Abstract

In this article, we introduce the BNPqte R package which implements the Bayesian nonparametric approach of Xu et al. (2018) for estimating quantile treatment effects in observational studies. This approach provides flexible modeling of the distributions of potential outcomes, so it is capable of capturing a variety of underlying relationships among the outcomes, treatments and confounders and estimating multiple quantile treatment effects simultaneously. Specifically, this approach uses a Bayesian additive regression trees (BART) model to estimate the propensity score and a Dirichlet process mixture (DPM) of multivariate normals model to estimate the conditional distribution of the potential outcome given the estimated propensity score. The BNPqte R package provides a fast implementation for this approach by designing efficient R functions for the DPM of multivariate normals model in joint and conditional density estimation. These R functions largely improve the efficiency of the DPM model in density estimation, compared to the popular DPpackage. BART-related R functions in the BNPqte R package are inherited from the BART R package with two modifications on variable importance and split probability. To maximize computational efficiency, the actual sampling and computation for each model are carried out in C++ code. The Armadillo C++ library is also used for fast linear algebra calculations.

Keywords: Bayesian additive regression trees (BART), Bayesian nonparametric (BNP), Dirichlet process mixture (DPM), Bayesian bootstrap, propensity score (PS), quantile treatment effect (QTE), R, C++, Rcpp, RcppArmadillo, OpenMP.

1. Introduction

Estimating causal effects is the objective of causal inference. Commonly used average treatment effects are often of less interest when the distribution of the outcome is skewed or multi-modal, and quantile treatment effects become more sensible and desirable. Under the potential outcome framework (Rubin (1978), Splawa-Neyman et al. (1990)) and the binary treatment setting, the \( p \)th quantile treatment effect (QTE) is defined as the difference between the \( p \)th population quantiles of the treated and untreated potential outcome distributions, i.e.,

\[
F_{1}^{-1}(p) - F_{0}^{-1}(p), \quad p \in (0, 1),
\]

where \( F_{t}^{-1}(p), t \in \{0, 1\} \), is the \( p \)th quantile for the cumulative distribution function (CDF) \( F_{t}(y) \) of the potential outcome \( Y(t) \) with \( Y(1) \) and \( Y(0) \) denoting the treated and untreated potential outcomes, respectively. There has been extensive work from both the frequentist and Bayesian perspectives (Chernozhukov and Hansen (2005), Zhang et al. (2012), Hoshino...
(2013), Linn et al. (2014), Karabatsos and Walker (2015), Díaz (2017)) on estimating QTEs for observational data. They typically develop their own identifying assumptions and many require different efficient estimating equations for different quantiles.

Xu et al. (2018) propose a fully Bayesian nonparametric (BNP) approach to estimate QTEs under a set of mild identifying assumptions. Specifically, they model the distributions of potential outcomes by first estimating the propensity score (PS) using a probit Bayesian additive regression trees (BART) model (Chipman et al. (2010)), then modeling the conditional distribution of the potential outcome given a BART posterior sample of the PS in each treatment group separately using a Dirichlet process mixture (DPM) of multivariate normals model (Müller et al. (1996)) and finally marginalizing the estimated conditional distribution over the population distribution of the confounders using Bayesian bootstrap (Rubin (1981)). The recovery of the distributions of potential outcomes enables the inference on any functionals of the distributions, including estimating multiple QTEs simultaneously. Additionally, the BNP methods provide a flexible approach to capture a wide range of relationships among the outcomes, treatments and confounders. Furthermore, modeling the distribution of the potential outcome conditional on the PS rather than on the confounders avoids potentially complex high-dimensional modeling and the two-stage approach of modeling the PS and the conditional distribution of the potential outcome on the PS separately averts the model feedback issue discussed in Zigler et al. (2013). Finally, the use of posterior samples of the PS rather than a point estimator of the PS propagates the uncertainty in the estimated PS. For convenience, throughout this article, we refer to this BNP approach as the BART-DPM approach.

On the Comprehensive R Archive Network (CRAN), there are many R packages implementing either the frequentist or Bayesian methods for estimating the average treatment effects, including (but not limited to) ipw (van der Wal et al. (2011)), pcalg (Kalisch et al. (2012)), CausalImpact (Brodersen et al. (2015)) and causaleffect (Tikka and Karvanen (2018)). However, only two R packages, qte (Callaway 2019) and Counterfactual (Chen et al. 2020), to our knowledge, are designed to estimate QTEs and the methods implemented are all frequentist. We bridge the gap by implementing the BART-DPM approach, a fully Bayesian nonparametric approach, in the BNPqte R (R Core Team 2017) package.

The BART-DPM approach includes the application of BART and DPM models. Currently, there are four CRAN packages available for the implementation of BART: bartMachine (Kapelner and Bleich (2016)), BayesTree (Chipman and McCulloch 2016), dbarts (Dorie 2020) and BART (Sparapani et al. (2021)). The bartMachine R package is written in JAVA, but the R to JAVA interface can be challenging to deal with as R is mainly written in C++ and Fortran. The BayesTree and dbarts (a clone of BayesTree interface) R packages are written in C++, but there are no future improvements planned for BayesTree so the packages following it, such as dbarts, are also strongly affected. The BART R package also chooses C++ as the main programming language, because both of R and C++ are object-oriented languages and seamless R and C++ integration can be provided by the Rcpp (Eddelbuettel and François (2011)) packages. Moreover, BART is actively maintained. As such, in the BNPqte package, we adopt BART (specifically, its functions wbart(), pbart() and lbart()) for the implementation of BART models. Slight modifications are applied to these functions to adjust for the data with mixed-type covariates and also to take into account the optimal posterior contraction for the BART prior, the latter of which is discussed in Ročková and Saha (2019).

Exact posterior distributions of DPM models are analytically intractable, so the implement-
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Implementations of DPM models heavily rely on the MCMC chain Monte Carlo (MCMC) samplers for the posterior distributions of DPM models. There are several CRAN packages implementing DPM models with different sampling algorithms and different purposes. DPpackage (Jara et al. (2011)), an archived CRAN package, implements Algorithm 4 and Algorithm 8 of Neal (2000), the former of which is essentially the "no-gaps" algorithm of MacEachern and Müller (1998). The dirichletprocess (Ross et al. 2020) R package also employs these two samplers but with a different purpose. Both the two samplers are based on the Pólya urn scheme and explore the marginal parameter space where some parameters are integrated out. Although these two samplers mitigate the slow mixing issue of the algorithm proposed in Escobar and West (1995), they do not have the direct access to the full posterior distribution and therefore require complicated algorithms to obtain it. Ishwaran and James (2001) consider a truncation approximation based on a mixture of Dirichlet process and suggest a blocked Gibbs sampling method that directly samples from the full posterior distribution of the truncated DPM model. This sampler leads to a rapidly mixing Markov chain and also permits direct inference on the full posterior distribution of the truncated DPM model. The PReMinM (Liverani et al. 2015) R package implements this sampler, but the application of DPM models in PReMinM is dedicated to the profile regression, which cannot be directly applied to other tasks such as density estimation which is relevant to the work here. Out of the consideration of the computational efficiency and the convergence speed of Markov chains, we implement the blocked Gibbs sampler of Ishwaran and James (2001) and Algorithm 8 (with \( m = 1 \)) of Neal (2000) in the BNPqte package for the DPM of multivariate normals model with application to nonparametric density estimation.

This article is organized as follows. In Section 2, we briefly review BART models and illustrate the modifications that we make for the R functions inherited from the BART package with a simulated example. In Section 3, we describe the DPM of multivariate normals model and two MCMC samplers implemented in the BNPqte package. We also demonstrate the usage of the DPM-related R functions in density estimation with simulated examples in Section 3. In Section 4, we introduce the BART-DPM approach for estimating QTEs, which is the focus of the BNPqte package, and present the usage of the BNPqte package in QTE estimation with a simulated example from Xu et al. (2018). We investigate the convergence of Markov chains from DPM models in Section 5 and finally conclude this article with a summary in Section 6. More computational details are provided in Appendix.

2. BNP Regression with BART Models

BART, built on the Bayesian classification and regression tree algorithm (Chipman et al. (1998)), is a Bayesian approach to nonparametric function estimation and inference using a sum of trees. Since Chipman et al. (2010), BART has been widely studied, including extensions to generalized regression and high-dimensional data, applications to variable selection and causal inference, theoretical studies and more. In this section, we first review the BART models for continuous and binary responses, BART-based variable importance and recent theoretical results, which are the implemented specification of BART in the BNPqte package, and then illustrate the usage of BART-related R functions with a simulated example.
2.1. BART Models Specification

Consider the regression problem of making inference about an unknown function $f_0$ that predicts a continuous response $Y_i$ using a $p$-dimensional vector of predictors $x_i = (x_{i1}, \ldots, x_{ip})^\top$ $(1 \leq i \leq n)$, 

$$Y_i = f_0(x_i) + \epsilon_i, \quad \epsilon_i \iid \text{Normal}(0, \sigma^2).$$  
(2)

BART models $f_0$ by a sum of $M$ Bayesian regression trees and can be expressed as 

$$f(x_i) = \sum_{m=1}^M g(x_i; T_m, \mu_m),$$  
(3)

where $g(x_i; T_m, \mu_m)$ is the output of $x_i$ from a single regression tree. Each $g(x_i; T_m, \mu_m)$ is determined by the binary tree structure $T_m$ that consists of a set of splitting rules and a set of terminal nodes and the vector of parameters $\mu_m = (\mu_{m,1}, \ldots, \mu_{m,b_m})$ associated with each of the $b_m$ terminal nodes of $T_m$, such that $g(x_i; T_m, \mu_m) = \mu_{m,l}$ if $x_i$ is associated with the $l$th terminal node of the tree $m$.

The prior of BART is specified for three components: (1) the $M$ independent trees structures $\{T_m\}_{m=1}^M$, (2) the parameters $\{\mu_m\}_{m=1}^M$ associated with the terminal nodes given $\{T_m\}_{m=1}^M$, and (3) the error variance $\sigma^2$ that is independent with the former two. A regularization prior is placed on the ensemble structure $\{T_m\}_{m=1}^M$. It consists of a Bernoulli distribution with probability 

$$p_{\text{split}}(d) = \frac{\gamma}{(1 + d)^\beta}, \quad \gamma \in (0, 1), \ \beta \in (0, \infty),$$  
(4)

for splitting a node at depth $d$ ($d \in \{0, 1, \ldots\}$) into two child nodes and two discrete uniform distributions for selecting a split variable and a split value given the selected split variable. This regularization prior keeps an individual tree from being too influential, thereby improving the overall fit and avoiding potential overfitting problems. Data-informed conjugate normal and inverse gamma priors are used for $\mu_m$’s and $\sigma^2$, respectively.

The posterior distribution is sampled through a Metropolis-within-Gibbs sampler (Hastings (1970), Geman and Geman (1984)) which uses Bayesian backfitting (Hastie et al. (2000)) to update each tree iteratively. Estimation of $f_0(x_i)$ is the average of BART posterior samples of $f_{\text{BART}}(x_i)$ after a burn-in period. More details of the BART prior, posterior and estimation computation can be found in the original BART paper (Chipman et al. (2010)).

The continuous BART model (3) has been extended to a variety of regression models for non-continuous responses, including probit BART (Chipman et al. (2010)) and logit BART (Sparapani et al. (2021)) for binary responses, which along with continuous BART, are the three BART models implemented in the BNPqte package.

Probit BART and logit BART specify 

$$P(Y_i = 1 \mid x_i) = H[f_{\text{BART}}(x_i)],$$  
(5)

where $f_{\text{BART}}(x_i)$ is the sum-of-trees function in (3) and $H$ is the link function with the probit link for probit BART and the logistic link for logit BART. Both of the models assign the same prior to the ensemble structure and the parameters of the terminal nodes, i.e., $\{T_m, \mu_m\}_{m=1}^M$, as continuous BART, but $\sigma^2$ is fixed due to identifiability.
Probit BART uses the data augmentation approach of Albert and Chib (1993) to adapt the Bayesian backfitting sampler of continuous BART. Specifically, a latent variable $Z_i$ such that $Y_i = 1(Z_i > 0)$ is first introduced for each response variable $Y_i$ and can be imputed by sampling from the full conditional distribution of $Z_i$ given $Y_i$ and other parameters at each iteration of the MCMC algorithm. The full conditional distribution essentially is a truncated normal distribution. The imputed $Z_i$’s are then modeled by the continuous BART model with $\sigma^2 = 1$, so the MCMC algorithm can be completed by performing the Bayesian backfitting algorithm of the continuous BART model on the imputed $Z_i$’s.

