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BAYESIAN NONPARAMETRIC INFERENCE FOR QUANTAL RESPONSE DATA

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The problem of nonparametric Bayes estimation of a tolerance distribution based on quantal response data has been considered previously with a prior distribution based on the Dirichlet process. In the present article, a broad class of priors is developed for this problem by allowing the hazard function of the tolerance distribution to be a realization of a nonnegative stochastic process with independent increments. This class includes the Dirichlet prior as a special case. In addition, priors over a space of absolutely continuous tolerance distributions, which includes IFR, DFR, and U-shaped failure rate distributions, are constructed by taking the failure rate to be the superposition of two processes with independent increments. Posterior Laplace transforms of the corresponding processes are obtained based on quantal response data with binomial sampling. These posterior Laplace transforms are then used to find Bayes estimates, and examples are given to illustrate the results.

1. Introduction. Recently, Bhattacharya (1981) and others have considered the problem of determining the posterior distributions of a Dirichlet process from quantal response data to estimate the distribution of the tolerance level to some drug in a population. As shown by Antoniak (1974), these posteriors are complicated mixtures of Dirichlet processes. Bhattacharya (1981) was able to express the finite-dimensional posterior distributions in terms of Markov chains which were then used to obtain the asymptotic posterior distributions.

In a reliability application, Doksum (1974) and Ferguson and Phadia (1979) constructed priors over a space of life distributions by taking the hazard function to be a completely random measure (called by Doksum a process neutral to the right). This results in priors over purely atomic life distributions. Dykstra and Laud (1981) constructed priors over a space of absolutely continuous life distributions by taking the failure rate function to be a completely random measure. Because the sample paths of such processes are nondecreasing a.s., the resulting life distributions are IFR. In the present article, the approaches of Doksum, Ferguson and Phadia, and Dykstra and Laud are used for the problem of Bayesian nonparametric inference of tolerance distributions based on quantal response data.

Section 2 discusses the model in which the hazard function is a completely random measure. This includes the special case in which the tolerance distribution has a Dirichlet process prior. Posterior Laplace transforms of the hazard

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function are obtained for binomial sampling, and Bayes estimates are obtained under squared error loss. These estimates are evaluated for the Dirichlet process prior and for the prior in which the hazard function is a gamma process.

In Section 3, the approach of Dykstra and Laud (1981) is expanded to include IFR, DFR, and U-shaped failure rate tolerance distributions by taking the failure rate function to be the superposition of two independent processes, one with nondecreasing sample paths and the other with nonincreasing sample paths. Joint posterior Laplace transforms of these processes are obtained for binomial sampling. These posterior Laplace transforms are then used to obtain Bayes estimates of the failure rate function, and an example is given to illustrate the evaluation of these estimates.

Specifically, let X denote the tolerance level of an individual to a drug and let F denote the population distribution function of X. The hazard function of F is defined to be

$$H(t) = -\log(1 - F(t)),$$

and the failure rate function, when it exists, is defined to be

$$h(t) = \frac{\partial}{\partial t} H(t).$$

Fix m dosage levels, $0 < z_1 < \cdots < z_m$, and for convenience, set $z_0 = 0$. Under binomial sampling, r_j individuals are randomly assigned to level z_j. This sampling scheme is denoted by $B(\mathbf{r}, \mathbf{z})$.

2. Random hazard functions. Ferguson and Phadia (1979) developed Bayesian nonparametric methods for some reliabilty problems by taking the hazard function H to be a nonnegative stochastic process with independent increments that has no deterministic component. Such processes generate random measures called completely random measures by Kingman (1967). In what follows, no notational distinction will be made between the stochastic process with independent increments and the generated random measure.

