(\alpha) + \nu_0 \delta - \varepsilon}{1 + \delta} \leq \theta(F) \leq \frac{\widehat{G}_n^{-1}(1 - \alpha) + \nu_0 \delta - \varepsilon}{1 + \delta}.$$

One can similarly handle parameters of the type  $g(\int f(x) dF(x))$ .

It should also be possible to construct a Bayesian skewness correction, cf. (2.3), but this is not pursued here.

- 5. Some exact calculations. This section looks briefly into the nature of the BB approximation method in two cases where exact calculations are possible.
  - 5A. A probability. If  $\theta(F) = F(A)$  for some set A of interest, then

$$\mathcal{L}_{B}\{\theta(F)|\mathrm{data}\} = \mathrm{Beta}\big\{aF_{0}(A) + \#(x_{i} \in A), a(1 - F_{0}(A)) + \#(x_{i} \notin A)\big\}.$$

Thus (1.3) and (1.4) can be obtained from tables of the incomplete Beta function. In this case the BB method amounts to approximating the Beta distribution  $G_n$  with that of Y/(n+a), where Y is binomial  $[n+a, \{aF_0(A) + \#(x_i \in A)\}/(a+n)]$ .

If U is Beta $\{mp, m(1-p)\}$  and V is Bin $\{m, p\}/m$ , then EU = EV = p, and

$$\operatorname{Var} U = \frac{p(1-p)}{m+1}, \quad \operatorname{Var} V = \frac{p(1-p)}{m}.$$

They differ in skewness and kurtosis, but not to any dramatic extent; for example,

$$\mathrm{skew}\, U = 2 \frac{(m+1)^{1/2}}{m+2} \frac{1-2p}{\{p(1-p)\}^{1/2}}, \quad \mathrm{skew}\, V = \frac{1}{m^{1/2}} \frac{1-2p}{\{p(1-p)\}^{1/2}}.$$

Brief investigations have shown the distributions of U and V, and therefore confidence intervals based on either the exact or BB approximated distributions, to be remarkably similar, even for moderate m. This holds provided p is not too close to zero or one, provided  $\alpha$  is not too close to zero, and finally provided the discrete distribution of V is interpolated. Rather than using  $\widehat{G}_m(t) = \Pr[\text{Bin}\{m,p\}/m \leq t]$ , which jumps at the points j/m, use  $\widetilde{G}_m(j/m) = \frac{1}{2}\Pr[\text{Bin}\{m,p\}/m \leq j/m] + \frac{1}{2}\Pr[\text{Bin}\{m,p\}/m \leq (j-1)/m]$ , and interpolate linearly in between. Similar modifications to  $\widehat{G}_n$  of (1.7) should also be used in other cases where it increases in sharp jumps.

5B. The median. The p-quantile functional is another example where it is possible to calculate the posterior distribution explicitly, but the resulting expressions are complex, and the BB would be much easier to carry out in practice. For simplicity only the median  $\theta(F) = F^{-1}(\frac{1}{2}) = \inf\{t: F(t) \ge \frac{1}{2}\}$  is considered here.

Assume for concreteness that the data points are distinct, with  $x_1 < \ldots < x_n$ . We shall find  $G_n(t) = \Pr\{\theta(F) \le t | \text{data}\}$ . For data point  $x_j$  one has

$$G_n\{x_j\} = \Pr\{F(-\infty, x_j) < \frac{1}{2}, F(-\infty, x_j] \ge \frac{1}{2}\}$$
  
=  $\Pr\{U < \frac{1}{2}, U + V \ge \frac{1}{2}\} = \Pr\{U < \frac{1}{2}, W < \frac{1}{2}\},$ 

in which (U, V, W) is Dirichlet with parameters  $\alpha = aF_0(x_j - 1) + j - 1$ ,  $\beta = aF_0\{x_j\} + 1$ , and  $\gamma = aF_0(x_j, \infty) + n - j$ . Taking the prior guess c.d.f. to be continuous we find

$$egin{aligned} G_n\{x_j\} &= rac{\Gamma(lpha+eta+\gamma)}{\Gamma(lpha)\Gamma(eta)\Gamma(eta)}rac{1}{lpha}\Big(rac{1}{2}\Big)^lpharac{1}{\gamma}\Big(rac{1}{2}\Big)^\gamma \ &= rac{\Gamma(a+n)}{\Gamma(aF_0(x_j)+j)\Gamma(a\{1-F_0(x_j)\}+n-j+1)}\Big(rac{1}{2}\Big)^{a+n-1}. \end{aligned}$$

Next consider  $G_n[t, t+dt]$  for some t outside the data points, and let for further convenience  $F_0$  be the integral of a prior guess density  $f_0$ . Following the reasoning above one may show that  $G_n$  has density at  $t \in (x_j, x_{j+1})$  given by

$$g_n(t) = rac{\Gamma(a+n)}{\Gamma(aF_0(t)+j)\Gamma(a\{1-F_0(t)\}+n-j)}\,af_0(t)\,Jig[aF_0(t)+j,a\{1-F_0(t)\}+n-jig],$$

where

$$J[lpha,\gamma] = \int_0^{rac{1}{2}} \int_0^{rac{1}{2}} u^{lpha-1} w^{\gamma-1} (1-u-w)^{-1} \ du dw.$$

It is in principle possible to compute for example the posterior expectation and the upper and lower 5 percent points for  $G_n$  based on this.