Logit BART also introduces latent $Z_i$’s but assumes them to follow a logistic distribution which has a heavier tail than a normal distribution, thereby improving the estimation for extreme $P(Y_i = 1|X_i)$. The latent $Z_i$’s are sampled using the technique of Gramacy et al. (2012) and conditional on the imputed $Z_i$’s, the continuous BART model with given heteroskedastic variance $\sigma_i^2$’s are fitted on $Z_i$’s, where $\sigma_i^2$’s are obtained by the method of Robert (1995). Details of the computation for probit and logit BART can be found in Sparapani et al. (2021). Though both probit BART and logit BART can be applied to the binary regression problem, it is important to recognize that probit BART is more computationally efficient than logit BART.

2.2. BART-Based Variable Importance

BART has also been applied to variable selection (Bleich et al. (2014), Linero (2018), Liu et al. (2018), Luo and Daniels (2021)). The BNPqte package provides five types of BART variable importance measures which can be used for variable selection; three of them are inherited from the BART package.

The three variable importance measures provided by the BART package are: variable inclusion proportion (VIP), marginal posterior variable inclusion probability (PVIP) and posterior split probability (PSP). VIP, proposed by Chipman et al. (2010), describes the average use per splitting rule for each predictor. The latter two variable importance measures are the products of the DART model (Linero (2018)) which modifies BART by replacing the discrete uniform distribution for selecting a split variable with a categorical distribution of which the event probabilities follow a Dirichlet distribution. PVIP estimates the average times that a predictor is included in an ensemble at least once and PSP suggests the probability that a predictor is selected as a split variable for a splitting rule. VIP and PSP are used as variable importance with the idea that predictors are important if they are used for many splitting rules. However, this idea fails in the presence of different types of predictors. For example, an important binary predictor can only be used once at most in each path of a tree because it only has two unique values. Also, the use of PVIP in variable selection often requires strong assumptions and the performance becomes unstable when predictors are correlated.

BNPqte also implements two variable importance measures proposed in Luo and Daniels (2021), which are designed for data with mixed-type predictors. The first one is the within-type variable inclusion proportion (within-type VIP) which describes the average use per splitting rule for a predictor, out of those splitting rules using the same type of predictors. Within-type VIP shows the relative importance of predictors within each type and improves the permutation-based variable selection approach (Bleich et al. (2014)). The second variable importance measure is the Metropolis importance (MI) which is defined as the average Metropolis acceptance ratio per splitting rule out of the splitting rules using the predictor.
This variable importance helps identify all the relevant predictors for data with general mixed-type predictors. More discussions on these variable importance measures can be found in Luo and Daniels (2021).

2.3. Theoretical Properties of BART Priors

Theoretical exploration of BART has begun in recent years, including Linero and Yang (2017), Ročková and Saha (2019), Ročková et al. (2020) and Jeong and Rockova (2020). Linero and Yang (2017) propose the soft BART prior to adapt to unknown smoothness and sparsity levels and show a near-optimal posterior contraction rate for sparse functions with an unknown smoothness level, or functions with additive structures. Ročková et al. (2020) develop the spike-and-tree prior which wraps the Bayesian CART prior (Denison et al. (1998)) with a spike-and-slab prior for dimension reduction and variable selection, and provide a near-optimal posterior contraction rate also for sparse function but with an unknown smoothness level up to 1, or functions with additive structures. Jeong and Rockova (2020) modify the spike-and-tree prior by split-nets which remove the prior dependence on the observed covariates values, and further establish theoretical results for a wide range of functions which can have anisotropic smoothness that possibly varies over the function domain. While these works study variants of the BART prior of Chipman et al. (2010), which is referred to as the 'exact BART' prior, only Ročková and Saha (2019) focus on the exact BART prior. They show that it is not clear whether the exact BART prior that uses (4) as the split probability has the optimal tail property of the number of terminal nodes and therefore that the optimal posterior contraction rate is not guaranteed. Instead, they show that the optimal tail property can be obtained if (4) is replaced by the split probability

$$p_{\text{split}}(d) = \gamma^d,$$

for some $\gamma \in [1/n, 1/2)$. As such, the model using the exact BART prior with the slightly modified split probability (6) can achieve the optimal posterior contraction (up to a log factor) for $\nu$-Hölder continuous regression functions with $0 < \nu \leq 1$, as shown in in Theorem 7.1 of Ročková and Saha (2019). The BNPqte package implements both the two types of split probability, (4) and (6), in the BART-related R functions.

2.4. Illustrations

The BART-related R functions in the BNPqte package are inherited from the BART package: \texttt{wbart()} for continuous BART, \texttt{pbart()} for probit BART and \texttt{lbart()} for logit BART. While the original features of these functions are preserved, two modifications are made. We illustrate the modifications by taking the function \texttt{wbart()} as an example. The usage of \texttt{pbart()} and \texttt{lbart()} is similar because the modifications are made only on trees structures which are shared by the three models.

The first modification is to add the split probability (6) as an alternative to the original split probability (4). When calling \texttt{wbart()}, one can specify the split probability to be either (4) by setting the argument \texttt{split.prob = "polynomial"} or (6) by setting \texttt{split.prob = "exponential"}. The character strings "polynomial" and "exponential" are named after the decreasing rate of the corresponding split probability with respect to the depth. The default values of the hyper-parameters $\gamma$ and $\beta$ in (4) are set the same as BART, i.e., \texttt{base = 0.95} for $\gamma$ and \texttt{power = 2} for $\beta$. When \texttt{split.prob = "exponential"}, the argument \texttt{power}
will not be used and the argument base is used to represent \( \gamma \) in (6). In this case, we set base = 0.5 by default. Other arguments of \texttt{wbart()} in our package are the same as that in the BART package.

The second modification is to add two new variable importance measures, within-type VIP and MI, to these functions, in order to improve variable selection in the presence of mixed-type predictors, as discussed in Section 2.2. The two new variable importance measures, similar to the original three variable importance measures, can be obtained from the output of \texttt{wbart()}, as shown below:

- \texttt{vip} is a vector of variable inclusion proportions (VIP) proposed in Chipman \textit{et al.} (2010)
- \texttt{within_type_vip} is a vector of within-type VIPs proposed in Luo and Daniels (2021)
- \texttt{mi} is a vector of Metropolis importance (MI) proposed in Luo and Daniels (2021)
- \texttt{pvip} is a vector of marginal posterior variable inclusion probabilities (PVIP) proposed in Linero (2018); only useful when DART is fit, i.e., \texttt{sparse = TRUE}
- \texttt{varprob.mean} is a vector of posterior split probabilities (PSP) proposed in Linero (2018); only useful when DART is fit, i.e., \texttt{sparse = TRUE}.

Now, we demonstrate the two newly added features with a simulated example. We simulate 500 observations with 5 binary predictors \( x_1, \ldots, x_5 \) from Bernoulli(0.5) and 5 continuous predictors \( x_6, \ldots, x_{10} \) from Uniform(0,1). The continuous response \( Y \) is sampled from Normal\( (f_0(x), 1) \), where

\[
  f_0(x) = 10 \sin(\pi x_1 x_6) + 20(x_8 - 0.5)^2 + 10x_2 + 5x_7. \tag{7}
\]

The data generation process described above can be done by using the function \texttt{MixData()} in our package as follows.

```r
R> library(BNPqte)
R> set.seed(0)
R> BartData = MixData(n = 500, p = 10, sigma = 1, binary = F)
```

We fit two BART models on the data (\texttt{BartData$Y, BartData$X}) with split probability (4) and (6), respectively. Specifically, the BART models are fit with 50 trees (i.e., \texttt{ntree = 50}) and 500 posterior samples are kept (i.e., \texttt{ndpost = 500}) after burning in 100 samples (i.e., \texttt{nskip = 100}). Other hyper-parameters are specified as default.

```r
R> BartPostP = wbart(BartData$X, BartData$Y, split.prob = "polynomial",
+     ntree = 50L, ndpost = 500L, nskip = 100L)
R> BartPostE = wbart(BartData$X, BartData$Y, split.prob = "exponential",
+     ntree = 50L, ndpost = 500L, nskip = 100L)
```

The results of running \texttt{wbart()} using split probability (4) and (6) are stored in the object \texttt{BartPostP} and \texttt{BartPostE}, respectively, both of which are of type \"wbart\". In a comparison with the root mean squared errors (RMSE), the BART model using the split probability (6) is slightly preferred, as shown below.
R> cat("RMSE of BartPostP: ",
+     sqrt(mean((BartData$Y - BartPostP$yhat.train.mean)^2)), "\n",
+     "RMSE of BartPostE: ",
+     sqrt(mean((BartData$Y - BartPostE$yhat.train.mean)^2)), sep = "")

RMSE of BartPostP: 0.9203228
RMSE of BartPostE: 0.8706075

The three BART-based variable importance measures, MI, VIP and within-type VIP, can be obtained from an object of type "wbart". In this example, MI, VIP and within-type VIP of the BART model using split probability (4) are stored in BartPostP$mi, BartPostP$vip and BartPostP$within_type_vip, respectively. We show the three variable importance measures for the object BartPostP in Figure 1. As shown in the figure, the relevant importance rankings of the predictors are similar when different types of variable importance are used. However, in the presence of mixed-type predictors, the permutation-based variable selection approach using either within-type VIP or MI improves the variable selection result of that using VIP, as shown in Luo and Daniels (2021).

Figure 1: BART-based variable importance measures, VIP, within-type VIP and MI, from the BART model using the split probability (4) for the example in (7). Solid points are for actual relevant predictors and empty points are for irrelevant predictors.

3. BNP Density Estimation with DPM Models

The DPM of multivariate normals model is a classic BNP model, which has been applied to density estimation in a variety of ways. The BART-DPM approach uses the approach of Müller et al. (1996) to estimate the conditional distribution of the outcome given the estimated PS, by first modeling the joint density of the outcome and the estimated PS using the DPM of multivariate normals and then deriving the conditional density of interest from the joint density. In this section, we describe the DPM of multivariate normals model, the two MCMC samplers implemented in the BNPqte package and (joint and conditional) density estimation based on the two samplers. Simulated examples are also provided to illustrate the features of the R functions in the BNPqte package for density estimation.

3.1. DPM of Multivariate Normals Model Specification
We follow the notation of (2) and further assume that all the predictors are continuous. For every $i = 1, \cdots, n$, let $z_i = (Y_i, x_i^T)$. According to Escobar and West (1995) and Müller et al. (1996), the DPM of multivariate normals model on data $\{z_i\}_{i=1}^n$ can be written as

\[
\begin{align*}
  z_i | \mu_i, \Sigma_i & \sim \text{Normal}(z_i | \mu_i, \Sigma_i) \\
  (\mu_i, \Sigma_i) | G & \sim G \\
  G | \alpha, G_0 & \sim \text{DP}(\alpha G_0)
\end{align*}
\]

where $\mu_i$ is a $d$-dimensional ($d = p + 1$) mean vector, $\Sigma_i$ is a $d \times d$ covariance matrix, $\alpha$ is the concentration parameter of the Dirichlet process (DP) prior $\text{DP}(\alpha G_0)$ and $G_0$ is the base distribution of the DP prior. The base distribution $G_0$ can be assumed as a conjugate normal-inverse-Wishart (NIW) distribution $G_0 \equiv \text{Normal}(m | \mu_0, \frac{1}{\lambda} \Sigma) \times \text{IW}(\Sigma | \nu, \Psi)$. (9)

Note that the inverse Wishart distribution $\text{IW}(\Sigma | \nu, \Psi)$ is parameterized such that $E(\Sigma) = \frac{\nu \Psi}{\nu - d - 1}$. A hierarchical DPM of multivariate normals can be obtained by further assuming hyper-priors for the hyper-parameters $m, \lambda, \Psi$ of $G_0$ and a prior for $\alpha$

\[
\begin{align*}
  \alpha | a_0, b_0 & \sim \text{Gamma}(\alpha | a_0, b_0) \\
  m | m_0, S_0 & \sim \text{Normal}(m | m_0, S_0) \\
  \lambda | \gamma_1, \gamma_2 & \sim \text{Gamma}(\lambda | \gamma_1, \gamma_2) \\
  \Psi | \nu_0, \Psi_0 & \sim \text{Wishart}(\Psi | \nu_0, \Psi_0)
\end{align*}
\]

where $\text{Gamma}(\alpha | a_0, b_0)$ and $\text{Wishart}(\Psi | \nu_0, \Psi_0)$ are parameterized such that $E(\alpha) = a_0/b_0$ and $E(\Psi) = \nu_0 \Psi_0$, respectively. To complete the model specification, hyper-parameters $\{\alpha, m, \lambda, \nu, \Psi\}$ for Model (8-9) and $\{a_0, b_0, m_0, S_0, \gamma_1, \gamma_2, \nu_0, \Psi_0\}$ for Model (8-10) need to be chosen. We choose these hyper-parameters according to Taddy (2008) and details can be found in Appendix A.

