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Abstract

Estimation of Kullback-Leibler information for assessing model fit requires a nonparametric estimate of entropy of the data-generating distribution. This paper develops a class of entropy estimates and provides a procedure for Bayesian inference on the entropy and a Kullback-Leibler information index of fit. We define a quantized entropy that approximates and converges to the entropy integral for the continuous case. The quantized entropy is a general representation that includes several entropy estimates that have been used for frequentist and Bayesian inferences. For inference about the fit, we use the candidate model as the expected distribution in the Dirichlet process prior for the unknown data-generating distribution. The maximum entropy characterization of the candidate model is then used to derive the prior and posterior distributions for the information index of fit. As by-products, the procedure also produces prior and posterior distributions for the model parameters and the moments. The posterior means of the quantized entropy and information index of fit are the Bayes estimates under quadratic loss. The consistency of the Bayes estimates for the entropy and for the information index are shown. The implementation steps are outlined and the performances of the Bayes estimates are illustrated using data sets simulated from exponential, gamma, and lognormal distributions.

Keywords: Nonparametric Bayes, Dirichlet process, Model selection, Kullback-Leibler.

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1 Introduction

Entropy and Kullback-Leibler information have been instrumental in the development of indices of fit of parametric models to the data. Frequentist inference procedures about entropy-based fit indices are abundant. Although use of a parametric model that fits the data is of paramount importance for Bayesian analysis, entropy based fit indices and Bayesian inference about them have not received much attention. In Bayesian statistics, Kullback-Leibler information and entropy are mainly used as descriptive measures for comparison of parametric models and many other purposes and as criteria for derivation of models; see, e.g., Clarke (1996), Clarke and Gustafson (1998), Yuan and Clarke (1999), Carota, Parmigiani, and Polson (1996), and Zellner (1991, 1996).

Given data x_1, \dots, x_n from a distribution F , we wish to assess whether the unknown $F(x)$ can be satisfactorily approximated by a parametric model $F^*(x|\boldsymbol{\theta})$. We measure the loss of approximating $F(x)$ by a parametric model $F^*(x|\boldsymbol{\theta})$ using the Kullback-Leibler discrimination information between the two distributions,

$$K(F : F^*|\boldsymbol{\theta}) = \int \log \frac{f(x)}{f^*(x|\boldsymbol{\theta})} dF(x), \quad (1)$$

where f and f^* are the respective probability density (mass) functions.

In model selection and parametric estimation problems, (1) is referred to as the entropy loss. Among the parametric models, the one that minimizes the expected loss $E[K(F : F^*|\boldsymbol{\theta})]$ is selected. The entropy loss has been used with frequentist and Bayesian risk functions in model selection and parametric estimation problems; see Soofi (1997) and references therein.

In general, estimation of (1) directly is formidable. Akaike (1974) observed that decomposing the log-ratio in (1) gives

$$K(F : F^*|\boldsymbol{\theta}) = -E_f[\log f^*(X|\boldsymbol{\theta})] - H(F), \quad (2)$$

where

$$H(F) = - \int \log f(x) dF(x) \quad (3)$$

is the entropy of F . Since the entropy of the data-generating distribution is free of the parameters, the second term in (2) is ignored in the derivation of the AIC for model selection. The AIC type measures are derived by minimizing the first term in (2) using the average likelihood of the sample. Consequently, the AIC type measures provide criteria for model comparison purposes only, and do not provide information diagnostic about the model fit. Spiegelhalter, Best, Carlin,

and van der Linde (2002) developed a generalization of the AIC for hierarchical Bayesian models using the posterior deviance concept proposed by Dempster (1974). The authors referred to this model comparison criterion as the Deviance Information Criterion (DIC) and showed that DIC is asymptotically equivalent to AIC for non-hierarchical models.

For developing information indices that assess whether the unknown F can be satisfactorily approximated by a parametric model F^* , estimation of the entropy integral (3) plays the pivotal role. In the discrete case, the problem leads to the quantities related to sample proportion and logit analysis. When F is absolutely continuous, information indices of fit and distributional tests require a nonparametric entropy estimate and an estimate for the entropy of a parametric model for F . This line of research began with Vasicek (1976) and continues to date. See for example, Vasicek (1976), Dudewicz and Van der Meulen (1981), Gokhale (1983), Arizono and Ohta (1989), Ebrahimi et al. (1992), Soofi et al (1995), deWaal (1996), Ebrahimi (1997, 1998, 2001), Mazzuchi et al. (2000), Mudholkar and Tian (2002), Taufer (2002), Inverardi (2003), Park and Park (2003), Park (1999, 2005), and Choi and Kim (2006). With the exception of Mazzuchi et al. (2000), all of these papers use frequentist procedures for nonparametric estimation of entropy. Several frequentist procedures for estimation of entropy are available in the literature, see Dudewicz and Van Der Meulen (1987), Ebrahimi et al. (1994), Beirlant et al. (1997), Kraskov et al (2004) and references therein.

Bayesian estimation of entropy has not received much attention. Gill and Joanes (1979) addressed Bayesian estimation of discrete entropy for the frequency data. Mazzuchi et al. (2000) proposed a computational procedure for Bayesian inference about the entropy and an information index of fit. The procedure was shown to be successful in identifying the correct model when fitting various models to a simulated example. Recently, Dadpay et al. (2007) have used a histogram-type entropy estimate for model fitting in generalized gamma family. Bayesian estimation of entropy is closely related to the notion of expected information in Bayesian analysis (Bernardo 1979 and Zellner 1991) and to the notion of average entropy in the communication theory (Campbell 1995).

For constructing information indices of fit, the parametric model $F^*(x|\boldsymbol{\theta})$ is selected based on the maximum entropy characterization of the densities of the parametric families. Consider the moment class of distributions:

$$\Omega_{\boldsymbol{\theta}} = \{F(x|\boldsymbol{\theta}) : E_F[T_j(X)|\boldsymbol{\theta}] = \theta_j, j = 1, \dots, J\}, \quad (4)$$

where $T_j(X)$ are integrable functions with respect to the density and $\boldsymbol{\theta} = (\theta_1, \dots, \theta_J)$ is a vector of moment parameters. The maximum entropy (ME) model in the moment class (4), if it exists, has the density in the following exponential form:

$$f^*(x|\boldsymbol{\theta}) = C(\boldsymbol{\eta})e^{-\eta_1 T_1(x) - \dots - \eta_J T_J(x)}, \quad (5)$$

where the model parameters $\boldsymbol{\eta} = (\eta_1, \dots, \eta_J)$ are the Lagrange multipliers in the ME procedure with

$$\eta_j = \eta_j(\boldsymbol{\theta}), \quad j = 1, \dots, J, \quad (6)$$

and $C(\boldsymbol{\eta}) = \eta_0^{-1}$ is the normalizing constant.

The entropy of ME model is given by

$$H[F^*(x|\boldsymbol{\theta})] = -\log C(\boldsymbol{\eta}) + \eta_1 \theta_1 + \dots + \eta_J \theta_J. \quad (7)$$

Soofi et al. (1995) showed that if $F \in \Omega_{\boldsymbol{\theta}}$ and F^* is the ME model in $\Omega_{\boldsymbol{\theta}}$, then the first term in (2) becomes the entropy of F^* and

$$K(F : F^*|\boldsymbol{\theta}) = H[F^*(x|\boldsymbol{\theta})] - H[F(x|\boldsymbol{\theta})]. \quad (8)$$

The first term is the entropy of the parametric ME model (5) and the second term is the entropy of a distribution which is unknown other than the density is a member of a general moment class, $F \in \Omega_{\boldsymbol{\theta}}$. This equality defines the information distinguishability (ID) between distributions in $\Omega_{\boldsymbol{\theta}}$. ID statistics are obtained by estimating (8).

The relation (8) reduces the problem of estimating $K(F : F^*|\boldsymbol{\theta})$ to the problem of estimating the two entropies shown in (8). Many known parametric families of distributions are in the form of (5) and therefore are ME subject to specific forms of moment constraints. For a parametric model, one may easily identify the moment class $\Omega_{\boldsymbol{\theta}}$ by writing the density in the exponential form (5); see, e.g., Soofi et al. (1995). The entropy expression for the well known parametric families are tabulated.

Two main issues remain: estimation of the entropy of the unknown distribution $H[F(x|\boldsymbol{\theta})]$ and maintaining the non-negativity of the estimate of (8).

This paper develops a class of entropy estimates and provides a procedure for Bayesian inference on the entropy and a fit index. We define a quantized approximation of (3), which for the continuous case converges to the entropy integral. The quantized entropy provides a general representation

for several existing entropy estimates, including Vasicek’s sample entropy, which has been the main vehicle for the frequentist entropy-based distributional tests, and the existing Bayes entropy estimates (Gill and Joanes 1979, Mazzuchi et al. 2000, Dadpay et al. 2007). We then derive a Bayes estimate of the quantized entropy, based on the Dirichlet process posterior for F , with the ME model as the prior expectation $E(F) = F^*$. We refer to this inferential procedure as the Maximum Entropy Dirichlet (MED). We explore the large sample properties of the Bayes estimates of entropy and the fit index.

For inference about the fit of the model F^* , we give an approximation of the posterior entropy loss, $K(F : F^*|\boldsymbol{\theta})$. The normalized estimated average entropy loss provides a Bayesian Information Distinguishability (BID) index of fit for the model. Inference about the fit is based on comparing the prior and posterior distributions of the normalized $K(F : F^*|\boldsymbol{\theta})$. As byproducts, the MED also provides priors and posteriors for the moment parameters $\boldsymbol{\theta}$ and the model parameters $\boldsymbol{\eta}$.