Now consider the BB method in this situation. Let for simplicity n + a = 2m + 1 be odd. The BB approximates the complicated  $G_n$  using  $X_i^*$ 's from  $F_{n,B}$ , as follows:

$$egin{aligned} \widehat{G}_n(t) &= \Pr_* ig[ heta_{BB}^* = \operatorname{median}\{X_1^*, \dots, X_{n+a}^*\} \leq t | \operatorname{data} ig] \ &= \Pr ig[ \operatorname{Bin}\{2m+1, F_{n,B}(t)\} \geq m+1 ig]. \end{aligned}$$

Expressions for  $\widehat{G}_n\{x_j\}$  and for the density  $\widehat{g}_n$  that the distribution has between data points can be worked out based on this, and they can be compared with  $G_n$  and  $g_n$  obtained above. Such a study is not pursued here. Note that the endpoints of the BB confidence interval (1.9) can be found using binomial tables. Note finally that in the non-informative case, where  $a \to 0$ , both  $G_n$  and  $\widehat{G}_n$  are supported on the data points.

- 6. Empirical Bayesian bootstrapping. The ideal Bayesian is able to specify a and  $F_0$  from the infamous but abstract 'prior considerations'. Results of Section 3 show that the importance of these parameters diminishes and disappears with growing n, but they do matter for small and moderate n. This section briefly discusses some empirical methods.
- 6A. Choosing a and parameters in  $F_0$ . In some situations previous data may be available that are either of the same type as the  $X_i$ 's or at least of a similar type. In the best case one has m previous measurements  $X_i^0$  that come from the same F as the new  $X_i$ 's. Then one may use a = m (indeed the 'prior sample size') and  $F_0$  equal to a smoothed empirical distribution or some fitted normal, say.

In other cases one might have a specified candidate  $F_0$  from previous similar data, but without knowing for certain that the new data are from the same distribution. Then the problem is to choose a, either from informal 'strength of belief' considerations, or from the new data. One wants to use a small a if data disagree with the old  $F_0$  and a larger one if they seem to fit. This can be done in a formal way by looking at moment properties of the empirical distribution  $F_n$ . We have  $E(F_n - F_0)^2 | F = (F - F_0)^2 + F(1 - F)/n$ , so that

$$E(F_n-F_0)^2=E(F-F_0)^2+\frac{1}{n}E\,F(1-F)=\Big(\frac{1}{n+1}+\frac{1}{n}\frac{a}{n+1}\Big)F_0(1-F_0),$$

and this can be used to fit a suitable a, for example via

$$E\int (F_n-F_0)^2 dW = \frac{1}{n} \left(1 + \frac{n-1}{a+1}\right) \int F_0(1-F_0) dW,$$

which holds for each weight measure W. Choosing  $W = F_0$  gives 1/6 for the last integral (in the continuous case).

There are other estimation methods for a with a fixed  $F_0$  and that to a larger extent uses properties of the Dirichlet process. The maximum likelihood estimator can be derived, see Hjort (1976). This and some other estimators depend however on the ties configurations in the data in a somewhat strange way, and the sufficient statistic is  $D_n$ , the number of distinct data points. This stems from some of the more esoteric and less satisfying mathematical properties of samples from a Dirichlet, and equating moments of natural quantities like above seems much more reasonable.

In still other cases there might be parameters in the prior guess  $F_0$  to specify, say  $F_0 = N\{\mu_0, \sigma_0^2\}$ . Then one is helped by  $E\bar{X}_n = E\int x\,dF(x) = \mu_0$  and

$$E\frac{1}{n-1}\sum_{i=1}^{n}(X_{i}-\bar{X}_{n})^{2}=E\sigma^{2}(F)=\frac{a}{a+1}\sigma_{0}^{2}.$$

If  $F_0$  is nonsymmetric one might fit parameters using also

$$Erac{n}{(n-1)(n-2)}\sum_{i=1}^{n}(X_i-ar{X}_n)^3=E\int\{x-\mu(F)\}^3dF(x) \ =rac{a}{a+1}rac{a}{a+2}\int\{x-\mu(F_0)\}^3dF_0(x).$$

All these moment methods should be used with care and sense. The moment formulae here have been proved using methods in Ferguson (1973) and Hjort (1976).

We mention finally that a frequentist inspired double bootstrap method for fitting a good weight  $\frac{a}{a+n}$  in the mixture  $\frac{a}{a+n}F_0 + \frac{n}{a+n}F_n$  was suggested in Hjort (1988).

- 6B. Cross validation and Rubin-Efron as empirical Bayes solutions. Observe that the kind of schemes described above can be used on the basis of only the given data set, by dividing it into a small training set and the remaining test set, or by some more elaborate cross validation strategy. A simple version of this is as follows: Pick a data points to constitute the training set, from which the nonparametric guess on F is  $F_a$ , the empirical c.d.f. for these. Since the remaining n-a data points come from the same F the considerations above suggest using a  $Dir(aF_a)$  as prior for F. But then the posterior becomes Dirichlet with  $aF_a + (n-a)F_{n-a} = nF_n = \sum_{i=1}^n \delta(x_i)$ . This is accordingly an empirical Bayes argument for using Rubin's method, and a fortiori for using its natural BB approximation, which is the classic Efron bootstrap.
- 7. BB in semiparametric regression. This section briefly discusses the extension of some of the previous methods and results to the semiparametric regression case. The model is

$$Y_{i} = \sum_{j=1}^{p} x_{i,j} \beta_{j} + \sigma \varepsilon_{i} = x'_{i} \beta + \sigma \varepsilon_{i}, \quad i = 1, \dots, n,$$
 (7.1)

where the standardised residuals  $\varepsilon_i = (Y_i - x_i'\beta)/\sigma$  are i.i.d. from F. The Bayesian version must have a prior distribution for the unknown parameters  $\beta$ ,  $\sigma$ , F. We stipulate that  $(\beta, \sigma)$  comes from some prior density  $\pi(\beta, \sigma)$  and that F, independently, comes from the