It is well-known that such processes, H, are infinitely divisible, and so their Laplace transforms have the special form given by

$$\Psi(\xi) = E \exp\left\{- \int_0^\infty \xi(t) H(dt)\right\} = \exp\left\{\int_0^\infty \int_0^\infty (e^{-v\xi(t)} - 1) Q(dv, dt)\right\},$$

where ξ is a Borel-measurable function on $[0, \infty)$ and Q is a measure on $(0, \infty) \times [0, \infty)$ that satisfies

$$\int_0^\infty (v \wedge 1) Q(dv, A) < \infty \tag{2.1}$$

for every compact Borel set $A \subset [0, \infty)$, where $a \wedge b = \min(a, b)$. The measure Q is called the Lévy measure of H. See Kallenberg (1976) for a thorough discussion of infinitely divisible processes.

For the binomial sampling scheme, define U_j to be the number of survivors at dosage z_j, $1 \le j \le m$. Then

$$P(U_1 = k_1, \cdots, U_m = k_m \mid H)$$

$$(2.2) \qquad = \sum_{n_1=0}^{r_1-k_1} \cdots \sum_{n_m=0}^{r_m-k_m} (-1)^n \binom{\mathbf{r}}{\mathbf{k},\ \mathbf{n}} \exp\{-\textstyle\sum_{j=1}^m (k_j + n_j)H(z_j)\},$$

where

$$\binom{\mathbf{r}}{\mathbf{k},\mathbf{n}} = \prod_{j=1}^m (r_j!)[k_j!n_j!(r_j - k_j - n_j)!]^{-1}.$$

In order to obtain the posterior Laplace transform of H given the complete observations,

$$(U_1 = k_1, \cdots, U_m = k_m),$$

define a functional μ_H by

$$(2.3) \quad \mu_H(\xi; \mathbf{k}) = EP(U_1 = k_1, \cdots, U_m = k_m \mid H)\exp\left\{-\int_0^\infty \xi(t)H(dt)\right\}.$$

Note that if ξ_0 denotes the zero function, then

$$\mu_H(\xi_0; \mathbf{k}) = P(U_1 = k_1, \cdots, U_m = k_m).$$

Hence, the posterior Laplace transform of H is given by

$$(2.4) \qquad \mu_H(\xi; \mathbf{k})/\mu_H(\xi_0; \mathbf{k}).$$

This posterior Laplace transform can be evaluated from Theorem 1.

THEOREM 1. *Under the $B(\mathbf{r}, \mathbf{z})$ sampling scheme,*

$$\mu_H(\xi; \mathbf{k}) = \sum_{n_1=0}^{r_1-k_1} \cdots \sum_{n_1=0}^{r_m-k_m} (-1)^n \binom{\mathbf{r}}{\mathbf{k},\mathbf{n}} \Psi(\xi + f),$$

where,

$$f(t; \mathbf{z}, \mathbf{k}, \mathbf{n}) = \begin{cases} \sum_{i=j}^m (k_i + n_i), & z_{j-1} < t \le z_j,\ 1 \le j \le m, \\ 0, & t > z_m. \end{cases}$$

The posterior Laplace transform of H for the special case in which no failures have been observed at all dosage levels can also be obtained from Theorem 3 of Ferguson and Phadia (1979) by noting that

$$P(U_j = r_j \mid H) = P(X(1) > z_j, \cdots, X(r_j) > z_j \mid H),$$

where $X(1), \cdots, X(r_j)$ are i.i.d. random variables with hazard function H and represent the tolerance levels of the r_j individuals who were exposed to, and survived, dosage level z_j. Theorem 1 can also be applied to a sequential sampling scheme in which individuals are assigned to the dosage levels until a specified number of failures have been observed.

