Nearest neighbor Dirichlet process

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Abstract

There is a rich literature on Bayesian nonparametric methods for unknown densities. The most popular approach relies on Dirichlet process mixture models. These models characterize the unknown density as a kernel convolution with an unknown almost surely discrete mixing measure, which is given a Dirichlet process prior. Such models are very flexible and have good performance in many settings, but posterior computation relies on Markov chain Monte Carlo algorithms that can be complex and inefficient. As a simple and general alternative, we propose a class of nearest neighbor-Dirichlet processes. The approach starts by grouping the data into neighborhoods based on standard algorithms. Within each neighborhood, the density is characterized via a Bayesian parametric model, such as a Gaussian with unknown parameters. Assigning a Dirichlet prior to the weights on these local kernels, we obtain a simple pseudo-posterior for the weights and kernel parameters. A simple and embarrassingly parallel Monte Carlo algorithm is proposed to sample from the resulting pseudo-posterior for the unknown density. Desirable asymptotic properties are shown, and the methods are evaluated in simulation studies and applied to a motivating dataset in the context of classification.

1 Introduction

Bayesian nonparametric methods provide a useful alternative to black box machine learning algorithms, having clear advantages in terms of their ability to characterize uncertainty in inferences and predictions. However, computation can be slow and unwieldy to implement. Hence, it is important to develop simpler and faster Bayesian nonparametric approaches, and hybrid methods that borrow the best of both worlds. For example, if one could use the Bayesian machinery for uncertainty quantification and reduction of mean square errors through shrinkage, while incorporating algorithmic aspects of machine learning approaches,
one may be able to engineer a highly effective hybrid. The focus of this article is on proposing such an approach for density estimation, motivated by the successes and limitations of nearest neighbor algorithms and Dirichlet process mixture models.

Nearest neighbor algorithms are popular due to a combination of simplicity and performance. Given a set of \( n \) observations \( \mathcal{X}^{(n)} = (X_1, \ldots, X_n) \) in \( \mathbb{R}^p \), the density at \( x \) is estimated as \( \hat{f}_{\text{knn}}(x) = k/(nV_p R_k^p) \), where \( k \) is the number of neighbors of \( x \) in \( \mathcal{X}^{(n)} \), \( R_k = R_k(x) \) is the distance of \( x \) from its \( k \)th nearest neighbor in \( \mathcal{X}^{(n)} \) and \( V_p \) is the volume of the \( p \)-dimensional unit ball (Loftsgaarden et al., 1965; Mack & Rosenblatt, 1979). Refer to Biau & Devroye (2015) for an overview of related estimators and corresponding theory.

Alternatively, following a Bayesian nonparametric approach, one can choose a prior \( f \sim \Pi \), with \( \Pi \) chosen to have large support over a set of densities \( \mathcal{F} \). It is important for \( \Pi \) to be interpretable and computationally tractable, and Dirichlet process mixture models provide a convenient choice (Ferguson, 1973; Lo, 1984; Escobar & West, 1995):

\[
f(x) = \int \mathcal{K}(x; \theta) dP(\theta), \quad P \sim \text{DP}(\alpha P_0),
\]

where \( \mathcal{K}(x; \theta) \) is a parametric density with parameters \( \theta \), and the mixing measure \( P \) is assigned a Dirichlet process prior with precision \( \alpha \) and base probability measure \( P_0 \). Under the stick-breaking representation (Sethuraman, 1994), (1) can be equivalently represented as

\[
f(x) = \sum_{h=1}^{\infty} \pi_h \mathcal{K}(x; \theta_h), \quad \theta_h \sim P_0, \quad (\pi_h)_{h=1}^{\infty} \sim \text{Stick}(\alpha),
\]

which corresponds to a discrete mixture. There are a rich variety of Markov chain Monte Carlo algorithms for posterior computation under (2) (Neal, 2000; Papaspiliopoulos & Roberts, 2008; Jain & Neal, 2004; Ishwaran & James, 2001), and a rich literature on frequentist asymptotic properties (Ghosal et al., 1999, 2007, 2001; Walker et al., 2007; Shen et al., 2013).

A disadvantage of (2) is inefficient posterior computation, particularly as \( n \) increases. This has motivated a literature on faster approaches, including sequential approximations (Wang & Dunson, 2011; Zhang et al., 2014) and variational Bayes (Blei & Jordan, 2006). These methods are order dependent, tend to converge to local modes, and/or lack theory support. Newton & Zhang (1999); Newton (2002) instead rely on predictive recursion. Such estimators are fast to compute and have theory support, but are also order dependent and do not provide a characterization of uncertainty. Alternatively, one can use a Polya tree as a conjugate prior (Lavine et al., 1992, 1994), and there is a rich literature on related multiscale and recursive partitioning approaches, such as the optional Polya tree (Wong & Ma, 2010). However, Polya trees have disadvantages in terms of sensitivity to a base partition and a tendency to favor spiky/erratic densities. These disadvantages are inherited by most of the computationally fast modifications.
Our proposed nearest neighbor-Dirichlet process has substantial advantages over current competitors. The basic idea is to rely on fast nearest neighbor search algorithms to group the data into local neighborhoods, and then condition on these neighborhoods in defining a Bayesian mixture model-based approach.

2 Methodology

2.1 Nearest neighbor Dirichlet process framework

Let $d(x_1, x_2)$ denote a distance metric between data points $x_1, x_2 \in \mathcal{X}$. For $\mathcal{X} = \mathbb{R}^p$, the Euclidean distance is typically chosen. For each $i \in \{1, 2, \ldots, n\}$, let $X_{i[j]}$ denote the $j$th nearest neighbor to $X_i$ in the data $\mathcal{X}^{(n)} = (X_1, \ldots, X_n)$, such that $d(X_i, X_{i[1]}) \leq \ldots \leq d(X_i, X_{i[n]})$, with ties broken by increasing order of indices. The indices on the $k$ nearest neighbors to $X_i$ are denoted as $N_i = \{j : d(X_i, X_j) \leq d(X_i, X_{i[k]})\}$, where by convention we define $X_{i[1]} = X_i$, for $i = 1, \ldots, n$.

Fix $x \in \mathcal{X}$. We model the density of the data within the $i$th neighborhood using

$$f_i(x) = \mathcal{K}(x; \theta_i), \quad \theta_i \sim P_0,$$

where $\theta_i$ are parameters specific to neighborhood $i$ that are given a common prior distribution $P_0$. The resulting posterior distribution of $\theta_i$ given data $\mathcal{X}^{(n)}$ and prior $P_0$ is

$$(\theta_i | \mathcal{X}^{(n)}, P_0) \sim P_0(\theta_i) \prod_{j \in N_i} \mathcal{K}(X_j; \theta_i).$$

This posterior is in a simple analytic form if $P_0$ is conjugate to $\mathcal{K}(x; \theta)$. The prior $P_0$ can involve unknown parameters and borrows information across neighborhoods; this reduces the large variance problem common to nearest neighbor estimators. Refer to the examples later in the paper.

To combine the $f_i(x)$s into a single global $f(x)$, similarly to equations (1)-(2), we let

$$f(x) = \sum_{i=1}^{n} \pi_i \mathcal{K}(x; \theta_i), \quad \pi = (\pi_i)_{i=1}^{n} \sim \text{Dirichlet} (\alpha, \ldots, \alpha), \quad \theta_i \sim P_0.$$

Here, there are two main differences with Dirichlet process mixture models. First, we use $k$-nearest neighbors to allocate data to local neighborhoods instead of allowing that allocation to be unknown. Second, we use an $n$-dimensional symmetric Dirichlet density for the weights instead of a stick-breaking process; it is common to approximate (2) using a finite Dirichlet motivated by the result of Ishwaran & Zarepour (2002).

In usual mixture models that choose a Dirichlet prior for the weights $\pi$, one obtains a conjugate conditional posterior for $\pi$ given latent variables indexing which component each data point is drawn from. Such conjugacy leads to a straightforward data augmentation.
Gibbs sampler, providing a routine approach for posterior computation in mixture models. Unfortunately, this and other samplers that rely on updating the allocation of data points to components tend to have famously poor performance as \( n \) increases. In our proposed approach, we avoid the need for Markov chain Monte Carlo by using nearest neighbor algorithms to allocate samples to clusters, defining a pseudo-posterior conditionally on the neighborhood structure.

Since the neighborhoods are overlapping, the conditional posterior for \( \pi \) under (5) is not exactly Dirichlet. However, since the radius of each neighborhood approaches zero as \( n \) increases (Biau & Devroye, 2015, Chapter 2), overlap becomes more and more minor, motivating the pseudo-posterior:

\[
(\pi \mid \mathcal{X}^{(n)}) \sim \text{Dirichlet}(\alpha + 1, \ldots, \alpha + 1). \tag{6}
\]

This distribution is centered on \((1/n, \ldots, 1/n)\) with concentration parameter \( n(\alpha + 1) \). In practice, \( \alpha \) is typically chosen to be close to zero and we let \( k = k_n \) increase slowly with the sample size. Section 3 provides a theoretical justification for this choice of pseudo-posterior.

Based on equations (3)-(6), our nearest neighbor-Dirichlet process produces a pseudo-posterior distribution for the unknown density \( f(x) \) through simple distributions for the parameters characterizing the density within each neighborhood and for the weights. To generate independent Monte Carlo samples from the pseudo-posterior for \( f \), one can simply draw samples from (4) and (6) independently and plug these samples into (5). Although this is not exactly a coherent fully Bayesian posterior distribution, we claim that it can be used as a simple alternative to such a posterior in practice. This claim is backed up by theoretical arguments, simulation studies and a real data application in the sequel.

### 2.2 Illustration with Gaussian kernels

Suppose we have independent and identically distributed observations \( \mathcal{X}^{(n)} \) from the density \( f \), where \( X_i \in \mathbb{R}^p \) for \( i = 1, \ldots, n \) and \( f \) is an unknown density function with respect to the Lebesgue measure on \( \mathbb{R}^p \) for \( p \geq 1 \). Let \( \mathbb{R}^{p \times p}_+ \) denote the set of all real-valued \( p \times p \) positive definite matrices. Fix \( x \in \mathbb{R}^p \). We will illustrate the method for a general \( p \geq 1 \) and note key changes for the special case \( p = 1 \). We proceed by setting \( \mathcal{K}(x; \theta) \) to be the multivariate Gaussian density \( \phi_p(x; \eta, \Sigma) = (2\pi)^{-p/2} \mid \Sigma \mid^{-1/2} \exp \left\{ -\frac{(x - \eta)^T \Sigma^{-1} (x - \eta)}{2} \right\} \), where \( \theta = (\eta, \Sigma), \eta \in \mathbb{R}^p \) and \( \Sigma \in \mathbb{R}^{p \times p}_+ \). We first compute the neighborhoods \( \mathcal{N}_i \) corresponding to \( X_i \) as in Section 2.1 and place a normal-inverse Wishart prior on \( \eta_i \mid \Sigma_i \sim N(\mu_0, \Sigma_i/\nu_0) \) independently for \( i = 1, \ldots, n \). That is, \( \eta_i \mid \Sigma_i \sim \mathcal{N}(\mu_0, \Sigma_i/\nu_0) \) and \( \Sigma_i \sim \mathcal{IW}(\gamma_0, \Psi_0) \) with \( \mu_0 \in \mathbb{R}^p, \nu_0 > 0, \gamma_0 > p - 1 \) and \( \Psi_0 \in \mathbb{R}^{p \times p}_+ \); for details about parametrization see Section S.9 of the Supplementary Material.

For \( p = 1 \), we have a univariate Gaussian density \( \phi(x; \eta_i, \sigma_i^2) \) in neighborhood \( i \) with normal-inverse gamma priors \( (\eta_i, \sigma_i^2) \sim \mathcal{NIG}(\mu_0, \sigma_i^2/\nu_0, \gamma_0/2, \gamma_0\delta_0^2/2) \) independently for \( i = \ldots, n \).
1, \ldots, n, with \( \mu_0 \in \mathbb{R} \) and \( \nu_0, \gamma_0, \delta_0^2 > 0 \). That is, \( \eta_i \mid \sigma_i^2 \sim N(\mu_0, \sigma_i^2/\nu_0) \) and \( \sigma_i^2 \sim IG(\gamma_0/2, \gamma_0\delta_0^2/2) \). When \( p = 1 \), the IW\(_p(\gamma_0, \Psi_0)\) density simplifies to an IG(\(\gamma_0/2, \gamma_0\delta_0^2/2\)) density with \( \delta_0^2 = \Psi_0/\gamma_0 \).

Monte Carlo samples from the pseudo-posterior of \( f(x) \) given the data \( X^{(n)} \) can be obtained using Algorithm 1. The corresponding steps for the univariate case are provided in Section S.8 of the Supplementary Material.

- **Step 1:** Compute the neighborhood \( N_i \) for data point \( X_i \in \mathbb{R}^p \) according to distance \( d(\cdot, \cdot) \) with \( (k - 1) \) nearest neighbors.
- **Step 2:** Update the parameters for neighborhood \( N_i \) to \((\mu_n^{(i)}, \nu_n, \gamma_n, \Psi_n^{(i)})\), where \( \nu_n = \nu_0 + k \), \( \gamma_n = \gamma_0 + k \), \( \mu_n^{(i)} = \nu_0\nu_n^{-1}\mu_0 + k\nu_n^{-1}\bar{X}_i \), \( \bar{X}_i = k^{-1}\sum_{j \in N_i} X_j \) and \( \Psi_n^{(i)} = \Psi_0 + \sum_{j \in N_i}(X_j - \bar{X}_i)(X_j - \bar{X}_i)^\top + k\nu_0\nu_n^{-1}(\bar{X}_i - \mu_0)(\bar{X}_i - \mu_0)^\top \).
- **Step 3:** To compute the \( t \)th Monte Carlo sample \( f^{(t)}(x) \) of \( f(x) \), sample Dirichlet weights \( \pi^{(t)} \sim \text{Dirichlet}(\alpha + 1, \ldots, \alpha + 1) \) and neighborhood specific parameters \((\eta_i^{(t)}, \Sigma_i^{(t)}) \sim \text{NIW}_p(\mu_n^{(i)}, \Sigma_n^{(i)}/\nu_n, \gamma_n, \Psi_n^{(i)})\), independently for \( i = 1, \ldots, n \), and set

\[
f^{(t)}(x) = \sum_{i=1}^n \pi_i^{(t)} \phi_p(x; \eta_i^{(t)}, \Sigma_i^{(t)}).
\]

**Algorithm 1:** Nearest neighbor-Dirichlet process algorithm to obtain Monte Carlo samples from the pseudo-posterior of \( f(x) \) given multivariate data \( X^{(n)} \) with Gaussian kernel and normal-inverse Wishart prior.