Dirichlet process with parameter  $a\Phi$ , where  $\Phi(.)$  is the standard normal. When a is large then the distribution of F becomes concentrated in  $\Phi$ , which gives us the familiar textbook normal regression model. This is accordingly a Bayesian generalisation with built-in uncertainty about the residual distribution. We are interested in Bayesian inference about parameters  $\theta = \theta(\beta, \sigma, F)$ , like regression deciles  $x'\beta + \sigma F^{-1}(j/10)$ , probabilities  $\Pr\{Y(x) \leq y\} = F((y-x'\beta)/\sigma)$ , expected distance  $E|Y(x)-x'\beta|$ , Eccetera. A BB strategy is arrived at below which makes it possible to get an approximation to the full posterior distribution of such parameters.

More general results of Hjort (1986, 1987) imply that the posterior density for  $(\beta, \sigma)$  becomes

$$\pi_n(\beta, \sigma | \text{data}) = \text{const.} \pi(\beta, \sigma) \prod_{i=1}^n \{ \sigma^{-1} \phi((y_i - x_i' \beta) / \sigma) \}, \tag{7.2}$$

provided the  $y_i$ 's are distinct, i.e., the posterior distribution for these parameters are as if F had been known to be  $\Phi$ . And F has a distribution being a mixture of Dirichlet processes, since

$$F|\{\beta,\sigma,\mathrm{data}\}\sim\mathrm{Dir}\big\{a\Phi+\sum_{i=1}^n\delta((y_i-x_i'\beta)/\sigma)\big\}.$$
 (7.3)

This makes it easy to write down  $E_B\{F(t)|\beta,\sigma,\text{data}\}$  and then integrating out  $(\beta,\sigma) \sim \pi_n(.)$  to reach the posterior expectation of F(t). Suppose for simplicity that  $\sigma$  is known and that  $\beta$  is given a flat prior on  $\mathbb{R}^p$ , which leads to  $\pi_n$  being quite simply  $N\{\widehat{\beta}, \frac{1}{n}\sigma^2M^{-1}\}$ , where  $M = \frac{1}{n}\sum_{i=1}^n x_i x_i'$  and  $\widehat{\beta} = M^{-1} \frac{1}{n}\sum_{i=1}^n x_i Y_i$  is the familiar least squares estimator (now seen also as the Bayes solution under the flat prior). Accordingly  $\varepsilon_i = (y_i - x_i'\beta)/\sigma$  has mean value  $e_i = (y_i - x_i'\widehat{\beta})/\sigma$ , the estimated residual, and variance  $h_i^2 = \frac{1}{n}x_i'M^{-1}x_i$ , giving

$$egin{aligned} F_{n,B}(t) &= E\{F(t)|\mathrm{data}\} \ &= E\Big[rac{a}{a+n}\Phi(t) + rac{n}{a+n}rac{1}{n}\sum_{i=1}^n I\{(y_i-x_i'eta)/\sigma \leq t\}\Big|\mathrm{data}\Big] \ &= rac{a}{a+n}\Phi(t) + rac{n}{a+n}rac{1}{n}\sum_{i=1}^n \Phi\Big(rac{t-e_i}{h_i}\Big). \end{aligned}$$

In constrast to the i.i.d. case, see (1.5), this is a continuous distribution with density

$$f_{n,B}(t) = \frac{a}{a+n}\phi(t) + \frac{n}{a+n}f_n(t) = \frac{a}{a+n}\phi(t) + \frac{n}{a+n}\frac{1}{n}\sum_{i=1}^n \phi\left(\frac{t-e_i}{h_i}\right)\frac{1}{h_i}.$$
 (7.4)

The second term  $f_n(t)$  is a variable kernel density estimate with smoothing parameters  $h_i$  smaller than the usual ones, i.e.  $f_n(t)$  follows the ups and downs of a fine histogram more than a typical kernel estimate would do. This particular result is implicit in Hjort (1987) and has also been found by Olaf Bunke (1988).

We can now describe the BB strategy. For a general prior  $\pi(\beta, \sigma)$ , work out the posterior  $\pi_n(\beta, \sigma|\text{data})$  and the corresponding generalisation of (7.4), with a  $f_n(t)$  that is potentially more complicated but still a variable kernel estimate for estimated residuals

 $e_i = (y_i - x_i'\tilde{\beta})/\tilde{\sigma}$ . Choose a random  $(\beta^*, \sigma^*)$  from  $\pi_n(.)$  and then a BB sample  $\varepsilon_1^*, \ldots, \varepsilon_{n+a}^*$  of size n+a from  $F_{n,B}(t|\beta^*, \sigma^*) = E\{F(t)|\beta^*, \sigma^*, \text{data}\}$ , cf. (7.3). Then compute the BB value  $\theta_{BB}^* = \theta(\beta^*, \sigma^*, F_{BB}^*)$ , where  $F_{BB}^*$  is the empirical distribution of the chosen  $\varepsilon_i^*$ 's. This is repeated a large number of times and gives  $\widehat{G}_n(t) = \Pr_*\{\theta_{BB}^* \leq t\}$ , proposed as an approximation to  $G_n(t) = \Pr_B\{\theta(\beta, \sigma, F) \leq t | \text{data}\}$ . BB-based point estimates and BB percentile intervals can then be computed. Bias corrections of some sort can be carried out using the exact information in (the parallel to) (7.4).