Section 2 presents the quantized entropy and the Bayes estimate of entropy for continuous case. Section 3 relates the entropy estimate to some measures for the discrete case. Section 4 presents estimation of the Kullback-Leibler function. Section 5 reports some results of a simulation study. Section 6 gives some concluding remarks. Technical details are given in an appendix.

2 The Continuous Case

For a real-valued random variable X with distribution function F , the probability integral transform gives a uniform random variable $U = F(X)$ over the unit interval and the quantile function is defined as $\xi = Q(u) = F^{-1}(u) = \inf\{x : F(x) \geq u\}$. Parzen (2004) gives an insightful discussion of quantile functions and the useful roles that they play in statistical data modeling, including quantile formula for mean and variance. Quantile formulas for sample moments use order statistics. Given a set of observations x_1, \dots, x_n from F , the sample quantiles are defined by the order statistics $y_{(1)} \leq y_{(2)} \leq \dots \leq y_{(n)}$ with $\hat{F}_i = \hat{P}(X \leq y_{(i)}) = \frac{i}{n}$, see Parzen (2004).

The quantile formula for entropy (3) is

$$H(F) = \int_0^1 \log \left[\frac{d}{du} Q(u) \right] du. \tag{9}$$

Vasicek (1976) noted this entropy representation and defined a sample entropy based on order

statistics as follows. At each sample point $\left(y_{(i)}, \frac{i}{n}\right)$, the derivative in (9) is estimated by

$$s_i(m, n) = \frac{y_{(i+m)} - y_{(i-m)}}{\hat{F}_{(i+m)} - \hat{F}_{(i-m)}} = \frac{y_{(i+m)} - y_{(i-m)}}{2m/n}, \quad (10)$$

where $m \in \left\{1, 2, \dots, \leq \frac{n}{2}\right\}$ is an estimation window size. Vasicek's sample entropy is defined by the average of (10),

$$H_v(m, n) = \frac{1}{n} \sum_{i=1}^n \log \left[\frac{n}{2m} (y_{(i+m)} - y_{(i-m)}) \right], \quad (11)$$

where $y_{i-m} = y_1$ for $i \leq m$ and $y_{i+m} = y_n$ for $i \geq n - m$.

We generalize Vasicek's sample entropy by a quantized entropy.

2.1 Quantized Entropy

Let $\xi_k = Q(u_k)$, $k = 0, 1, \dots, q$ be a set of quantiles of F and let $F_k = F(\xi_k)$. Each set of quantiles define a partition of the real line \mathfrak{R} ,

$$-\infty < \xi_0 < \xi_1 < \dots < \xi_q < \infty. \quad (12)$$

At each point (ξ_k, F_k) , we estimate the derivative in (9) by

$$s_k(m, q) = \frac{\Delta \xi_{m,k}}{\Delta F_{m,k}}, \quad (13)$$

where $m \in \left\{0, 1, 2, \dots, \leq \frac{q}{2}\right\}$ is an estimation window size, $\Delta \xi_{m,k}$ is spacing of order $2m$ defined by

$$\Delta \xi_{m,k} = \begin{cases} \xi_k - \xi_{k-1} \equiv \Delta \xi_k & \text{for } m = 0 \\ \xi_{k+m} - \xi_{k-m} = \sum_{\ell=-m}^m \Delta \xi_{k+\ell} & \text{otherwise,} \end{cases} \quad (14)$$

and

$$\Delta F_{m,k} = \begin{cases} F_k - F_{k-1} \equiv \Delta F_k & \text{for } m = 0 \\ F_{k+m} - F_{k-m} = \sum_{\ell=-m}^m \Delta F_{k+\ell} & \text{otherwise,} \end{cases} \quad (15)$$

with $\xi_{k-m} = \xi_0$, $k < m$ and $\xi_{k+m} = \xi_q$, $k > q - m$ are set such that $F_0 < \epsilon_0$ and $F_q < 1 - \epsilon_q$.

Figure 1 depicts estimation of the derivative of the quantile function $\frac{dQ(u)}{du}$. Figure 1a shows five quantiles $\xi_{k-2}, \xi_{k-1}, \xi_k, \xi_{k+1}, \xi_{k+2}$ and the probabilities on the distribution function $F(x)$. Figure 1b shows the quantile function $\xi = Q(u)$, which is the mirror image of the $u = F(x)$ on the rotated axis. At point (F_k, ξ_k) , the derivative $\frac{dQ(u)}{du}$ may be estimated by any of the slopes computed by the following ratios of the spacings to the corresponding probability increments:

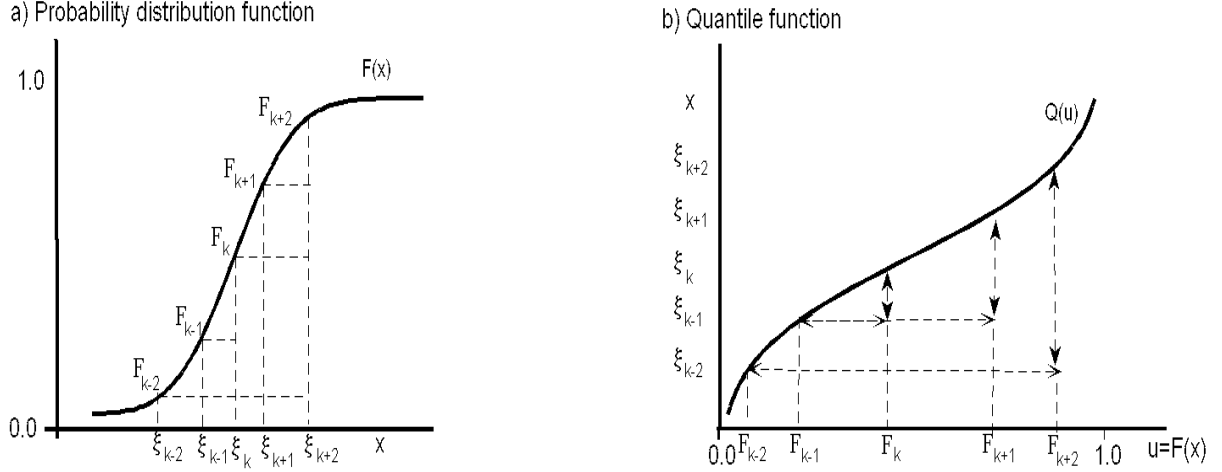


Figure 1: Probability distribution function and quantile function

- (a) Ratio of the spacings of order one to the corresponding probability increments. $s_k(0, q) = \frac{\xi_k - \xi_{k-1}}{F_k - F_{k-1}}$;
- (b) Ratio of the spacings of order two to the corresponding probability increments. $s_k(1, q) = \frac{\xi_{k+1} - \xi_{k-1}}{F_{k+1} - F_{k-1}}$;
- (c) Ratio of the spacings of order four to the corresponding probability increments. $s_k(2, q) = \frac{\xi_{k+2} - \xi_{k-2}}{F_{k+1} - F_{k-1}}$.

Other plausible alternatives include $\frac{\xi_{k+1} - \xi_k}{F_{k+1} - F_k}$ and a combination of $s_k(m, q)$, $m = 1, 2$.

The roles of spacing $\Delta\xi_{m,k}$ and window size m are to smooth the slope estimate (13). With $m > 0$ the derivative is estimated based on the spacings of order $2m$ and the corresponding probability increments. Due to the relationship between the single and higher order spacings and probability increments shown in (14) and (15), the case of $m > 0$ provides a “moving average” type estimate for $\frac{dQ(u)}{du}$ in the form of

$$s_k(m, q) = \frac{\overline{\Delta\xi_k}}{\overline{\Delta F_k}}, \quad m > 0,$$

where $\overline{\Delta\xi_k} = \sum_{\ell=-m}^m \frac{\Delta\xi_{k+\ell}}{2m}$ and $\overline{\Delta F_k} = \sum_{\ell=-m}^m \frac{\Delta F_{k+\ell}}{2m}$ are the moving averages of spacings of order one and the corresponding probability increments defined by $m = 0$. If the spacings of order one are all equal, then the case of $m > 0$ is simply the moving average of the case of $m = 0$, i.e.,

$$s_k(m, q) = \bar{s}_k(0, q)^*.$$

The quantized entropy is defined by the average of the logarithm of the slopes (13):

$$H_{m,q}(F) = - \sum_{k=1}^q \Delta F_k \log \frac{\Delta F_{m,k}}{\Delta \xi_{m,k}}. \quad (16)$$

For a distribution with an absolutely continuous density, $H_{m,q}(F)$ provides a quantized approximation for the entropy integral (3). Note that $H_{m,q}(F)$ has the scale property of the differential entropy $H(F)$. That is for a constant a , $H_{m,q}(F_{aX}) = H_{m,q}(F_X) + \log |a|$.

$H_{m,q}(F)$ is a general representation that includes several entropy estimates proposed in the literature. For $m = 0$, the quantized entropy (16) gives a modification of the quantized approximation of the differential entropy (3) by the discrete entropy proposed by Cover and Thomas (1991). This case was used in Mazzuchi et al (2000). The modification resolve the convergence problem of the quantized approximation of Cover and Thomas (1991).

Lemma 1 *Let F be a distribution with an absolutely continuous density f . Then,*

$$H_{m,q}(F) \rightarrow H(F), \quad \text{as } q \rightarrow \infty, \quad \Delta \xi_{m,k} \rightarrow 0 \quad \forall k.$$

Proofs of this and other results are given in the Appendix.