To complete this section, Theorem 1 is applied to an estimation problem. Suppose that the loss function has the form

$$L(H, \hat{H}) = \int_0^\infty [\hat{H}(t) - H(t)]^2 W(dt),$$

where W is a measure which satisfies

$$\int_0^\infty \operatorname{var} H(t) W(dt) < \infty.$$

The Bayes estimate of $H(s)$ for this loss function is the mean of $H(s)$ with respect to the posterior distribution. This estimate can be obtained from Theorem 1 by setting

$$\xi(t) = \begin{cases} \theta, & 0 \le t \le s, \\ 0, & t > s, \end{cases}$$

and then evaluating the derivative of the posterior Laplace transform with respect to θ at $\theta = 0$. The Bayes estimate, $\hat{H}(s)$, based on $B(\mathbf{r}, \mathbf{z})$ sampling is given by

$$(2.5) \qquad \hat{H}(s) = \frac{\sum_{0 \le n_j \le r_j - k_j} \cdots \sum (-1)^n \binom{\mathbf{r}}{\mathbf{k}, \mathbf{n}} \int_0^s \int_0^\infty v e^{-vf(t;\mathbf{z},\mathbf{k},\mathbf{n})} Q(dv, dt) \Psi(f)}{\sum_{0 \le n_j \le r_j - k_j} \cdots \sum (-1)^n \binom{\mathbf{r}}{\mathbf{k}, \mathbf{n}} \Psi(f)}.$$

Bayes estimates for other loss functions can also be obtained from (2.4) and Theorem 1. Suppose for example, that the loss function has the form

$$L(F, \hat{F}) = \int (\hat{F}(t) - F(t))^2 W(dt),$$

where W is a finite measure. Then the Bayes estimate is

$$\hat{F}(s) = 1 - E(e^{-H(t)} \mid \mathbf{U} = \mathbf{k}),$$

which can be obtained from (2.4) and Theorem 1 by setting

$$\xi(t) = \begin{cases} 1, & 0 \le t \le s, \\ 0, & t > s. \end{cases}$$

EXAMPLES. As noted by Ferguson (1974), the Dirichlet process prior for F can be obtained by taking H to have Lévy measure

$$Q(dv, dt) = e^{-v[\alpha(R) - \alpha(t)]}(1 - e^{-v})^{-1} \alpha(dt)\, dv,$$

where $\alpha(t)$ is a nondecreasing function with $\alpha(0) = 0$ and $\alpha(t) \to \alpha(R) < \infty$. From Lemma 1 of Ferguson (1974),

$$(2.6) \qquad \Psi(f) = \prod_{j=1}^m \frac{\Gamma(\alpha(R) - \alpha(z_{j-1}))\Gamma(\alpha(R) - \alpha(z_j) + c_j)}{(\alpha(R) - \alpha(z_j))\Gamma(\alpha(R) - \alpha(z_{j-1}) + c_j)},$$

where

$$c_j = \sum_{i=j}^{m} (k_i + n_i).$$

Also,

$$(2.7)\quad \int_0^s \int_0^\infty v e^{-vf(t;\mathbf{z},\mathbf{k},\mathbf{n})} Q(dv, dt)$$
$$= \sum_{j=1}^{r} [di(\alpha(R) - \alpha(s_{j-1}) + c_j) - di(\alpha(R) - \alpha(s_j) + c_j)],$$

where $s_1, \cdots, s_{m+1}$ denote the ordered values of $s, z_1, \cdots, z_m$, r denotes the rank of s in this set, $c_{m+1} = 0$, and di denotes the digamma function,

$$di(\alpha) = \frac{\partial}{\partial u} \log\Gamma(u)\,|_{u=\alpha}.$$

The Bayes estimate of H can be evaluated by substituting (2.6) and (2.7) into (2.5). Bhattacharya (1981) has expressed $\hat{H}$ in terms of Markov chains and obtained large sample approximations for this estimate.

An alternative prior to the Dirichlet process can be obtained by allowing H to be a gamma process. This process has Lévy measure given by

$$Q(dv, dt) = v^{-1} e^{v/\beta} \alpha(dt)\, dv,$$

where $\beta > 0$ and $\alpha(t)$ is a nondecreasing function with $\alpha(0) = 0$, $\alpha(t) \to \infty$ as $t \to \infty$. In this case,

$$Ee^{-\theta H(s)} = (1 + \theta\beta)^{-\alpha(s)}, \quad EH(s) = \alpha(s)\beta, \quad \text{var } H(s) = \alpha(s)\beta^2.$$