### 3.2. Gibbs Sampler Based on Pólya Urn Scheme

The MCMC sampler of Escobar and West (1995) for the posterior distribution of the DPM model (8) iteratively draws each pair of $(\mu_i, \Sigma_i)$ from its conditional distribution given both the data $\{z_i\}_{i=1}^n$ and the other pairs of $\{(\mu_j, \Sigma_j)\}_{j \neq i}$. This algorithm yields an ergodic Markov chain; however, it mixes poorly, because it updates each $(\mu_i, \Sigma_i)$ one at a time and a value of $(\mu_i, \Sigma_i)$ that is shared with many observations is hard to change.

Algorithm 8 of Neal (2000) solves this problem by first constructing an equivalent model of (8), which is the limit of a finite mixture model with $N$ components as $N$ goes to infinity.
The finite mixture model has the following form

\[
\begin{align*}
  z_i \mid \kappa_i, \phi & \overset{\text{iid}}{\sim} \text{Normal}(z_i \mid \zeta_{\kappa_i}, \Omega_{\kappa_i}) \\
  \kappa_i \mid \omega & \overset{\text{iid}}{\sim} \sum_{k=1}^{N} \omega_k \delta_k(\cdot) \\
  \omega \mid \alpha & \sim \text{Dirichlet}(\frac{\alpha}{N}, \cdots, \frac{\alpha}{N}) \tag{11}
\end{align*}
\]

where \(\delta_k\) is a degenerate distribution at \(k\), \(\omega\) is a set of \(N\) mixing weights that sum to 1, \(\kappa_i\) is the latent cluster indicator for the observation \(z_i\), \(\phi\) is the collection of all \(\phi_k\)'s and \((\zeta_{\kappa_i}, \Omega_{\kappa_i})\) for \(1 \leq k \leq N\) and \(1 \leq i \leq n\).

The Gibbs sampler of Algorithm 8 is applied to the limit of (11) with the mixing weights \(\omega\) integrated out, so the permanent state of the Markov chain only consists of \(\{\kappa_i\}_{i=1}^{n}\) and \(\phi_k\)'s that are currently associated with some observations. Specifically, at each iteration of MCMC, they sample each \(\kappa_i\) from the conditional distribution of \(\kappa_i\) given \(Y_i, \kappa_{-i}\) and \(\phi\), where \(\kappa_{-i} = \{\kappa_j\}_{j \neq i}\) and \(\phi\) represents the set of \(\phi_k\) currently associated with at least one observation. This conditional distribution can be obtained by taking the limit of the corresponding conditional distribution under the finite mixture model (11) and has the following form

\[
P(\kappa_i = k \mid \kappa_{-i}, z_i, \phi) \propto n_{-i,k} f(z_i \mid \phi_k) \quad \text{if } k = \kappa_j \text{ for some } j \neq i,
\]

\[
\propto \alpha \int f(z_i \mid \phi)dG_0(\phi) \quad \text{if } k \neq \kappa_j \text{ for all } j \neq i, \tag{12}
\]

where \(n_{-i,k}\) is the number of \(\kappa_j\) that are equal to \(k\) for \(j \neq i\) and \(f(z_i \mid \phi_k)\) is the normal likelihood. Since the conditional distribution of \(\kappa_i\) in (12) has the form of the Pólya urn scheme, we refer to this sampler as the Pólya urn Gibbs sampler for convenience. To avoid potentially complex or intractable integration over \(G_0\) in (12), Algorithm 8 introduces \(m\) auxiliary parameters \(\phi\) from \(G_0\) with the idea that sampling \(x\) from a distribution \(\pi_x\) can be accomplished by sampling \((x, y)\) from some distributions \(\pi_{xy}\) as long as the marginal distribution of \(x\) from \(\pi_{xy}\) is \(\pi_x\). The auxiliary parameters are discarded after the update of \(\kappa_i\). Once \(\kappa_i\)'s are updated, every \(\phi_k \in \phi\) for the cluster \(k\) is simply sampled from the posterior distribution of the prior \(G_0\) and the likelihood of the observations \(\{z_i : \kappa_i = k, 1 \leq i \leq n\}\) in that cluster. Algorithm 8 (with \(m = 1\)) of Neal (2000) is restated in Algorithm 1 below and detailed computation for \(\phi_k\)'s and other hyper-parameters can be found in Appendix B.

### 3.3. Blocked Gibbs Sampler Based on Truncated DPM

The Pólya urn Gibbs sampler of Neal (2000) discussed above is the first sampler implemented in the **BNPqte** package and we refer to it as **neal** in the related R functions. We also implement the blocked Gibbs sampler of Ishwaran and James (2001), which is referred to as **truncated** in the related R functions. The blocked Gibbs sampler is more efficient in density estimation than the Pólya urn Gibbs sampler, because it has the direct access to the full posterior distribution.

We first recall the stick-breaking representation of the Dirichlet process which can be expressed

\[
B \overset{\text{dist}}{\sim} \text{Dirichlet} \left( \frac{\alpha}{N}, \ldots, \frac{\alpha}{N} \right)
\]
Algorithm 1 Algorithm 8 of Neal (2000) with $m = 1$ auxiliary parameter.

1: procedure ONE ITERATION OF MARKOV CHAIN$((\kappa_i)_{i=1}^n, \{\phi_k\}_{k \in \{\kappa_i\}_{i=1}^n})$
2: for $i = 1, \ldots, n$ do
3: Let $k^-$ be the number of distinct $\kappa_j$ for $j \neq i$
4: Label $\kappa_{-i}$ with values in $\{1, \ldots , k^-\}$
5: if $\kappa_i = \kappa_j$ for some $j \neq i$ then
6: Draw $\phi_{k^-+1}$ from $G_0$
7: else
8: Set $\phi_{k^-+1} = \phi_{\kappa_i}$
9: end if
10: Draw a new value for $\kappa_i$ from $\{1, \ldots , k^-+1\}$ with the following probabilities:
11: \[
P(\kappa_i = k | \kappa_{-i}, z_i, \phi_1, \ldots , \phi_{k^-+1}) \propto \begin{cases} n_{-i,k}f(z_i | \phi_k) & \text{if } 1 \leq k \leq k^- \\ \alpha f(z_i | \phi_{k^-+1}) & \text{if } k = k^- + 1 \end{cases}
\]
12: end for
13: for $k \in \{\kappa_1, \ldots, \kappa_n\}$ do
14: Draw a new value for $\phi_k$ from the posterior distribution $\phi_k | \{z_i : \kappa_i = k\}$
15: end for
16: Draw new values for $\alpha$ or hyper-parameters if they are assumed to be random
17: end procedure

as
\[
P_{\infty}(\cdot) = \sum_{k=1}^{\infty} \omega_k \delta_{(\mu_k, \Sigma_k)}(\cdot), \quad (13)
\]
where $\omega_1 = V_1$, $\omega_k = (1 - V_1) \cdots (1 - V_{k-1}) V_k$ for $k \geq 2$ and $V_k \overset{iid}{\sim} \text{Beta}(1, \alpha)$ for $k \geq 1$. Therefore, $G | \alpha, G_0 \sim \text{DP}(\alpha G_0)$ in model (8) can be rewritten as $G \sim P_{\infty}$.

Based on the representation (13), Ishwaran and Zarepour (2000) and Ishwaran and James (2001) find a random probability measure, denoted by $P_N$, almost surely converging to $P_{\infty}$. The random probability measure $P_N$ is obtained by truncating the higher-order terms in the representation (13) and has the following form
\[
P_N(\cdot) = \sum_{k=1}^{N} \omega_k \delta_{(\mu_k, \Sigma_k)}(\cdot), \quad (14)
\]
where
\[
\omega_1 = V_1, \quad \omega_k = V_k \prod_{j=1}^{k-1} (1 - V_j) \quad \text{for } 2 \leq k \leq N, \\
V_N = 1, \quad V_k \overset{iid}{\sim} \text{Beta}(1, \alpha) \quad \text{for } 1 \leq k \leq N - 1.
\]

The weights $\omega = \{\omega_k\}_{k=1}^N$ constructed by (15) essentially follow a generalized Dirichlet distribution $\text{GD}(1, \alpha, \cdots, 1, \alpha)$.

They then build an efficient MCMC algorithm for the DPM model (8) with the DP prior $P_{\infty}$ replaced by $P_N$, i.e., the truncated DPM model. Similar to Algorithm 8 of Neal (2000),
they also include latent cluster indicators and the truncated DPM model can be expressed as follows

\[ z_i \mid \kappa_i, \phi \overset{iid}{\sim} \text{Normal}(z_i \mid \zeta_{\kappa_i}, \Omega_{\kappa_i}) \]

\[ \kappa_i \mid \omega \overset{iid}{\sim} \sum_{k=1}^{N} \omega_i \delta_k(\cdot) \quad (16) \]

\[ \omega \mid \alpha \sim \text{GD}(1, \alpha, \cdots, 1, \alpha) \]

\[ \phi_k \triangleq (\zeta_k, \Omega_k) \overset{iid}{\sim} G_0. \]

Model (16) allows block updates for all the parameters in a Gibbs sampler, which leads to rapid mixing of the Markov chain. Also, there is no need to integrate any parameters out, which permits direct inference for the posterior \( P_N \mid \{z_i\}_i=1 \).

The blocked Gibbs sampler for the truncated DPM model (16) is based on the following form of the full posterior distribution

\[
f(\{\phi_k\}_k=1, \{\kappa_i\}_i=1, \omega \mid \{z_i\}_i=1, \alpha) \propto \left[ \prod_{j=1}^{K^*} f(\phi_{\kappa_j^*}) \prod_{\{i: \kappa_i = \kappa_j^*\}} f(z_i \mid \phi_{\kappa_j^*}) \right] \times \left[ \prod_{k \notin K^*} f(\phi_k) \right] \times \left[ \prod_{i=1}^{n} f(\kappa_i \mid \omega) \right] \times f(\omega \mid \alpha), \quad (17)
\]

where \( K^* = \{\kappa_j^*\}_{j=1}^{K^*} \) is the collection of unique values in \( \{\kappa_i\}_i=1 \). Hyper-priors can also be included in (17) if the hierarchical structure (10) is assumed. The algorithm for the truncated DPM model (16) is summarized in Algorithm 2 and details of the posterior computation can be found in Appendix C.

The posterior samples obtained from Algorithm 2 are used for approximating posterior samples of the DPM model (8). To achieve an adequate approximation of the Dirichlet process, we need to choose a reasonably large \( N \). Theorem 2 of Ishwaran and Zarepour (2000) provides guidance to select \( N \). In the BNPqte package, we set \( N = 50 \) by default.

### 3.4. Density Estimation Based on Blocked Gibbs Sampler

The DPM of multivariate normals model can be used to estimate the density for continuous data. Consider the problem of estimating the predictive density for a future observation \( z_{n+1} \) given the observations \( \{z_i\}_{i=1}^{n} \). Let \( f(z_{n+1} \mid \{z_i\}_{i=1}^{n}) \) be the predictive density of \( z_{n+1} \) given the observations \( \{z_i\}_{i=1}^{n} \) under the DPM of multivariate normals model. Based on the stick-breaking representation of the DP prior in (13), we have that

\[
f(z_{n+1} \mid \{z_i\}_{i=1}^{n}) = \int \int f(z_{n+1} \mid \mu_{n+1}, \Sigma_{n+1}) dF(\mu_{n+1}, \Sigma_{n+1} \mid P_\infty) dF(P_\infty \mid \{z_i\}_{i=1}^{n}), \quad (18)
\]

where \( f(z_{n+1} \mid \mu_{n+1}, \Sigma_{n+1}) \) is the assumed normal likelihood and \( F(P_\infty \mid \{z_i\}_{i=1}^{n}) \) in the outer integral is the posterior distribution of the Dirichlet process.