When the partition (12) is defined in terms of the order statistics, $\xi_k = y_i$, $k = i = 1, \dots, n$, then $H_{m,n}(F)$ with $\xi_1 = y_1, \dots, \xi_q = y_n$, and the empirical distribution $\Delta F_n = \Delta \hat{F}_n = 1/n$ gives Vasicek's sample entropy $H_v(m, n)$. Ebrahimi et al. (1994) observed that (10) does not define correct measures of the slope when $i \leq m$ or $i \geq n - m + 1$ and provided two modifications of $H_v(m, n)$ which are asymptotically equivalent to $H_v(m, n)$. The quantized entropy (16) includes both of these modifications.

Hall and Morton (1993) proposed estimating $H(f)$ by the entropy of a histogram,

$$H_q^h(F) = - \sum_{k=1}^q \Delta \hat{F}_k \log \frac{\Delta \hat{F}_k}{h},$$

where $\Delta \hat{F}_k = \frac{n_k}{n}$, $k = 1, \dots, q$ are the relative frequencies in the bin width $h = \Delta \xi_{m,k}$. $H_{m,q}(F)$ gives the histogram entropy when $m = 0$, $\Delta \xi_k = h$, and $\Delta F_k = \Delta \hat{F}_k$ $k = 1, \dots, q$.

Another useful partition is given by the Dirichlet tessellation (Bowyer 1981) defined by

$$\mathcal{T}_k = \{x : |x - \xi_k| < |x - \xi_j|, \forall j \neq k\}.$$

*Interpretation of this special case is due to a referee

In this case each data point x_i , $i = 1, \dots, n$ is placed in an interval (ξ_i, ξ_{i+1}) , $i = 0, \dots, n - 1$. The boundaries are given by the data midpoints

$$\xi_i = \frac{1}{2} (y_{(i)} + y_{(i+1)}), \quad i = 1, \dots, n - 1, \quad (17)$$

where $y_{(1)} \leq \dots \leq y_{(n)}$ are the order statistics; ξ_0 and ξ_n are defined as above.

Theil (1980) used the midpoints (17) for derivation of a mass and mean preserving ME (MMME) density estimate f_n^* , which is piecewise uniform over the intervals $[\xi_i, \xi_{i+1}]$, $i = 1, \dots, n - 1$ and exponential over $(-\infty, \xi_1]$, and $[\xi_n, \infty)$. Its entropy, given by

$$H(F_n^*) = - \sum_{i=1}^n \Delta \hat{F}_i \log \frac{\Delta \hat{F}_i}{\Delta \xi_i} + \frac{2}{n} (1 - \log 2).$$

This entropy is a nonparametric entropy (Dudewicz and Van Der Meulen 1987, Soofi and Retzer 2002) and is a special case of the quantized entropy (16) with $F = F^*$, $m = 1$, and $q = n$ as $n \rightarrow \infty$.

In case of histogram partition, where $h = \Delta \xi_{m,k}$, $\forall k$ and $m = 0$, smoothing is done only through the binwidth h . Whereas in the case of a partition defined by order statistics (e.g., Vasicek's sample entropy and Dirichlet tessellation) smoothing is done through the window size. The choice of $m \geq 1$ for Vasicek's sample entropy and its modifications has been studied via simulation in terms of frequentist criteria such as bias and mean squared error of estimation and power of the distributional tests (see, e.g., Ebrahimi et al 1992, Ebrahimi et al 1994, Mudholkar and Tian 2002, and Park and Park 2003). Choice of m for the quantized entropy requires simulation study in the context of its applications to various statistical problems. Section 5 reports some results for Bayesian estimation of entropy and inference about the fit.

2.2 Bayes Estimate of Entropy

Given a sample $\mathbf{x} = (x_1, \dots, x_n)$ from unknown F , the Bayes entropy estimate is defined by the mean of a posterior distribution of the quantized entropy (16),

$$\tilde{H}_{m,q}(F) \equiv E[H_{m,q}(F)|\mathbf{x}].$$

We use the Dirichlet process prior (Ferguson 1973) for the unknown F ,

$$F(\xi_k)|\mathcal{B}, F^* \sim \mathcal{D}(\mathcal{B}, F^*), \quad (18)$$

where F^* is a prior mean of F and $\mathcal{B} > 0$ is the strength of belief parameter. We use F^* , the ME distribution in Ω_{θ} , as the best guess distribution of the Dirichlet prior. In this context, \mathcal{B} is

the degree of belief in the ME distribution F^* and we refer to $\mathcal{D}(\mathcal{B}, F^*)$ as the *maximum entropy Dirichlet (MED)* prior.

For any partition (12) of \mathfrak{R} , the increments ΔF_k , $k = 1, \dots, q$ have the Dirichlet distribution

$$\pi(\mathbf{\Delta F}) \propto (\Delta F_1)^{\alpha(\xi_1)-1} (\Delta F_2)^{\alpha(\xi_2)-\alpha(\xi_1)-1} \dots (\Delta F_q)^{\mathcal{B}-\alpha(\xi_{q-1})-1}. \quad (19)$$

The parameters of the Dirichlet distribution (19) are given by $\alpha(\xi_k) \equiv \alpha((-\infty, \xi_k])$, a measurable function defined over \mathfrak{R} such that $\lim_{\xi \rightarrow \infty} \alpha(\xi) = \mathcal{B}$, and

$$E[F(\xi_k)] = \frac{\alpha(\xi_k)}{\mathcal{B}} = F^*(\xi_k).$$

The prior variance of $F(\xi)$ is given by

$$V[F(\xi)|F^*, \mathcal{B}] = \frac{\alpha(\xi)[\mathcal{B} - \alpha(\xi)]}{\mathcal{B}^2(\mathcal{B} + 1)} = \frac{F^*(\xi)[1 - F^*(\xi)]}{\mathcal{B} + 1},$$

reinforcing the notion of F^* being the best guess and \mathcal{B} being the strength of belief parameter.

It is well-known that the posterior distribution of F is also Dirichlet process with parameters updated by the data as:

$$F(\xi)|F^*, \mathcal{B}, \mathbf{x} \sim \mathcal{D}(\tilde{\mathcal{B}}, \tilde{F}), \quad (20)$$

with the parameters updated by

$$\tilde{\mathcal{B}} = \mathcal{B} + n, \quad \text{and} \quad \tilde{\alpha}(\xi_k) = \alpha(\xi_k) + \sum_{i=1}^q \delta[x_i \leq \xi_k] \quad (21)$$

where $\delta[\cdot]$ is the indicator function of the set.

The posterior mean of F_k is given by

$$\tilde{F}_k = E[F(\xi_k)|F^*, \mathcal{B}, \mathbf{x}] = \frac{\mathcal{B}}{\tilde{\mathcal{B}}} F^*(\xi_k) + \frac{n}{\tilde{\mathcal{B}}} \hat{F}(\xi_k), \quad (22)$$

where $\hat{F}(\xi_k)$ is an empirical distribution.

The natural choice for empirical distribution is the cumulative distribution (piece-wise uniform). For the Dirichlet tessellation with $m = 0$, the empiric distribution function of order one (piecewise uniform over intervals $(\xi_{k-1} < x \leq \xi_{k+1}]$, $k = 1, \dots, n$) developed by Dudewicz and Van Der Meulen (1987) and the cumulative distribution of Theil's MMME (piece-wise uniform over intervals $(\xi_{k-1} < x \leq \xi_{k+1}]$, $k = 1, \dots, n$ with exponential tails) are also applicable. For Dirichlet tessellation with $m \geq 1$ the higher order empiric distribution developed by Dudewicz and Van Der Meulen (1987) and the distribution function associated with Vasicek's sample entropy developed by Park and Park (2003) are applicable.

Theorem 1 For each given partition (12) with the Dirichlet prior (19) the following results hold.

(i) The posterior average quantized entropy is

$$\tilde{H}_{m,q}(F) = \psi(\tilde{\mathcal{B}} + 1) - \sum_{k=1}^q \Delta \tilde{F}_k [\psi(\tilde{\mathcal{B}} \Delta \tilde{F}_{m,k} + 1) - \log \Delta \xi_{m,k}], \quad (23)$$

where $\psi(z) = \frac{d \log \Gamma(z)}{dz}$ is the digamma function.

(ii) For large $\tilde{\mathcal{B}}$ such that $\Delta \tilde{F}_k / (\tilde{\mathcal{B}} \Delta \tilde{F}_{m,k}) \approx 0$,

$$\tilde{H}_{m,q}(F) \approx - \sum_{k=1}^q \Delta \tilde{F}_k \log \frac{\Delta \tilde{F}_{m,k}}{\Delta \xi_{m,k}}. \quad (24)$$

Since the Dirichlet prior (19) requires specification of a parametric first guess distribution F^* , for $\mathcal{B} > 0$ the posterior mean $\tilde{H}_{m,q}(F)$ is a *semiparametric Bayes entropy estimate* under quadratic loss. For the case of the improper prior $\mathcal{B} = 0$, or when $n \rightarrow \infty$, the posterior mean $\tilde{H}_{m,q}(F)$ is a *nonparametric Bayes entropy estimate* under quadratic loss.

In practice, the posterior mean will be computed by the average of a large number of replications of posterior Dirichlet vectors generated from (20) and computing (16) for each run, and then taking the average. By the law of large numbers, the simulated Bayes estimate should be close to (23), which may be used for the simulation accuracy as well.

Next result shows the consistency of the Bayes entropy estimate for the histogram partition.

Theorem 2 Let F be a distribution with an absolutely continuous density f . Then $\tilde{H}_{m,q}(F)$ based on a histogram type partition is consistent.