An interesting bootstrapping strategy emerges in the case of vague prior information. This would mean a flat prior for  $\beta$ , a flat prior for  $\log \sigma$ , and  $a \to 0$  for the Dirichlet. The steps above take this form: Draw first  $\sigma^*$  from the distribution that corresponds to  $1/\sigma^2$  being Gamma with parameters  $\frac{1}{2}(n-p)$  and  $\frac{1}{2}(n-p)\widehat{\sigma}^2$ , where  $\widehat{\sigma}^2 = \sum_{i=1}^n (y_i - x_i'\widehat{\beta})^2/(n-p)$  is the usual estimate. Then draw  $\beta^*$  from  $N\{\widehat{\beta}, \frac{1}{n}(\sigma^*)^2M^{-1}\}$ , and then  $\varepsilon_1^*, \ldots, \varepsilon_n^*$  from the empirical distribution of  $\varepsilon_i = (y_i - x_i'\beta^*)/\sigma^*$ . Finally compute  $\theta^* = \theta(\beta^*, \sigma^*, \varepsilon_1^*, \ldots, \varepsilon_n^*)$  based on these, i.e., based on pairs  $(x_i, y_i^*)$  where  $y_i^* = x_i'\beta^* + \sigma^*\varepsilon_i^*$ . This constitutes an alternative frequentist way of bootstrapping in the semiparametric regression model.

- 8. Bootstrapping schemes in hazard rate models. To what extent do methods and results of the previous sections generalise to situations with censored data, and to more general models for survival data analysis? This section deviates somewhat from the rest of the article and reports on a brief investigation into frequentist and Bayesian bootstrapping schemes for such problems, where it is natural to shift attention from cumulative distribution functions (c.d.f.'s) to cumulative hazard rates (c.h.r.'s).
- 8A. From c.d.f. F to c.h.r. A. For concreteness we concentrate on the random censorship model here. Generalisations to counting process models should not be difficult. Life-times  $X_i^0$  from a distribution F on  $[0,\infty)$  may be censored on the right, so that only  $X_i = \min\{X_i^0, c_i\}$  and  $\delta_i = I\{X_i \leq c_i\}$  are observed. It is assumed that  $X_i^0$ 's and censoring times  $c_i$ 's are independent, and that the  $c_i$ 's come from some H. The c.h.r. A is defined via  $A[s, s+ds] = F[s, s+ds]/F[s, \infty)$ , or  $dA(s) = dF(s)/F[s, \infty)$  for short, which leads to

$$A(t) = \int_0^t \frac{dF(s)}{F(s,\infty)}$$
 and  $F(t) = 1 - \prod_{[0,t]} \{1 - dA(s)\}.$  (8.1)

When F is continuous then  $A = -\log(1 - F)$ , but we will encounter non-continuous c.d.f.'s and c.h.r.'s, for which the product integral representation (8.1) is appropriate; see for example Hjort (1990). Parameters defined in terms of F can equally be represented as functions of A, say  $\theta = \theta_{\rm cdf}(F) = \theta_{\rm chr}(A)$ .

Introduce  $N_n(t) = \sum_{i=1}^n I\{X_i \leq t, \delta_i = 1\}$ , counting the number of observed events in [0,t], and  $Y_n(t) = \sum_{i=1}^n I\{X_i \geq t\}$ , the number at risk just before time t. The Kaplan-Meier and the Nelson-Aalen estimator are respectively

$$F_n(t) = 1 - \prod_{[0,t]} \{1 - dN_n(s)/Y_n(s)\}$$
 and  $A_n(t) = \int_0^t dN_n(s)/Y_n(s)$ . (8.2)

Here  $dN_n(s)$  jumps only at observed life-times, with jump  $\Delta N_n(x_i) = 1$  if these are distinct. In particular  $A_n$  is the c.h.r. associated with  $F_n$ , and  $dA_n(s) = dN_n(s)/Y_n(s)$ .

In the uncensored case  $\Delta A_n(x_i) = 1/(n-i+1)$ , assuming  $x_1 < \ldots < x_n$ , and then  $F_n$  becomes the usual empirical c.d.f. Traditional nonparametric inference is based on the fact that for large n,  $A_n(.)$  has approximately independent increments with

$$EdA_n(s) \doteq dA(s), \quad \text{Var } dA_n(s) = EY_n(s)^{-1} dA(s) \{1 - dA(s)\}.$$
 (8.3)

A precise large-sample statement is that  $\mathcal{L}[\sqrt{n}\{A_n(.) - A(.)\}] \to V(.)$ , in which V(.) is a Gaußian martingale with independent increments and  $\operatorname{Var} dV(s) = dA(s)\{1 - dA(s)\}/y(s)$ . Here y(s) is the limit in probability of  $Y_n(s)/n$ , that is  $y(s) = F[s, \infty)G[s, \infty)$  under present circumstances. See Hjort (1991), for example. In the continuous case dA(1 - dA) = dA, of course.