When the truncated DPM model (16) is used to approximate the exact DPM model (8), the inside integral in (18) can be estimated by

\[
\sum_{k=1}^{N} \omega_k^{(l)} f(z_{n+1} \mid \zeta_k^{(l)}, \Omega_k^{(l)}), \quad (19)
\]
Algorithm 2 Blocked Gibbs Sample of Ishwaran and James (2001)

1: procedure One Iteration of Markov Chain(\(\{\kappa_i\}_{i=1}^N, \{\phi_k\}_{k=1}^N, \{\omega_k\}_{k=1}^N\))
2: for \(k = 1, \cdots, N\) do
3: if \(k \in \kappa^*\) then
4: Sample a new value for \(\phi_k\) from the posterior distribution \(\phi_k | \{z_i : \kappa_i = k\}\)
5: else
6: Sample a new value for \(\phi_k\) from the prior distribution of \(\phi_k\)
7: end if
8: end for
9: Sample a vector of new values for \(\{\omega_k\}_{k=1}^N\) from \(GD(a_1, b_1, \cdots, a_{N-1}, b_{N-1})\) with
10: \(a_k = n_k + 1\) and \(b_k = N_k + \alpha\), where \(n_k = |\{i : \kappa_i = k\}|\) for \(1 \leq k \leq N\) and \(N_k = n_{k+1} + \cdots, n_N\) for \(1 \leq k \leq N - 1\)
11: for \(i = 1, \cdots, n\) do
12: Sample a new value for \(\kappa_i\) from \(\{1, \cdots, N\}\) with probabilities proportional to \(\omega_1 f(z_i | \phi_1), \cdots, \omega_N f(z_i | \phi_N)\)
13: end for
14: Draw new values for \(\alpha\) or hyper-parameters if they are assumed to be random
15: end procedure

where \(\{\omega^{(l)}(\kappa^*_l), \kappa^{(l)}_k, \Omega^{(l)}_k\}_{k=1}^N\) is the \(l^{th}\) posterior sample from MCMC. The predictive density \(f(z_{n+1} | \{z_i\}_{i=1}^n)\) can then be estimated by the average of (19) across all the MCMC samples.

We can also estimate the predictive conditional density of \(Y_{n+1}\) given \(x_{n+1}\) based on the DPM model (8) on the joint data \(\{z_i = (Y_i, x_i^\top)\}_{i=1}^n\). Let \(f(Y_{n+1} | x_{n+1}, \{z_i\}_{i=1}^n)\) be the predictive conditional density of interest under the DPM model. It can be directly derived from (18) and has the following form

\[
f(Y_{n+1} | x_{n+1}, \{z_i\}_{i=1}^n) = \int f(Y_{n+1}, x_{n+1} | P_\infty) \frac{f(x_{n+1} | P_\infty)}{f(x_{n+1} | P_\infty)} dF(P_\infty | \{z_i\}_{i=1}^n). \tag{20}\]

The numerator of the fraction in (20) is the inside integral in (18), so the estimation is simply (19) if the blocked Gibbs sampler is used. The denominator of the fraction is the marginal density of \(x_{n+1}\), which can be obtained by integrating the numerator over \(Y_{n+1}\), so it can be estimated by the integral of (19) over \(Y_{n+1}\). In conclusion, the integrand in (20) can be estimated by

\[
\sum_{k=1}^N \omega^{(l)}_k(x_{n+1}) f_{\text{Normal}}(Y_{n+1} | \beta^{(l)}_{0k} + x_{n+1}^\top \beta^{(l)}_k, \sigma^{(l)}_k^2), \tag{21}\]
where $f_{\text{Normal}}(\cdot | \beta, \sigma^2)$ represents a univariate normal density with mean $\beta$ and variance $\sigma^2$,

$$
\beta_k^{(l)} = \Omega_{12k}^{(l)} \Omega_{22k}^{(l)-1}, \quad \beta_{0k}^{(l)} = \zeta_{1k}^{(l)} - \beta_k^{(l)} \Omega_{22k}^{(l)}, \quad \sigma_k^{2(l)} = \Omega_{11k}^{(l)} - \beta_{0k}^{(l)} \Omega_{22k}^{(l)}.
$$

(22)

The estimator in (21) induces an estimator for the predictive conditional mean of $Y$ given a future $x_{n+1}$, which can be expressed as

$$
\hat{E}(Y | x_{n+1}) = \frac{\sum_{k=1}^{N} \omega_k^{(l)}(x_{n+1}) (\beta_{0k}^{(l)} + x_{n+1}^\top \beta_k^{(l)})}{\sum_{k=1}^{N} \omega_k^{(l)} f(x_{n+1} | \zeta_k^{(l)}, \Omega_k^{(l)})}.
$$

The predictive conditional CDF of $Y_{n+1}$ given $x_{n+1}$ can be similarly estimated by an estimator which has the form of (21) with the normal density $f_{\text{Normal}}$ replaced by the corresponding normal CDF.

Density estimation based on the Pólya urn Gibbs sampler is more complicated than that based on the blocked Gibbs sampler, because it samples from the marginal posterior distribution and does not have the access to the mixing weights $\omega_k$’s. We implement the approach of Müller et al. (1996), when the Pólya urn Gibbs sampler is employed for the MCMC sampling. We describe the details in Appendix D.

3.5. Illustrations

The BNPqte package implements joint density estimation by the R function DPMdensity() and conditional density estimation by the R function DPMcdensity(). Arguments of the two functions can be divided into five components: data inputs, prediction inputs, model specification, MCMC parameters and diagnostics setting, the last three of which are shared between the two functions. We first introduce the three shared components.

In the model specification part, two important arguments are updateAlpha and useHyperpriors, which are described below.

- updateAlpha = TRUE implies that the concentration parameter $\alpha$ is assumed to be random as (10), otherwise it is assumed to be a fixed value

- useHyperpriors = TRUE implies that the hyper-parameters of the base distribution $G_0$ are assumed to be random as (10), otherwise they are assumed to be fixed values

By setting these two arguments to different values, both hierarchical and non-hierarchical DPM models can be fit in our package. Other arguments for specifying hyper-parameters can often be omitted since the default values are adequate for most purposes.

Arguments for MCMC parameters include those for specifying the sampling algorithm and those for setting the number of posterior samples burned, kept and thinned. We list these arguments below.

- method is a character string; the Pólya urn Gibbs sampler is chosen if method = "neal" and the blocked Gibbs sampler is chosen if method = "truncated"
- **nclusters** is the number of clusters \(N\) pre-specified for the blocked Gibbs sampler if `method = "truncated"

- **nskip**, **ndpost** and **keepevery** are the number of posterior samples burned, kept and thinned, respectively

The last part of arguments shared between `DPMdensity()` and `DPMcdensity()` includes an argument **diag** of boolean type. By setting **diag = TRUE**, logarithm likelihood and logarithm marginal partition posterior (only for the blocked Gibbs sampler) are calculated at each iteration of the Markov chain and are returned to users for further diagnostics analysis. We discuss this in Section 5.

Unlike the three parts of arguments discussed above, arguments for data and prediction are different for `DPMdensity()` and `DPMcdensity()` and they are either always or frequently needed from users. The data and prediction inputs of `DPMdensity()` are as follows.

- **y** is a matrix giving the data from which the density estimate is to be computed

- **ngrid** and **grid** produce the grid points where the density estimate is evaluated; they are only used when **y** is bivariate and nothing is evaluated when **ngrid = 0** and **grid = NULL**

The data and prediction inputs of `DPMcdensity()` are slightly different from above, as shown below.

- **y** is a vector giving the values for which the conditional density (and/or conditional mean and/or conditional CDF) estimate is to be computed

- **x** is a vector or matrix specifying the predictors

- **ngrid** and **grid** produce the grid points where the conditional density (and/or conditional mean and/or conditional CDF) estimate is evaluated; nothing is evaluated when **ngrid = 0** and **grid = NULL**

- **xpred** is a vector or matrix giving the values of the predictors for prediction

- **type.pred** is a vector of strings; the conditional density (and/or conditional mean and/or conditional CDF) is estimated if "pdf" (and/or "meanReg" and/or "cdf") is included in **type.pred**

- **compute.band** is a boolean argument indicating whether a credible band for the conditional density (and/or conditional mean and/or conditional CDF) is computed and **type.band** is a string indicating the type of credible bands to be computed; 95\% point-wise highest posterior interval (or Bayesian credible interval) (Chen and Shao (1999)) is computed if **type.band = "HPD"** (or **type.band = "BCI"**) 

The result of running `DPMdensity()` (or `DPMcdensity()`) is returned in an object of class "DPMdensity" (or "DPMcdensity") which essentially is a list. Besides the prediction results, the posterior samples are stored in a sub-list called **posterior** and the latest posterior sample is stored in a sub-list called **state** which can be used as initial values for a new Markov chain. We illustrate these outputs with simulated examples later.
We also provide S3 method `predict()` and `plot()` functions for classes "DPMdensity" and "DPMcdensity". Users can use `predict()` to obtain the prediction of the grid points provided by them and use `plot()` to visualize the prediction results from objects of class "DPMdensity" and "DPMcdensity".

Next, we illustrate the usage of the R functions `DPMdensity()` and `DPMcdensity()` with two simulated examples.

**Joint density estimation**

We simulate $n = 500$ independent and identically distributed (i.i.d.) observations $\{y_i\}_{i=1}^n$ from a mixture of three bivariate normal distributions with equal weights. The mean vectors of the three normals are $\zeta_0^\top_1 = (2, -1)$, $\zeta_0^\top_2 = (1, 0)$ and $\zeta_0^\top_3 = (-1, -1)$, respectively; the three normals share the same covariance matrix which is a 2 by 2 diagonal matrix with diagonal elements equal to 0.5, i.e., $\Sigma_0 = 0.5I_2$. The true density function of $y$ is given below

$$f(y) = \frac{1}{3}f_{\text{Normal}}(y | \zeta_0^1, \Sigma_0) + \frac{1}{3}f_{\text{Normal}}(y | \zeta_0^2, \Sigma_0) + \frac{1}{3}f_{\text{Normal}}(y | \zeta_0^3, \Sigma_0).$$  (23)

BNPqte provides the R function `ThreeNormals()` to generate the data described above. As shown below, besides the observations (i.e., $y$), the true density function (i.e., $dtrue$) is also returned by the function.

R> set.seed(0)
R> DpmData1 = ThreeNormals(n = 500)
R> names(DpmData1)
[1] "y"     "dtrue"

We model the joint density of $y$ by fitting a hierarchical DPM of multivariate normals model on the observations $\{y_i\}_{i=1}^n$. Specifically, we run the R function `DPMdensity()` on the data `DpmData1$y`. The Pólya urn Gibbs sampler (i.e., `method = "neal"`) and the blocked Gibbs sampler (i.e., `method = "truncated"`) are used, respectively, and the corresponding results are returned in the objects `JtDpmP` and `JtDpmB`. We burn in the first 5000 posterior samples (i.e., `nskip = 5000`) and then save 5000 posterior samples (i.e., `ndpost = 5000`) by keeping every 3rd sample (i.e., `keepevery = 3`). The estimated density is evaluated at 1000 grid points (i.e., `ngrid = 1000`) generated from the observed data.

R> t1 = Sys.time()
R> JtDpmB = DPMdensity(y = DpmData1$y, ngrid = 1000,
+                   method = "truncated", nclusters = 50,
+                   nskip = 5000, ndpost = 5000, keepevery = 3)
R> t2 = Sys.time()
R> JtDpmP = DPMdensity(y = DpmData1$y, ngrid = 1000, method = "neal",
+                   nskip = 5000, ndpost = 5000, keepevery = 3)
R> t3 = Sys.time()

The returned object `JtDpmB` is a list and has the following components.

R> names(JtDpmB)
Posterior samples of (hyper-)parameters are returned in the component \$posterior, as follows.

```r
R> names(JtDpmB$posterior)
```

```
[1] "Zeta" "Omega" "lw" "kappa" "alpha" "m" "lambda" [8] "Psi"
```

Prediction results are returned in the components \$predict.pdfs and \$predict.pdf.avg. The component \$predict.pdfs is a list of length \texttt{ndpost}. Each element of the list is a matrix of the estimated density evaluated at grid points (\$grid1, \$grid2), using a single MCMC sample. The component \$predict.pdf.avg is the averaged \$predict.pdfs across the MCMC samples.