In the case of Dirichlet tessellation partition, $q = n$ and $\tilde{H}_{m,q}(F) = \tilde{H}_{m,n}(F)$. Note that use of the Dirichlet tessellation partition circumvents the empty cell problem that usually is encountered in applications of the Dirichlet process prior. Next result shows the consistency of the Bayes entropy estimate for the Dirichlet tessellation partition.

Theorem 3 Let F be a distribution with an absolutely continuous density f . Let (12) be the partition with ξ_i defined by the Dirichlet tessellation (17). Then as $n \rightarrow \infty$, $m \rightarrow \infty$, and $\frac{m}{n} \rightarrow 0$,

$$\tilde{H}_{m,n}(F) \xrightarrow{P} H_v(m, n) \xrightarrow{P} H(F),$$

where $H_v(m, n)$ is the Vasicek's entropy estimate.

According to Theorem 2 and Theorem 3 consistency may be achieved by smoothing, either through the binwidth h or through increasing the window size m . Consistency can also be proved for the case of $m = 0$, however, under a very stringent requirement of $\Delta\xi_i \rightarrow 0 \forall i = 1, \dots, n$, which is hardly implementable. We therefore present it as a remark.

Remark 1 *Let F be a distribution with an absolutely continuous density f . Let (12) be the partition with ξ_i defined by the Dirichlet tessellation (17). Then as $\Delta\xi_i \rightarrow 0 \forall i = 1, \dots, n$, $\tilde{H}_{0,n}(F) \xrightarrow{p} H(F)$.*

As a final point, we also should note that the posterior variance of quantized entropy is available. Since derivation is tedious and the variance expression is messy it is not reported here. It can be shown that the posterior variance goes to zero as $n \rightarrow \infty$.

3 The Discrete Case

We have discussed the problem when F has a continuous density. However, with some modifications, the procedure is applicable when F is discrete or a distribution over q categories. Let

$$H(\Delta F) = - \sum_{k=1}^q \Delta F_k \log \Delta F_k, \quad (25)$$

where $\Delta F_k = f_k$ is probability assigned to the k th category, $k = 1, \dots, q$ by F . Then under the Dirichlet prior (19) for F , the posterior average discrete entropy is

$$\tilde{H}(\Delta F) = \psi(\tilde{\mathcal{B}} + 1) - \sum_{k=1}^q \Delta \tilde{F}_k [\psi(\tilde{\mathcal{B}} \Delta \tilde{F}_k + 1)]. \quad (26)$$

This is obtained by using part (ii) of Lemma 2 with $u = \tilde{\mathcal{B}} \Delta \tilde{F}_k$ and $v = \tilde{\mathcal{B}}(1 - \Delta \tilde{F}_k)$.

Specific cases of (26) have been used previously. Gill and Joanes (1979) used the symmetric Dirichlet prior distribution

$$\pi(f_1, \dots, f_q) \propto f_1^{\rho-1} \dots f_q^{\rho-1}, \quad \rho > 0 \quad (27)$$

and found the posterior mean of $H(f)$. This prior reduces to the uniform prior when $\rho = 1$ and to the Jeffreys invariant prior when $\rho = 1/2$.

Campbell (1995) obtained simple expressions for the prior average entropy and the prior entropy variance using (27). The following theorem characterizes the results based on (27) in terms of the Dirichlet prior (19).

Theorem 4 Let F be a distribution with probability mass function f_1, \dots, f_q over q points $y_1 < \dots < y_q$. Then the average entropy based on the symmetric Dirichlet prior (27) is given by (26) if and only if the prior guess for the Dirichlet prior (19) is uniform, $F^*(y_k) = k/q$, $k = 1, \dots, q$.

Let $\Delta \hat{F}_k = n_k/n$, where $n_k = \sum_{i=1}^q \delta[x_i = y_k]$. Then with the uniform best guess, the posterior average entropy (26) gives the Bayes estimate of the discrete entropy obtained by Gill and Joanes (1979).

4 Information Index of Fit

The entropy-difference tests of distributional hypotheses are based on the right-hand-side of (8) and the Kullback-Leibler tests arrive at (8) from (1). The tests were constructed using an estimate $\hat{\eta}_j$ in the expression for the parametric entropy $H[F^*(x|\boldsymbol{\theta})]$ and a sample entropy (usually Vasicek's entropy $H_v(m, n)$) as the nonparametric estimate of $H[F(x|\boldsymbol{\theta})]$ in (8). Often these tests are computed without imposing the constraints (4) on the two entropy estimates. When F is not constrained to be in $\Omega_{\hat{\theta}}$ with $F^*(x|\hat{\theta})$ as the ME model in the moment class, the entropy difference in (8) does not measure disparity between F and F^* . Moreover, without the constraints the procedure may produce a negative estimate of the discrimination information function $K(F : F^*|\boldsymbol{\theta})$. Soofi et al (1995) and Park and Park (2003), developed distributional fit indices and tests that ensure non-negativity of $K(F : F^*|\boldsymbol{\theta})$.

In order to ensure the non-negativity of $K(F : F^*|\boldsymbol{\theta})$, the parameters of the ME model (hyperparameters) are determined by the moments of the quantized F . Quantized approximations of the moment are obtained by

$$\theta_{q,j} = \sum_{k=1}^q T_j(\bar{\xi}_{k,m})(\Delta F_k), \quad j = 1, \dots, J, \quad (28)$$

where

$$\bar{\xi}_{k,m} = \begin{cases} \frac{\xi_k + \xi_{k-1}}{2} & \text{for } m = 0 \\ \frac{\xi_{k-m} + \xi_{k+m}}{2} & \text{for } m \geq 1. \end{cases}$$

The quantized moments (28) are approximations of the moments $\theta_j = \theta_j(F) \approx \theta_j(\boldsymbol{\Delta F}) = \theta_{q,j}$ in (4). We then use the maximum entropy $H(F^*|\boldsymbol{\theta}_q)$, where $\boldsymbol{\theta}_q$ is the vector of quantized moments, and the quantized entropy $H_{m,q}(F)$ in the decomposition (8). By using (28), in addition to ensuring

non-negativity of the Kullback-Leibler function, we can draw prior and posterior for $\boldsymbol{\theta}$ from the Dirichlet prior and posterior for F . Then the priors and posteriors for the model parameters $\eta_j(\boldsymbol{\theta})$ are obtained.

The priors and posteriors of $H(f^*|\boldsymbol{\theta})$ are obtained using $\theta_{q,j}$ and $\eta_j(\boldsymbol{\theta}_q)$ in the general form of the entropy of ME model $f^* \in \Omega_{\boldsymbol{\theta}}$ given by

$$H[f^*(x|\boldsymbol{\theta}_q)] = -\log C(\boldsymbol{\eta}_q) - \sum_{j=1}^J \eta_{q,j} \theta_{q,j}.$$

Then the prior and posterior distributions for $K(F : F^*|\boldsymbol{\theta})$ are induced by

$$K_{m,q}(F : F^*) = H(F^*|\boldsymbol{\theta}_q) - H_{m,q}(F)$$

Note that $K_{m,q}(F : F^*)$ is scale invariant and $P(K_{m,q}F : F^*) \geq 0) = 1$.

Using the posterior mean of the entropy of the ME model $\tilde{H}[f^*(x|\boldsymbol{\theta}_q)]$, (23) and (24) in (8) gives the posterior mean of $K_{m,q}$

$$\begin{aligned} \tilde{K}_{m,q}(F : F^*) &= \tilde{H}[F^*(x|\boldsymbol{\theta}_q)] + \psi(\tilde{B} + 1) - \sum_{k=1}^q \Delta \tilde{F}_k [\psi(\tilde{B} \Delta \tilde{F}_{m,k} + 1) - \log \Delta \xi_{m,k}] \\ &\approx \tilde{H}[F^*(x|\boldsymbol{\theta}_q)] - \sum_{k=1}^q \Delta \tilde{F}_k \log \frac{\Delta \tilde{F}_{m,k}}{\Delta \xi_{m,k}}. \end{aligned} \quad (29)$$

This approximation of the expected entropy loss provides an *Information Distinguishability (ID) index* for assessing the fit of the parametric model F^* .

The ID index can be normalized as:

$$\begin{aligned} ID_{m,q}(F : F^*) &= 1 - \exp[-K_{m,q}(F : F^*)] \\ &= 1 - \exp[H_{m,q}(F) - H(F^*|\boldsymbol{\theta}_q)]. \end{aligned} \quad (30)$$

Note that $0 \leq ID_{m,q}(F : F^*) \leq 1$, and $ID_{m,q}(F : F^*) = 0$ if and only if $F(x|\boldsymbol{\theta}) = F^*(x|\boldsymbol{\theta})$ with probability 1. The posterior mean $\tilde{ID}_{m,q}(F : F^*)$ of the $ID_{m,q}(F : F^*)$ index will be referred to as *Bayesian Information Discrimination (BID) index*. We compare the posterior and prior distributions of the ID index for inference about the fit. If the posterior distribution of $ID_{m,q}(F : F^*)$ shifts to the left of the prior, then data provide support for the ME model. If the posterior shifts to the right of the prior or concentrates around the prior mean then the data and model are not compatible.

Next result shows the consistency of the information index of fit for the histogram and tessellation partitions.

Theorem 5 Let F^* be a distribution with an absolutely continuous density f^* . If the data is generated from F^* , then the following results hold.

(i) For the histogram type partition $\tilde{K}_{m,q}(F : F^*) \xrightarrow{p} 0$.