Also,

$$(2.8)\quad \Psi(f) = \prod_{j=1}^{m} (1 + \beta c_j)^{-[\alpha(z_j) - \alpha(z_{j-1})]},$$

and

$$(2.9)\quad \int_0^s \int_0^\infty v e^{-vf} Q(dv, dt) = \sum_{j=1}^{r} \beta(1 + \beta c_j)^{-1}[\alpha(s_j) - \alpha(s_{j-1})].$$

The Bayes estimates for the gamma process prior can be obtained by substituting (2.8) and (2.9) into (2.5). To implement this prior, the statistician can specify the expected prior hazard function, $H_0(t)$, and the variance of the prior hazard function, $\sigma^2(t)$, by

$$H_0(t) = \alpha(t)\beta, \quad \sigma^2(t) = \alpha(t)\beta^2 = \beta H_0(t).$$

Note that in this case the coefficient of variation,

$$\sigma(t)/H_0(t) = \beta^{1/2}[H_0(t)]^{-1/2} \to \infty \quad \text{as} \quad t \to 0.$$

This implies that the relative uncertainty regarding the hazard function (and hence the tolerance distribution) is high for low dosage levels, which is often the case in applications.

3. Random failure rates. Since the processes used to generate priors in the preceding section are purely atomic, then the resulting tolerance distributions are discrete with probability one. In a reliability application, Dykstra and Laud (1981) constructed priors over a space of absolutely continuous life distributions by taking the failure rate function to be a gamma process. Since the sample paths of gamma processes are nondecreasing a.s., then this prior chooses IFR tolerance distributions a.s. In this section the approach of Dykstra and Laud is expanded to include IFR, DFR, and U-shaped failure rate tolerance distributions by taking the failure rate to be the superposition of two completely random measures. Specifically, let X_1 and X_2 be two independent completely random measures with Lévy measures Q_1 and Q_2 respectively, where Q_1 satisfies (2.1) and Q_2 satisfies

$$\int_0^\infty (v \wedge 1) Q_2(dv, [0, \infty)) < \infty. \tag{3.1}$$

Note that (3.1) implies that $X_2[0, \infty) < \infty$ a.s. Next, let the failure rate of the tolerance distribution be given by

$$h(t) = X_1[0, t] + X_2(t, \infty). \tag{3.2}$$

Here X_1 represents the increasing component of the failure rate and X_2 represents the decreasing component.

Under $B(\mathbf{r}, \mathbf{z})$ sampling,

$$\begin{aligned} &P(U_1 = k_1, \cdots, U_m = k_m \mid X_1, X_2) \\ &\quad = \sum_{n_1=0}^{r_1-k_1} \cdots \sum_{n_m=0}^{r_m-k_m} (-1)^n \binom{\mathbf{r}}{\mathbf{k}, \mathbf{n}} \exp\left\{-\sum_{j=1}^m (k_j + n_j) \int_0^{z_j} h(t)\, dt\right\}. \end{aligned} \tag{3.3}$$

As in Section 2, define a functional $\mu_{1,2}$ by

$$\begin{aligned} \mu_{1,2}(\xi_1, \xi_2; \mathbf{k}) &= EP(U_1 = k_1, \cdots, U_m = k_m \mid X_1, X_2) \\ &\quad \cdot \exp\left\{-\int_0^\infty \xi_1(t) X_1(dt) - \int_0^\infty \xi_2(t) X_2(dt)\right\}. \end{aligned}$$

For the purpose of evaluating this functional, define g_1 and g_2 by

$$g_1(t; \mathbf{z}, \mathbf{k}, \mathbf{n}) = \sum_{j=1}^m (k_j + n_j)(z_j - t)^+,$$

$$g_2(t; \mathbf{z}, \mathbf{k}, \mathbf{n}) = \sum_{j=1}^m (k_j + n_j)(z_j \wedge t),$$

where $a^+ = \max(a, 0)$.