We can visualize the prediction results by applying the \texttt{plot()} function to the object \texttt{JtDpmB}, as shown in Figure 2. Note that if the \texttt{true_density_fun} is not provided to the \texttt{plot()} function, only the posterior mean estimate is plotted.

```r
R> plot(JtDpmB, diff = TRUE, true_density_fun = DpmData1$dtrue, + type.plot="contour")
```

![Figure 2](image_url)

Figure 2: From left to right, subfigures are contours of the difference between the estimated density and the true density, the estimated density, and the true density, respectively, for the DPM of multivariate normals model using the blocked Gibbs sampler for the example in (23).

The DPM model using the Pólya urn Gibbs sampler has similar prediction results, as shown in Figure 10 in Appendix F. The \texttt{plot()} function in \texttt{BNPqte} also provides \texttt{plotly} 3D-surface (HTML output) for the estimated density from \texttt{DPMdensity}(). Users can obtain the 3D-surface by setting \texttt{type.plot = "surface"}, if working in a HTML environment.

The run times of the blocked Gibbs sampler and the Pólya urn Gibbs sampler are similar, when the DPM model is applied to the joint density estimation.
$tB = \text{difftime}(t2, t1)$
$tP = \text{difftime}(t3, t2)$

Run time of Blocked Gibbs Sampler: 1.19mins
Run time of Pólya urn Sampler: 1.1mins

With a fitted object like $JtDpmB$ and $JtDpmP$, users can evaluate the estimated density at some given grid points by plugging the object in the `predict()` function. The returned object from the `predict()` function is also of class "DPMdensity", so the prediction result can be viewed by the `plot()` function as well. We show the syntax of the `predict()` function below.

```r
grids = matrix(runif(10), ncol = 2)
predict(object = JtDpmB, grid = grids)
```

**Conditional density estimation**

We show the usage of the R function `DPMcdensity()` with a simulated example from Dunson et al. (2007), which is also replicated by the `DPpackage` R package. We first sample $n = 500$ i.i.d. covariate values $\{x_i\}_{i=1}^n$ from Uniform(0,1), and then for each $x_i$, generate the response $y_i$ from a mixture of a normal linear regression model and a normal non-linear regression model, with the mixture weights depending on the predictor $x_i$. The true conditional density of $y$ given $x$ can be expressed as follows:

$$f(y \mid x) = \exp(-2x)f_{\text{Normal}}(y \mid x, 0.01) + (1 - \exp(-2x))f_{\text{Normal}}(y \mid x^4, 0.04). \quad (24)$$

The data described above can be generated by the R function `DunsonExample()` in our package. Besides the data (i.e., $y$ and $x$), the density function (i.e., $dtrue$), mean (i.e., $mtrue$) and CDF (i.e., $ptrue$) of the true conditional distribution are also returned by the function, as shown below.

```r
set.seed(0)
DpmData2 = DunsonExample(n = 500)
names(DpmData2)
```

```
[1] "y"   "x"   "mtrue" "dtrue" "ptrue"
```

We model the conditional density of $y$ given $x$ by fitting a hierarchical DPM of multivariate normals model on the joint data $\{y_i, x_i\}_{i=1}^n$ and then calculating the conditional density from the estimated joint density, as described in Section 3.4 and Appendix D. Specifically, we run the function `DPMcdensity()` twice with the Pólya urn Gibbs sampler and the blocked Gibbs sampler, respectively. The corresponding returned objects are `CdDpmP` and `CdDpmB`, which are of class "DPMcdensity". MCMC settings are the same as those in the joint density estimation above. Some arguments set to their default values are omitted in the following code chunk.
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R> type.pred = c("pdf", "meanReg", "cdf")
R> xpred = seq(0, 1, 0.02)
R> t4 = Sys.time()
R> CdDpmB = DPMcdensity(y = DpmData2$y, x = DpmData2$x,
+     xpred = xpred, ngrid = 100, type.pred = type.pred,
+     nskip = 5000, ndpost = 5000, keepevery = 3)
R> t5 = Sys.time()
R> CdDpmP = DPMcdensity(y = DpmData2$y, x = DpmData2$x, method = "neal",
+     xpred = xpred, ngrid = 100, type.pred = type.pred,
+     nskip = 5000, ndpost = 5000, keepevery = 3)
R> t6 = Sys.time()

The returned object CdDpmB has similar components to the object JtDpmB obtained in joint density estimation, except those about prediction results. The component $predict.pdfs consists of the estimated conditional density at each MCMC iteration, and $predict.pdf.avg is the average of $predict.pdfs across MCMC iterations. The components $predict.pdf.lower and $predict.pdf.upper are the lower and upper bounds of the pointwise 95% credible intervals of $predict.pdfs. The estimated conditional mean and CDF have similar names of return values as the estimated conditional density, except that the pdf in the name of a return value for the estimated conditional density is replaced by meanReg (or CDF) for the estimated conditional mean (or CDF), as shown below.

R> names(CdDpmB)
[1] "updateAlpha"         "useHyperpriors"
[3] "status"               "state"
[5] "posterior"            "predict.meanRegs"
[7] "predict.meanReg.avg"  "predict.meanReg.lower"
[9] "predict.meanReg.upper" "predict.pdfs"
[11] "predict.pdf.avg"      "predict.pdf.lower"
[13] "predict.pdf.upper"    "predict.cdfs"
[15] "predict.cdf.avg"      "predict.cdf.lower"
[17] "predict.cdf.upper"    "proc.time"
[19] "prediction"           "type.pred"
[21] "compute.band"         "type.band"
[23] "xpred"                "grid"

Like the function DPMdensity(), we can also visualize the prediction results of the function DPMcdensity() via the function plot() as below. The prediction results of the DPM model using the blocked Gibbs sampler are shown in Figure 3, Figure 4 and Figure 5 and those using the Pólya urn Gibbs sampler can be found in Appendix F. The two Gibbs samplers produce similar prediction results.

R> plot(CdDpmB, xpred.idx = c(20, 30), true_pdf_fun = DpmData2$dtrue,
+     true_cdf_fun = DpmData2$ptrue, true_meanReg_fun = DpmData2$mtrue)

However, the run time of the function DPMcdensity() using the Pólya urn Gibbs sampler is much longer (7 times longer in this example) than that using the blocked Gibbs sampler. This
is because the Pólya urn Gibbs sampler does not have the direct access to the full posterior distribution and requires a complicated algorithm to obtain it. We discuss this in detail in Appendix D.

```
R> ctB = difftime(t5, t4)
R> ctP = difftime(t6, t5)
R> cat("Run time of blocked Gibbs Sampler: ", round(ctB, 2), units(ctB), ",\n" + "Run time of Pólya urn Sampler: ", round(ctP, 2), units(ctP), sep = ")

Run time of blocked Gibbs Sampler: 3.19mins
Run time of Pólya urn Sampler: 23.96mins
```

When using the Pólya urn Gibbs sampler, the function DPMcdensity() implements the exact same model as the function DPcdensity() in the DPPackage R package, except that the latter does not provide conditional CDF estimation. We examine the run time of these two functions by running DPcdensity() and DPMcdensity() with different samplers, respectively, on Dunson’s example (24). Only conditional density and conditional mean are
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estimated and the same grid points, hyper-parameters and MCMC settings as \( \text{CdDpmB} \) are used. Table 1 shows the run time of different functions. As we can see, the \( \text{DPMcdensity()} \) with \texttt{method = "truncated"} is the most efficient and the \( \text{DPMcdensity()} \) with \texttt{method = "neal"} is much faster than its competitor \( \text{DPcdensity()} \). In addition to the usage of the \texttt{Armadillo} C++ library which provides efficient linear algebra calculations, the fast run time of \( \text{DPMcdensity(method = "neal")} \) is due to the optimization of the algorithm for the estimated conditional density evaluation. Algorithm 4 in Appendix D shows the algorithm that we use for the estimated conditional density evaluation. Step 5 in Algorithm 4 evaluates the marginal and conditional density using the clusters parameters currently associated with at least one observation and saves the result, before the stick-breaking weights generation and clusters sampling. This avoids repeatedly evaluating the density evaluated at step 5, thereby improving the efficiency of \( \text{DPcdensity()} \). Hence, our package provides a fast implementation of the DPM of multivariate normals model in conditional density estimation, compared to the popular \texttt{DPpackage}. This is critical to the computational efficiency of the BART-DPM approach, because this approach involves multiple runs of the function \( \text{DPMcdensity()} \).

| Function          | \text{DPMcdensity()} | \text{DPcdensity()} |
|-------------------|----------------------|---------------------|
| Gibbs Sampler     | 1.88 min             | 13.58 min           |
| Blocked           | Pólya urn             | Pólya urn            |
| Run Time          |                      |                     |

Table 1: Run time of the function \( \text{DPMcdensity()} \) in \texttt{BNPqte} and the function \( \text{DPcdensity()} \) in \texttt{DPpackage} for the example in (24). Only conditional density and mean are estimated. Other settings are the same across different functions. The estimated density is evaluated at 5100 grid points. The number of total MCMC iterations is 20000, out of which 5000 posterior samples are kept.

4. BNP QTE Estimation with BART-DPM Approach
In this section, we first present the BART-DPM approach to estimate QTEs for observational data and then demonstrate the corresponding R function in the BNPqte package with a simulated example.

### 4.1. BART-DPM Approach Specification

Consider a data framework $\{Y_i, x_i, T_i\}_{i=1}^{n}$ in causal inference, where $Y_i$ is the observed outcome, $x_i = (x_{i1}, \cdots, x_{ip})^\top$ is the observed confounders and $T_i$ is the treatment assigned to the $i$th subject with $T_i = 1$ for the active treatment and $T_i = 0$ for the control treatment. We assume the outcome to be continuous and allow the $p$ confounders to be of any type. Let $(Y_i(0), Y_i(1))$ be the potential outcomes for the $i$th subject under the control and active treatment, respectively. Under the consistency assumption, we have $Y_i = Y_i(T_i)$. The propensity score (PS) for the $i$th subject, denoted by $e(x_i)$, is defined as the probability of the subject being assigned to the active treatment group given a set of observed confounders, i.e., $P(T_i = 1 | x_i)$.

To make inference in observational studies, Xu et al. (2018) use three identifying assumptions, i.e., the stable unit treatment value assumption, the strong ignorability assumption and the overlap assumption, under which the treatment assignment is independent of potential outcomes given PS. As such, the CDF of the potential outcome $Y(t)$, $t \in \{0, 1\}$, is identified as

$$F_t(y) = \int P(Y < y | e(X) = e(x), T = t) dR(e(x)),$$

where $R$ is the distribution of PS in the population of interest and can be induced by the distribution of the confounders in the population of interest. The BART-DPM approach to model $F_t(y)$ is built based on the identification above.

The BART-DPM approach first fits a binary BART model (5) on the observations $\{T_i, x_i\}_{i=1}^{n}$ to model the regression of the treatment assignment on confounders, i.e.,

$$T_i = 1 | x_i \overset{\text{i.i.d}}{\sim} \text{Bernoulli} \left( H \left( \sum_{m=1}^{M} g(x_i; T_m, \mu_m) \right) \right),$$

where the link function $H$ is the CDF of the standard normal distribution for the probit BART model and the CDF of the logistic distribution for the logit BART model. $K$ posterior samples of the set of PS $\{e(x_i)\}_{i=1}^{n}$ can be calculated by $e^{(k)}(x_i) = H(\sum_{m=1}^{M} g(x_i; T_m^{(k)}, \mu_m^{(k)}))$, $1 \leq k \leq K$, where $\{T_m^{(k)}, \mu_m^{(k)}\}_{m=1}^{M}$ is the $k$th posterior sample from the binary BART model. For simplicity, we denote $e^{(k)}(x_i)$ by $e_i^{(k)}$ for $1 \leq k \leq K$ and $1 \leq i \leq n$.