(ii) Let (12) be the partition with ξ_i defined by the Dirichlet tessellation (17). Then as $n \rightarrow \infty$, $m \rightarrow \infty$, and $\frac{m}{n} \rightarrow 0$, $\tilde{K}_{m,q}(F : F^*) \xrightarrow{p} 0$.

Thus if F^* is not a suitable approximation for the true data-generating distribution F , then for large n , we can generally expect large values of $\tilde{K}_{m,q}$. The next remark gives the consistency for the case of $m = 0$ under the stringent requirement of $\Delta\xi_i \rightarrow 0 \forall i = 1, \dots, n$.

Remark 2 Let F be a distribution with an absolutely continuous density f . Let (12) be the partition with ξ_i defined by the Dirichlet tessellation (17). Then as $\Delta\xi_i \rightarrow 0 \forall i = 1, \dots, n$, and as $n \rightarrow \infty$, $\tilde{K}_{0,q}(F : F^*) \xrightarrow{p} 0$.

5 Implementation and Examples

This section outlines the computational steps and reports results of a simulation study for the proposed Bayes entropy estimate and information index of fit.

5.1 Implementation

Computation of the entropy estimate and the fit index for the case of $m = 0$ is discussed in Mazzuchi et al. (2000). The procedure is adjusted for general m as follows.

1. Specification of the MED inputs:

- (a) Identify the moment constraints (4) for which the likelihood function is the ME model $F^*(x|\boldsymbol{\theta})$; for a table of ME distributions see, e.g., Soofi et al. (1995).
- (b) Set up the moment equations (28), the model parameter equations (6), and the entropy expression for $F^*(x|\boldsymbol{\theta})$. Use an entropy table (see e.g., Ebrahimi et al. (1999)) or (7).
- (c) Specify the uncertainty about the ME distribution $F^*(x|\boldsymbol{\theta})$ as the prior expected distribution via the degree of belief parameter \mathcal{B} .

- (d) Set the best guess moment parameter $\boldsymbol{\theta}^0$; in the absence of prior values use the data moments.
- (e) Set ξ_0 and ξ_q as suitable percentiles of $F^*(x|\boldsymbol{\theta}^0)$ and compute data midpoints ξ_i for the Dirichlet tessellation partition.

2. Simulation of the MED priors:

- (a) Simulate n -dimensional Dirichlet vectors, $\mathbf{F}^s = (\Delta F_1^s, \dots, \Delta F_n^s)$, $s = 1, \dots, S$, $S \gg n$, according to 1(a)-1(e) and obtain the Dirichlet prior (18) for the quantized distribution \mathbf{F} .
- (b) For each Dirichlet vector \mathbf{F}^s , $s = 1, \dots, S$, use (16) to compute $H_{m,q}^s(F)$ and obtain the prior distribution for the unknown entropy $H(F)$.
- (c) For each Dirichlet vector \mathbf{F}^s , $s = 1, \dots, S$, use (28) to compute the quantized moment parameters $\boldsymbol{\theta}_q^s$ and obtain the prior distributions of the moment parameters $\boldsymbol{\theta}$.
- (d) For each vector of moment parameters $\boldsymbol{\theta}_q^s$, $s = 1, \dots, S$, use (6) to compute the model parameters $\boldsymbol{\eta}_q^s$ and obtain the prior distributions of $\boldsymbol{\eta}$.
- (e) For each vector of model parameters $\boldsymbol{\eta}_q^s$, $s = 1, \dots, S$, use the entropy expression to compute the ME model entropy $H(F^*|\boldsymbol{\theta}_q^s)$ and obtain the prior for $H(F^*|\boldsymbol{\theta})$.
- (f) Use each pair of $H_{m,q}^s(F)$ and $H(F^*|\boldsymbol{\theta}_q^s)$, $s = 1, \dots, S$ in (30) to compute $ID_{m,q}^s(F : F^*; \boldsymbol{\theta}_q)$ and obtain the prior distribution for the ID index,
- (g) The simulation accuracy can be checked as follows.
 - i. Compute the prior mean of the quantized entropy using (23) with $n = 0$ in (22) and compare it with the simulated mean $\bar{H}_{m,q}^s = S^{-1} \sum_{s=1}^S H_{m,q}^s$. If the two quantities are not satisfactorily close, increase the number of simulations S .
 - ii. Compare the quantized moments with the corresponding moments of $F^*(x|\boldsymbol{\theta}^0)$. If there is a large discrepancy, adjust ξ_q (h for histogram partition).

3. Simulation of the MED posteriors:

- (a) Update the Dirichlet prior parameters to obtain the posterior parameters of (21).
- (b) Simulate S posterior Dirichlet vectors using 1(a)-1(d) with the updated Dirichlet parameters and obtain the posterior distribution of the quantized distribution \mathbf{F} .

Table 1. Maximum entropy models used for simulated data

ME Model	Exponential	Gamma	Log-normal
Distribution	$1 - e^{-\lambda x}$	$\int_{\infty}^x \frac{\lambda^{\alpha}}{\Gamma(\alpha)} t^{\alpha-1} e^{-\lambda t} dt$	$\int_{\infty}^x \frac{1}{\sqrt{2\pi\sigma x}} e^{-\frac{1}{2\sigma^2}(\log t - \nu)^2} dt$
Moment class	$E(X) = \mu$	$\begin{cases} E(X) = \mu \\ E(\log X) = \nu \end{cases}$	$\begin{cases} E(\log X) = \nu \\ E(\log X)^2 = \tau \end{cases}$
Model Entropy	$1 + \log \mu$	$\log \frac{\Gamma(\alpha)}{\lambda} + (1 - \alpha)\psi(\alpha) + \alpha$	$\frac{1}{2} \log(2\pi\sigma^2) + \nu$
Quantized moments	$\sum \Delta F_k \bar{\xi}_{k,m} = \mu_q$	$\begin{cases} \sum \Delta F_k \bar{\xi}_{k,m} = \mu_q \\ \sum \Delta F_k \log \bar{\xi}_{k,m} = \nu_q \end{cases}$	$\begin{cases} \sum \Delta F_k \log \bar{\xi}_{k,m} = \nu_q \\ \sum \Delta F_k (\log \bar{\xi}_{k,m})^2 = \tau_q \end{cases}$

- (c) Obtain the MED posterior distributions using the posterior Dirichlet vectors as in 2(a) and then follow 2(b)-2(g).

5.2 Example

We present the results for three sets of data generated from exponential, gamma, and lognormal distributions. For each set of data, we consider all three distributions as the ME models. These are typical results that may be viewed as prototypes of MED analysis for these types of data and models.

For each model, Table 1 shows the distribution function $F^*(x|\boldsymbol{\theta})$ of each candidate model used as the best guess in the Dirichlet prior for unknown distribution F , the moment class (4) in which it is the ME model, and the expression for the entropy of the ME model. The table also shows the quantized moment equations (28) which link the ingredients of the MED procedure.

We report on the results based on the histogram partition and the Dirichlet tessellation. We complete the MED prior specification for each model by setting $\mathcal{B} = 6$ to reflect a very weak degree of belief in the ME distribution.

We report the results for the Dirichlet tessellation for $q = n = 500$ and window sizes $m = 0, 1, 2, 5, 10$, which depict the general patterns in light of the theoretical results. For the distributions under consideration here, the natural choice for $\xi_0 = 0$. We set ξ_q such that $F^*(\xi_q) \geq .99$, adjusted to obtain moment estimates close to sample moments, and hence to prevent negative BID values. Computation times on a desk top varied between 20-30 seconds for various values of m .

In choosing the histogram's number of bins (h), we started with a standard rule (Sturges'

rule $h = 1 + 3.322 \log(500)$, which gives approximately 10 classes. But then this was adjusted for accuracy in moment fitting. We used 12-15 classes in most cases. However, for lognormal alternative sometimes a much large number of classes were needed to obtain moment estimates close to sample moments, and hence to prevent negative BID values. Computation time on a desk top for histogram partition was about 10 seconds.

The exponential data were generated using $\lambda = 1$. Thus, the model entropy is $H(F^*) = 1$. The sample mean is $\bar{x} = 1.03$. The gamma data were generated using $\alpha = 2$ and $\lambda = 1$. Thus, the model entropy is $H(F^*) = 1.577$. The sample moments are $\bar{x} = 1.99$ and $\overline{\log x} = .41$, which give moment estimates (MLE) $\hat{\alpha} = 1.950$ and $\hat{\lambda} = .980$. The lognormal were data generated using $\nu = 0$ and $\sigma^2 = 1$. Thus, the model entropy is $H(F^*) = 1.419$. The sample moments are $\overline{\log x} = -0.012$ and $\overline{(\log x)^2} = 0.957$, which give MLE $\hat{\nu} = 1.950$ and $\hat{\sigma}^2 = .975$.

Table 2 shows the results for entropy estimation. The maximum likelihood method gives estimate $\hat{H}(F^*)$ for entropies of the parametric models. The MED method gives estimates of entropies of the parametric models H^* and a nonparametric estimate $H_{m,q}$ for each class of distributions where the model is ME. Table 2 shows the prior and posterior means and standard deviations for the model and quantized entropies. The table shows the following general patterns, typically found in the simulation runs. Estimates of model entropy given by MLE, MED with histogram partition and tessellation for all m are all similar. For the exponential data, the model entropy estimates are close to the actual value. For gamma and lognormal data the model entropies are underestimated by these methods. The quantized entropy estimates with histogram partition are close to the actual model entropies, thus verifying the result of Theorem 2. The quantized entropy estimates with tessellation partition move closer to the actual model entropies as m increases. For $m = 10$, the estimates are close to the actual model entropies, verifying the result of Theorem 3. The results for $m = 0$ are not satisfactory because the condition of $\Delta\xi_i \rightarrow 0 \forall i = 1, \dots, 500$ is violated; in general it is difficult to achieve. Smoothing by $m > 0$ substantially improves the estimates.