8B. The weird bootstrap. Let us make the following introductory remark, which applies to both frequentist and Bayesian bootstrapping: There is nothing particularly magic about resampling data per se, and other data-conditional simulation schemes might easily work as well. In the classical i.i.d. framework, for example, resampling from  $F_n$  creates a  $F_n^*$  with the properties

$$E_*F_n^*(t) = F_n(t)$$
 and  $cov_*\{F_n^*(s), F_n^*(t)\} = n^{-1}F_n(s)\{1 - F_n(t)\}$  for  $s \le t$ , (8.4)

which properly match

$$EF_n(t) = F(t)$$
 and  $cov\{F_n(s), F_n(t)\} = n^{-1}F(s)\{1 - F(t)\}$  for  $s \le t$ .

This almost suffices for  $\mathcal{L}_*\{\sqrt{n}(F_n^* - F_n)|\text{data}\}$  to be close to  $\mathcal{L}\{\sqrt{n}(F_n - F)\}$ , and (3.7)–(3.8) make this precise. But other simulation schemes that in one way or another create some artificial  $F_n^*(.)$  with properties like (8.4) can also be expected to work. That is, even if the random  $F_n^*$  is created from other means than actual sampling, one would expect  $\mathcal{L}_*[\sqrt{n}\{\theta_{\text{cdf}}(F_n^*) - \theta_{\text{cdf}}(F_n)\}|\text{data}]$  to be close to  $\mathcal{L}[\sqrt{n}\{\theta_{\text{cdf}}(F_n) - \theta_{\text{cdf}}(F)\}]$ .

In view of this remark and of (8.3) we should look for data-conditional simulation strategies that produce some random c.h.r.  $A_n^*$  with approximately independent increments and with

$$E_*\{dA_n^*(s)|\text{data}\} \doteq dA_n(s), \quad \text{Var}_*\{dA_n^*(s)|\text{data}\} \doteq Y_n(s)^{-1} dA_n(s)\{1 - dA_n(s)\}.$$
 (8.5)

Such schemes will succeed in the required

$$\mathcal{L}_* \left[ \sqrt{n} \{ \theta_{\text{chr}}(A_n^*) - \theta_{\text{chr}}(A_n) \} | \text{data} \right] \doteq \mathcal{L} \left[ \sqrt{n} \{ \theta_{\text{chr}}(A_n) - \theta_{\text{chr}}(A) \} \right], \tag{8.6}$$

or  $\mathcal{L}_*\{\sqrt{n}(\widehat{\theta}_n^* - \widehat{\theta}_n)|\text{data}\} \doteq \mathcal{L}\{\sqrt{n}(\widehat{\theta}_n - \theta)\}$  for short, with few extra requirements. One very simple way of achieving this is to let  $A_n^*(.)$  have independent increments and

$$dA_n^*(s) = Y_n(s)^{-1} \operatorname{Bin}\{Y_n(s), dA_n(s)\}.$$
(8.7)

So  $A_n^*(.)$  is flat between observed life times, and at such a point  $x_i$ , say, the hazard jump  $\Delta A_n^*(x_i)$  is a relative frequency from a binomial with parameters  $Y_n(x_i)$  and  $1/Y_n(x_i)$ . This is Richard Gill's 'weird bootstrap' (1990, personal communication).

Note that  $A_n^*$  corresponds to a random  $F_n^*(x_i) = 1 - \prod_{x_j \leq x_i} \{1 - \Delta A_n^*(x_j)\}$ , which is different from that obtained through resampling from  $F_n$ . The weird bootstrap does not resample any data set, but it works, with and without censoring. A precise asymptotic result about (8.6) can be proved. In particular the weird bootstrap can be seen as an alternative to Efron's bootstrap in the uncensored case, developed from the hazard rate point of view.

8C. Exact nonparametric Bayesian analysis. Now we can embark on Bayesian issues. The canonical analogue to a Dirichlet process for F is a Beta process for A. Let A be such a process with parameters c(.) and  $A_0(.)$ , which means that A has independent increments that are approximately Beta distributed,

$$dA(s) \approx \operatorname{Beta}\left[c(s)dA_0(s), c(s)\{1 - dA_0(s)\}\right].$$

Note that

$$E_B dA(s) = dA_0(s) \quad ext{and} \quad ext{Var}_B dA(s) = rac{dA_0(s)\{1 - dA_0(s)\}}{c(s) + 1},$$

so  $A_0$  is the prior guess and c(s) is related to the concentration of the prior measure around this prior guess. When  $c(s) = aF_0[s,\infty)$ , where  $F_0 = 1 - \prod_{[0,\cdot]} (1-dA_0)$ , then  $F = 1 - \prod_{[0,\cdot]} (1-dA)$  is Dirichlet with parameter  $aF_0$ . See Hjort (1990) about further properties for Beta processes.

Given data A is still a Beta process, with parameters  $c + Y_n$  and  $A_{n,B}$ , where

$$A_{n,B}(t) = \int_0^t \frac{c(s)dA_0(s) + dN_n(s)}{c(s) + Y_n(s)}$$

is the Bayes estimate. So A given data has independent increments with

$$dA(s)|\mathrm{data} \approx \mathrm{Beta} \big[c(s)dA_0(s) + dN_n(s),\ c(s)\{1 - dA_0(s)\} + Y_n(s) - dN_n(s)\big].$$
 (8.8)  
In particular

$$E_B\{dA(s)|{
m data}\} = dA_{n,B}(s) \quad {
m and} \quad {
m Var}_B\{dA(s)|{
m data}\} = rac{dA_{n,B}(s)\{1-dA_{n,B}(s)\}}{c(s)+Y_n(s)+1}.$$

Full Bayesian posterior analysis is now theoretically possible, via simulation of the independent increment process A and then calculation of  $\theta_{\rm chr}(A)$ , leading in the end to  $G_n(t) = \Pr_B\{\theta_{\rm chr}(A) \le t | {\rm data}\}$ , cf. (1.3). And in view of (8.3) and (8.9) we would get the pleasing result

$$\mathcal{L}_{B}ig\{\sqrt{n}(A-A_{n,B})|\mathrm{data}ig\}pprox \mathcal{L}ig\{\sqrt{n}(A_{n}-A)ig\},$$

i.e. frequentists and Bayesians would agree for large sample sizes. The full Bayesian simulation method is cumbersome, however, and requires a fine partitioning of the halfline.