Given each posterior sample $\{e_i^{(k)}\}_{k=1}^{n}$ of PS, the BART-DPM approach estimates the conditional CDF $P(Y < y | e(X) = e(x), T = t)$ in (25) by fitting a DPM of bivariate normals model (8) on the observations $\{Y_i, H^{-1}(e_i^{(k)})\}_{i \in \{i : T_i = t\}}$, i.e., $\{Y_i, \sum_{m=1}^{M} g(x_i; T_m^{(k)}, \mu_m^{(k)})\}_{i \in \{i : T_i = t\}}$, in treatment group $T = t$. The specific DPM model can be expressed as

$$\begin{align*}
(Y_i, H^{-1}(e_i^{(k)}))^\top | \mu_i, \Sigma_i & \overset{\text{i.i.d}}{\sim} \text{Normal} \left( (Y_i, H^{-1}(e_i^{(k)}))^\top | \mu_i, \Sigma_i \right), \\
(\mu_i, \Sigma_i) | G & \overset{\text{i.i.d}}{\sim} G, \quad G | \alpha, G_0 \sim \text{DP}(\alpha G_0), \quad i \in \{i : T_i = t\}.
\end{align*}$$

Posterior samples of Model (27) are obtained by using either the Pólya urn Gibbs sampler discussed in Section 3.2 or the blocked Gibbs sampler discussed in Section 3.3. The conditional
CDF $P(Y < y | e(X) = e(x), T = t)$ can be estimated by either (39) or (21) depending on which Gibbs sampler is used.

Once the estimated conditional CDF $P(Y < y | e(X) = e(x), T = t)$ in (25) is obtained, the CDF $F_t(y)$ of the potential outcome $Y(t)$ can be approximated by integrating the estimated conditional CDF over the distribution $R$ of PS in the population of interest. If the true distribution of the confounders is known, we can estimate the CDF $F_t(y)$ by averaging the estimated conditional CDFs which are evaluated at the estimated PS of the confounders generated from its true distribution. If the true distribution of the confounders is unknown, the BNPqte package estimates the distribution $R$ by either the empirical distribution $R_{n,k}^{(k)}(\cdot) = \sum_{i=1}^{n} \delta_{\epsilon_i}^{(k)}(\cdot)/n$ or the distribution $R_{n,k}^{(k)}(\cdot) = \sum_{i=1}^{n} u_i \delta_{\epsilon_i}^{(k)}(\cdot)$ obtained from Bayesian bootstrap, where the weights $(u_1, \cdots, u_n)$ follows a Dirichlet$(1, \cdots, 1)$ distribution. Quantiles of interest and QTEs can be computed from the estimated distributions of potential outcomes. Since we estimate the entire distributions of potential outcomes, we are able to estimate multiple QTEs simultaneously. We summarize the complete approach in Algorithm 3.

4.2. Illustrations

The ultimate goal of the BNPqte package is to implement the BART-DPM approach of Xu et al. (2018). The R function qte() does this. The main arguments of qte() can be divided into three parts: data inputs, prediction settings and models specification.

The data is entered into the function qte() through the following three arguments.

- $y$ is a vector of continuous observed outcomes
- $x$ is a vector or matrix of observed confounders of any type
- treatment is a vector of binary observed treatment assignments

The quantiles of interest are specified via the argument probs which is a vector of real numbers between 0 and 1. Similar to the two DPM functions, users can obtain credible intervals of the estimated distributions of potential outcomes through the arguments compute.band and type.band. Moreover, users can specify the confidence levels by setting different values to the argument alphas.

The BART and DPM models, as well as the distribution of PS in the population of interest, are specified by the following arguments.

- bart.link is a string indicating the link used in the binary BART model (26); probit BART is used if bart.link = "probit" and logit BART is used if bart.link = "logit"
- bart.params is a list containing arguments in pbart() or lbart(); a default value will be used for an argument if it is not provided to bart.params
- dpm.params is a list containing arguments in DPMcdensity(); a default value will be used for an argument if it is not provided to dpm.params
Algorithm 3 BART-DPM Approach to Estimate QTEs

procedure QTE(\(\{Y_i, T_i, x_i\}_{i=1}^n\), \(p\))

1. Fit a binary BART model (26) on \(\{T_i, x_i\}_{i=1}^n\) and obtain \(K\) posterior samples \(\{H^{-1}(e_i^{(k)})\}_{i,k=1}^{n,K}\)
2. Create a set of grid points of \(Y\) values: \((g_1, \ldots, g_S)\)
3. if \(R\) is known then
   4. Generate \(\tilde{n}\) i.i.d. \(\tilde{x}_i\) from the true distribution of the confounders
   5. Obtain the prediction \(\{H^{-1}(e_i^{(k)}(\tilde{x}_i))\}_{i,k=1}^{n,K}\)
else
   6. Find a grid point \(\tilde{x}_i\) from the BART model in Step 2
   7. Set \(\tilde{n} = n\) and \(\{H^{-1}[(e_i^{(k)}(\tilde{x}_i))]\}_{i,k=1}^{n,K} = \{H^{-1}(e_i^{(k)})\}_{i,k=1}^{n,K}\)
end if

for \(k = 1, \ldots, K\) do
   for \(t = 0, 1\) do
      12. Fit a DPM of bivariate normals (27) on \(\{Y_i, H^{-1}(e_i^{(k)})\}_{i \in \{i: T_i = t\}}\)
      if Blocked Gibbs sampler is used then
         14. Use Algorithm 2 to obtain \(L\) posterior samples
         15. Use (21-22) to calculate \(\{F^{[kl]}(g_s | H^{-1}[e^{(k)}(\tilde{x}_i)]) , T = t\}_{i,s,l=1}^{\tilde{n},S,L}\)
      end if
      if Pólya urn Gibbs sampler is used then
         17. Use Algorithm 1 to obtain \(L\) posterior samples
         18. Use Algorithm 4 to calculate \(\{F^{[kl]}(g_s | H^{-1}[e^{(k)}(\tilde{x}_i)]) , T = t\}_{i,s,l=1}^{\tilde{n},S,L}\)
      end if
   end if
end for

if \(R\) is known or Empirical distribution is used then
   22. Set \((u_1^{(k)}, \ldots, u_{\tilde{n}}^{(k)}) = (1/\tilde{n}, \ldots, 1/\tilde{n})\)
else
   24. Sample \((u_1^{(k)}, \ldots, u_{\tilde{n}}^{(k)})\) from Dirichlet(1, \ldots, 1)
end if

for \(l = 1, \ldots, L\) do
   27. Calculate the CDF of \(Y(t)\) as follows:
   \[F^{[kl]}_t(g_s) = \sum_{i=1}^{\tilde{n}} u_i^{(k)} F^{[kl]}_t(g_s | H^{-1}[e^{(k)}(\tilde{x}_i)], T = t), \quad 1 \leq s \leq S, t \in \{0, 1\}\]
   29. Find a grid point \(g_{t,p}^{[kl]}\) such that \(F^{[kl]}_t(g_{t,p}^{[kl]}) = p\) for \(t \in \{0, 1\}\)
   30. The \(p^{th}\) quantile from the CDF \(F_t^{[kl]}(\cdot)\) is \(g_{t,p}^{[kl]}\) for the treatment group \(T = t\)
end for
end for

The estimated CDF of \(Y(t)\) on a grid point \(g_s\) is \(F_t(g_s) = \frac{1}{K} \sum_{k,l=1}^{K,L} F^{[kl]}_t(g_s)\)
33. The estimated \(p^{th}\) quantile for the treatment group \(T = t\) is \(\frac{1}{K} \sum_{k,l=1}^{K,L} g_{t,p}^{[kl]}\)
35. The estimated \(p^{th}\) QTE is \(\frac{1}{K} \sum_{k,l=1}^{K,L} (g_{1,p}^{[kl]} - g_{0,p}^{[kl]})\)
end procedure
• **Rdist** is a string indicating whether the distribution of PS is known or estimated; it is known if Rdist = "known"; it is estimated by the empirical distribution if Rdist = "empirical"; it is estimated by Bayesian bootstrap if Rdist = "bootstrap" which is the default value;

• **xpred** is a vector or matrix giving the confounders values sampled from the true distribution of the confounders; the binary BART model makes prediction at xpred and the resulting values are used to evaluate the estimated conditional distributions in the DPM models; only used when Rdist = "known"

As seen in Algorithm 3, multiple DPM models need to be fit to obtain the conditional distributions of potential outcomes given the estimated PS. We provide parallel computing for fitting multiple DPM models in the function `qte()` by setting the argument `mc.cores` greater than 1.

The object returned by the function `qte()` belongs to the class "qte", which essentially is an R list containing predictions results and parameters used in the analysis. The functions `predict()` and `plot()` are also available for objects of class "qte", through S3 Method.

In the following, we illustrate the usage of the function `qte()` with a simulated example from Xu et al. (2018) and present the prediction results for the BART-DPM approach using probit BART and logit BART respectively by generating 100 replicated datasets and then running `qte()` with different `bart.link` on each dataset.

We simulate n = 2000 subjects with 10 confounders x₁, ⋯, x₁₀ sampled from Uniform(−2, 2).

The treatment assignment T and the outcome Y are generated from the following data generation process

\[ T \mid x \sim \text{Bernoulli} \left( 0.3 \sum_{j=1}^{10} x_j \right) \]

\[ Y \mid x, T = 1 \sim \text{expit} \left( 0.5x_3x_4 \right) \text{Normal} \left( 3 + 0.5x_2x_5 + 0.5x_1^2, 0.5^2 \right) \]

\[ + \left[ 1 - \text{expit} \left( 0.5x_3x_4 \right) \right] \text{Normal} \left( -0.5 + 0.5x_2^2 - 0.5x_1x_3, 0.8^2 \right) \quad (28) \]

\[ Y \mid x, T = 0 \sim \exp \left( -|x_5| \right) \text{Normal} \left( \sum_{j=1}^{5} 0.2x_j^4, 1 \right) \]

\[ + \left( 1 - \exp \left( -|x_5| \right) \right) \text{Normal} \left( 2 + \sum_{j=1}^{5} 0.2x_j^2, 1 \right). \]

This process can be done by using the function `QteExample()` in our package. Apart from the data (i.e., $x$, $treatment$, $y$), this function also returns the true conditional density function of the outcome given the confounders in each treatment group: $fy1$ for the active treatment group and $fy0$ for the control treatment group.

R> set.seed(0)
R> qteData = QteExample(n = 2000)
R> names(qteData)
[1] "x" "treatment" "y0" "y1" "y" [6] "fy1" "fy0"
We run the function `qte()` on the data (qteData$y, qteData$x, qteData$ treatment) to estimate the 10th, 25th, 50th, 75th and 90th QTEs (i.e., probs = c(0.1, 0.25, 0.50, 0.75, 0.90)) simultaneously. Specifically, we use the probit BART model (i.e., bart.link = "probit") to estimate the PS. We use 50 trees (i.e., bart.params$ntree = 50) in the BART model and run the MCMC for 1000 iterations and keep every 10th posterior sample (i.e., bart.params$keepevery = 100) after the first 500 iterations (i.e., bart.params$nskip = 500). Other hyper-parameters of BART are set to default values. For the DPM model, we use the blocked Gibbs sampler (i.e., dpm.params$method = "truncated") with 50 clusters (i.e., dpm.params$nclusters = 50) and run 900 MCMC iterations with the first 500 samples burned in (i.e., dpm.params$nskip = 500) and every 2nd sample saved (i.e., dpm.params$keepevery = 2). Other hyper-parameters of the DPM model are set as suggested in Appendix A. Besides the estimated quantiles, we require the function to return the estimated density and CDF of potential outcomes by setting dpm.params$type.pred = c("cdf", "pdf") and their 95% pointwise credible intervals are also returned via the setting compute.band = TRUE, type.band = "HPD", alphas = c(0.05). We use Bayesian bootstrap (i.e., Rdist = "bootstrap") to estimate the distribution of PS in the population of interest. The following code realizes the settings described above.

```r
> qteFit = qte(y = qteData$y, x = qteData$x, treatment = qteData$treatment, 
+   probs = c(0.1, 0.25, 0.50, 0.75, 0.90), 
+   compute.band = TRUE, type.band = "HPD", alphas = c(0.05), 
+   bart.link = "probit", 
+   bart.params = list(ntrees = 50, nskip = 500, ndpost = 5, 
+     keepevery = 100), 
+   dpm.params = list(method = "truncated", nclusters = 50, 
+     type.pred = c("cdf", "pdf"), ngrid = 100, 
+     nskip = 500, ndpost = 200, keepevery = 2), 
+   Rdist = "bootstrap", mc.cores = 1)
```