Although the pseudo-posterior distribution of \( f(x) \) lacks an analytic form, we can obtain a simple form for its pseudo-posterior mean by integrating over the pseudo-posterior distribution of \((\theta_i)_{i=1}^n\) and \( \pi \). Recall the definitions of \( \mu_n^{(i)} \) and \( \Psi_n^{(i)} \) from Step 2 of Algorithm 1 and define \( \Lambda_n^{(i)} = \{\nu_n(\gamma_n - p + 1)\}^{-1}(\nu_n + 1) \Psi_n^{(i)} \). Then the pseudo-posterior mean of \( f(x) \) is given by

\[
\hat{f}_n(x) = \frac{1}{n} \sum_{i=1}^n t_{\gamma_n-p+1}(x; \mu_n^{(i)}, \Lambda_n^{(i)}).
\]

Here \( t_{\gamma}(x; \mu, \Lambda) = [\Gamma((\gamma+p)/2)/\Gamma(\gamma/2)](\gamma\pi)^{-\gamma/2} |\Lambda|^{-1/2} [1+(x-\mu)^\top(\gamma\Lambda)^{-1}(x-\mu)]^{-(\gamma+p)/2} \) for \( x \in \mathbb{R}^p \) is the \( p \)-dimensional Student’s t-density with degrees of freedom \( \gamma > 0 \), location \( \mu \in \mathbb{R}^p \) and \( \Lambda \in \mathbb{R}_+^{p \times p} \). For the univariate case, we have \( \gamma_n \) and \( \nu_n \) as in Algorithm 1. The pseudo-posterior mean of \( f(x) \) is given by

\[
\hat{f}_n(x) = \frac{1}{n} \sum_{i=1}^n \frac{1}{\lambda_n^{(i)}} t_{\gamma_n}\left(\frac{x - \mu_n^{(i)}}{\lambda_n^{(i)}}\right),
\]

where \( \mu_n^{(i)} = \nu_0\nu_n^{-1}\mu_0 + k\nu_n^{-1}\bar{X}_i \), \( \bar{X}_i = k^{-1}\sum_{j \in N_i} X_j \), \( \lambda_n^{(i)} = \delta_n^{(i)} (\nu_n + 1)/\nu_n, \sigma_n^{(i)} = \)
\[ \gamma_n^{-1}\{\gamma_0\delta_0^2 + \sum_{j \in \mathcal{N}_i}(X_j - \bar{X}_i)^2 + k\nu_0\nu_n^{-1}(\mu_0 - \bar{X}_i)^2\} \]. Here \( t_{\gamma_n}(. \cdot) \) represents the univariate Student's t-density with \( \gamma_n \) degrees of freedom.

### 2.3 Cross validation for hyperparameter choice

The hyperparameters in the prior for the neighborhood-specific parameters need to be chosen carefully - we found results to be sensitive to \( \gamma_0 \) and \( \Psi_0 \). If non-informative values are chosen for these key hyperparameters, we tend to inherit problems of typical nearest neighbor estimators including lack of smoothness and high variance. Suppose \( \Sigma \sim \text{IW}_p(\gamma_0, \Psi_0) \) and for \( i, j = 1, \ldots, p \), let \( \Sigma_{ij} \) and \( \Psi_{0,ij} \) denote the \( i, j \)th entry of \( \Sigma \) and \( \Psi_0 \), respectively. Then \( \Sigma_{jj} \sim \text{IG}(\gamma_* / 2, \Psi_{0, jj} / 2) \) where \( \gamma_* = \gamma_0 - p + 1 \). Thus borrowing from the univariate case, we set \( \Psi_{0, jj} = \gamma_*\delta_0^2 \) and \( \Psi_{0, ij} = 0 \) for all \( i \neq j \), which implies that \( \Psi_0 = (\gamma_*\delta_0^2)I_p \) and we use leave-one-out cross validation to select the optimum \( \delta_0^2 \). With \( p \) dimensional data, we recommend fixing \( \gamma_0 = p \) which implies a multivariate Cauchy prior predictive density. We choose the leave-one-out log likelihood as the criterion function for cross-validation, which is closely related to minimizing the Kullback-Leibler divergence between the true and estimated density (Hall et al., 1987; Bowman, 1984). The explicit expression for the pseudo-posterior mean in equations (8) and (9) makes cross-validation computationally efficient. A description of a fast implementation is provided in Section S.7 of the Supplementary Material.

### 3 Theory

#### 3.1 Asymptotic properties

There is a rich literature on asymptotic properties of the exact posterior for an unknown density under Dirichlet process mixtures; refer, for example to Ghosal et al. (1999), Ghosal et al. (2007). Unfortunately, the tools used for studying frequentist asymptotic properties of Bayesian posteriors do not apply to the pseudo-posterior produced by the nearest neighbor-Dirichlet process. Instead, we focus on analyzing the pseudo-posterior mean and variance at a fixed test point \( x \). The key idea behind our proofs is to show that the pseudo-posterior mean is asymptotically close to a kernel density estimator with suitably chosen bandwidth. We then leverage on existing arguments establishing consistency of kernel density estimators. To accomplish this, we carry out a detailed study of the neighborhood specific parameters \( \mu_n^{(i)} \) and \( \lambda_n^{(i)} \) which are closely related to the neighborhood mean and variance, respectively.

We first consider the univariate case with Gaussian kernel. Consider independent and identically distributed data \( \mathcal{X}^{(n)} \) from a fixed unknown density \( f_0 \) on \( \mathbb{R} \) with the Euclidean metric, inducing the measure \( P_{f_0} \) on \( \mathcal{B}(\mathbb{R}) \). Hereby, we will use \( E\{f(x) \mid \mathcal{X}^{(n)}\} \), \( \text{var}\{f(x) \mid \mathcal{X}^{(n)}\} \) and \( \text{pr}\{f(x) \in B \mid \mathcal{X}^{(n)}\} \) to denote the mean of \( f(x) \), variance of \( f(x) \) and probability of the event \( \{f(x) \in B\} \) for \( B \in \mathcal{B}(\mathbb{R}) \), respectively, under the pseudo-posterior distribution.
of \( f(x) \) implied by equations (3)-(6). We make the following regularity assumptions on \( f_0 \):

**Assumption 3.1** (Support). \( f_0(x) > 0 \) for all \( x \in [0,1] \) and \( \int_{[0,1]} f_0(x) \, dx = 1 \).

**Assumption 3.2** (Continuity). \( f_0 \) is continuous on \([0,1]\).

**Assumption 3.3** (Bounded curvature). \(| f''_0(x) | \leq L \) for all \( x \in (0,1) \) and some finite \( L \geq 0 \).

Such assumptions are common in the nearest neighbor literature (Evans et al., 2002). Assumption 3.3 ensures that the first derivative \( f'_0(\cdot) \) is also bounded on \((0,1)\), and Assumptions 3.1 and 3.2 imply that there exist positive constants \( l_1 \) and \( l_2 \) such that for all \( x \in [0,1] \),

\[
0 < l_1 \leq f_0(x) \leq l_2 < \infty. \tag{10}
\]

Recall the definition of \( \mu^{(i)}_n \) and \( \lambda^{(i)}_n \) from equation (9) for \( i = 1, \ldots, n \). Define \( h_n \) by

\[
h_n = (\nu_n + 1)^{1/2}(\nu_n \gamma_n)^{-1/2} (\gamma_0 \delta_0^2)^{1/2}. \]

For ease of exposition, we suppress the dependence of \( \mu^{(i)}_n \), \( \lambda^{(i)}_n \) and \( h_n \) on the sample size \( n \) and instead write \( \mu_i \), \( \lambda_i \) and \( h \), respectively. From the definition of \( \lambda_i \) it is immediate that \( \lambda_i \geq h \) for all \( i = 1, \ldots, n \). It also follows that \( (\lambda_i)_{i=1}^n \) are identically distributed under \( P_{f_0} \) and so are \( (\mu_i)_{i=1}^n \). We then have the following result.

**Lemma 3.4.** Define \( \xi_1(f_0) = \int_0^1 [f'_0(y)/\{12 f_{x_0}^2(y)\}] \, dy \) and \( \xi_2(f_0) = \int_0^1 \{12 f_0(y)\}^{-1} \, dy \) and let \( \nu_0 = o(n^{-2}k^3) \). Then for sufficiently large \( n \), we have

\[
E_{P_{f_0}}(| \mu_1 - X_1 |) \leq \xi_1(f_0) \frac{k^2}{n^2} + o\left( \frac{k^2}{n^2} \right), \quad E_{P_{f_0}}(\lambda_1^2 - h^2) \leq \xi_2(f_0) \frac{k^2}{n^2} + o\left( \frac{k^2}{n^2} \right). \tag{11}
\]

The proof of Lemma 3.4 is provided in Section S.2 of the Supplementary Material. Equation (10) ensures that the quantities \( \xi_1(f_0) \) and \( \xi_2(f_0) \) in Lemma 3.4 are finite. Using Lemma 3.4 we approximate (9) by a kernel density estimator \( f_K(x) = (nh)^{-1} \sum_{i=1}^n t_{n_i} (h^{-1}(x - X_i)) \).

Weak consistency of this estimator is established in Lemma S.3.1 of the Supplementary Material. We are now ready to state a theorem on weak consistency of the pseudo-posterior mean \( E\{f(x) \mid X(n)\} = \hat{f}_n(x) \).

**Theorem 3.5.** Fix \( x \in \mathbb{R}, x \notin \{0,1\} \). Suppose \( k_n = k \to \infty \) with \( n^{-4/9}k \to 0 \) and \( \nu_0 = o(n^{-2}k^3) \) as \( n \to \infty \). Then, \( \hat{f}_n(x) \to f_0(x) \) in \( P_{f_0} \)-probability under Assumptions 3.1-3.3.

The proof of Theorem 3.5 is provided in the Appendix. We now look at the pseudo-posterior variance of \( f(x) \). In equation (6), we let \( \omega = \alpha + 1 \). Define \( r_n = \{2\pi^{1/2}(\gamma_n + 1)^{1/2}\Gamma(\gamma_n/2)\}^{-1} \{1 + (2/\nu_n)\}^{-1/2} \) and \( D_n = \{(\gamma_n + 1)(\nu_n + 1)\}^{-1/2} \). For \( i = 1, \ldots, n \), let \( b_i = \lambda_i(D_n/2)^{1/2} \) and define \( \tilde{f}_1(x) = (1/n) \sum_{i=1}^n b_i^{-1} t_{n+1} \{b_i^{-1}(x - \mu_i)\} \). As \( n \to \infty \), analogous steps to the ones used in the proof of Theorem 3.5 can be used to imply that \( \tilde{f}_1(x) \to f_0(x) \) in \( P_{f_0} \)-probability. Also, \( r_n \to (8\pi)^{-1/2} \) by Stirling’s approximation and \( D_n \to 1 \) as \( n \to \infty \). Finally, let \( a_n = a_n(x) = \{(2/D_n)^{1/2} r_n\} \tilde{f}_1(x) \). We now provide an upper bound on the pseudo-posterior variance of \( f(x) \).
Lemma 3.6. Under Assumptions 3.1-3.3 with $x, k$ and $\nu_0$ as in Theorem 3.5, we have
\[
\text{var}\{f(x) \mid \mathcal{X}(\alpha)\} \leq a_n \left\{ \frac{1}{(n\omega + 1)h} + \frac{1}{nh} \right\}.
\] (12)

The proof of Lemma 3.6 is provided in Section S.4 of the Supplementary Material. Since $\hat{f}_1(x) \to f_0(x)$ in $P_{f_0}$-probability under the conditions of Theorem 3.5, we have $a_n \to (2\pi^{1/2})^{-1} f_0(x)$ in $P_{f_0}$-probability as $n \to \infty$. Combining this with Lemma 3.6 and the fact that $nh \to \infty$ as $n \to \infty$, we have the following result for the pseudo-posterior variance of $f(x)$.

Theorem 3.7. Under the conditions of Lemma 3.6, $\text{var}\{f(x) \mid \mathcal{X}(\alpha)\} \to 0$ in $P_{f_0}$-probability as $n \to \infty$.

Fix $\epsilon > 0$ and consider the $\epsilon$-ball $U_\epsilon = \{y_\ast : |y_\ast - f_0(x)| \leq \epsilon\}$. Then by Chebychev’s inequality, we have $\text{pr}(f(x) \in U_\epsilon \mid \mathcal{X}(\alpha)) \leq \frac{\text{var}\{f(x) \mid \mathcal{X}(\alpha)\}}{\epsilon^2} \to 0$ in $P_{f_0}$-probability, using Theorems 3.5 and 3.7. This implies concentration of the pseudo-posterior measure of $f(x)$ around the true value $f_0(x)$.

Theorem 3.8. Let Assumptions 3.1-3.3 be satisfied with $x, k$ and $\nu_0$ as in Theorem 3.5. Fix $\epsilon > 0$ and define the $\epsilon$-ball around $f_0(x)$ by $U_\epsilon = \{y_\ast : |y_\ast - f_0(x)| \leq \epsilon\}$. Then, $\text{pr}(f(x) \in U_\epsilon \mid \mathcal{X}(\alpha)) \to 0$ in $P_{f_0}$-probability as $n \to \infty$.

Related results in the general $p$ multivariate case are provided in Section S.6 of the Supplementary Material.

3.2 Choice of Dirichlet prior parameter

Although Theorem 3.8 implies consistency of the pseudo-posterior for fixed $x$ and any $\omega = \alpha + 1$, the choice of $\alpha$ impacts frequentist coverage of the pseudo-posterior credible intervals as it directly influences the pseudo-posterior variance of $f(x)$ through Lemma 3.6. We now describe a data-dependent method to choose $\alpha$ using Bernstein-von Mises results for linear functionals of Bayesian density estimators in the univariate setup (Rivoirard et al., 2012).

Suppose $f$ is a density on $\mathbb{R}$ and we define the linear functional $\mathcal{P}(f) = \int \tilde{p}(u) f(u) \, du$ where $\tilde{p}(\cdot)$ satisfies conditions in Rivoirard et al. (2012). Suppose $X_1, \ldots, X_n$ are independent and identically distributed data from a compactly supported density $f_0$ with cumulative distribution function $F_0$. Define $q(u) = \tilde{p}(u) - \int \tilde{p}(v) f_0(v) \, dv$ and let $\mathcal{F}_n$ be the empirical distribution function of $X_1, \ldots, X_n$. Then under a suitable prior distribution of $f(\cdot)$, Rivoirard et al. (2012) show that the centered posterior distribution of $n^{1/2} \{\mathcal{P}(f) - \mathcal{P}(\mathcal{F}_n)\}$ with $\mathcal{P}(\mathcal{F}_n) = n^{-1} \sum_{i=1}^n \tilde{p}(X_i)$ behaves asymptotically like a Gaussian distribution with mean 0 and variance $\Omega = \int q^2(x) f_0(x) \, dx$. When $\tilde{p}(u) = u$, we have $\Omega = \int (u - m_{f_0})^2 f_0(u) \, du = \sigma_{f_0}^2$, where $m_{f_0}$ is the mean of $f_0$.
where \( m_{f_0} = \int u f_0(u) \, du \) and \( \sigma^2_{f_0} \) is the population variance of \( f_0 \). Setting \( \bar{p}(u) = u \), our strategy for finding a value of \( \alpha \) when \( f \) has the nearest neighbor-Dirichlet process formulation involves equating the pseudo-posterior variance of \( n^{1/2}P(f) \) with \( \sigma^2_{f_0} \) and letting \( n \to \infty \). The variance of \( n^{1/2}P(f) = n^{1/2} \int u f(u) \, du \) is provided below.