THEOREM 2. *The joint posterior Laplace transform of X_1 and X_2 under $B(\mathbf{r}, \mathbf{z})$ sampling is given by*

$$\mu_{1,2}(\xi_1, \xi_2; \mathbf{k}) / \mu_{1,2}(\xi_0, \xi_0; \mathbf{k}),$$

where

$$\mu_{1,2}(\xi_1, \xi_2; \mathbf{k}) = \sum_{n_1=0}^{r_1-k_1} \cdots \sum_{n_m=0}^{r_m-k_m} (-1)^n \binom{\mathbf{r}}{\mathbf{k}, \mathbf{n}} \Psi_1(\xi_1 + g_1) \Psi_2(\xi_2 + g_2), \tag{3.4}$$

and Ψ_i denotes the Laplace transform of X_i, $i = 1, 2$.

PROOF. The proof follows directly from (3.3) by noting that

$$E \exp\left\{-\sum_{j=1}^m (k_j + n_j) \int_0^{z_j} h(t)\,dt - \int_0^\infty \xi_1(t)X_1(dt) - \int_0^\infty \xi_2(t)X_2(dt)\right\}$$

$$= E \exp\left\{-\sum_{j=1}^m (k_j + n_j) \left[\int_0^{z_j}\int_0^t X_1(ds)\,dt + \int_0^{z_j}\int_t^\infty X_2(ds)\,dt\right] - \int_0^\infty \xi_1(t)X_1(dt) - \int_0^\infty \xi_2(t)X_2(dt)\right\}$$

$$= E \exp\left\{-\sum_{j=1}^m (k_j + n_j) \left[\int_0^\infty (z_j - s)^+X_1(ds) + \int_0^\infty (z_j \wedge t)X_2(ds)\right] - \int_0^\infty \xi_1(t)X_1(dt) - \int_0^\infty \xi_2(t)X_2(dt)\right\}$$

$$= \Psi_1(\xi_1 + g_1)\Psi_2(\xi_2 + g_2).$$

The interchange of integrals above is justified by Tonelli's Theorem (see Royden, 1968, page 270).

This posterior Laplace transform is next applied to an estimation problem. Suppose that the loss function for h satisfies

$$L(h, \hat{h}) = \int_0^\infty [\hat{h}(t) - h(t)]^2W(dt).$$

Then the Bayes estimate of h is

$$\hat{h}(s) = E(h(s) \mid U_1 = k_1, \cdots, U_m = k_m).$$

This estimate can be obtained from Theorem 2 by setting

$$\xi_1(t) = \begin{cases}\theta, & 0 \le t \le s,\\ 0, & t > s,\end{cases} \qquad \xi_2(t) = \begin{cases}0, & 0 \le t \le s,\\ \theta, & t > s,\end{cases}$$

and then evaluating the derivative of the posterior Laplace transform with respect to θ at $\theta = 0$. This gives

$$\hat{h}(s) = \sum_{0 \le n_j \le r_j - k_j} \cdots \sum (-1)^n \binom{\mathbf{r}}{\mathbf{k}, \mathbf{n}}$$

$$\left[\int_0^s \int_0^\infty ve^{-vg_1(t)}Q_1(dv, dt) + \int_s^\infty \int_0^\infty ve^{-vg_2(t)}Q_2(dv, dt)\right]$$

$$\Psi_1(g_1)\Psi_2(g_2)\left[\sum \cdots \sum (-1)^n \binom{\mathbf{r}}{\mathbf{k}, \mathbf{n}} \Psi_1(g_1)\Psi_2(g_2)\right]^{-1}.$$