Some general remarks are in order.

1. Entropy estimation procedures underestimate the entropy. This point has been noted in previous studies (e.g. Ebrahimi et al 1994) and is observed for all procedures used in the present study, as noted in Table 2 .
2. Table 2 shows substantial shifts from the prior means (highly negative) toward the actual

Table 2. Posterior means and standard deviations of entropies for exponential, gamma, and lognormal data

		Exponential $H = 1.000$		Gamma $H = 1.722$		Lognormal $H = 1.419$	
		Mean	S.D.	Mean	S.D.	Mean	S.D.
<u>Maximum Likelihood</u>							
	Model entropy \hat{H}^*	1.030	---	1.579	---	1.385	---
<u>Histogram</u>							
	Prior model entropy H^*	1.001	.348	1.478	.304	1.276	.437
	Posterior model entropy H^*	1.037	.040	1.607	.035	1.376	.052
	Prior quantized entropy $H_{m,q}$.659	.254	.952	.230	.780	.253
	Posterior quantized entropy $H_{m,q}$	1.005	.039	1.568	.033	1.350	.044
<u>Tessellation</u>							
$m = 0$							
	Prior model entropy H^*	.979	.371	1.480	.313	1.240	.449
	Posterior model entropy H^*	1.032	.042	1.605	.037	1.387	.054
	Prior quantized entropy $H_{m,q}$	-2.487	.529	-1.944	.499	-2.155	.615
	Posterior quantized entropy $H_{m,q}$.320	.061	.906	.054	.667	.069
$m = 1$							
	Prior model entropy H^*	.961	.362	1.454	.321	1.262	.444
	Posterior model entropy H^*	1.033	.041	1.604	.036	1.388	.055
	Prior quantized entropy $H_{m,q}$	-1.891	.507	-1.366	.468	-1.536	.587
	Posterior quantized entropy $H_{m,q}$.604	.055	1.172	.051	.951	.064
$m = 2$							
	Prior model entropy H^*	.948	.357	1.468	.302	1.253	.448
	Posterior model entropy $H_{m,q}$	1.031	.041	1.603	.036	1.386	.055
	Prior quantized entropy H^*	-1.304	.489	-.751	.421	-.928	.576
	Posterior quantized entropy $H_{m,q}$.797	.051	1.355	.046	1.147	.062
$m = 5$							
	Prior model entropy H^*	.957	.372	1.478	.298	1.251	.453
	Posterior model entropy H^*	1.031	.041	1.604	.037	1.386	.055
	Prior quantized entropy $H_{m,q}$	-.566	.482	-.021	.422	-.198	.555
	Posterior quantized entropy $H_{m,q}$.942	.047	1.499	.042	1.299	.060
$m = 10$							
	Prior model entropy H^*	.962	.384	1.461	.309	1.258	.439
	Posterior model entropy $H_{m,q}$	1.032	.042	1.602	.035	1.384	.056
	Prior quantized entropy H^*	-.045	.490	.489	.402	.335	.536
	Posterior quantized entropy $H_{m,q}$	1.002	.047	1.556	.040	1.364	.058

model entropies for the MED procedures with histogram partition and tessellation for every m .

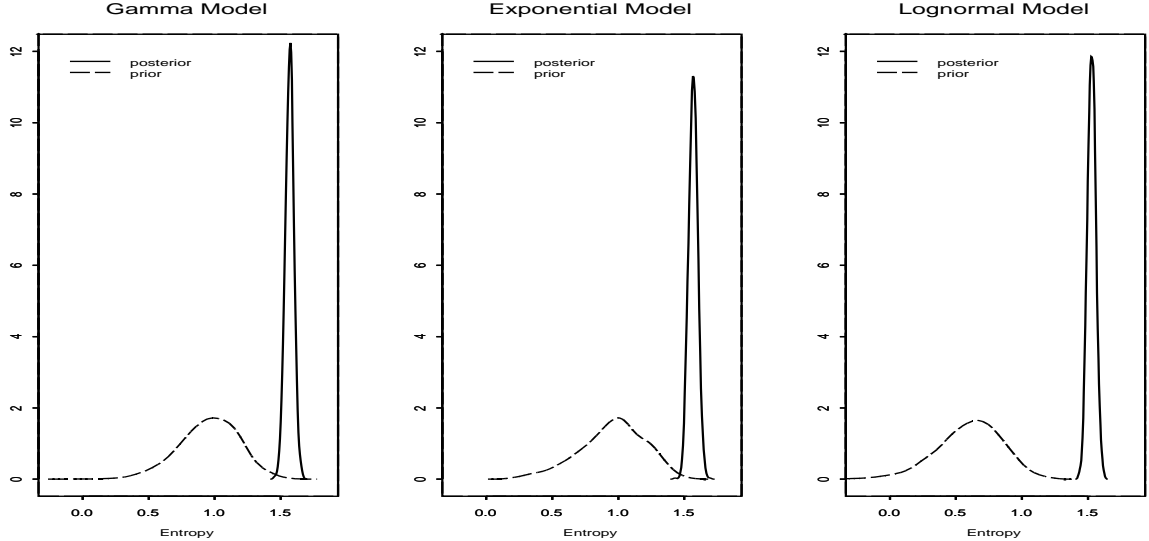


Figure 2: MED prior and posterior distributions of quantized entropy based on the histogram partition for gamma data with three best guess models for the prior.

3. When the sample size is large and the prior is weak, by Theorems 2 and 3, the sample dominates the first guess model F^* , and this makes the MED a robust procedure for inference about entropy. Our simulation studies confirm this. Figure 2 shows the prior and posterior distributions of quantized entropy for gamma data when the gamma, exponential, and lognormal distributions described above are used as the best guess models in the prior. With $n = 500$ and $\mathcal{B} = 6$, the MED prior and posterior distributions are quite similar in all three cases. The factor that makes a difference in the information fit measure $\tilde{K}_{m,q}(F : F^*)$ for these models is the parametric model entropy.

Table 3 shows the prior and posterior means and standard deviations of the normalized information fit index for three candidate models for the exponential data. Since exponential is gamma with shape parameter one (estimate based on exponential data is close to one), the values of posterior mean (BID) index should be similar for the two models. This is the case in Table 3. The exponential BID is always lower than the lognormal BID. The consistency of the BID estimate is observed in the cases of histogram partition and tessellation partition with $m = 10$. In these cases the BID indices of the exponential and gamma models are relatively much lower than the BID index of lognormal model.

Tables 4 shows the prior and posterior means and standard deviations of the normalized information fit index for three candidate models for the gamma and lognormal data. For each data

Table 3. Prior and Posterior means and standard deviations of fit indices for exponential data

		Candidate Models					
		Exponential		Gamma		Lognormal	
		Mean	S.D.	Mean	S.D.	Mean	S.D.
<u>Histogram</u>							
	Prior	.274	.136	.319	.152	.542	.152
	Posterior	.032	.006	.023	.008	.082	.013
<u>Tessellation</u>							
$m = 0$							
	Prior	.967	.012	.964	.014	.961	.016
	Posterior	.509	.021	.508	.021	.555	.021
$m = 1$							
	Prior	.939	.021	.934	.025	.929	.029
	Posterior	.349	.023	.347	.023	.406	.025
$m = 2$							
	Prior	.889	.034	.878	.047	.875	.040
	Posterior	.209	.022	.208	.022	.279	.026
$m = 5$							
	Prior	.773	.067	.755	.072	.745	.068
	Posterior	.085	.017	.084	.019	.164	.025
$m = 10$							
	Prior	.623	.100	.596	.108	.598	.096
	Posterior	.030	.015	.030	.015	.108	.024

set, the BID for the true model is the lowest among the three candidate models. Again, for the histogram and tessellation with $m = 10$, differences between the BID indices of gamma and other two models are relatively substantial.

Figure 3 shows the MED prior and posterior distributions of the information fit index of the gamma and exponential models for the gamma data. We note that in all cases the posterior distributions shift toward zero and concentrate relative to the prior, and more so for the gamma model than for the exponential. That is, the fit index favors the correct model for any partition type and window size. The posterior distributions for the gamma based on the histogram and tessellation partition with $m = 10$ depict the consistency of MED for estimation of Kullback-Leibler information encapsulated in of Theorem 5. The consistency for the case of $m = 0$ is not achieved due to the lack of the required condition $\Delta\xi \rightarrow 0, \forall i = 1, \dots$.

Figure 4 shows the MED prior and posterior for the gamma model parameters based on the gamma data, which is produced through the quantized moment estimation. We note that the posterior distributions are almost symmetric and concentrate on the true values of the parameters.