**Theorem 3.9.** Suppose \( f_0 \) satisfies Assumptions 3.1-3.3, \( f \) has the nearest neighbor-Dirichlet process formulation, and \( k, \nu_0 \) are chosen as in Theorem 3.5. Let \( \Theta = \int u f(u) \, du = \sum_{i=1}^{n} \pi_i \eta_i \) as in Section 2.2. For \( \gamma_n > 2 \), define \( v_i = \{(\nu_n + 1)(\gamma_n - 2)\}^{-1} \gamma_n \lambda_i^2 \) for \( i = 1, \ldots, n \), \( \bar{v} = n^{-1} \sum_{i=1}^{n} v_i \), \( \bar{\mu} = n^{-1} \sum_{i=1}^{n} \mu_i \) and \( S^2_\mu = n^{-1} \sum_{i=1}^{n} (\mu_i - \bar{\mu})^2 \). Then \( \text{var}(n^{1/2} \Theta \mid X^{(n)}) = \bar{v} + ((n\omega + 1)^{-1} n S^2_\mu + (n-1)\bar{v}) \).

Equating the above with \( \sigma^2_{f_0} \) and letting \( n \to \infty \), we get the following choice of \( \alpha \) given by:

\[
\alpha = \frac{\gamma_n \sigma^2_0}{\sigma^2_{f_0} \gamma_n \nu_n}. \tag{13}
\]

The proof of Theorem 3.9 and derivation of equation (13) are in Section S.5 of the Supplementary Material. Let \( H_n \) be the \( p \times p \) matrix given by \( H_n = \{\nu_n (\gamma_n - p + 1)\}^{-1} \{\nu_n + 1)(\gamma_n - p + 1)\sigma^2_0\} I_p \) and \( \Sigma_{f_0} \) be the unknown population covariance matrix of \( f_0 \). Then, a natural extension of equation (13) to the multivariate scenario is \( \alpha = \nu_n^{-1} \mid H_n \Sigma_{f_0}^{-1} \mid \). Once \( \sigma^2_0 \) is estimated according to Section 2.3 and the underlying population variance is estimated, one can use equation (13) or its multivariate analogue to select an appropriate value of \( \alpha \).

### 4 Simulation experiments

#### 4.1 Preliminaries

In this section, we compare the performance of the proposed density estimator with the frequentist kernel density estimator and the Dirichlet process mixture through several numerical experiments. Specifically, we will compare the pseudo-posterior mean \( \hat{f}_0 \) with the frequentist kernel density estimator \( \hat{f}_{\text{KDE}} \) and the posterior mean \( \hat{f}_{\text{DP}} \) of the Dirichlet process mixture model. We evaluate performance based on the expected \( L_1 \) distance (Devroye & Gyorfi, 1985). For the pair \( (f_0, \hat{f}) \), where \( f_0 \) is the true data generating density and \( \hat{f} \) is an estimator, the expected \( L_1 \) distance is defined as \( L_1(f_0, \hat{f}) = E_{P_{f_0}} \{ \int \mid f_0(x) - \hat{f}(x) \mid \, dx \} \). Given a sample size \( n \), we compute an estimate \( \hat{L}_1(f_0, \hat{f}) \) of \( L_1(f_0, \hat{f}) \) in two steps. First, we sample \( X_1, \ldots, X_n \sim f_0 \) and obtain \( \hat{f} \) based on this sample, and then further sample \( n_t \) independent test points \( X_{n+1}, \ldots, X_{n+n_t} \sim f_0 \) and compute \( \hat{L} = n_t^{-1} \sum_{i=1}^{n_t} \mid 1 - \{ \hat{f}(X_{n+i}) / f_0(X_{n+i}) \} \mid \). In the second step, to approximate the expectation with respect to \( P_{f_0} \), the first step is repeated \( R \) times. Letting \( \hat{L}_r \) denote the estimate for the \( r \)th replicate, we compute the final estimate as \( \hat{L}_1(f_0, \hat{f}) = R^{-1} \sum_{r=1}^{R} \hat{L}_r \). Then, it follows that \( \hat{L}_1(f_0, \hat{f}) \to L_1(f_0, \hat{f}) \) as \( n_t, R \to \infty \), by the law of large numbers. In our experiments, we set \( n_t = 500 \) and \( R = 20 \).
All simulations were carried out using the R programming language (R Core Team, 2018). For Dirichlet process mixture models, we collect 1,000 Markov chain Monte Carlo samples after discarding a burn-in of 1,500 samples using the package dirichletprocess (J. Ross & Markwick, 2019) with default choices of prior hyperparameters. For the nearest neighbor-Dirichlet process, 1,000 Monte Carlo samples are taken. For the kernel density estimator, we select the bandwidth by the default plug-in method hpi for univariate cases and Hpi for multivariate cases (Sheather & Jones, 1991; Wand & Jones, 1994) using the package ks (Duong, 2020). We denote the nearest neighbor-Dirichlet process, Dirichlet process mixture and the kernel density estimator by NN-DP, DP and KDE, respectively, in tables and figures.

4.2 Univariate cases

We set \( n = 200, 500 \) with \( k_n = \lceil n^{1/3} \rceil + 1 \) where \( \lceil n_0 \rceil \) denotes the greatest integer less than or equal to \( n_0 \). We consider 10 choices of \( f_0 \) from the R package benchden; the specific choices are double exponential (DE), logistic (LO), Cauchy (CA), symmetric Pareto (SP), Gaussian (GS), lognormal (LN), inverse exponential (IE), skewed bimodal (SB), claw (CW) and sawtooth (ST) with default choices of the corresponding parameters. The prior hyperparameter choices for our experiments are \( \mu_0 = 0, \nu_0 = 0.001, \gamma_0 = 1; \delta_0^2 \) is chosen via the cross-validation algorithm of Section 2.3. The results are summarized in Table 1.

In general, kernel density estimates struggle when data are generated from a heavy-tailed distribution so much that we have to omit results for some of the cases in Table 1. For instance, when \( n = 500 \) and \( f_0 \) is the standard Cauchy (CA) density, the estimated \( L_1 \) error we obtain is 38501.85. For very spiky multi-modal densities, such as the claw (CW) and sawtooth (ST), both the Dirichlet process mixture and the kernel density estimator struggle. The pseudo-posterior mean \( \hat{f}_n \) performs very well across all the settings considered in Table 1, seemingly achieving the best of both worlds; comparable with the Dirichlet process mixture for heavy-tailed densities and with the kernel density estimator for smooth densities. Moreover, it exhibits superior performance to both competitors in very spiky multi-modal cases.

In Figure 1, we show the performance of the proposed pseudo-posterior mean estimate \( \hat{f}_n \) along with the posterior mean under a Dirichlet process mixture model with 500 samples generated from the sawtooth (ST) density. The Dirichlet process mixture is unable to detect the multiple spikes, merging adjacent modes to form larger clusters, perhaps due to inadequate mixing of the Markov chain Monte Carlo sampler or to the Gaussian kernels used in the mixture. The nearest neighbor-Dirichlet process has dramatically better performance. We also compare the performance of the two methods with a smoother test density in Figure 2, where the data are generated from a skewed bimodal (SB) distribution. Both the estimates are comparable, but the nearest-neighbor Dirichlet process provides better uncertainty quantification. Similar results are obtained for \( n = 1,000 \), and hence are omitted.
Table 1: Comparison of the three methods in terms of the expected $L_1$ distance in the univariate case. Number of test points and replications considered are $n_t = 500$ and $R = 20$

| Sample size | Estimator | DE | LO | CA | SP | GS | LN | IE | SB | CW | ST |
|-------------|------------|----|----|----|----|----|----|----|----|----|----|
| 200         | NN-DP      | 0.19 | 0.13 | 0.22 | 0.33 | 0.12 | 0.20 | 0.39 | 0.17 | 0.32 | 0.31 |
|             | DP         | 0.16 | 0.13 | 0.19 | 0.27 | 0.10 | 0.22 | 0.36 | 0.23 | 0.37 | 0.56 |
|             | KDE        | 0.16 | 0.11 | -    | -    | 0.12 | 0.18 | -   | 0.18 | 0.37 | 0.52 |
| 500         | NN-DP      | 0.13 | 0.10 | 0.16 | 0.25 | 0.08 | 0.17 | 0.31 | 0.11 | 0.18 | 0.21 |
|             | DP         | 0.12 | 0.09 | 0.12 | 0.22 | 0.08 | 0.19 | 0.27 | 0.13 | 0.35 | 0.53 |
|             | KDE        | 0.11 | 0.08 | -    | -    | 0.08 | 0.15 | -   | 0.11 | 0.32 | 0.51 |

Figure 1: Plot comparing density estimates for nearest neighbor-Dirichlet process and Dirichlet process mixtures for data of sample size $n = 500$ generated from the Sawtooth (ST) density. Shaded regions correspond to 95% (pseudo) posterior credible intervals.

4.3 Multivariate cases

For the multivariate cases, we consider $n = 200$ and 1,000. The number of neighbors is set to $k = 10$ and the dimension $p$ is chosen from $\{2, 3, 4, 6\}$. Recall the definition of $\phi_p(x; \mu, \Sigma)$ from Section 2.2 and let $\Phi(x)$ be the cumulative distribution function of the standard Gaussian density. Let $0_p$ and $1_p$ denote the vector of all 0s and 1s in $\mathbb{R}^p$ for $p \geq 1$, respectively. We now describe the test cases. (1) Mixture of Gaussians (MG): $f_0(x) = 0.4 \phi_p(x; m_1, S_0) + 0.6 \phi_p(x; m_2, S_0)$, where $m_1 = -2 \times 1_p, m_2 = 2 \times 1_p$ and the matrix $S_0 = \rho 1_p 1_p^T + (1 - \rho) I_p$ with $\rho = 0.8$. (2) Skew normal (SN): $f_0(x) = 2\phi_p(x; m_0, S_0)\Phi\{s_0^T W^{-1}(x - m_0)\}$ (Azzalini, 2005), where $W$ is the diagonal matrix with diagonal entries $W_{ii}^2 = S_{0,ii}$ for $i = 1, \ldots, p$. We choose $m_0 = 0_p$ and the skewness parameter vector $s_0 = 0.5 \times 1_p$. $S_0$ is as defined
Figure 2: Similar to Figure 1, with data of sample size $n = 500$ generated from the skewed bimodal (SB) density.

above. (3) **Multivariate t-distribution (T):** $f_0(x) = t_{d_0}(x; m_*, S_0)$ is the density of the $p$-dimensional multivariate Student’s t-distribution as in Section 2.2. We set $d_0 = 10$, $m_* = 1_p$ and $S_0$ as before. (4) **Mixture of multivariate skew t-distributions (MST):** We consider a two component mixture of the multivariate skew t-distribution (Azzalini, 2005) given by $f_0(x) = 0.25 t_{d_0}(x; m_1, S_0, s_0) + 0.75 t_{d_0}(x; m_2, S_0, s_0)$. Here, $t_d(\cdot; \mu, S, s)$ is the skew t-density with parameters $d, \mu, S, s$ as in Azzalini (2005), with $d_0, s_0, S_0$ are as defined before and $m_1, m_2$ the same as in the first case. The hyperparameters for the nearest neighbor-Dirichlet process are chosen as $\mu_0 = 0_p, \nu_0 = 0.001, \gamma_0 = p$ and $\Psi_0 = \{(\gamma_0 - p + 1) \delta_0^2 I_p = \delta_0^2 I_p$, where the optimal $\delta_0^2$ is chosen via cross-validation. Results are reported in Table 2.

The $L_1$ error of the nearest neighbor-Dirichlet process scales nicely with the dimension for all the cases considered. For some cases however, the Dirichlet process mixture shows sudden increase in $L_1$ error with increasing dimension. For example, with 200 samples drawn from the mixture of two Gaussians (MG), the $L_1$ error for the Dirichlet process mixture jumps from 0.20 to 0.53 when $p$ increases from 2 to 3. The kernel density estimator shows the sharpest decline in performance - when the dimension is changed from 2 to 6, the average increase in $L_1$ error is by factors of about 5 and 7 for sample sizes 200 and 1,000, respectively. This is possibly due to lack of adaptive density estimation in higher dimensions using a single bandwidth matrix, since data in $\mathbb{R}^p$ become increasingly sparse with increasing $p$. The Dirichlet process mixture performs better than the nearest neighbor-Dirichlet process when the true density is unimodal, such as the skew-normal (SN) or the multivariate t-distribution (T), while having inferior performance for the discrete mixture cases.
Table 2: Comparison of the three methods in terms of the $L_1$ distance in the multivariate case. Number of test points and replications considered are $n_t = 500$ and $R = 20$

| Density | Dimension | 2 | 3 | 4 | 6 | 2 | 3 | 4 | 6 | 2 | 3 | 4 | 6 |
|---------|-----------|---|---|---|---|---|---|---|---|---|---|---|---|
| NN-DP   |           | 0.29 | 0.41 | 0.47 | 0.68 | 0.24 | 0.33 | 0.42 | 0.58 | 0.27 | 0.34 | 0.40 | 0.53 | 0.28 | 0.38 | 0.45 | 0.60 |
| DP      |           | 0.20 | 0.53 | 0.62 | 0.67 | 0.16 | 0.19 | 0.27 | 0.34 | 0.21 | 0.26 | 0.35 | 0.44 | 0.42 | 0.55 | 0.68 |
| KDE     |           | 0.28 | 0.52 | 0.79 | 1.29 | 0.22 | 0.50 | 0.78 | 1.26 | 0.26 | 0.53 | 0.74 | 1.21 | 0.27 | 0.55 | 0.72 | 1.21 |

4.4 Frequentist coverage

In this section, we assess frequentist coverage of the 95% pseudo-posterior credible intervals for the nearest neighbor-Dirichlet process and compare it with coverage based on the 95% posterior credible intervals for the Dirichlet process mixture. We consider the cases $p \in \{1, 2\}$ for the true data generating density $f_0$ on $\mathbb{R}^p$. For $p = 1$, we take $f_0$ to be the standard Gaussian density (GS) and inspect coverage at the points $x_0 \in \{-1, 0, 1\}$. For $p = 2$, we take the bivariate Gaussian (BG) having density $f_0(x) = \phi_2(x; 0, S)$ for $x \in \mathbb{R}^2$, where $S$ has diagonal elements equal to 1 and off-diagonal elements equal to 0.25, and inspect coverage at $x_0 \in \{-1, 0, 1\}$. We implement the Dirichlet process mixture as before, while for the nearest neighbor-Dirichlet process, we take $k = [500^{1/3}] + 1 = 8$ in the univariate case, $k = 5$ in the bivariate case, $\alpha$ as in Section 3.2 and other hyperparameters chosen as before. For each choice of $f_0$ we generate $R_{cov} = 200$ replicates of the data, each of sample size $n_{cov} = 500$. The results are summarised in Table 3.