EXAMPLE. Let X_1 and X_2 be independent gamma processes with Lévy measures

$$Q_1(dv, dt) = \alpha v^{-1} e^{-v/\beta} dt\, dv,$$

$$Q_2(dv, dt) = \lambda v^{-1} e^{-v/\delta} (1 + t)^{-2} dt\, dv,$$

where $\alpha, \beta, \lambda, \delta > 0$. Note that Q_2 satisfies (3.1). Now, if $z_{r-1} < s \le z_r$, $1 \le r \le m$, then

$$\int_0^s \int_0^\infty v \exp\{-v g_1(t)\} Q_1(dv, dt)$$

$$= \alpha \sum_{i=1}^{r-1} c_i^{-1} [\log(1 + \beta \sum_{j=i}^m (k_j + n_j)(z_j - z_{i-1})) - \log(1 + \beta \sum_{j=i}^m (k_j + n_j)(z_j - z_i))]$$

$$+ \alpha c_r^{-1} [\log(1 + \beta \sum_{j=r}^m (k_j + n_j)(z_j - z_{r-1})) - \log(1 + \beta \sum_{j=r}^m (k_j + n_j)(z_j - s))],$$

and if $s > z_m$, then

$$\int_0^s \int_0^\infty v \exp\{-v g_1(t)\} Q_1(dv, dt)$$

$$= \alpha \sum_{i=1}^m c_i^{-1} [\log(1 + \beta \sum_{j=i}^m (k_j + n_j)(z_j - z_{i-1})) - \log(1 + \beta \sum_{j=i}^m (k_j + n_j)(z_j - z_i))] + \alpha\beta(s - z_m).$$

Also,

$$\Psi_1(g_1) = \exp\{-\alpha \sum_{i=1}^m \int_{z_{i-1}}^{z_i} \log[1 + \beta \sum_{j=i}^m (k_j + n_j)(z_j - t)] dt\},$$

which can be evaluated from the indefinite integral,

$$\int \log(a + bx) dx = b^{-1}[(a + bx)\log(a + bx) - (a + bx)].$$

Finally, note that if $z_{r-1} < s \le z_r$, $1 \le r \le m$, then

$$\int_s^\infty \int_0^\infty v \exp\{-v g_2(t)\} Q_2(dv, dt)$$

$$= \lambda \sum_{i=r}^m \int_{u_{i-1}}^{u_i} \delta [1 + \delta \sum_{j=1}^{i-1} (k_j + n_j) z_j + \delta c_i t]^{-1} (1 + t)^{-2} dt$$

$$+ \lambda\delta [1 + \delta \sum_{j=1}^m (k_j + n_j) z_j]^{-1} (1 + z_m)^{-1},$$

where $u_{r-1} = s$, $u_j = z_j$, $r \le j \le m$. This can be evaluated from the indefinite integral,

$$(a-b)^2 \int (a+bt)^{-1}(1+t)^{-2}\,dt = b^2\log(a+bt) - (a-2b)(1+t)^{-1} + bt(1+t)^{-1} - b\log(1+t), \quad a \neq b.$$

If $s \geq z_m$, then

$$\int_s^\infty \int_0^\infty v \exp\{-vg_2(t)\}Q_2(dv, dt) = \lambda\delta(1+z_m)^{-1}[1+\delta \textstyle\sum_{j=1}^m (k_j+n_j)z_j]^{-1}.$$

Also,

$$\Psi_2(g_2) = \exp\left\{-\lambda \sum_{i=1}^m \int_{z_{i-1}}^{z_i} \log[1+\delta \textstyle\sum_{j=1}^{i-1}(k_j+n_j)z_j + \delta c_j t](1+t)^{-2}dt + \delta(1+z_m)^{-1}\log[1+\delta \textstyle\sum_{j=1}^m (k_j+n_j)z_j]\right\},$$

which can be evaluated from the indefinite integral,

$$\int (1+t)^{-2}\log(a+bt)\,dt = b(a-b)^{-1}\log\left(\frac{1+t}{a+bt}\right) - (1+t)^{-1}\log(a+bt), \quad a \neq b.$$

For this example, the expected failure rate, $h_0(t)$, satisfies

$$h_0(t) = EX_1[0, s] + EX_2(s, \infty) = \alpha\beta s + \lambda\delta(1+s)^{-1},$$

so that if $\lambda\delta > \alpha\beta$, then $h_0(s)$ initially decreases but eventually increases.

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