Table 4. Prior and Posterior means and standard deviations of fit indices for gamma and lognormal data

		Candidate Models					
		Exponential		Gamma		Lognormal	
		Mean	S.D.	Mean	S.D.	Mean	S.D.
Gamma data							
<u>Histogram</u>							
	Prior	.448	.144	.391	.139	.541	.138
	Posterior	.113	.014	.038	.008	.089	.013
<u>Tessellation</u>							
<i>m</i> = 0							
	Prior	.960	.021	.965	.012	.965	.013
	Posterior	.542	.020	.503	.021	.506	.021
<i>m</i> = 1							
	Prior	.930	.031	.937	.021	.936	.021
	Posterior	.403	.022	.350	.022	.355	.023
<i>m</i> = 2							
	Prior	.878	.046	.887	.032	.886	.033
	Posterior	.282	.022	.219	.021	.229	.022
<i>m</i> = 5							
	Prior	.765	.072	.769	.060	.765	.057
	Posterior	.175	.019	.099	.016	.125	.018
<i>m</i> = 10							
	Prior	.627	.097	.611	.092	.611	.087
	Posterior	.130	.018	.044	.013	.086	.013
Lognormal data							
<u>Histogram</u>							
	Prior	.169	.083	.339	.154	.361	.174
	Posterior	.118	.026	.105	.034	.026	.017
<u>Tessellation</u>							
<i>m</i> = 0							
	Prior	.963	.015	.960	.023	.964	.013
	Posterior	.553	.022	.552	.023	.513	.021
<i>m</i> = 1							
	Prior	.933	.026	.927	.032	.936	.023
	Posterior	.407	.025	.404	.026	.354	.024
<i>m</i> = 2							
	Prior	.878	.046	.887	.032	.886	.033
	Posterior	.282	.022	.219	.021	.229	.022
<i>m</i> = 5							
	Prior	.765	.066	.744	.079	.756	.066
	Posterior	.159	.029	.157	.027	.083	.019
<i>m</i> = 10							
	Prior	.619	.098	.588	.107	.591	.095
	Posterior	.097	.029	.094	.029	.020	.013

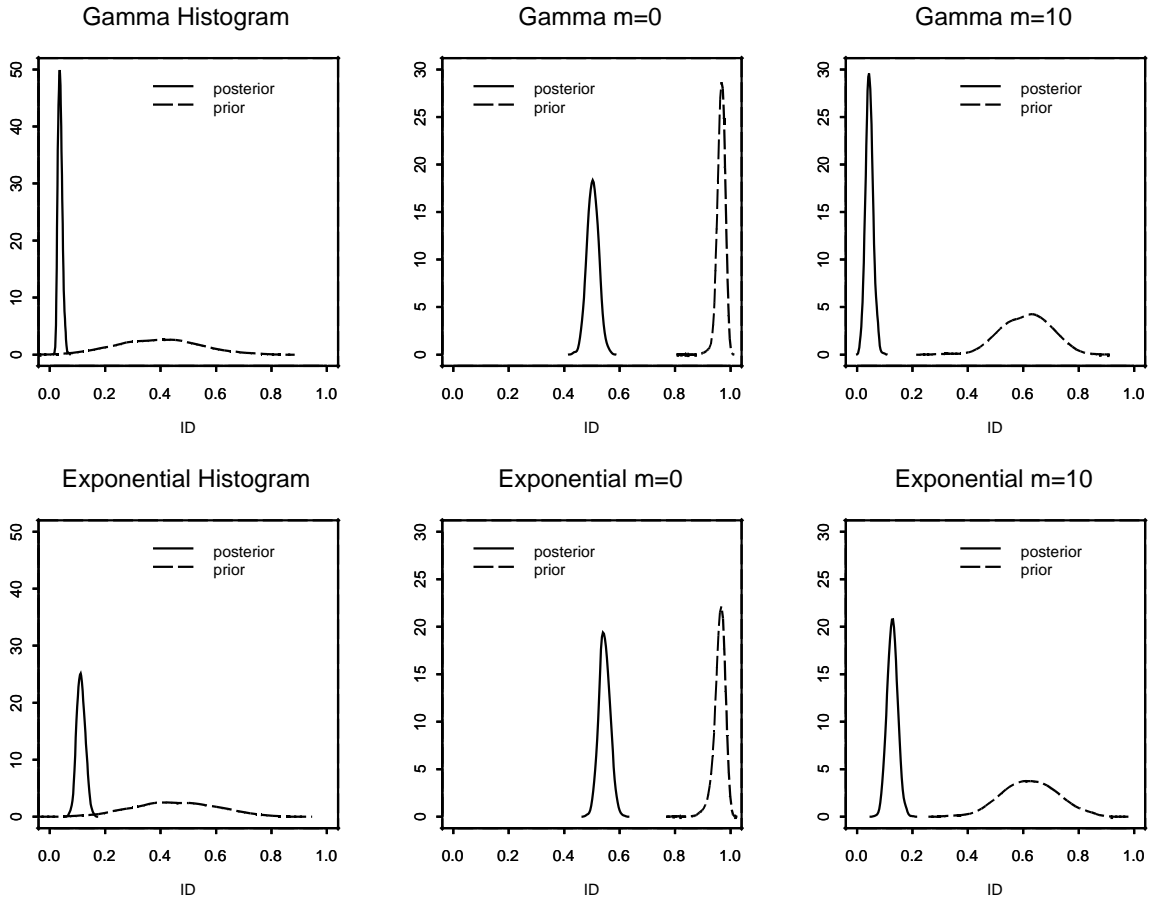


Figure 3: MED prior and posterior distributions of information index of fit for two alternative models for gamma data

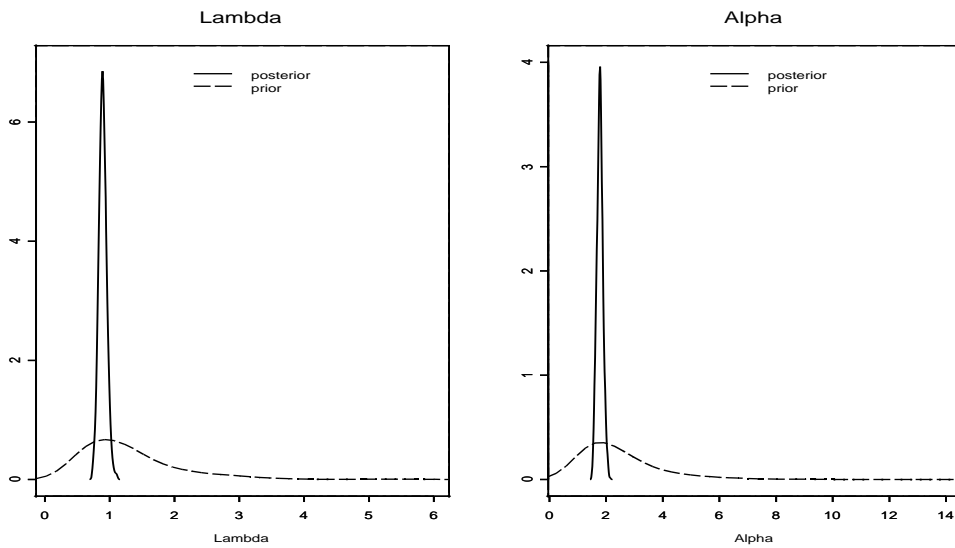


Figure 4: MED prior and posterior distributions of parameters of gamma distribution

6 Concluding Remarks

We have introduced a quantized entropy which provides a general representation of various versions of sample entropy measures found in the literature. We have developed a Bayesian alternative to the sampling theory entropy based approach for assessing the fit of parametric models. The fit is measured by an estimate of a Kullback-Leibler information. Prior and posterior distributions for the quantized entropy are obtained from the Dirichlet process prior for the unknown data generating distribution. We then showed how prior and posterior distributions for the information index can be obtained based on the maximum entropy characterization of the parametric model. The ME model is used as the expectation in the Dirichlet prior. In addition to providing Bayesian inference for the entropy and information index of fit, the MED procedure produces prior and posterior distributions for the model parameters and the moments.

We have derived the exact expression and a simple approximate formula for the posterior mean of the quantized entropy. The posterior mean provides a semiparametric Bayes estimate of entropy, which becomes nonparametric when the data dominate the prior. The posterior variance is also available, but is not included in this paper because the expression for the variance and its derivation are cumbersome. We have shown that the Bayes estimates of entropy and the Kullback-Leibler information possess appropriate consistent properties. The inference is computer-intensive. All prior and posterior distributions are found via simulations.

We have reported results of examples of some simulation runs for exponential, gamma, and lognormal data, where for each set of data, all three distributions were considered as the ME models. The findings, which are prototypes of MED analysis for these types of data and models shed some lights on the theoretical results. The examples indicated that MED is as good as the MLE for producing estimates of parametric model entropy. In addition, MED produces nonparametric estimate and Bayesian inference of entropy, which for large sample is robust against the best guess model in the Dirichlet prior. The proposed Kullback-Leibler information index, BID, favored the correct model in every case. The simulation results indicated that smoothing (through histogram or large window size) is important for consistency of the Bayes entropy estimate and the Kullback-Leibler information index. The specific case of $m = 0$, used in Mazzuchi (2000), although selected the correct model in all three cases, it failed to verify the its consistency results with a sample as large as $n = 500$ and a Dirichlet prior as weak as one signified by $\mathcal{B} = 6$.

Finally, two points are noteworthy regarding our formulation of the Dirichlet prior. First, in the MED prior, the initial best guess model is formulated systematically according to the maximum entropy formalism. Second, the MED formulation extends the traditional maximum entropy approach by associating uncertainty with the ME model. We therefore have bridged the maximum entropy and Bayesian approaches in a new context.