The returned object `qteFit` is of class "qte" and has the following components.

```r
> names(qteFit)
[1] "propensity"       "bart.parmas"
[3] "grid"             "xpred"
[5] "type.pred"        "compute.band"
[7] "type.band"        "alphas"
[9] "probs"            "control.cdfs"
[11] "treatment.cdfs"   "control.quantiles.avg"
[13] "treatment.quantiles.avg" "qtes.avg"
[15] "control.quantiles.ci" "treatment.quantiles.ci"
[17] "qtes.ci"          "control.pdfs.avg"
[19] "treatment.pdfs.avg" "control.pdfs.ci"
[21] "treatment.pdfs.ci" "n0"
[23] "n1"               "p"
[25] "dpm.params"
```

Let us look at a couple of key components.
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- \$qtes.avg is a vector of the averaged QTEs and the \( i^{th} \) $qtes.avg corresponds to the \( i^{th} \) probs
- $qtes.ci is a matrix representing the credible intervals of estimated QTEs; the \( i^{th} \) row corresponds to the \( i^{th} \) probs; the first (second) column refers to the lower (upper) bound; other returns with "$\cdot ci" suffix have similar definitions
- $control.pdfs.avg ($treatment.pdfs.avg) is a vector of the averaged estimated density of the potential outcome under the control (active) treatment group, which is evaluated at $grid
- $control.cdfs ($treatment.cdfs) is a matrix of the estimated CDF of the potential outcome under the control (active) treatment group, which is evaluated at $grid; each row is for a posterior sample and each column is for a grid point

The prediction results of qte() can be visualized by simply applying the plot() function to the object qteFit, i.e., plot(qteFit). The estimated density of potential outcomes (see Figure 6) and the width of the credible intervals of the estimated QTEs (see Figure 8) are plotted by plot(). If the true quantiles of interest are provided, the plot() function also returns a Q-Q plot (see Figure 7) and a plot for the bias of the estimated QTEs (see Figure 8). The following code shows the usage of the plot() function for objects of class "qte". Since the true density and the true quantiles of the potential outcomes for the example in (28) are not analytically achievable, we use the functions qteData$fy0 and qteData$fy0 to simulate the true density at grid points and generate the true quantiles from a large sample data.

R> truefy0 = truefy1 = c()
R> for (i in 1 : 100) {
+   truefy0[i] = qteData$fy0(qteFit$grid[i], 10000)
+   truefy1[i] = qteData$fy1(qteFit$grid[i], 10000)
+ }
R> Data0 = SampleFun5(n = 10000000)
R> q0 = quantile(x = Data0$y0, probs = c(0.1, 0.25, 0.5, 0.75, 0.9))
R> q1 = quantile(x = Data0$y1, probs = c(0.1, 0.25, 0.5, 0.75, 0.9))
R> plot(qteFit, true.fy1 = truefy1, true.fy0 = truefy0,
+       true.quantile1 = q1, true.quantile0 = q0, true.qte = q1 - q0)

We also provide the S3 predict() function for objects of class "qte". Given the fitted object from the qte() function, users can estimate more quantiles as well as QTEs from the estimated CDFs of potential outcomes. Taking the object qteFit as an example, we show the syntax of the predict() function for objects of class "qte" as follows.

R> predict(object = qteFit, probs = seq(0.1, 0.99, 100))

We conclude this section with simulation results based on 100 repeatedly simulated datasets for the BART-DPM approach using probit BART and logit BART respectively. Specifically, we generate 100 datasets according to the data generation process in (28) and run the qte() function on each dataset with probit BART, i.e., bart.link = "probit", and logit BART, i.e., bart.link = "logit", respectively. Arguments except bart.link are set the same as
Figure 6: Estimated density of potential outcomes for the example in (28).

Figure 7: Q-Q plots of potential outcomes for the example in (28).

Figure 8: Left subfigure is the bias of the averaged estimated QTEs for one replication of the example in (28) and right subfigure is the width of the 95% credible intervals of the estimated QTEs for one replication of the example in (28). True 10th, 25th, 50th, 75th and 90th QTEs are $-0.22$, $-0.18$, $-0.13$, 0.04 and 0.05, respectively.
Table 2: Comparison of the average QTEs and 95% CIs across 100 replications between the BART-DPM approaches using probit BART and logit BART for the example in (28).

the example above. Table 2 shows the result. We can see that the two models yield similar estimation for QTEs.

5. Convergence Diagnostics for DPM Models

In this section, we empirically compare the convergence of the MCMC chains between the Pólya urn Gibbs sampler (Algorithm 1) and the blocked Gibbs sampler (Algorithm 2). The cluster-specific parameters such as $\zeta_k$, $\Omega_k$ and $\omega_k$ cannot be directly used for assessing the convergence due to label switching. Thus, it is more appropriate to examine a quantity that is not affected by the issue, such as a global (hyper-)parameter. In the following analysis, we investigate the autocorrelation of the global parameter $\alpha$, the global hyper-parameters $\lambda$, $m$ and $\Psi$ and the logarithm likelihood, to assess the mixing of the MCMC chains generated by different Gibbs samplers. The posterior samples of the global (hyper-)parameters can be found in the sub-list $\texttt{posterior}$ of an object returned by the DPMdensity() or DPMcdensity() function and the posterior samples of the logarithm likelihood are calculated and returned to the sub-list $\texttt{posterior}$ when the argument diag of the function DPMdensity() or DPMcdensity() is set to TRUE. When diag = TRUE and method = "truncated", the posterior samples of the logarithm marginal partition posterior $\log(f(\{\kappa_i\}_{i=1}^n | \{z_i\}_{i=1}^n))$ suggested by Hastie et al. (2015) are also returned to the sub-list $\texttt{posterior}$. This quantity represents the posterior distribution of the allocations, with all the other parameters integrated out. However, the marginal partition posterior does not have a closed form for the limit model of Model (11), so we do not provide it for the Pólya urn Gibbs sampler, nor investigate it here. We show the calculation of the marginal partition posterior as well as the likelihood in Appendix E.

For more convergence diagnostics, we recommend using the coda R package (Plummer et al. (2006)) which provides functions for summarizing and plotting the outputs from a MCMC chain and diagnostics tests of convergence for a MCMC chain.

Now, we revisit the simulation example in the joint density estimation, i.e., the mixture of three bivariate normals. We run the function DPMdensity() with the Pólya urn Gibbs sampler and the blocked Gibbs sampler respectively on the data DpmData1$y generated from (23). For the blocked Gibbs sampler, we run the function four times with different number of clusters: $N \in \{20, 30, 50, 100\}$. For each MCMC chain, we skip the first 10000 iterations and save the subsequent 10000 posterior samples.

R> BFit = list()
R> Nvec = c(20, 30, 50, 100)
R> for (i in 1:4) {

| Quantiles | Truth | Probit BART | Logit BART |
|-----------|-------|-------------|------------|
| 10th      | -0.22 | -0.22(-0.44, 0.01) | -0.22(-0.44, 0.01) |
| 25th      | -0.18 | -0.18(-0.44, 0.08) | -0.18(-0.44, 0.09) |
| 50th      | -0.13 | -0.11(-0.51, 0.29) | -0.12(-0.52, 0.28) |
| 75th      | 0.04  | 0.06(-0.16, 0.28)  | 0.05(-0.17, 0.26)  |
| 90th      | 0.05  | 0.06(-0.16, 0.28)  | 0.05(-0.16, 0.27)  |
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```r
+ BFit[[i]] = DPMdensity(DpmData1$y, ngrid = 0, method = "truncated",
+ nclusters = Nvec[i], diag = TRUE,
+ nskip = 10000, ndpost = 10000, keepevery = 1)
+ }
R> PFit = DPMdensity(DpmData1$y, ngrid = 0, method = "neal", diag = TRUE,
+ nskip = 10000, ndpost = 10000, keepevery = 1)

Taking the object PFit as an example, the parameters of interest can be obtained by the following code.

```r
R> alpha = PFit$posterior$alpha
R> lambda = PFit$posterior$lambda
R> m = PFit$posterior$m
R> Psi = PFit$posterior$Psi
R> llik = PFit$posterior$ylogliks
R> length(alpha)

[1] 10000
```

Figure 9 shows the autocorrelation for different parameters and different samplers. In general, the MCMC chains generated by the Pólya urn Gibbs sampler mix better than those generated by the blocked Gibbs sampler. From the first row of Figure 9, we can see that as \( N \) increases, the autocorrelation of \( \alpha \) sampled by the blocked Gibbs sampler decreases fast and becomes similar to that sampled by the Pólya urn Gibbs sampler. This is because as \( N \) increases, the mixing weights (15) used to update \( \alpha \) converge to the stick-breaking weights of DP (13) and therefore the distribution used to update \( \alpha \) in the blocked Gibb sampling becomes similar to that in the Pólya urn Gibbs sampling. From the second to the fourth row of Figure 9, we find that the chains of hyper-parameters based on the blocked Gibbs sampling mix better for a smaller \( N \). Let \( \eta \) denote a hyper-parameter of the base distribution \( G_0 \). Both of the two samplers update \( \eta \) based on the product distribution of the hyper-prior on \( \eta \) and the base distribution \( G_0 \), except that the Pólya urn Gibbs sampler only includes \( G_0 \) of the parameters associated with some observations while the blocked Gibbs sampler includes \( G_0 \) of all the parameters. The parameters included by the blocked Gibbs sampler but not related to any observation are sampled from their prior distributions and shared by different \( \eta \)’s across the MCMC iterations, thereby making the chain of the hyper-parameter mix slowly. As \( N \) decreases, there are fewer empty clusters, so the chain mixes better. The fifth row of Figure 9 shows the autocorrelation of logarithm likelihood. As we can see, when \( N \) gets greater, the autocorrelation of the log likelihood of the blocked Gibbs sampler becomes similar to that of the Pólya urn Gibbs sampler, which can be explained by the almost sure convergence of the truncated DPM model.

6. Summary

This article reviews the models and algorithms implemented in the BNPqte R package, introduces the usage of the R functions with simulated examples, and assesses the mixing properties of the two Gibbs sampling algorithms used for the DPM models. As software for
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Causal inference, **BNPqte** implements a Bayesian approach to estimate QTEs and provides **R** users who are interested in QTE estimation with an alternative **R** package to those **R** packages implementing frequentist methods. Moreover, **BNPqte** provides a fast implementation of the DPM of multivariate normals model in density estimation, especially in conditional estimation, compared to the popular **DPpackage** **R** package. Finally, **BNPqte** modifies the functions from the **BART** **R** package to improve them for data with mixed-type predictors and to obtain the optimal posterior contraction rate.

### Computational Details

The results in this article were obtained using **R** 3.6.0 with the **BNPqte** **R** package. **R** itself and all packages used, except **BNPqte** and **DPpackage**, are available from the Comprehensive **R** Archive Network (CRAN) at [https://CRAN.R-project.org/](https://CRAN.R-project.org/). **BNPqte** is available at [https://github.com/chujiluo/BNPqte](https://github.com/chujiluo/BNPqte). **DPpackage** is archived from CRAN, but the source
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code is available at https://github.com/cran/DPpackage.

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A. Hyper-Parameters Specification for DPM Models

We adopt the specification of Taddy (2008) to choose hyper-parameters, which ensures that the hyper-priors are appropriately diffuse, are scaled to the data, and provide minimal prior information.

Following the notation of Section 3, let \(c_y\) and \(c_{xj}\) denote the mean of \(\{Y_i\}_{i=1}^n\) and \(\{x_{ij}\}_{i=1}^n\), \(j = 1, \ldots, p\), and also \(\tau_y\) and \(\tau_{xj}\) be the corresponding range, i.e., difference between the max and min values. Let \(c = (c_y, c_{x_1}, \ldots, c_{xp})\) and denote by \(R\) the \(d \times d\) diagonal matrix with diagonal elements \((r_y/4)^2, (r_{x_1}/4)^2, \ldots, (r_{xp}/4)^2\), which represent prior guesses for the mean and variability of the data, respectively.