For the univariate case, both the Dirichlet process mixture and the nearest neighbor-Dirichlet process have lower coverage at the mode 0, compared to the other two points. The nearest neighbor-Dirichlet process exhibits nearly 95% frequentist coverage at $x_0 = 1$ and $x_0 = -1$. However, the coverage provided by the Dirichlet process mixture falls far from the nominal coverage - the maximum coverage is 43% for $x_0 = -1$. For the bivariate case, we see a similar pattern.

4.5 Runtime comparison

We also compare runtimes of the proposed nearest neighbor-Dirichlet process and Dirichlet process mixture for dimensions 1 and 4. For the univariate case, the sample size is varied
Table 3: Comparison of the frequentist coverage of 95% (pseudo) posterior credible intervals of the nearest neighbor-Dirichlet process and the Dirichlet process mixture. $\bar{C}$ and $\bar{L}$ denote the average coverage and the average length of intervals, respectively. Number of replications and sample size are $R_{cov} = 200$ and $n_{cov} = 500$, respectively.

| True density | Dimension ($p$) | Method | $-1_p$ | $0_p$ | $1_p$ | $\bar{C}$ | $\bar{L}$ |
|--------------|----------------|--------|--------|--------|--------|----------|----------|
| GS 1         | NN-DP          | 0.97   | 0.86   | 0.97   | 0.93   | 0.08     |          |
|              | DP             | 0.43   | 0.29   | 0.38   | 0.37   | 0.02     |          |
| BG 2         | NN-DP          | 0.98   | 0.74   | 0.95   | 0.89   | 0.05     |          |
|              | DP             | 0.13   | 0.08   | 0.16   | 0.12   | 0.004    |          |

from $n = 200$ to $n = 3,000$ in increments of 100, with data generated from the standard Gaussian density (GS). In the multivariate case, data are generated from a four dimensional mixture of skew t-distributions with the parameters the same as described for the case MST in Section 4.3 with the sample size varied from $n = 200$ to $n = 1,500$ in increments of 100. The simulations were carried out on an i7-8700K processor with 16 gigabytes of memory.

In the left panel of Figure 3 we plot the average run time of each approach for 10 independent replications. The corresponding average $L_1$ error of the two methods is also included in the right panel of Figure 3. The proposed method is an order of magnitude faster. The time saved becomes more pronounced in the multivariate case, shown in the bottom left of Figure 3, where for sample size 1,500 the proposed method is $\sim$ 15 times faster. The gain in computing time does not come at the cost of accuracy as can be seen from the right panel; the proposed method maintains the same order of $L_1$ error as the Dirichlet process mixture in the univariate case and often outperforms the Dirichlet process mixture in the multivariate case. We did not implement the Monte Carlo sampler for the proposed algorithm in parallel, but such a modification would substantially improve runtime.

5 Application

We apply the proposed density estimator to binary classification. Consider data $D = \{(X_i, Y_i) : i = 1, \ldots, n\}$, where $X_i \in \mathbb{R}^p$ are $p$-dimensional feature vectors and $Y_i \in \{0, 1\}$ are binary class labels. To predict the probability that $y_0 = 1$ for a test point $x_0$, we use Bayes rule:

$$
\text{pr}(y_0 = 1 | x_0) = \frac{f_1(x_0) \text{pr}(y_0 = 1)}{f_0(x_0) \text{pr}(y_0 = 0) + f_1(x_0) \text{pr}(y_0 = 1)},
$$

(14)

where $f_j(x_0)$ is the feature density at $x_0$ in class $j$ and $\text{pr}(y_0 = j)$ is the marginal probability of class $j$, for $j = 0, 1$. Based on $n_t$ test data, we let $\hat{\text{pr}}(y_0 = 1) = (1/n_t) \sum_{i=1}^{n_t} Y_i$, with
Figure 3: Left panel shows run times of competing methods vs sample size for univariate (top row) and multivariate data (bottom row). $\ell_1$ errors are shown in the right panel.
\(\hat{p}\mathcal{r}(y_0 = 0) = 1 - \hat{p}\mathcal{r}(y_0 = 1)\), and use either the nearest neighbor-Dirichlet process pseudo-posterior mean \(\hat{f}_n(\cdot)\) or the Dirichlet process mixture posterior mean \(\hat{f}_{DP}(\cdot)\) for estimating the within class densities. We omit the kernel density estimator as no routine \text{R} implementation is available for data having more than 6 dimensions. We compare the resulting classification performances in terms of sensitivity and specificity.

The high time resolution universe survey data (Keith et al., 2010) contain information on sampled pulsar stars. Pulsar stars are a type of neutron star and their radio emissions are detectable from the Earth. These stars have gained considerable interest from the scientific community due to their several applications (Lorimer & Kramer, 2012). The data are publicly available from the University of California at Irvine machine learning repository. Stars are classified into pulsar and non-pulsar groups according to 8 attributes (Lyon, 2016). There are a total of 17,898 instances of stars, among which 1,639 are classified as pulsar stars.

We create a test data set of 200 stars, among which 23 are pulsar stars. The training size is then varied from 300 to 1,800 in increments of 300, each time adding 300 training points by randomly sampling from the entire data leaving out the initial test set. In Figure 4, we plot the sensitivity and specificity of the proposed method and the Dirichlet process mixture. Both the methods exhibit similar sensitivity across various training sizes; the Dirichlet process mixture has marginally better specificity for training sizes 1, 200 and 1, 500, while the nearest neighbor-Dirichlet process has better specificity for training sizes 300 and 600. In the left panel of Figure 5, the receiver operating characteristic curve of the two methods is shown for 1,800 training samples. The area under the curve (AUC) for the nearest neighbor-Dirichlet process and the Dirichlet process mixture are 0.96 and 0.95, respectively.

We also compare the methods using the Brier score, a proper scoring rule (Gneiting & Raftery, 2007) for probabilistic classification. Suppose for \(n_t\) test points and the \(i\)th Monte Carlo sample, \(p_1^{(i)} = (p_1^{(i)} j)_{j=1}^{n_t}\) and \(p_2^{(i)} = (p_2^{(i)} j)_{j=1}^{n_t}\) denote the \(n_t \times 1\) probability vectors for the nearest neighbor-Dirichlet process and the Dirichlet process mixture, respectively. We compute the normalized Brier score for the \(i\)th sample as \((1/n_t) \sum_{j=1}^{n_t} (p_{c j}^{(i)} - Y_j)^2\) for \(c = 1, 2\). Then with \(T\) samples of \(p_1^{(i)}\) and \(p_2^{(i)}\), we compute the average Brier score and 95% credible interval. The average Brier score for each training size is shown in the right panel of Figure 5, which naturally shows a declining trend with increasing training size. The average length of 95% credible intervals for the Brier scores across the training sizes for the proposed method and Dirichlet process mixture are 0.03 and 0.02, respectively. For 1,800 training samples, the computation time for the proposed method is about 13 minutes while for the Dirichlet process mixture it is approximately 5 hours. Hence, the proposed method is much faster, even without exploiting parallel computation. We also fitted the proposed method using the training set of all 17,698 points; Dirichlet process mixtures were too slow in this case. The sensitivity and specificity increased to 0.99 and 0.91, respectively.
Figure 4: Sensitivity and specificity of the nearest neighbor-Dirichlet process and the Dirichlet process mixture classifiers for the universe survey data.

Figure 5: On the left, we show the receiver operating characteristic curve of the nearest neighbor-Dirichlet process and the Dirichlet process mixture classifiers with 1,800 training samples. Area under the curve is abbreviated as AUC. Normalized Brier scores for the two methods are shown on the right for varying training size.
6 Discussion

The proposed nearest neighbor-Dirichlet process seems to provide a practically useful alternative to Dirichlet process mixtures with much faster computational speed and stability in avoiding Markov chain Monte Carlo algorithms. Such algorithms can have very poor performance in mixture models and other multimodal cases, due to difficulty in mixing, and hence can lead to posterior inferences that are unreliable. The main conceptual disadvantage of the proposed approach is the lack of a coherent Bayesian posterior updating rule. However, we have shown that nonetheless the resulting pseudo-posterior can have appealing behavior in terms of frequentist asymptotic properties, finite sample performance, and accuracy in uncertainty quantification. In addition, it is important to keep in mind that Dirichlet process mixtures and other related Bayesian nonparametric models have key disadvantages that are difficult to remove within a fully coherent Bayesian modeling framework. These include a strong sensitivity to the choice of kernel and prior on the weights on these kernels; refer, for example to Miller & Dunson (2019).

There are several important next steps. The first is to develop fast and robust algorithms for using the nearest neighbor-Dirichlet process not just for density estimation but also as a component of more complex hierarchical models. For example, one may want to model the residual density in regression nonparametrically or treat a random effects distribution as unknown. In such settings, one can potentially update other parameters within a Bayesian model using Markov chain Monte Carlo, while using algorithms related to those proposed in this article to update the nonparametric part conditionally on these other parameters.

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Supplementary Material

In the Supplementary Material we provide proofs of Lemmas 3.4 and 3.6, Theorem 3.9 and equation (13), a multivariate extension of Theorem 3.5 and other required technical results. We also provide an algorithm for univariate implementation of the nearest neighbor-Dirichlet process, details on faster implementation of leave-one-out cross validation and a note on the inverse Wishart density. Code for implementing the proposed method is available at https://github.com/shounakchattopadhyay/NN-DP.
Appendix

Lemmas and Propositions numbered as S1, S2 and so on are stated and proven in the Supplementary Materials.

Proof of Theorem 3.5

Fix $x \in \mathbb{R}, x \not\in \{0, 1\}$. Recall $f_K(x) = (nh)^{-1} \sum_{i=1}^{n} t_{\gamma_n}(x-X_i)/h$ from Section 3 and define another function $f_V(x) = n^{-1} \sum_{i=1}^{n} \lambda_i^{-1} t_{\gamma_n}(x-X_i)/\lambda_i$. By triangle inequality and linearity of expectations, we get

$$E_{P_{f_0}}( | \hat{f}_n(x) - f_K(x) | ) \leq E_{P_{f_0}}( | \hat{f}_n(x) - f_V(x) | ) + E_{P_{f_0}}( | f_V(x) - f_K(x) | ).$$

We now analyze the two terms in equation (15) separately. For the first term, we immediately have by the triangle inequality

$$E_{P_{f_0}}( | \hat{f}_n(x) - f_V(x) | ) \leq E_{P_{f_0}}( \lambda_i^{-1} | t_{\gamma_n}(x-\mu_1)/\lambda_1 - t_{\gamma_n}(x-X_1)/\lambda_1 | ),$$

since the random variables $\lambda_i^{-1}(x-\mu_i)$ are identically distributed under $P_{f_0}$ for $i = 1, \ldots, n$. Using Proposition S1 in conjunction with Lemma 3.4 we get existence of $L_1 = L_{1,n} > 0$ such that

$$E_{P_{f_0}}( | \hat{f}_n(x) - f_V(x) | ) \leq L_1 E_{P_{f_0}}( \lambda_i^{-2} | X_1 - \mu_1 | ) \leq L_1 \xi_1(f_0)(\gamma_0 \delta_0)^{-1}(n^{-2}k^3) + o(n^{-2}k^3).$$

(16)

The expression on the right hand side of (16) goes to 0 since $k = o(n^{4/9})$ and $L_1 \to (2\pi)^{-1/2}$ as $n \to \infty$. We now consider the second term. Again, applying the triangle inequality and the mean value theorem, there exists $\sigma \in [h^2, \lambda_2^2]$ such that

$$E_{P_{f_0}}( | f_V(x) - f_K(x) | ) \leq E_{P_{f_0}}( | \lambda_i^{-1} t_{\gamma_n}(\lambda_1^{-1}(x-X_1)) - h^{-1} t_{\gamma_n}(h^{-1}(x-X_1)) | )$$

$$= E_{P_{f_0}}( | g_{\gamma_n}(\sigma) | (\lambda_2^2 - h^2) ),$$

where $g_{\beta}(u) = u^{-1/2} t_{\beta}(c u^{-1/2})$ for $u > 0$, $\beta = \gamma_n$ and $c = (x-X_1)$. Routine calculations, the triangle inequality and $\sigma \geq h^2$ imply that $| g_{\gamma_n}(\sigma) | \leq h^{-3} c_{\gamma_n}(\gamma_n + 2)$, where $c_{\gamma_n} = \{(\gamma_n \pi)^{1/2} \Gamma((\gamma_n + 1)/2)\}^{-1} \Gamma((\gamma_n + 1)/2)$. Using Lemma 3.4, we get

$$E_{P_{f_0}}( | f_V(x) - f_K(x) | ) \leq c_{\gamma_n} \xi_2(f_0)(\gamma_0 \delta_0)^{-3/2}(n^{-2}k^{9/2}) + o(n^{-2}k^{9/2}),$$

(17)

where $\xi_1(f_0) = \int_0^1 \{ f_0(y)/\{12 f_0^2(y)\} \} dy$, $\xi_2(f_0) = \int_0^1 \{12 f_0(y)\}^{-1} dy$ are finite by equation (10). The expression on the right hand side of equation (17) goes to 0 since $k/n^{4/9} \to 0$ and $c_{\gamma_n} \to (2\pi)^{-1/2}$ as $n \to \infty$. Hence, $E_{P_{f_0}}( | \hat{f}_n(x) - f_K(x) | ) \to 0$ as $n \to \infty$ from equation (15). Combining this with the fact that $f_K(x) \to f_0(x)$ in $P_{f_0}$-probability as $n \to \infty$ from Lemma S3, the theorem is proved. □
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Supplementary Material for
Nearest neighbor Dirichlet process

Convention

Equations defined in this document are numbered (S1), (S2) etc, while (1), (2) etc refer to those defined in the main document. Similar for lemmas, theorems, sections etc. We list the assumptions we make on the true density $f_0$ for the sake of completeness.

- **Assumption 3.1** (Support). $f_0$ is supported on $[0, 1]$ with $f(x) > 0$ for all $x \in [0, 1]$.
- **Assumption 3.2** (Continuity). $f_0$ is continuous on $[0, 1]$.
- **Assumption 3.3** (Bounded curvature). $|f''_0(x)| \leq L$ for all $x \in (0, 1)$ and some finite $L \geq 0$.

S.1 Prerequisites

We start with a proposition showing Lipschitz continuity of the $t$ kernel used to prove weak consistency of the pseudo-posterior mean of the nearest neighbor-Dirichlet process.