8D. A weird Bayesian bootstrap. In view of the relative complexity of the full Bayesian Beta process approach one may look for approximating BB-strategies, perhaps generalising our basic BB of (1.5)-(1.7). One way is to sample  $X_1^{0*}, \ldots, X_{n+a}^{0*}$  from the Bayes estimate

$$F_{n,B}(t) = 1 - \prod_{[0,t]} \Big\{ 1 - \frac{cdA_0 + dN_n}{c + Y_n} \Big\},$$

then pairing them with simulated censoring times  $c_i^*$  from the Kaplan-Meier estimate  $H_n$  for H, and then treating  $X_i^* = \min\{X_i^{0*}, c_i^*\}$  and  $\delta_i^* = I\{X_i^{0*} \leq c_i^*\}$  as a new BB-data set. Here a is related to the c(.) function, for example being taken to be its maximum value. This works, asymptotically, under some conditions, but not particularly well under non-negligible censoring. So in this sense there does not seem to be a natural generalisation of this article's full data BB to hazard rate models with Beta process priors. The approximation suggested here does however work best when  $c(s) = aF_0[s, \infty)$ , which is the Dirichlet $(aF_0)$  prior for F, and indeed with BB sample size n + a.

A simpler second solution which both works better and has a nice interpretation of its own is to generate  $A_{BB}^*$  with independent binomial frequencies increments

$$dA_{BB}^{*}(s) = \{c(s) + Y_{n}(s)\}^{-1} \operatorname{Bin}\{c(s) + Y_{n}(s), dA_{n,B}(s)\}.$$
(8.10)

This manages to almost match (8.9), and the small difference disappears asymptotically. At observed life times the jump  $\Delta A_{BB}^*(x_i)$  is a binomial  $[c(x_i)+Y_n(x_i),1/\{c(x_i)+Y_n(x_i)\}]$  divided by  $c(x_i)+Y_n(x_i)$ . Again, this scheme does not correspond to data resampling, but weirdly kills and reincarnates individuals at each time point.

8E. Exact Bayesian and BB analysis under a noninformative reference prior. Let c(.) go to zero in the above constructions. The exact Bayesian solution is then a Beta process A with parameters  $Y_n$  and  $A_n$ , i.e.

$$dA(s)|\text{data} \sim \text{Beta}\{dN_n(s), Y_n(s) - dN_n(s)\}, \tag{8.11}$$

with independent jumps only at observed life times. Note that

$$E_B\{dA(s)|\mathrm{data}\}=dA_n(s) \quad ext{and} \quad \mathrm{Var}_B\{dA(s)|\mathrm{data}\}=rac{dA_n(s)\{1-dA_n(s)\}}{Y_n(s)+1}.$$

Observe also that letting  $c(.) \to 0$  in the posterior distributions is the same as letting  $a \to 0$  in the posterior distribution with a Dirichlet $(aF_0)$ . In this way we have arrived at a generalisation to censored data for Rubin's noninformative Bayesian bootstrap. In addition to being a natural limit of proper Bayes solutions it can be given an empirical Bayesian interpretation. The (8.11) method is also the method proposed by Lo (1991); see his paper for further properties.

Letting  $c(.) \to 0$  in the weird BB of 8D gives Gill's weird bootstrap of 8B. The latter can therefore be seen as the noninformative limit of a natural simulation-based approximation to a full Bayesian method.

One can prove that all the schemes described here are first order equivalent. In particular each scheme will reach confidence intervals asymptotically equivalent to (3.11).

8F. Cox regression. Let us finally note that the methods above can be extended and used in the semiparametric Cox regression model. Suppose individual no. i has covariate  $z_i$  and c.h.r.  $A_i$ , and that

$$1 - dA_i(s) = \{1 - dA(s)\}^{\exp(\beta z_i)}, \quad i = 1, \dots, n.$$

If the Bayesian prior is that  $\beta$  comes from some  $\pi(\beta)$  and that A independently is a Beta process  $(c, A_0)$ , then the posterior distributions can be worked out, making a full semi-parametric Bayesian analysis awkward but possible, through cumbersome simulations. See Hjort (1990, Section 6). Simulation-based approximations to this scheme can be developed, with ideas as above, giving in particular a weird BB scheme, but requiring more involved distributions than the simple binomial. Let us merely report on the noninformative limit version of the exact Bayes solution, as  $c(.) \to 0$ . First draw a  $\beta$  from

$$\pi_n(eta) = \mathrm{const.} \ \prod_{i=1}^n ig\{ \psiig( R_n(x_i,eta) ig) - \psiig( R_n(x_i,eta) - \exp(eta z_i) ig) ig\}^{\delta_i}.$$