Appendix

Proof of Lemma 1. We show the result along the lines of Cover and Thomas (1991, pp. 228-229). Since the density is absolutely continuous, by the mean value theorem, there exists a point $\xi_k^* \in (\xi_{k-m}, \xi_{k+m})$ such that

$$\Delta F_{m,k} = \int_{\xi_{k-m}}^{\xi_{k+m}} f(x) dx = \Delta \xi_{m,k} f(\xi_k^*).$$

In particular, $\Delta F_k = \Delta \xi_k f(\xi_k^*)$. Substituting in (16), we have

$$\begin{aligned} H_{m,q}(F) &= - \sum_{k=1}^q \Delta \xi_k f(\xi_k^*) \log \frac{\Delta \xi_{m,k} f(\xi_k^*)}{\Delta \xi_{m,k}} \\ &= - \sum_{k=1}^q \Delta \xi_k f(\xi_k^*) \log f(\xi_k^*) \\ &\rightarrow - \int f(x) \log f(x) dx \quad \text{as } \Delta \xi_{m,k} \rightarrow 0 \quad \forall k. \end{aligned}$$

The limit is due to the fact that since the integral (3) exists, $f(x) \log f(x)$ is Riemann integrable.

The following results are needed for proof of Theorem 1.

Lemma 2 *Let X be a random variable with Beta density*

$$g(x) = \frac{\Gamma(u+v)}{\Gamma(u)\Gamma(v)} x^{u-1} (1-x)^{v-1}, \quad 0 \leq x \leq 1, \quad u > 0, \quad v > 0.$$

Then

- (i) $E(\log X) = [\psi(u) - \psi(u+v)];$
- (ii) $E(X \log X) = \frac{u}{u+v} [\psi(u+1) - \psi(u+v+1)];$

Proof. Part (i) is well known. For (ii) note that for $\alpha = 1, 2, \dots$,

$$\begin{aligned}
E[(X \log X)^\alpha] &= \frac{\Gamma(u+v)}{\Gamma(u)\Gamma(v)} \int_0^1 (\log x)^\alpha x^{u+\alpha-1} (1-x)^{v-1} dx \\
&= \frac{\Gamma(u+v)}{\Gamma(u)\Gamma(v)} \int_0^1 \frac{\partial^\alpha}{\partial u^\alpha} [x^{u+\alpha-1} (1-x)^{v-1}] dx \\
&= \frac{\Gamma(u+v)}{\Gamma(u)\Gamma(v)} \frac{\partial^\alpha}{\partial u^\alpha} \int_0^1 x^{u+\alpha-1} (1-x)^{v-1} dx \\
&= \frac{\Gamma(u+v)}{\Gamma(u)\Gamma(v)} \frac{\partial^\alpha}{\partial u^\alpha} \left[\frac{\Gamma(u+\alpha)\Gamma(v)}{\Gamma(u+v+\alpha)} \right].
\end{aligned}$$

The result is obtained upon differentiation and simplification and letting $\alpha = 1$.

Lemma 3 Let $\mathbf{X} = (X_1, \dots, X_{q-1})'$ be a Dirichlet vector with density

$$g(\mathbf{x}|\mathbf{u}) = \frac{\Gamma\left(\sum_{k=1}^q u_k\right)}{\prod_{k=1}^q \Gamma(u_k)} \prod_{k=1}^{q-1} x_k^{u_k-1} \left\{1 - \sum_{k=1}^{q-1} x_k\right\}^{u_q-1}, \quad \sum_{k=1}^{q-1} x_k \leq 1, \quad x_k \geq 0, \quad u_k > 0, \quad k = 1, \dots, q.$$

Then

$$E_{g(\cdot|\mathbf{u})}[X_k \log T_k(\mathbf{X})] = \frac{u_k}{\sum_{k=1}^q u_k} E_{g(\cdot|\mathbf{v})}[\log T_k(\mathbf{X})],$$

where $T_k(\mathbf{X}) = \sum_{j=k-a}^{k+b} X_j$ and the expectation in the right hand side is with respect to the Dirichlet density with parameters $v_j = u_k + \delta(j=k)$, δ being the indicator function.

Proof. Since $v_j = u_k + 1$ when $j = k$ and $v_j = u_k$ for all $j \neq k$, we have $\prod_{j=1}^{q-1} x_j^{v_j-1} = x_k \prod_{j=1}^{q-1} x_j^{u_j-1}$ and $\sum_{j=1}^q v_j = 1 + \sum_{k=1}^q u_k$. By recursion of the gamma function we have,

$$\begin{aligned}
\Gamma\left(\sum_{k=1}^q v_k\right) &= \Gamma\left(1 + \sum_{k=1}^q u_k\right) = \left(\sum_{k=1}^q u_k\right) \Gamma\left(\sum_{k=1}^q u_k\right) \\
\prod_{k=1}^q \Gamma(v_k) &= u_k \prod_{j=1}^q \Gamma(u_j).
\end{aligned}$$

Using the above relations in the expectation integral gives the result.

Proof of Theorem 1.

(i) Write the quantized entropy as

$$H_{m,q}(F) = \sum_{k=1}^q \Delta F_k \log \Delta \xi_{m,k} - \sum_{k=1}^q \Delta F_k \log \Delta F_{m,k}.$$

The expected value of the first summation is obtained by noting that the increments ΔF_k , $k = 1, \dots, q$ are distributed as Beta with parameters $\tilde{\mathcal{B}}\Delta\tilde{F}_k$ and $\tilde{\mathcal{B}}(1-\Delta\tilde{F}_k)$. Thus $E(\Delta F_k) = \Delta\tilde{F}_k$.

The expected value of the second summation is obtained as follows. For $m = 0$, using part (ii) of Lemma 2 with $u = \tilde{\mathcal{B}}\Delta\tilde{F}_k$ and $v = \tilde{\mathcal{B}}(1 - \Delta\tilde{F}_k)$ gives the result. For $m \neq 0$, first use Lemma 3 with $\Delta F_{m,k} = \sum_{j=k-m+1}^{k+m} \Delta F_j = T_k(\Delta\mathbf{F})$. Then use the fact that the distribution of $T_k(\mathbf{X})$ is Beta with parameters $T_k(\mathbf{u})$ and $\sum_{k=1}^q u_k - T_k(\mathbf{u})$ and part (i) of Lemma 2. The result is obtained upon some simplifications.

(ii) Using the recursion $\psi(z+1) = \psi(z) + z^{-1}$ (Abramowitz and Stegun 1970) we can write (23) as

$$\tilde{H}_{m,q}(F) = \psi(\tilde{\mathcal{B}}) + \frac{1}{\tilde{\mathcal{B}}} - \sum_{k=1}^q \frac{\Delta\tilde{F}_k}{\tilde{\mathcal{B}}\Delta\tilde{F}_{m,k}} - \sum_{k=1}^q \Delta\tilde{F}_k [\psi(\tilde{\mathcal{B}}\Delta\tilde{F}_{m,k}) - \log \Delta\xi_{m,k}].$$

For large $\tilde{\mathcal{B}}$ the second and third terms vanish. Also for large $\tilde{\mathcal{B}}$, $\psi(\tilde{\mathcal{B}}) \approx \log \tilde{\mathcal{B}}$ (Abramowitz and Stegun 1970), so

$$\tilde{H}_{m,q}(F) \approx \log \tilde{\mathcal{B}} - \sum_{k=1}^q \Delta\tilde{F}_k (\log \tilde{\mathcal{B}} + \log \Delta\tilde{F}_{m,k} - \log \xi_{m,k}),$$

which gives the result.

Proof of Theorem 2. For large n the sample dominates the prior in (22) and $\Delta\tilde{F}_{0,k} \rightarrow \Delta\hat{F}_k$ as $n \rightarrow \infty$. Then the consistency of the histogram entropy (Hall and Morton 1993) gives the result.

Proof of Theorem 3. For large n the sample dominates the prior in (22), i.e., $\Delta\tilde{F}_{m,i} \rightarrow \Delta\hat{F}_{m,i} = (2m)/n$ as $n \rightarrow \infty$. Since $n \rightarrow \infty$ and $m/n \rightarrow 0$, we can use the approximation (24) with $\Delta\tilde{F}_{m,i} = (2m)/n$ which gives $\tilde{H}_{m,n}(F) \xrightarrow{P} H_v(m, n)$. Then the result follows from the consistency of $H_v(m, n)$; see Vasicek (1976).

Proof of Remark 1. Since for $m = 0$, $\Delta F_{m,i} = \Delta F_i$ and n is large, the approximation (24) is applicable. Then the consistency of the empirical distribution implies

$$\tilde{H}_{m,n}(F) \xrightarrow{P} H_{m,n}(F), \quad \text{as } n \rightarrow \infty.$$

Lemma 1 gives the result.

Proof of Theorem 4. Let $\xi_k = y_k$, $k = 1, \dots, q$. Then $H(\Delta\mathbf{F}) = H(f_1, \dots, f_q)$. To see that the uniform prior guess is sufficient, let $n = 0$ and $\Delta F_k^* = q^{-1}$ in (26) and obtain the prior average entropy obtained by Campbell (1995), $E[H(\Delta\mathbf{F}) | F_k^* = k/q, \mathcal{B}] = \psi(\mathcal{B} + 1) - \psi(\mathcal{B}/q + 1)$; i.e., $\rho = \mathcal{B}/q$. Also note that with the uniform best guess, $\alpha(y_k) = k\mathcal{B}/q$, thus $\alpha(y_k) - \alpha(y_{k-1}) = \mathcal{B}/q \equiv \rho$; i.e. (19) reduces to the symmetric Dirichlet prior (27). Conversely, the uniform distribution is implied by letting $\alpha(y_k) - \alpha(y_{k-1}) = \rho$ in (19) which implies that $\alpha(y_k) = k\rho$ and $\mathcal{B} = q\rho$.

Proofs of Theorem 5. As $n \rightarrow \infty$ the quantized moments approach to the sample moments. The consistency of the sample moments implies the consistency of $H(F^*|\theta_q)$. Then results follow from the uniqueness of the ME density and Theorems 2 and 3.

Proof of Remark 2. Use the same argument as proof Theorem 5.

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