**Proposition S.1.1.** Consider the $t$ density with $\beta > 0$ degrees of freedom: $t_\beta(u) = c_\beta(1 + u^2/\beta)^{-(\beta+1)/2}$ for $u \in \mathbb{R}$ where $c_\beta = (\beta\pi)^{-1/2}\Gamma(\beta/2)^{-1}\Gamma((\beta+1)/2)$. Then $t_\beta(\cdot)$ is Lipschitz continuous, so that there exists $L_1 = L_1(\beta) > 0$ such that for any $u, v, \in \mathbb{R}$,

$$|t_\beta(u) - t_\beta(v)| \leq L_1|u - v|. \quad (S.1)$$

**Proof.** Fix any arbitrary $u, v \in \mathbb{R}$. Then $|t_\beta(u) - t_\beta(v)| \leq \{\sup_x |t'_\beta(x)|\} |u - v|$ by the mean value theorem. It is then enough to show that $\sup_x |t'_\beta(x)|$ is finite. Straightforward arguments show that (S.1) is satisfied for $L_1 = \sup_x |t'_\beta(x)| = c_\beta((\beta+1)/\beta)\{\beta/(\beta+2)\}^{1/2}\{1 + (\beta + 2)^{-1}\}^{-(\beta+3)/2}$. \hfill $\square$

Now consider independent and identically distributed data $X_1, \ldots, X_n \sim f_0$ supported on the interval $[0, 1]$ in $\mathbb{R}$ and satisfying Assumptions 3.1-3.3. Let $\mathcal{X}^{(n)} = (X_1, \ldots, X_n)$ and suppose $f_0$ induces the measure $P_{f_0}$ on the Borel $\sigma$-field on $\mathbb{R}$. We form the $k$-nearest neighborhood of $X_i$ using the Euclidean norm for $i = 1, \ldots, n$. For a generic $X_i$, let $Q_i$ be its $k$-th nearest neighbor in $\mathcal{X}^{-i} = (X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_n)$ and let $R_i$ be the distance between $X_i$ and $Q_i, R_i = |X_i - Q_i|$. Define the ball $B_i = \{y \in [0, 1] : 0 < |y - X_i| < R_i\}$

S.1
and the probability $G(X_i, R_i) = \int_{B_i} f_0(u) \, du$ of the ball $B_i$. Let $Y^{(i)}_1 = X_i$ and $Y^{(i)}_2, \ldots, Y^{(i)}_{k-1}$ denote the observations from the data which fall in $B_i$. Then, we define the neighborhood specific mean and variance as $\bar{X}_i = k^{-1}\{\sum_{j=1}^{k-1} Y^{(i)}_j + Q_i\}$ and $S_i^2 = k^{-1}\{\sum_{j=1}^{k-1} (Y^{(i)}_j - \bar{X}_i)^2 + (Q_i - \bar{X}_i)^2\}$, respectively. Under this setup, the neighborhood specific summary statistics, such as the neighborhood mean and neighborhood variance, are identically distributed but not independent. Hence in our subsequent results we consider the neighborhood specific mean and variance for $i = 1$ only.

Given $X_1 = x_1$ and $R_1 = r_1$, following Mack & Rosenblatt (1979) the conditional joint density of $Y^{(1)}_2, \ldots, Y^{(1)}_{k-1}$ and $Q_1$ is

$$f(y_2, \ldots, y_{k-1}, q \mid x_1, r_1) = \left\{ \prod_{j=2}^{k-1} \frac{f_0(y_j)}{G'(x_1, r_1)} \mathbb{I}(y_j \in B_1) \right\} \frac{f_0(q)}{G'(x_1, r_1)} \mathbb{I}(|q - x_1| = r_1), \tag{S.2}$$

where $G'(x_1, r_1) = \partial G(x_1, r_1)/\partial r_1$ and $\mathbb{I}_A$ denotes the indicator function of the event $A$. Thus conditional on $X_1$ and $R_1$, the random variables $Y^{(1)}_2, \ldots, Y^{(1)}_{k-1}$ are independent and identically distributed, and independent of $Q_1$. Also, Mack & Rosenblatt (1979) states that under Assumptions 3.1-3.2 which imply $f_0$ is bounded and continuous on $[0, 1]$, we have,

$$G(x_1, r_1) = 2f_0(x_1)r_1 + o(r_1). \tag{S.3}$$

Let the function $\rho(x_1, r_1) = \{G(x_1, r_1)\}^{-\kappa_2} r_1^{\kappa_1}$ where $\kappa_1$ and $\kappa_2$ are non-negative integers. This function can be identified as $\phi(\cdot)$ in equation (11) of Mack & Rosenblatt (1979). In the following propositions we will require the expected values of $\rho(x_1, r_1)$ for different choices of $\kappa_1$ and $\kappa_2$. To that end, we shall repeatedly make use of the equation (12) from Mack & Rosenblatt (1979) adapted to our setting:

$$E_{P_{f_0}}(\rho(x_1, R_1) \mid X_1 = x_1) = \frac{(n - 1)!}{(k-2)!(n-k)!} \int_0^1 \left\{ \left( \frac{t}{C_1 f_0(x_1)} \right)^{\kappa_1} + o(t^{\kappa_1}) \right\} t^{k-2-\kappa_2} (1 - t)^{n-k} \, dt, \tag{S.4}$$

where $C_1$ is the volume of the unit ball in $\mathbb{R}$ so $C_1 = 2$; see Section 2 in Mack & Rosenblatt (1979) for sufficient conditions to ensure existence of expectations of $\rho(\cdot, \cdot)$.

**Proposition S.1.2.** Given $X_1$, the conditional expected value of the random variable $Y^{(1)}_j - X_1$ for any $j = 2, \ldots, k-1$ is

$$E(Y^{(1)}_j - X_1 \mid X_1) = \frac{1}{12} \frac{f'_0(X_1)}{f^3(X_1)} \frac{k^2}{n^2} + o \left( \frac{k^2}{n^2} \right). \tag{S.5}$$


Proof. For any \( j = 2, \ldots, k-1 \), using the law of iterated expectations, the conditional expected value of \( Y_j^{(1)} - X_1 \) given \( X_1 \) is,

\[
E(Y_j^{(1)} - X_1 \mid X_1) = E\{E(Y_j^{(1)} - X_1 \mid X_1, R_1) \mid X_1\}. \tag{S.6}
\]

Then we obtain,

\[
E(Y_j^{(1)} - X_1 \mid X_1, R_1) = \int_{|y-X_1| < R_1} (y - X_1) \frac{f_0(y)}{G(X_1, R_1)} \, dy
\]

\[
= \frac{1}{G(X_1, R_1)} \left[ \int_{|y-X_1| < R_1} (y - X_1) \left\{ f_0(X_1) + (y - X_1)f_0'(X_1) + \frac{(y - X_1)^2}{2}f_0''(\xi) \right\} \, dy \right] 
\]

\[
= \frac{1}{G(X_1, R_1)} \left\{ \frac{2f_0'(X_1)R_1^3}{3} + \int_{|y-X_1| < R_1} \frac{(y - X_1)^3}{2}f_0''(\xi) \, dy \right\},
\]

using the second order mean value theorem for \( f_0(y) \), where \( \xi \) lies between \( y \) and \( X_1 \) in the integral. We now proceed to bound the absolute value of the second term in brackets in the above expression. We have,

\[
\int_{|y-X_1| < R_1} \frac{|y - X_1|^3}{2} | f_0''(y) | \, dy \leq \frac{L}{4} R_1^4,
\]

following Assumption 3.3 on \( f_0(\cdot) \). Thus, we get,

\[
E\{Y_j^{(1)} - X_1 \mid X_1, R_1\} = \frac{2f_0'(X_1)R_1^3}{3G(X_1, R_1)} + O\left( \frac{R_1^4}{G(X_1, R_1)} \right). \tag{S.7}
\]

The proof is then completed using (S.4) with \( \kappa_1 = 3 \) and \( \kappa_2 = 1 \). \( \square \)

**Proposition S.1.3.** Given \( X_1 \), the conditional expected value of the random variable \( Q_1 - X_1 \) for sufficiently large \( n \) is

\[
E(Q_1 - X_1 \mid X_1) = \frac{f_0'(X_1)}{2f_0^3(X_1)} \frac{k^2}{n^2} + o\left( \frac{k^2}{n^2} \right). \tag{S.8}
\]

**Proof.** Using the law of iterated expectations, we have \( E(Q_1 - X_1 \mid X_1) = E\{E(Q_1 - X_1 \mid X_1, R_1) \mid X_1\} \). We first consider \( E(Q_1 - X_1 \mid X_1, R_1) \). Given \( X_1 \) and \( R_1 \), the random variable \( Q_1 \) has the following distribution:

\[
Q_1 = \begin{cases} 
X_1 + R_1 & \text{with probability } p(X_1, R_1) \\
X_1 - R_1 & \text{with probability } 1 - p(X_1, R_1).
\end{cases} \tag{S.9}
\]

Thus, \( E(Q_1 - X_1 \mid X_1, R_1) = 2R_1 \{ p(X_1, R_1) - (1/2) \} \). Now, we have

\[
p(X_1, R_1) - \frac{1}{2} = \frac{f_0(X_1 + R_1) - f_0(X_1 - R_1)}{2\{f_0(X_1 + R_1) + f_0(X_1 - R_1)\}} \leq R_1 \frac{f_0'(X_1)}{f_0(X_1)} + L \frac{R_1^2}{f_0(X_1)},
\]

S.3
for sufficiently large $n$, using the fact that $f_0(X_1 + R_1) + f_0(X_1 - R_1) \geq f_0(X_1)$ since $R_1 \to 0$ $P_{f_0}$-almost surely (Biau & Devroye, 2015), and $f_0(X_1 + R_1) - f_0(X_1 - R_1) \leq 2R_1f_0'(X_1) + LR_1^2$ by the mean value theorem and Assumption 3.3. The proof is completed upon invoking equation (S.4).

\[ \text{Lemma S.1.4.} \text{ Given } X_1 \text{ and for sufficiently large } n, \text{ we have} \]
\[ E(\hat{X}_1 - X_1 \mid X_1) = \frac{f_0'(X_1)}{12f_0^2(X_1)} \frac{k^2}{n^2} + o \left( \frac{k^2}{n^2} \right). \]  
\[ \text{(S.10)} \]

\[ \text{Proof.} \text{ We have,} \]
\[ E(\hat{X}_1 - X_1 \mid X_1) = \frac{1}{k} E \left[ \left\{ \sum_{j=2}^{k-1} (Y_j^{(1)} - X_1) + (Q - X_1) \right\} \mid X_1 \right] \]
\[ = \frac{f_0'(X_1)}{12f_0^2(X_1)} \frac{k^2}{n^2} + o \left( \frac{k^2}{n^2} \right), \]

following Propositions S.1.2 and S.1.3. \hfill \Box

Next, we study the neighborhood variance in terms of $k$, $n$ and terms involving $f_0$. For $j = 1, \ldots, k - 1$, we define the random variables $Z_j^{(1)} = Y_j^{(1)} - X_1$, and let $q_1 = Q_1 - X_1$. By definition of $Y_1^{(1)}$, we have $Z_1^{(1)} = 0$. Since $|Q_1 - X_1| = R_1$, we trivially obtain that $E(q_1^2 \mid X_1, R_1) = R_1^2$.

\[ \text{Proposition S.1.5.} \text{ Given } X_1, \text{ the conditional second moment of the random variable } Z_j^{(1)} \]
\[ \text{for any } j = 2, \ldots, k - 1 \text{ is given by} \]
\[ E\{Z_j^{(1)} \mid X_1\} = \frac{1}{12f_0^2(X_1)} \frac{k^2}{n^2} + o \left( \frac{k^2}{n^2} \right). \]  
\[ \text{(S.11)} \]

\[ \text{Proof.} \text{ We have, for } j = 2, \ldots, k - 1, \]
\[ E\{(Y_j^{(1)} - X_1)^2 \mid X_1, R_1\} = \int_{|y - X_1| < R_1} (y - X_1)^2 \frac{f_0(y)}{G(X_1, R_1)} dy \]
\[ = \frac{2f_0(X_1)R_1^3}{3G(X_1, R_1)} + O \left( \frac{R_1^4}{G(X_1, R_1)} \right), \]

using the mean value theorem as in Proposition S.1.2 and the fact that $f_0'(\cdot)$ is also bounded using Assumptions 3.1-3.3. The proof is then completed using (S.4) with $\kappa_1 = 3$ and $\kappa_2 = 1$. \hfill \Box

\[ \text{Proposition S.1.6.} \text{ Given } X_1, \text{ the conditional second moment of the random variable } q_1 \text{ is} \]
\[ \text{given by} \]
\[ E(q_1^2 \mid X_1) = E(R_1^2 \mid X_1) = \frac{1}{4f_0^2(X_1)} \frac{k^2}{n^2} + o \left( \frac{k^2}{n^2} \right). \]  
\[ \text{(S.12)} \]
Proof. The proof is immediate by using $\kappa_1 = 2$ and $\kappa_2 = 0$ in equation (S.4).

\textbf{Lemma S.1.7.} Let $V_1 = kS_1^2$. Given $X_1$ and sufficiently large $n$, the conditional expected value of $V_1$ given $X_1$ is given by

\[ E(V_1 \mid X_1) = \frac{1}{12} f_0^2(X_1) n^2 + o\left(\frac{k^3}{n^2}\right). \]  

(S.13)

Proof. We first start out by observing $V_1 = \sum_{j=1}^{k-1}(V_j - \bar{X}_1)^2 + (Q_1 - \bar{X}_1)^2 = \sum_{j=1}^{k-1}(Z_j^1 - \bar{Z}_1)^2 + (q_1 - \bar{Z}_1)^2$, where $\bar{Z}_1 = \bar{X}_1 - X_1$. This immediately implies that $V_1 = (\sum_{j=1}^{k-1}Z_j^1 + q_1^2) - k\bar{Z}_1^2 \leq (\sum_{j=1}^{k-1}Z_j^1 + q_1^2)$. Propositions S.1.5 and S.1.6 complete the proof.

\textbf{S.2 Proof of Lemma 3.4}

Using Assumptions 3.1-3.3 we obtain $\xi_1(f_0), \xi_2(f_0) < \infty$. We have $E_{P_0}(\mid \mu_1 - X_1 \mid) \leq E_{P_0}(\mid \mu_1 - \bar{X}_1 \mid) + E_{P_0}(\mid \bar{X}_1 - X_1 \mid)$, using the triangle inequality. Since $\mid \bar{X}_1 \mid \leq 1$ and $\nu_0 = o(n^{-2}k^3)$, we get $E_{P_0}(\mid \mu_1 - \bar{X}_1 \mid) \leq \nu_0 \nu_0^{-1}\{E_{P_0}(\mid \bar{X}_1 \mid) + \mid \mu_0 \mid\} \leq \nu_0 \nu_0^{-1}(1 + \mid \mu_0 \mid) = o(k^2/n^2)$. Using Lemma S.1.4, we get

\[ E_{P_0}(\mid \mu_1 - X_1 \mid) \leq \xi_1(f_0) \frac{k^2}{n^2} + o\left(\frac{k^2}{n^2}\right). \]  

(S.14)

For the approximation of the neighborhood specific bandwidth parameter $\lambda_1$, we have,

\[ \lambda_1^2 - h^2 = \frac{\nu_n + 1}{\nu_n} \frac{1}{\gamma_n} \left( V_1 + \frac{k\nu_0}{\nu_n} \bar{X}_1^2 \right). \]  

(S.15)

This implies that

\[ E(\lambda_1^2 - h^2 \mid X_1) \leq \frac{1}{12} f_0^2(X_1) n^2 + o\left(\frac{k^2}{n^2}\right), \]  

(S.16)

using Lemma S.1.7 and $\bar{X}_1^2 \leq 1$. Taking another expectation over $X_1$ yields the result.