Then let A be flat between observed life times, and have independent jumps

$$\Delta A(x_i) \sim rac{z^{-1} \left\{ (1-z)^{R_n(x_i,eta) - \exp(eta z_i) - 1} - (1-z)^{R_n(x_i,eta) - 1} 
ight\}}{\psi(R_n(x_i,eta)) - \psi(R_n(x_i,eta) - \exp(eta z_i))}, \quad 0 < z < 1,$$

for those  $x_i$  with  $\delta_i = 1$ . In these expressions  $R_n(s,\beta) = \sum_{i=1}^n Y_i(s) \exp(\beta z_i)$ , where  $Y_i(s) = I\{X_i^0 \geq s, c_i \geq s\}$  is the at-risk indicator for individual i. And any sensible simpler way of simulating  $\Delta A_{BB}^*(x_i)$  instead, with asymptotically correct matching for the two first moments, defines a weird BB.

- 9. Supplementing results and remarks. This final section offers some concluding comments and mentions some extensions of previous results.
- 9A. Two viewpoints. There are presumably two ways to approach the problem of handling  $\theta(F)$  in a Bayesian nonparametric way. One way is to ignore the underlying F and concentrate on  $\theta(F)$  and what the prior information on this particular parameter is. In the end some Bayesian calculations are carried out for  $\theta$  given data. In this mode each parameter must be treated separately, and inconsistencies can occur, since Bayesians are nonperfect. The second way is the one chosen in this article, where information is expressed in terms of the underlying F once and for all, after which analysis can proceed on an automatic basis for every conceivable  $\theta(F)$ .

9B. Exact simulation. There are actually ways of simulating almost exactly from  $G_n = \mathcal{L}_B\{\theta(F)|\text{data}\}$ , cf. remarks made at the start of 2A, where one such method was described, using a fine partition of the real line and finite-dimensional Dirichlet distributions. Another way would be through simulation of F via its product integral representation in terms of the cumulative hazard process A, which is a Beta process, see Section 8 above. This remark and results there show that such posterior simulation of  $\theta(F)$  is possible even with censored data, and in more complex models for survival data.

A third possibility is to use Sethuraman's constructive definition of an arbitrary Dirichlet process, see Sethuraman and Tiwari (1982). The present  $Dir(aF_0+nF_n)$  case (see (1.2)) can be represented as follows. Generate an infinite i.i.d. sequence  $\{x_i'\}$  from  $F_{n,B}$  of (1.5), and an infinite i.i.d. sequence  $\{B_i\}$  from Beta $\{1, a+n\}$ . Then let  $A_i = B_i \prod_{j=1}^{i-1} (1-B_j)$  and use

$$F = \sum_{i=1}^{\infty} A_i \delta(x_i'), \tag{9.1}$$

where  $\delta(x)$  means unit point mass at position x. To see how this can be used, consider the mad-parameter  $\theta(F) = \int |x - \text{med}(F)| dF(x)$ , for example. Approximate F by using a large number I instead of  $\infty$  in (9.1), perhaps I = 1000. Order the  $x_i'$  points and determine the one for which the cumulative probability mass  $\sum_{i=1}^{j} A_i$  first exceeds  $\frac{1}{2}$ ; this gives an approximation med' to  $F^{-1}(\frac{1}{2})$ . Some care is required since there will be heavy ties in the  $x_i'$  data. Then compute  $\theta' = \sum_{i=1}^{I} |x_i' - \text{med}'| A_i$ , all in all giving an approximation to one particular  $\theta$  drawn from F. This algorithm must then be repeated a large number of times to form  $\mathcal{L}\{\theta(F)|\text{data}\}$ . — This elaborate strategy makes almostexact Bayesian caculations possible, and in a certain sense makes the BB less necessary. But arguments still favouring the BB include (i) that it is much simpler to use, regarding both programming, simulation, and cpu-use, (ii) that it is less functional-dependent, (iii) that BB and almost-exact simulation are first order equivalent, by Section 3, and (iv) that the BB perhaps is more trustworthy and realistic than the almost-exact version in that it only exploits the first and second order characteristics of the Dirichlet process structure, and not the more esoteric ones, like the inherent discreteness of its sample paths, visible in (9.1). In any case the (9.1)-based method does make almost-exact posterior Dirichlet analysis possible and should be included in any serious comparison between the various strategies.

9C. Invariance under transformations. Both the nonparametric Bayesian confidence interval  $[\theta_L, \theta_U]$  of (1.4) and its BB approximation  $[\widehat{\theta}_L, \widehat{\theta}_U]$  of (1.9) transform very neatly, with respect to both data-transformations and parameter-transformations. (i) Suppose  $\nu = g(\theta)$  is a new parameter, with a smooth and increasing g(.). The (1.4) scheme uses  $H_n(t) = \Pr_B\{\nu(\theta(F)) \le t\} = G_n(g^{-1}(t))$ , and the (1.9) uses  $\widehat{H}_n(t) = \Pr_*\{\nu_{BB}^* \le t\} = \widehat{G}_n(g^{-1}(t))$ . It follows that

$$[
u_L, \nu_R] = [g(\theta_L), g(\theta_R)], \quad [\widehat{\nu}_L, \widehat{\nu}_R] = [g(\widehat{\theta}_L), g(\widehat{\theta}_R)].$$
 (9.2)

(ii) Suppose  $Y_i = h(X_i)$  for a smooth increasing h(.). If F for  $X_i$  is Dirichlet  $aF_0$ , then  $\widetilde{F} = Fh^{-1}$  for  $Y_i$  is Dirichlet  $a\widetilde{F}_0 = aF_0h^{-1}$ . Write  $\nu(\widetilde{F}) = \theta(F)$  for the old parameter seen in the context of  $Y_i$ 's from  $\widetilde{F}$ . Then  $H_n(t) = \Pr_B\{\nu \leq t\} = G_n(t)$  and the Dirichlet transformation property implies  $\widehat{H}_n(t) = \Pr_*\{\nu_{BB}^* \leq t\} = \widehat{G}_n(t)$ . So (1.4) and (1.9) are invariant under data transformations.