\textbf{S.3 Proof of consistency of $f_K(x)$}

Recall $f_K(x) = (nh)^{-1} \sum_{i=1}^{n} t_{\gamma_n}(h^{-1}(x - X_i))$ from Section 3 of the main document, where $h = h_n = (\nu_n + 1)^{1/2}(\nu_n \gamma_n)^{-1/2}(\gamma_0^3)^{1/2}$. Here, the bandwidth $h_n$ satisfies $h_n \to 0$ and $nh_n \to \infty$ as $n \to \infty$. The following lemma proves the consistency of any such generic estimator $f_K(x) = (nw)^{-1} \sum_{i=1}^{n} t_{\gamma_n}(w^{-1}(x - X_i))$, where the bandwidth $w = w_n$ satisfies $w_n \to 0$ and $nw_n \to \infty$ as $n \to \infty$, with independent and identically distributed data $X_1, \ldots, X_n \sim f_0$ satisfying Assumptions 3.1-3.3.
Lemma S.3.1. Suppose $w = w_n$ is a sequence satisfying $w \to 0$ and $n\,w \to \infty$ as $n \to \infty$. Let $f_K(x) = (n\,w)^{-1} \sum_{i=1}^{n} t_{\gamma_n} \{ w^{-1}(x - X_i) \}$. Then $f_K(x) \to f_0(x)$ in $P_{f_0}$-probability for each $x \in \mathbb{R}, x \neq 0, 1$.

Proof. First we prove the result for any $x \in (0, 1)$. It is enough to show that $E_{P_{f_0}} \{ f_K(x) \} \to f_0(x)$ and $\text{var}_{P_{f_0}} \{ f_K(x) \} \to 0$ as $n \to \infty$. Let us start first with $E_{P_{f_0}} \{ f_K(x) \}$. We have

$$E_{P_{f_0}} \{ f_K(x) \} = E_{P_{f_0}} \left\{ \frac{1}{w} t_{\gamma_n} \left( \frac{x - X_1}{w} \right) \right\} = \int_0^{1/w} \frac{1}{w} t_{\gamma_n} \left( \frac{y - x}{w} \right) f_0(y) \, dy$$

where the second from the last expression is obtained by applying the mean value theorem. Suppose $\Phi_n$ and $\Phi$ are the cumulative distribution functions of the $t_{\gamma_n}$ density and the standard Gaussian density, respectively. Then, $\int_{-\infty}^{1/w} t_{\gamma_n}(u) \, du = \Phi_n \{ (1 - x)/w \} - \Phi_n(-x/w)$. But $\Phi_n$ converges weakly to $\Phi$ and $\Phi$ is continuous, so by Polya's theorem (Pólya, 1920), $\Phi_n$ converges uniformly to $\Phi$. Since $(1 - x)/w \to \infty$ and $-x/w \to -\infty$ for $x \in (0, 1)$, we get $\int_{-\infty}^{1/w} t_{\gamma_n}(u) \, du \to 1$ as $n \to \infty$. To bound the second term, observe that $| w \int_{-\infty}^{1/w} u t_{\gamma_n}(u) f_0'(\xi) \, du | \leq w \{ \sup_{\xi} f_0'(\xi) \} \int_{-\infty}^{\infty} | u | \, t_{\gamma_n}(u) \, du \to 0$ as $n \to \infty$, using the fact that as $\gamma_n \to \infty$, $f_0(\cdot)$ is bounded and $w \to 0$ as $n \to \infty$.

Before we look at the variance, we observe that for any $u \in \mathbb{R}, t_{\gamma_n}^2(u) = c_{\gamma_n}^2 (c_{2\gamma_n+1}^2)^{-1} t_{2\gamma_n+1} \{ 2 + (1/\gamma_n) \}^{1/2} u$. We then have

$$\text{var}_{P_{f_0}} \{ f_K(x) \} = \frac{1}{n} \text{var}_{P_{f_0}} \left\{ \frac{1}{w} t_{\gamma_n} \left( \frac{x - X_1}{w} \right) \right\} \leq \frac{1}{n} E_{P_{f_0}} \left\{ \frac{1}{w^2} t_{\gamma_n}^2 \left( \frac{x - X_1}{w} \right) \right\} \leq \frac{1}{nw^2} \int_{-\infty}^{w} t_{\gamma_n}^2 \left( \frac{y - x}{w} \right) f_0(y) \, dy$$

where $l_{1,n} = -(x/w) \{ 2 + (1/\gamma_n) \}^{1/2}, l_{2,n} = \{ 2 + (1/\gamma_n) \}^{1/2}(1 - x)/w$ and we have applied the mean value theorem to obtain the second to last expression. The final expression in the above display can be shown to go to 0 with analogous arguments as before, using uniform
convergence of \( \Phi_n \) to \( \Phi \) (Pólya, 1920) and the fact that \( l_{1,n} \to -\infty, l_{2,n} \to \infty, nw \to \infty \) as \( n \to \infty \). This proves the result for \( x \in (0, 1) \).

To prove the result for \( x \) outside \([0, 1]\), we show the result for any \( x < 0 \) and observe that identical arguments lead to the proof for any \( x > 1 \) by symmetry. For \( x < 0 \), one has \( f_0(x) = 0 \) using Assumption 3.1, so it is enough to show that both \( E_{P_{f_0}} \{ f_K(x) \} \) and \( \text{var}_{P_{f_0}} \{ f_K(x) \} \to 0 \) as \( n \to \infty \). Since we have

\[
E_{P_{f_0}} \{ f_K(x) \} = \int_{-x/w}^{(1-x)/w} t_{\gamma_n}(u) f_0(x + wu) \, du,
\]

it follows using equation (10) that \( E_{P_{f_0}} \{ f_K(x) \} \leq l_2 \{ \Phi_n \{(1-x)/w\} - \Phi_n(-x/w) \} \). Since \( x < 0 \), we have both \( -x/w, (1-x)/w \to \infty \) as \( n \to \infty \). Observing that \( \Phi_n \) converges uniformly to \( \Phi \) as \( n \to \infty \) by Pólya (1920), we obtain that

\[
\lim_{n \to \infty} E_{P_{f_0}} \{ f_K(x) \} \leq l_2 \{ \Phi(\infty) - \Phi(\infty) \} = 0.
\]

The variance can be shown to go to 0 analogously, proving the result for any \( x < 0 \). \( \square \)

The above result can be extended to the multivariate scenario using identical arguments as described above when the random sample \( X_1, \ldots, X_n \sim f_0 \) for \( f_0 \) a density on \( \mathbb{R}^p \). Suppose \( f_0 \) is supported on \([0, 1]^p\), continuous on \([0, 1]^p\) and \( \| \nabla f_0(x) \|_2 < \infty \) for all \( x \in (0, 1)^p \). Define the multivariate kernel density estimator by \( f_K(x) = (nw^p)^{-1} \sum_{i=1}^n t_{\gamma_n-p+1}(w^{-1}(x - X_i)) \) where \( w \to 0 \) and \( nw^p \to \infty \) as \( n \to \infty \). Then one has \( f_K(x) \to f_0(x) \) in \( P_{f_0} \)-probability for all \( x \in \{(z_1, \ldots, z_p)^T : z_i \in \mathbb{R}, z_i \notin \{0, 1\}, \text{ for all } i = 1, \ldots, p\} \).

### S.4 Proof of Lemma 3.6

Fix \( x \in (0, 1) \). For \( i = 1, \ldots, n \), let \( z_i = \phi(x ; \eta_i, \sigma_i^2) \) and suppose \( z^{(n)} = (z_1, \ldots, z_n)^T \). Then, we have \( f(x) = \sum_{i=1}^n \pi_i z_i = z^{(n)^T} \pi^{(n)} \) where \( \pi^{(n)} = (\pi_1, \ldots, \pi_n)^T \sim \text{Dirichlet}(\omega, \ldots, \omega) \) given \( \chi^{(n)} \), with \( \omega = \alpha + 1 \). We begin with the identity

\[
\text{var}\{ f(x) \mid \chi^{(n)} \} = \text{var}[E\{ f(x) \mid \chi^{(n)}, z^{(n)} \} \mid \chi^{(n)}] + E[\text{var}\{ f(x) \mid \chi^{(n)}, z^{(n)} \} \mid \chi^{(n)}]. \quad (S.17)
\]

For \( i = 1, \ldots, n \), we have

\[
E(z_i^2 \mid \chi^{(n)}) = \frac{r_n}{b_i} t_{\gamma_n+1} \left( \frac{x - \mu_i}{b_i} \right), \quad (S.18)
\]

where \( r_n = \{2\Gamma(\gamma_n/2)\pi^{1/2}(\gamma_n+1)^{1/2}\}^{-1} \left[ \Gamma\left\{(\gamma_n+1)/2\right\}\{1+(2/\nu_n)\}^{1/2} \right] \), \( b_i = \lambda_i(D_n/2)^{1/2} \) and \( D_n = \{(\gamma_n+1)(\nu_n+1)\}^{-1} \gamma_n(\nu_n+2) \). Equation (S.18) is obtained by integrating over the
pseudo-posterior distribution of \((\eta_i, \sigma_i^2)_{i=1}^n\) given \(\mathcal{X}^{(n)}\), namely \(\text{NIG}(\mu_i, \sigma_i^2/\nu_i, \gamma_n/2, \gamma_n\delta_i^2/2)\), where for ease of exposition we have suppressed the dependence of \(\delta_n^{(i)}\) on \(n\) and have represented it as \(\delta_i\). Moreover, \(z_1, \ldots, z_n\) are conditionally independent given the data \(\mathcal{X}^{(n)}\).

We first start with the first term on the right hand side of equation (S.17). We have

\[
\text{var}[E\{f(x) \mid \mathcal{X}^{(n)}, z^{(n)}\} \mid \mathcal{X}^{(n)}] = \text{var}\left(\frac{1}{n} \sum_{i=1}^n z_i \mid \mathcal{X}^{(n)}\right) \\
= \frac{1}{n^2} \sum_{i=1}^n \text{var}(z_i \mid \mathcal{X}^{(n)}) \\
\leq \frac{1}{n^2} \sum_{i=1}^n E(z_i^2 \mid \mathcal{X}^{(n)}) \\
= \frac{1}{n^2} \sum_{i=1}^n \frac{1}{b_i} \frac{r_n}{b_i} t_{\gamma_n+1} \left(\frac{x - \mu_i}{b_i}\right),
\]

where the first equality is obtained using \(E(\pi_i \mid \mathcal{X}^{(n)}) = 1/n\) for each \(i = 1, \ldots, n\) and the last equality is obtained using equation (S.18). For \(i = 1, \ldots, n\), since \(\lambda_i \geq h\), we have \(b_i \geq h(D_n/2)^{1/2}\). Letting \(\hat{f}_1(x) = (1/n) \sum_{i=1}^n b_i^{-1} t_{\gamma_n+1} \{b_i^{-1}(x - X_i)\}\) and \(a_n = a_n(x) = (2/D_n)^{1/2} r_n \hat{f}_1(x)\), we have,

\[
\text{var}[E\{f(x) \mid \mathcal{X}^{(n)}, z^{(n)}\} \mid \mathcal{X}^{(n)}] \leq \frac{a_n}{nh}.
\]

We now analyze the second term on the right hand side of equation (S.17). Recall that \(\pi^{(n)}\) is conditionally independent of \(z^{(n)}\) given the data \(\mathcal{X}^{(n)}\) following from the nearest-neighbor Dirichlet process framework as discussed in Section 2.1 of the main document. Let \(\Sigma_\pi\) denote the pseudo-posterior covariance matrix of \(\pi^{(n)}\). Given \(\mathcal{X}^{(n)}\), since \(\pi^{(n)} \sim \text{Dirichlet}(\omega, \ldots, \omega)\) where \(\omega = \alpha + 1\), standard results yield that \(\Sigma_\pi = V_n \{(1 - C_n)I_n + C_n J_n\}\), where \(V_n = (n-1)/\{n^2(n\omega+1)\}\), \(C_n = -1/(n-1)\), \(I_n\) is the \(n \times n\) identity matrix, and \(J_n = 1_n 1_n^T\) where \(1_n = (1, \ldots, 1)^T \in \mathbb{R}^n\). Then, we have

\[
E[\text{var}\{f(x) \mid \mathcal{X}^{(n)}, z^{(n)}\} \mid \mathcal{X}^{(n)}] = E[z^{(n)^T} \Sigma_\pi z^{(n)} \mid \mathcal{X}^{(n)}].
\]

Using the expression for \(\Sigma_\pi\) along with equation (S.20), we obtain,

\[
E[\text{var}\{f(x) \mid \mathcal{X}^{(n)}, z^{(n)}\} \mid \mathcal{X}^{(n)}] = \frac{1}{(n\omega + 1)} E \left\{ \frac{1}{n} \sum_{i=1}^n (z_i - \bar{z})^2 \mid \mathcal{X}^{(n)} \right\},
\]

(S.21)
where \( \bar{z} = (1/n) \sum_{i=1}^{n} z_i \). We now have

\[
E[\var\{f(x) | \mathcal{X}^{(n)}, z^{(n)}\} | \mathcal{X}^{(n)}] = \frac{1}{n(n\omega + 1)} \left\{ \sum_{i=1}^{n} E(z_i^2 | \mathcal{X}^{(n)}) - nE(\bar{z}^2 | \mathcal{X}^{(n)}) \right\}
\]
\[
\leq \frac{1}{n(n\omega + 1)} \sum_{i=1}^{n} E(z_i^2 | \mathcal{X}^{(n)})
\]
\[
\leq \frac{1}{n(n\omega + 1)} \sum_{i=1}^{n} \frac{r_i}{b_i^2} \left( \frac{x - \mu_i}{b_i} \right),
\]

where the last inequality is obtained using equation (S.18). Using \( b_i \geq h(D_n/2)^{1/2} \) for \( i = 1, \ldots, n \) as before, we have

\[
E[\var\{f(x) | \mathcal{X}^{(n)}, z^{(n)}\} | \mathcal{X}^{(n)}] \leq \frac{a_n}{(n\omega + 1)h}. \tag{S.22}
\]

Combining equations (S.19) and (S.22) and putting the results back in equation (S.17), we have the result. □