9D. Boot sample size. The bootstrap sample size 'boot' in (1.8) should of course be large in order for (1.8) and (1.9) to work well, i.e. for functions of  $\widehat{G}_{n,\text{boot}}(.)$  to be close to the same functions of  $\widehat{G}_n$ . The investigation of Efron (1987, Section 9), albeit for a different bootstrap, is relevant here, and indicates that boot = 1000 may be a rough minimum for quantiles in the tail, required in (1.9), but that boot = 100 may suffice for average operations like the mean, required in (1.8).

9E. Highest posterior density. The starting point for our confidence intervals has been (1.4). Sometimes in the Bayesian literature highest posterior density regions are advocated instead. In the present case this would involve approximating the posterior distribution  $G_n$  with one with a density  $g_n$ , and then letting  $\{t: g_n(t) \geq g_0\}$  be the confidence region, for appropriate level  $g_0$ . This approach makes most sense when  $g_n$  is unimodal, which it would not necessarily be in applications of the present kind, due to the fact that the posterior

distribution of F places extra weight on the observed data points. This is illustrated in Section 5 for the case of the median.

9F. Data-dependent functionals. The functional  $\theta = \theta(F)$  can depend on the sample size; the described BB procedure works specifically for the given n. It is also allowed to depend upon the actual data sample, say  $\theta = \theta(F, x_1, \dots, x_n)$ . Let us illustrate this comment with a description of how a nonparametric Bayesian might construct a simultaneous confidence band for F. Consider

$$\theta_{\min} = \min_{a \le t \le b} \frac{F(t) - F_{n,B}(t)}{[F_{n,B}(t)\{1 - F_{n,B}(t)\}]^{1/2}} \quad \text{and} \quad \theta_{\max} = \max_{a \le t \le b} \frac{F(t) - F_{n,B}(t)}{[F_{n,B}(t)\{1 - F_{n,B}(t)\}]^{1/2}}.$$

The natural band is

$$F_{n,B}(t) - c[F_{n,B}(t)\{1 - F_{n,B}(t)\}]^{1/2} \le F(t) \le F_{n,B}(t) + d[F_{n,B}(t)\{1 - F_{n,B}(t)\}]^{1/2}$$

for  $a \leq t \leq b$ , where c and d ideally would be determined by

$$\Pr_{B}\left\{-c \leq \theta_{\min}(F, x_1, \dots, x_n), \, \theta_{\max}(F, x_1, \dots, x_n) \leq d \, \middle| \, \mathrm{data} \right\} = 0.90,$$

say (with an additional condition to make them unique, like requiring minimisation of c+d). The BB method consists of generating perhaps 1000 values of

$$\theta_{\min,BB}^* = \min_{a \le t \le b} \frac{F_{BB}^*(t) - F_{n,B}(t)}{[F_{n,B}(t)\{1 - F_{n,B}(t)\}]^{1/2}}, \ \theta_{\max,BB}^* = \max_{a \le t \le b} \frac{F_{BB}^*(t) - F_{n,B}(t)}{[F_{n,B}(t)\{1 - F_{n,B}(t)\}]^{1/2}},$$

and using the correspondingly defined  $\widehat{c}$  and  $\widehat{d}$ . One may prove that  $(n+a)^{1/2}(\widehat{c}-c)$  and  $(n+a)^{1/2}(\widehat{d}-d)$  go to zero in probability, by methods and results of Section 3. [Strictly speaking, this is true provided boot<sub>n</sub> realisations are generated instead of 1000 and boot<sub>n</sub>/(n log n) grows with towards infinity.] It could be advantageous to use this asymmetric band instead of the simpler symmetric one since the distribution of  $F - F_{n,B}$  is typically skewed.

9G. Two-sample BB. The BB method can be generalised to two-sample situations, and indeed to more general non-i.i.d. models, as shown in Section 7. To illustrate, let  $x_1, \ldots, x_n$  and  $y_1, \ldots, y_m$  be samples from respectively  $F_1$  and  $F_2$ , assume  $\theta = F_1^{-1}(\frac{1}{2}) - F_2^{-1}(\frac{1}{2})$  is of interest, and suppose  $F_1 \sim \text{Dir}(aF_{1,0})$  and  $F_2 \sim \text{Dir}(bF_{2,0})$ . A Bayes estimate and confidence interval for this difference of population medians can be obtained by generating perhaps 1000 realisations of  $\theta_{BB}^* = \text{med}\{X_1^*, \ldots, X_{n+a}^*\} - \text{med}\{Y_1^*, \ldots, Y_{m+b}^*\}$ , where the  $X_i^*$ 's are drawn from  $(aF_{1,0} + nF_{1,n})/(a+n)$  and the  $Y_i^*$ 's from  $(bF_{1,0} + mF_{2,m})/(b+m)$ , and then treating the resulting histogram (or smoothed density estimate) as the posterior distribution of  $\theta$ .

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