### S.5 Proof of Theorem 3.9 and choice of \( \alpha \)

#### S.5.1 Proof of Theorem 4

Let \( \eta^{(n)} = (\eta_1, \ldots, \eta_n)^T \). Then, we have \( \Theta = \sum_{i=1}^{n} \pi_i \eta_i = \eta^{(n)^T} \pi^{(n)} \) where \( \pi^{(n)} = (\pi_1, \ldots, \pi_n)^T \sim \text{Dirichlet}(\omega, \ldots, \omega) \) given \( \mathcal{X}^{(n)} \), with \( \omega = \alpha + 1 \). We start out by observing that

\[
\var(\Theta | \mathcal{X}^{(n)}) = \var[E(\Theta | \eta^{(n)}, \mathcal{X}^{(n)}) | \mathcal{X}^{(n)}] + E[\var(\Theta | \eta^{(n)}, \mathcal{X}^{(n)}) | \mathcal{X}^{(n)}]. \tag{S.23}
\]

Let \( n \) be sufficiently large so that \( k > 2 - \gamma_0 \), since \( k \to \infty \) as \( n \to \infty \). For \( i = 1, \ldots, n \), let \( v_i = \var(\eta_i | \mathcal{X}^{(n)}) = \gamma_n \delta_i^2 / \{\nu_n(\gamma_n - 2)\} \), and \( \bar{v} = (1/n) \sum_{i=1}^{n} v_i \). Since \( E(\Theta | \eta^{(n)}, \mathcal{X}^{(n)}) = (1/n) \sum_{i=1}^{n} \eta_i \) and \( \eta_1, \ldots, \eta_n \) are conditionally independent given the data \( \mathcal{X}^{(n)} \), we have

\[
\var[E(\Theta | \eta^{(n)}, \mathcal{X}^{(n)}) | \mathcal{X}^{(n)}] = \frac{\bar{v}}{n}. \tag{S.24}
\]

Since the pseudo-posterior covariance matrix of \( \pi^{(n)} \) is \( \Sigma_{\pi} = V_n \{ (1 - C_n) I_n + C_n J_n \} \), we obtain that

\[
\var(\Theta | \eta^{(n)}, \mathcal{X}^{(n)}) = \frac{1}{n(n\omega + 1)} \sum_{i=1}^{n} (\eta_i - \bar{\eta})^2
\]
\[
= \frac{1}{n(n\omega + 1)} \left( \sum_{i=1}^{n} \eta_i^2 - n \bar{\eta}^2 \right). \tag{S.25}
\]
Thus, we have
\[ E(\eta_i^2 | X^{(n)}) = \mu_i^2 + \nu_i, \]
and multiplying both sides by \( \bar{\nu} / n \) yields
\[ E(\eta_i^2 | X^{(n)}) = (\bar{\nu}/n) + \bar{\mu}^2. \]
Putting these back in equation (S.25) we get that
\[ E[\text{var}\{\Theta | \eta^{(n)}(\mu), X^{(n)}\} | \mathcal{X}^{(n)}] = \frac{1}{n(n\omega + 1)} \left\{ \sum_{i=1}^{n} (\mu_i - \bar{\mu})^2 + (n - 1) \bar{\nu} \right\}. \] (S.26)

Combining the results of equations (S.24) and (S.26), putting them back in equation (S.23), and multiplying both sides by \( n \), we get the result. \( \square \)

S.5.2 Choice of \( \alpha \)

Suppose \( \sigma^2_{f_0} \) is the variance of the underlying true density \( f_0 \) satisfying Assumptions 3.1-3.3. Let \( S^2_{\mu} = (1/n) \sum_{i=1}^{n} (\mu_i - \bar{\mu})^2 \) and \( S^2 = (1/n) \sum_{i=1}^{n} (X_i - \bar{X})^2 \). We start out by observing that, \( EP_{f_0}(\mid S^2_{\mu} - S^2 \mid) \leq (1/n) EP_{f_0}(\sum_{i=1}^{n} (\mu_i - X_i + \bar{X} - \bar{\mu})(\mu_i + X_i - \bar{\mu} - \bar{X})) \leq (4/n) EP_{f_0}(\sum_{i=1}^{n} (\mid \mu_i - X_i \mid + | \bar{X} - \bar{\mu} |)) \) by the triangle inequality and the fact that \( | \mu_i |, | X_i | \leq 1 \) for \( i = 1, \ldots, n \). Since \( (\mu_i)_{i=1}^{n} \) are identically distributed and \( (X_i)_{i=1}^{n} \) are identically distributed, we have \( EP_{f_0}(\mid S^2_{\mu} - S^2 \mid) \leq 4(EP_{f_0}(\mid \mu_1 - X_1 \mid) + EP_{f_0}(\mid \bar{\mu} - \bar{X} \mid)) \). But \( EP_{f_0}(\mid \bar{\mu} - \bar{X} \mid) \leq (1/n) \sum_{i=1}^{n} EP_{f_0}(\mid \mu_i - X_i \mid) \) by the triangle inequality, from which it follows that \( EP_{f_0}(\mid \bar{\mu} - \bar{X} \mid) \leq EP_{f_0}(\mid \mu_1 - X_1 \mid) \) since \( (\mu_i - X_i)_{i=1}^{n} \) are identically distributed. Thus, we have
\[ EP_{f_0}(\mid S^2_{\mu} - S^2 \mid) \leq 8 EP_{f_0}(\mid \mu_1 - X_1 \mid) \]
\[ \leq 8\xi_1(f_0) \frac{k^2}{n^2} + o \left( \frac{k^2}{n^2} \right), \] (S.27)
using Lemma 3.4. Since \( S^2 \to \sigma^2_{f_0} \) in \( P_{f_0} \)-probability as \( n \to \infty \) by the weak law of large numbers, we get that \( S^2_{\mu} \to \sigma^2_{f_0} \) in \( P_{f_0} \)-probability as \( n \to \infty \) as well. Equating the pseudo-posterior variance of \( n^{1/2} \Theta \) from Theorem 3.9 with \( \sigma^2_{f_0} \), we get after some rearranging,
\[ \omega + \frac{1}{n} = \frac{S^2_{\mu} + \{(n-1)\bar{\nu}/n\}}{\sigma^2_{f_0} - \bar{\nu}}. \] (S.28)
As \( n \to \infty \), since each \( \lambda_i \) satisfies \( \lambda_i^2 - h^2 \to 0 \) in \( P_{f_0} \)-probability for \( i = 1, \ldots, n \) using Lemma 3.4, \( \bar{\nu} \) is well approximated by \( (\gamma_0 \nu_\infty)^{-1}(\gamma_0 \delta_0^2) \) in the sense that \( \{\bar{\nu} - (\gamma_0 \nu_\infty)^{-1}(\gamma_0 \delta_0^2)\} \to 0 \) in \( P_{f_0} \)-probability as \( n \to \infty \). In particular, we have \( \bar{\nu} \to 0 \) in \( P_{f_0} \)-probability. Combining these with the fact that \( S^2_{\mu} \to \sigma^2_{f_0} \) in \( P_{f_0} \)-probability as \( n \to \infty \), we obtain,
\[ \omega = \alpha + 1 \approx 1 + \frac{\bar{\nu}}{\sigma^2_{f_0}} - \frac{1}{n}. \] (S.29)
Since \( 1/n \) can be asymptotically neglected in comparison to \( \bar{\nu}/\sigma^2_{f_0} \) owing to the fact that \( k^2/n \to 0 \) as \( n \to \infty \), equation (S.29) implies the choice of \( \alpha \) as described in equation (13).
S.6 Extension of Theorem 3.5 to multivariate case

In the multivariate case, carrying out a detailed study of the neighborhood mean and variance proved more challenging than in the univariate scenario. For this reason, we did not take the same path as described in Sections S.1-S.2, instead relying on simpler inequalities to prove results. We assume multivariate analogues of Assumptions 3.1-3.3 on the underlying continuous true density $f_0$, assumed to be supported on $[0,1]^p$ and having bounded gradient.

Suppose $X_1, \ldots, X_n$ are independent and identically distributed random variables generated from the density $f_0$. For $i = 1, \ldots, n$, recall the definitions of $\mu_n^{(i)} = \mu_i$ and $\Lambda_n^{(i)} = \Lambda_i$ from equation (8):

$$
\mu_i = \frac{\nu_0}{\nu_n} \mu_0 + \frac{k}{\nu_n} \hat{X}_i, \quad \Lambda_i = \frac{\nu_n + 1}{\nu_n(\gamma_n - p + 1)} \Psi_i,
$$

where we have suppressed the dependence of $\mu_n^{(i)}, \Lambda_n^{(i)}$ and $\Psi_n^{(i)}$ on $n$ and expressed them as $\mu_i, \Lambda_i$ and $\Psi_i$, respectively. The expression for $\Psi_i$ is as described in Algorithm 1.

We want to show that, $\hat{f}_n(x) = (1/n) \sum_{i=1}^n t_{\gamma_n-p+1}(x; \mu_i, \Lambda_i) \to f_0(x)$ in $P_{f_0}$-probability as $n \to \infty$ for any $x \in (0,1)^p$, where $\hat{f}_n(x)$ is as described in equation (8). We first prove two propositions involving successive mean value type approximations to $\hat{f}_n(x)$ in the same spirit as outlined in the Appendix of the main document, which will imply the final result.

To that end, we introduce some notation with accompanying technical details which will be used hereafter. We define the Frobenius norm of the $p \times p$ matrix $A$ with real-valued entries by $\| A \|_F = \{ \text{tr}(A^T A) \}^{1/2}$. We observe that, for a vector $v \in \mathbb{R}^p$, one has $\| vv^T \|_F = \| v \|_2^2$ where $\| a \|_2 = (a^T a)^{1/2}$ is the Euclidean norm of $a$. For two symmetric $p \times p$ matrices $A$ and $B$, we say that $A \succeq B$ if $A - B$ is positive semi-definite, that is $x^T (A-B)x \geq 0$ for all $x \in \mathbb{R}^p, x \neq 0_p$ where $0_p = (0, \ldots, 0)^T$. For a matrix $A_*$, let the eigenvalues of $A_*$ be denoted by $e_1(A_*), \ldots, e_p(A_*)$, arranged such that $e_1(A_*) \geq \ldots \geq e_p(A_*)$. If $A \succeq B$, then it follows by the min-max theorem (Teschl, 2009) that, for each $j = 1, \ldots, p$, we have $e_j(A) \geq e_j(B)$.

In particular, we have $| A | \geq | B |$ and $\| A \|_F \geq \| B \|_F$. We now state the two propositions, with accompanying proofs, before stating the final theorem.

**Proposition S.6.1.** Fix $x \in (0,1)^p$. Let $f_1(x) = n^{-1} \sum_{i=1}^n t_{\gamma_n-p+1}(x; \mu_i, \Lambda_i)$. Also, let $k = o(n^{i_1})$ with $i_1 = 2/(p^2 + p + 2)$ and $\nu_0 = o(n^{-1/pk^{(1/p)+1}})$. Then, we have $E_{P_{f_0}}( | \hat{f}_n(x) - f_1(x) | ) \to 0$ as $n \to \infty$.

**Proof.** Since the $(\Lambda_i)_{i=1}^n$ are identically distributed and $(\mu_i)_{i=1}^n$ are identically distributed, we have $E_{P_{f_0}}( | \hat{f}_n(x) - f_1(x) | ) \leq E_{P_{f_0}}( | t_{\gamma_n-p+1}(x; \mu_1, \Lambda_1) - t_{\gamma_n-p+1}(x, X_1, \Lambda_1) | )$. The
multivariate mean value theorem now implies that

\[
E_{P_0}( | \hat{f}_n(x) - f_1(x) | ) \leq E_{P_0} \left\{ | \Lambda_{i} |^{-1/2} | t'_{\gamma_{n-p+1}}(x; \mu, I_{p}) ||_2 \Lambda_{i}^{-1/2} (X_1 - \mu) \right\},
\]

(S.30)

where \( t'_{\gamma_{n-p+1}}(x; \mu, I_{p}) = [\nabla \{ t_{\gamma_{n-p+1}}(x; \mu, I_{p}) \}]_\xi \) for some \( \xi \) in the convex hull of \( \Lambda_{i}^{-1/2} (x - X_1) \) and \( \Lambda_{i}^{-1/2} (x - \mu) \). Using standard results and the min-max theorem, we have \( | \Lambda_{i}^{-1/2} (X_1 - \mu) ||_2 \leq || \Lambda_{i}^{-1/2} ||_F X_1 - \mu ||_2 \). If we let \( H_n = H = \{ \nu_{n} (\gamma_n - p + 1) \}^{-1} (\nu_{n} + 1) \Psi_0 = h^2 I_p \) where \( h^2 = \{ \nu_{n} (\gamma_n - p + 1) \}^{-1} \{ (\nu_{n} + 1) (\gamma_o - p + 1) \} \delta_0 \) following the choice of \( \Psi_0 \) from Section 2.3, then it is clear that \( \Lambda_{i} \geq H \). Therefore, we have \( | \Lambda_{i}^{-1/2} (X_1 - \mu) \right||_2 \leq \| H^{-1/2} \|_F = h^{-1/2} \) and \( | X_1 - \mu \right||_2 \leq R_1 + \{ \nu_{n}^{-1} (1 + \mu_0 \| \nu \|_2) \nu_0 \} \) where \( R_1 = \| X_1 - X_{1[k]} \|_2 \). Using Theorem 2.4 from Biau & Devroye (2015), we have \( E_{P_0}(R_1) \leq \{ E_{P_0}(R_1^2) \}^{1/2} \leq d_p (k/n)^{1/p} \) where \( d_p = C_p^{-1/p} (2.5)^{p-1} (1 + p^{1/2}) \) for \( p \geq 2 \) and \( C_p = \int_{\| x \|_2 \leq 1} dx_1 \) is the volume of the unit ball in \( \mathbb{R}^p \). We also have \( | \Lambda_{i}^{-1/2} \|_F \leq H \|^{-1/2} \leq h^{-p} \). Finally, simple calculations yield that \( | t'_{\gamma_{n-p+1}}(x; 0, I_{p}) \right||_2 \leq L_{1,n,p} \) where \( L_{1,n,p} > 0 \) satisfies \( L_{1,n,p} \rightarrow (2\pi)^{-p/2} e^{-1/2} \) as \( n \rightarrow \infty \). Plugging all these back in equation (S.30), we obtain a finite constant \( L_{2,n,p} > 0 \) such that

\[
E_{P_0}( | \hat{f}_n(x) - f_1(x) | ) \leq L_{2,n,p} (n^{-i_2} k (p^{2+p^2}/2p) + o \{ (n^{-i_2} k)^{(2^p+p^2)/(2p)} \}),
\]

(S.31)

which goes to 0 as \( n \rightarrow \infty \), completing the proof.

We now provide the second mean value approximation which approximates the random bandwidth matrix \( \Lambda_{i} \) in \( f_1(x) \) by \( H \) for each \( i = 1, \ldots, n \).

**Proposition S.6.2.** Fix \( x \in (0, 1)^p \). Let \( f_K(x) = n^{-1} \sum_{i=1}^{n} t_{\gamma_{n-p+1}}(x; X_i, H) \). Also, let \( k = o(n^{i_2}) \) with \( i_2 = 4/p + 2 \) and \( \nu_0 = o(n^{-2/p} k^{2/p+1}) \). Then, we have \( E_{P_0}( | \hat{f}_1(x) - f_K(x) | ) \rightarrow 0 \) as \( n \rightarrow \infty \).

**Proof.** Using the identically distributed properties of \( (\Lambda_{i})_{i=1}^{n} \) and \( (X_i)_{i=1}^{n} \), we obtain \( E_{P_0}( | \hat{f}_1(x) - f_K(x) | ) \leq E_{P_0}( | t_{\gamma_{n-p+1}}(x; X_1, \Lambda_1) - t_{\gamma_{n-p+1}}(x; X_1, H) | ) \). Using the multivariate mean value theorem, we obtain that

\[
E_{P_0}( | t_{\gamma_{n-p+1}}(x; X_1, \Lambda_1) - t_{\gamma_{n-p+1}}(x; X_1, H) | ) \leq E_{P_0}( | M_1 || F \| \Lambda_1 - H \|_F \),
\]

(S.32)

where \( M_1 = [\partial t_{\gamma_{n-p+1}}(x; X_1, \Sigma)]/\partial \Sigma \Sigma_0 \) with \( \Sigma_0 \) in the convex hull of \( \Lambda_1 \) and \( H \). Since \( \Lambda_1 \geq H \), we immediately have \( \Sigma_0 \geq H \) as well. Using the definitions of \( \Lambda_1 \) and \( H \), we have \( | \Lambda_1 - H \|_F \leq \{ \nu_0 (\gamma_n - p + 1) \}^{-1} (\nu_0 + 1) \{ | \sum_{j \in N}(X_j - X_1)(X_j - X_1)^{\top} \|_F + \nu_0^{-1} k \nu_0 \| X_1 X_1^{\top} \|_F \} \). Therefore, we get \( E_{P_0}( | \Lambda_1 - H \|_F ) \leq E_{P_0}(R_1^2 + o(n^{-2/p} k^{2/p})) \). Using Theorem 2.4
from Biau & Devroye (2015), we get that \( E_{P_{f_{0}}} (R^2_{p}) \leq d^2_{p} (k/n)^{2/p} \) where \( d_p \) is as in Proposition S.6.1. We now observe that, \( t_{\gamma_i-p+1}(x; X_1, \Sigma) \leq c_{p,\gamma_i-p+1} \mid \Sigma \mid^{-1/2} \leq c_{p,\gamma_i-p+1} \mid H \mid^{-1/2} = h^{-p} c_{p,\gamma_i-p+1} \) for any \( p \times p \) positive definite \( \Sigma \), where \( c_{p,\beta} = (\pi \beta)^{-p/2} (\Gamma(\beta/2))^{-1} \Gamma((\beta + p)/2) \) for \( p \geq 1, \beta > 0 \). It is immediate that \( c_{p,\beta} \rightarrow (2\pi)^{-p/2} \) as \( \beta \rightarrow \infty \) for any \( p \geq 1 \). Taking partial derivatives of \( \log(t_{\gamma_i-p+1}(x; X_1, \Sigma)) \) with respect to \( \Sigma \) evaluated at \( \Sigma_0 \) and taking Frobenius norm of both sides, we obtain that \( || t_{\gamma_i-p+1}^{-1}(x; X_1, \Sigma_0) M_1 ||_F \leq h^{-2}(\gamma_i + 1) \) for sufficiently large \( n \). This immediately implies that \( || M_1 ||_F \leq h^{-(p+2)} c_{p,\gamma_i-p+1}(\gamma_i + 1) \) for sufficiently large \( n \), since \( \nu_0 = o(n^{-2/p}k(2/p)^{+1}) \). Plugging all these back in equation (S.32), we obtain for sufficiently large \( n \), a finite \( L_{3,n,p} > 0 \) such that
\[
E_{P_{f_{0}}} (| \hat{f}_1(x) - f_K(x) |) \leq L_{3,n,p}(n^{-i_2}k((p+2)^2/(2p)) + o\{(n^{-i_2}k((p+2)^2/(2p))\},
\]
which goes to 0 as \( n \rightarrow \infty \), proving the proposition.

Since \( i_1 \leq i_2 \) for all \( p \geq 2 \), we require \( k = o(n^{i_1}) \) for both Propositions S.6.1 and S.6.2 to hold, along with \( \nu_0 = o(n^{-2/p}k(2/p)^{+1}) \). Since \( E_{P_{f_{0}}} (| \hat{f}_n(x) - f_K(x) |) \leq E_{P_{f_{0}}} (| \hat{f}_n(x) - f_1(x) |) + E_{P_{f_{0}}} (| f_1(x) - f_K(x) |) \) by the triangle inequality and \( f_K(x) \rightarrow f_0(x) \) in \( P_{f_{0}} \)-probability following the arguments of Section S.3, we state our final theorem on weak consistency of \( \hat{f}_n(x) \) below.

**Theorem S.6.3.** Fix \( x \in (0,1)^p \) for \( p \geq 2 \). Let \( k = o(n^{i_1}) \) with \( i_1 = 2/(p^2 + p + 2) \) and \( \nu_0 = o(n^{-2/p}k((2/p)^{+1}) \). Then, \( \hat{f}_n(x) \rightarrow f_0(x) \) in \( P_{f_0} \)-probability as \( n \rightarrow \infty \).

### S.7 Cross-validation

Consider independent and identically distributed data \( X_1, \ldots, X_n \in \mathbb{R}^p \sim f \) with \( f \) having the nearest neighbor-Dirichlet process formulation. In the univariate setting, the prior for each of the neighborhood specific parameters is \( \theta_i = (\eta_i, \sigma_i^2) \sim \text{NIG}(\mu_0, \sigma_i^2/\nu_0, \gamma_0/2, \gamma_0 \delta_0^2/2) \). The equivalent prior in the general multivariate setting following Sections 2.2 and 2.3 is \((\eta_i, \Sigma_i) \sim \text{NIW}(\mu_0, \Sigma_i/\nu_0, \gamma_0, \Psi_0) \) where \( \Psi_0 = (\gamma_0 \delta_0^2) I_p \). We use the pseudo-posterior mean in equations (8) and (9) to compute leave-one-out log likelihoods \( \mathcal{L}(\delta_0^2) \) for different choices of the hyperparameter \( \delta_0^2 \), choosing \( \delta_0^2_{\text{CV}} = \arg\sup_{\delta_0^2} \mathcal{L}(\delta_0^2) \) to maximize this criteria. The details of the computation of \( \mathcal{L}(\delta_0^2) \) for a fixed \( \delta_0^2 \) are provided in Algorithm 2.

In Algorithm 2, the nearest neighborhood specification for each \( X^{-i} \) is different. However, we bypass this computation by initially forming a neighborhood of size \((k+1)\) using the entire data for each data point and storing the respective neighborhood means and variances. We describe the approach for univariate data. Suppose for \( X_i \), the \((k+1)\)-nearest neighbors are
• Consider data \( \mathcal{X}^{(n)} = (X_1, \ldots, X_n) \) where \( X_i \in \mathbb{R}^p, p \geq 1 \). Fix the number of neighbors \( k \) and other hyperparameters \( \mu_0, \nu_0, \gamma_0 \).

• For \( i \in \{1, \ldots, n\} \), consider the dataset leaving out the \( i \)th data point, given by \( \mathcal{X}^{-i} = (X_1, \ldots, X_{i-1}, X_{i+1}, \ldots, X_n) \). Compute the pseudo-posterior mean density estimate at \( X_i \) using \( \mathcal{X}^{-i} \) and equation (9) when \( p = 1 \), or equation (8) when \( p \geq 2 \). Write this as \( \mathcal{L}^{(i)}(\delta_0^2) = \hat{f}^{-i}(X_i) \). Finally, compute the leave-one-out log likelihood given by

\[
\mathcal{L}(\delta_0^2) = \frac{1}{n} \sum_{i=1}^{n} \log \{ \mathcal{L}^{(i)}(\delta_0^2) \}. \tag{S.34}
\]

• For \( \delta_0^2 \geq 0 \), obtain \( \delta_0^2, \text{CV} = \arg \sup_{\delta_0^2} \mathcal{L}(\delta_0^2). \)

**Algorithm 2:** Leave-one-out cross-validation for choosing the hyperparameter \( \delta_0^2 \) in nearest neighbor-Dirichlet process method.

given by \( \mathcal{N}_i = \{ X_{i[1]}, \ldots, X_{i[k+1]} \} \), arranged in increasing order according to their distance from \( X_i \) with \( X_{i[1]} = X_i \). Define the neighborhood mean \( m_i = \{1/(k+1)\} \sum_{j \in \mathcal{N}_i} X_{ij} \) and the neighborhood variance \( s_i^2 = \{ \sum_{j \in \mathcal{N}_i} X_{ij}^2 \}/(k+1) - m_i^2 \). Then, to form a \( k \)-nearest neighborhood for the new data \( \mathcal{X}^{-i} \), a single pass over the initial neighborhoods \( \mathcal{N}_i \) is sufficient to update the new neighborhood means and variances. Below, we describe the update for the neighborhood means \( m_{j^{(-i)}} \) and variances \( s_{j^{(-i)}}^2 \) for \( j = 1, \ldots, n \) and \( j \neq i \), considering the data \( \mathcal{X}^{-i} \). For \( j = 1, \ldots, n \) and \( j \neq i \), we have,

\[
m_{j^{(-i)}} = \begin{cases} 
(1/k)\{(k+1)m_j - X_{j[k+1]}\} & \text{if } X_i \notin \mathcal{N}_j \\
(1/k)\{(k+1)m_j - X_i\} & \text{if } X_i \in \mathcal{N}_j,
\end{cases}
\]

\[
s_{j^{(-i)}}^2 = \begin{cases} 
\delta_j^2 - \{(k+1)/k\}(m_j - X_{j[k+1]}^2) & \text{if } X_i \notin \mathcal{N}_j \\
\delta_j^2 - \{(k+1)/k\}(m_j - X_i)^2 & \text{if } X_i \in \mathcal{N}_j.
\end{cases} \tag{S.35}
\]

The corresponding multivariate update for \( m_{j^{(-i)}} \) is the same as in equation (S.36), and that of the neighborhood covariance matrix \( S_{j^{(-i)}} \) is given by

\[
S_{j^{(-i)}} = \begin{cases} 
S_j - \{(k+1)/k\}(m_j - X_{j[k+1]})(m_j - X_{j[k+1]^T}) & \text{if } X_i \notin \mathcal{N}_j \\
S_j - \{(k+1)/k\}(m_j - X_i)(m_j - X_i^T) & \text{if } X_i \in \mathcal{N}_j.
\end{cases} \tag{S.36}
\]

**S.8 Algorithm with Gaussian kernels for univariate data**

Suppose we have independent and identically distributed observations \( \mathcal{X}^{(n)} = (X_1, \ldots, X_n) \) from the density \( f \), where \( X_i \in \mathbb{R}, i = 1, \ldots, n \). In the nearest neighbor-Dirichlet process
framework for univariate data with the Gaussian kernel $\phi(\cdot; \eta, \sigma^2)$, neighborhood specific parameters $\theta_i = (\eta_i, \sigma^2_i) \sim \text{NIG}(\mu_0, \sigma^2_0/\nu_0, \gamma_0/2, \gamma_0\delta_0^2/2)$ apriori independently for $i = 1, \ldots, n$. Monte Carlo samples for the estimated density at any point $x$ can be generated following the steps of Algorithm 3.

- **Step 1:** Compute the neighborhood $\mathcal{N}_i$ for data point $X_i$ with $X_{i[1]} = X_i$, according to distance $d(\cdot, \cdot)$ with $(k-1)$ nearest neighbors.
- **Step 2:** Update the parameters for neighborhood $\mathcal{N}_i$ to $(\mu_n^{(i)}, \nu_n, \gamma_n, \delta_n^{(i)2})$ where
  
  $\nu_n = \nu_0 + k, \gamma_n = \gamma_0 + k, \mu_n^{(i)} = \nu_0^{-1}\mu_0 + k\nu_n^{-1}X_i, X_i = k^{-1}\sum_{j \in \mathcal{N}_i} X_j$ and

  $\delta_n^{(i)2} = \gamma_n^{-1}\{\gamma_0\delta_0^2 + \sum_{j \in \mathcal{N}_i} (X_j - X_i)^2 + k\nu_0^{-1}(\mu_0 - X_i)^2\}$.
- **Step 3:** To compute the $t$th Monte Carlo sample of $f(x)$, sample Dirichlet weights $\pi^{(t)} \sim \text{Dirichlet}(\alpha + 1, \ldots, \alpha + 1)$ and neighborhood-specific parameters $(\eta_i^{(t)}, \sigma_i^{(t)2}) \sim \text{NIG} \left( \mu_n^{(i)}, \sigma_n^{(i)2}/\nu_n, \gamma_n/2, \gamma_n\delta_n^{(i)2}/2 \right)$ independently for $i = 1, \ldots, n$, and set

  \[
  f^{(t)}(x) = \sum_{i=1}^{n} \pi_i^{(t)} \phi(x; \eta_i^{(t)}, \sigma_i^{(t)2}). \tag{S.37}
  \]

**Algorithm 3:** Nearest neighbor-Dirichlet process algorithm to obtain Monte Carlo samples from the pseudo-posterior of $f(x)$ given univariate data $\mathcal{X}^{(n)}$ with Gaussian kernel and normal-inverse gamma prior.

### S.9 Inverse Wishart Parametrization

The parametrization of the inverse Wishart density defined on the set of all $p \times p$ matrices with real entries used in this article is given as follows. Suppose $\gamma > p - 1$ and $\Psi$ is a $p \times p$ positive definite matrix. If $\Sigma \sim \text{IW}_p(\gamma, \Psi)$, then $\Sigma$ has the following density function:

\[
g(\Sigma) = \begin{cases} 
\frac{1}{2^{\gamma/2}P(\gamma/2)^{\gamma/2}\text{etr}(-\Psi\Sigma^{-1}/2)} |\Sigma|^{-(\gamma+p+1)/2} \text{etr}(-\Psi\Sigma^{-1}/2) & \text{if } \Sigma \text{ is positive definite,} \\
0 & \text{otherwise},
\end{cases}
\]

where $\Gamma_p(\cdot)$ is the multivariate Gamma function defined by $\Gamma_p(a) = \pi^{p(p-1)/4} \prod_{j=1}^{p} \Gamma[a + \{(1-j)/2\}]$ for $a \geq (p-1)/2$ and the function $\text{etr}(A) = \exp\{\text{tr}(A)\}$ for a square matrix $A$. 

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**S.15**