We first specify the hyper-parameters for the DPM model without hyper-priors, i.e., Model (8-9). Based on the form of \(G_0\), we can obtain the marginal prior moments for \(\mu\), i.e., \(E(\mu) = m\) and \(\text{Cov}(\mu) = \frac{\Psi}{\lambda^2} \cdot 1\), as well as the marginal mean for \(\Sigma\), i.e., \(E(\Sigma) = \frac{\Psi}{\nu - d - 1}\). We take \(E(\mu) = c\), set \(\text{Cov}(\mu) = 2R\) using a variance inflation factor of 2, specify \(E(\Sigma) = R\), and finally choose a value of \(\nu\) which yields a more dispersed prior for \(\Sigma\). Hence, by default, we set the hyper-parameters of Model (8-9) as follows:

\[
m = c, \quad \lambda = 0.5, \quad \nu = d + 2, \quad \Psi = R.
\]

For the hierarchical model (8-10), the marginal prior moments for \(\mu\) and \(\Sigma\) are slightly changed by the hyper-priors in (10), i.e., \(E(\mu) = m_0\), \(\text{Cov}(\mu) = S_0 + \frac{\gamma_2}{\gamma_1 - 1} \cdot \frac{\nu_0 \Psi_0}{\nu - d - 1}\) and \(E(\Sigma) = \frac{\nu_0 \Psi_0}{\nu - d - 1}\). With the same idea to estimate \(E(\mu)\) by \(c\), \(\text{Cov}(\mu)\) by \(2R\) and \(E(\Sigma)\) by \(R\), we obtain \(m_0 = c, S_0 + \frac{\gamma_2}{\gamma_1 - 1} \cdot \frac{\nu_0 \Psi_0}{\nu - d - 1} = 2R\) and \(\nu_0 \Psi_0 = R\). By setting \(S_0 = R\), we have \(\frac{\gamma_2}{\gamma_1 - 1} = 1\) and \(\nu_0 \Psi_0 = R\).

By default, we let \(\gamma_1 = 3\) and \(\gamma_2 = 2\) to satisfy \(\frac{\gamma_2}{\gamma_1 - 1} = 1\). We also set \(\nu = \nu_0 = d + 2\) to allow the largest dispersion. In conclusion, by default, we specify the hyper-parameters for Model (8-10) as follows:

\[
m_0 = c, \quad S_0 = R, \quad \gamma_1 = 3, \quad \gamma_2 = 2, \quad \nu = \nu_0 = d + 2, \quad \Psi_0 = R/\nu_0.
\]

Regarding the choice of the concentration parameter \(\alpha\), we set \(\alpha = 10\) for the Model (8-9) and \(a_0 = 10, b_0 = 1\) for the hierarchical model (8-10), to allow higher prior probability for larger number of distinct clusters (Antoniak (1974)).

B. Posterior Computation for Pólya Urn Gibbs Sampling

In this section, we provide the details for sampling the posterior distribution of \(\phi_k = (\zeta_k, \Omega_k)\)'s, \(\alpha\) and other hyperparameters for the DPM of multivariate normals model (Model (8-9) or Model (8-10)), using Algorithm 1, i.e., Algorithm 8 of Neal (2000).

It is not possible to explicitly represent the infinite number of \((\zeta_k, \Omega_k)\)'s for the DPM model, so instead, Algorithm 1 updates only those \((\zeta_k, \Omega_k)\)'s currently associated with some observations. Based on (8) and (9), we sample \((\zeta_k, \Omega_k)\) \((\kappa \in \{\kappa_1, \ldots, \kappa_n\})\) from their conjugate posterior distribution:

\[
f(\zeta_k, \Omega_k | \{z_i : \kappa_i = k\}) \propto f_{\text{Normal}}(\zeta_k | m_*, \frac{1}{\lambda^*} \Omega_k) \times f_{\text{IW}}(\Omega_k | \nu, \Psi^*) \times \prod_{\{i : \kappa_i = k\}} f_{\text{Normal}}(z_i | \zeta_k, \Omega_k)
\]

\[
\qquad \propto f_{\text{Normal}}(\zeta_k | m_*, \frac{1}{\lambda^*} \Omega_k) \times f_{\text{IW}}(\Omega_k | \nu^*, \Psi^*), \tag{29}
\]
\[ m^* = \frac{\lambda m + n_k \bar{z}_k}{\lambda + n_k}, \quad \lambda^* = \lambda + n_k, \quad \nu^* = \nu + n_k, \]

\[ \Psi^* = \Psi + \sum_{\{i: \kappa_i = k\}} (z_i - \bar{z}_k)(z_i - \bar{z}_k)^\top + \frac{\lambda n_k}{\lambda + n_k}(\bar{z}_k - m)(\bar{z}_k - m)^\top, \tag{30} \]

\[ n_k = |\{i : \kappa_i = k\}|, \quad \bar{z}_k = \frac{1}{n_k} \sum_{\{i: \kappa_i = k\}} z_i. \]

Note that \( f \) without a subscript in (29) represents a general density and that \( f \) with a subscript represents a specific density specified by the subscript. Parameters after | are parameterized as usual. For example, \( f_{\text{Normal}}(z | \zeta, \Omega) \) means a normal density with mean equal to \( \zeta \) and covariance matrix equal to \( \Omega \) for the observation \( z \). We follow this notation in this section and subsequent sections.

If the hierarchical structure (10) is assumed for the DPM model, we update \( \alpha, m, \lambda \) and \( \Psi \) sequentially at each iteration of MCMC as follows.

1. The concentration parameter \( \alpha \) is updated in two steps, using the approach of Escobar and West (1995):
   
   (a) sample \( \eta \) from Beta(\( \alpha + 1, n \)) and calculate a weight \( \pi_\eta \) such that \( \frac{\pi_\eta}{1 - \pi_\eta} = \frac{a_\eta + K^* - 1}{\eta_0(\eta_0 - \log(\eta))} \), where \( K^* \) is the number of distinct values in \( \{\kappa_i\}_{i=1}^n \);
   
   (b) sample a new value for \( \alpha \) from a mixture of gamma distribution:
   
   \[ \pi_\eta \Gamma(\alpha_0 + K^*, b_0 - \log(\eta)) + (1 - \pi_\eta) \Gamma(\alpha_0 + K^* - 1, b_0 - \log(\eta)). \]

2. Sample a new value for the mean vector \( m \) of the base distribution \( G_0 \) from
   
   \[ f(m | \{\zeta_k, \Omega_k\}_{k \in \{\kappa_i\}_{i=1}^n}, \{\kappa_i\}_{i=1}^n, \lambda, m_0, S_0) \]
   
   \[ \propto f_{\text{Normal}}(m | m_0, S_0) \times \prod_{k \in \{\kappa_i\}_{i=1}^n} f_{\text{Normal}}(\zeta_k | m, \frac{1}{\lambda} \Omega_k) \]
   
   \[ \propto f_{\text{Normal}}(m | m_0^*, S_0^*) \tag{31} \]

   where \( (S_0^*)^{-1} = \lambda \left( \sum_{k \in \{\kappa_i\}_{i=1}^n} \Omega_k^{-1} \right) + S_0^{-1} \) and \( m_0^* = \]

   \[ S_0^* \left[ \lambda \left( \sum_{k \in \{\kappa_i\}_{i=1}^n} \Omega_k^{-1} \zeta_k \right) + S_0^{-1} m_0 \right]. \]

3. Sample a new value for the scale parameter \( \lambda \) of the base distribution \( G_0 \) from
   
   \[ f(\lambda | \{\zeta_k, \Omega_k\}_{k \in \{\kappa_i\}_{i=1}^n}, \{\kappa_i\}_{i=1}^n, m, \gamma_1, \gamma_2) \]
   
   \[ \propto f_{\Gamma}(\lambda | \gamma_1, \gamma_2) \times \prod_{k \in \{\kappa_i\}_{i=1}^n} f_{\text{Normal}}(\zeta_k | m, \frac{1}{\lambda} \Omega_k) \]
   
   \[ \propto f_{\Gamma}(\lambda | \gamma_1^*, \gamma_2^*) \tag{32} \]

   where \( \gamma_1^* = \gamma_1 + \frac{dK^*}{2} \) and \( \gamma_2^* = \gamma_2 + \frac{1}{2} \sum_{k \in \{\kappa_i\}_{i=1}^n} (\zeta_k - m)^\top \Omega_k^{-1}(\zeta_k - m). \)
Similar to (17), the full posterior distribution of model (16, 9, 10) can be expressed as follows.

\[
dpm \text{ of multivariate normals model.}
\]

Algorithm 2, i.e., the blocked Gibbs sampler of Ishwaran and James (2001). The posterior to be (9) and the hyper-parameters of 

In this section, we provide details for posterior sampling for model (16) with 

parameters. 

where \( \phi \) 


\[
\begin{align*}
\text{Note that the auxiliary parameters created during the update of } \kappa_i \text{'s are neither updated nor involved in the update of hyper-parameters, which facilitates fast convergence of hyper-parameters.}
\end{align*}
\]

C. Posterior Computation for Blocked Gibbs Sampling

In this section, we provide details for posterior sampling for model (16) with \( G_0 \) assumed to be (9) and the hyper-parameters of \( G_0 \) and the parameter \( \alpha \) assumed to be (10), using Algorithm 2, i.e., the blocked Gibbs sampler of Ishwaran and James (2001). The posterior samples from this sampler are used for approximating posterior samples of the corresponding DPM of multivariate normals model.

Similar to (17), the full posterior distribution of model (16, 9, 10) can be expressed as follows

\[
f(\{\phi_k\}_{i=1}^{N}, \kappa_i, \omega, \alpha, m, \lambda, \Psi \mid \{z_i\}_{i=1}^{n}, a_0, b_0, m_0, S_0, \gamma_1, \gamma_2, \nu, \nu_0, \Psi_0) 
\]

\[
\propto f_{\text{Wishart}}(\Psi \mid \nu_0, \Psi_0) \prod_{k \in \kappa} f_{\text{Wishart}}(\Psi_k \mid \nu, \Psi) 
\]

\[
\propto f_{\text{Wishart}}(\Psi \mid \nu_0^*, \Psi_0^*) \tag{33}
\]

\[
\text{where } \nu_0^* = \nu K^* + \nu_0 \text{ and } \Psi_0^* = \left( \Phi_0^{-1} + \sum_{k \in \kappa} \Omega_k^{-1} \right)^{-1}.
\]

Note that the auxiliary parameters created during the update of \( \kappa_i \)'s are neither updated nor involved in the update of hyper-parameters, which facilitates fast convergence of hyper-parameters.

1. Sample a new value for each \( (\zeta_k, \Omega_k) \) \( (1 \leq k \leq N) \) from the posterior distribution

\[
f_{\text{Normal}}(\zeta_k \mid m, \frac{1}{\lambda} \Omega_k) \times f_{\text{Wishart}}(\Omega_k \mid \nu, \Psi) \times \prod_{\{i: \kappa_i = k\}} f_{\text{Normal}}(z_i \mid \zeta_k, \Omega_k)
\]

which essentially is (29-30), if \( k \in \kappa^* \), and sample a new value for each \( (\zeta_k, \Omega_k) \) from the prior distribution \( f_{\text{Normal}}(\zeta_k \mid m, \frac{1}{\lambda} \Omega_k) \times f_{\text{Wishart}}(\Omega_k \mid \nu, \Psi) \) otherwise.

2. Sample a vector of new values for \( \{\omega_k\}_{k=1}^{N} \) from

\[
f(\omega \mid \kappa_i, \alpha) \propto f_{\text{GD}}(\omega \mid 1, \alpha, \ldots, 1, \alpha) \times \prod_{i} f_{\text{Discrete}}(\kappa_i \mid \omega)
\]

\[
\propto f_{\text{GD}}(\omega \mid a_1, b_1, \ldots, a_{N-1}, b_{N-1})
\]

using two steps:
(a) sample a value for $V_k$ from Beta($a_k, b_k$) for $1 \leq k \leq N - 1$ and set $V_N = 1$,
(b) compute $\omega_1 = V_1$ and $\omega_k = (1 - V_1) \cdots (1 - V_{k-1})V_k$ for $2 \leq k \leq N$,
where $a_k = n_k + 1$, $b_k = N_k + \alpha$, $N_k = n_{k+1} + \cdots + n_N$ for $1 \leq k \leq N - 1$ and $n_k = |\{i : \kappa_i = k\}|$ for $1 \leq k \leq N$.

3. Sample a new value for each $\kappa_i (1 \leq i \leq n)$ from a discrete distribution

$$P(\kappa_i = k | \omega, \{(\zeta_k, \Omega_k)\}_{k=1}^N, \{z_i\}_{i=1}^n) \propto P(\kappa_i = k) \times f_{\text{Normal}}(z_i | \zeta_k, \Omega_k)$$

where $k = 1, \cdots, N$. In practice, Gumbei-max trick (Maddison et al. (2014)) is used to help sample the discrete distribution in log-space and avoid potentially floating point inaccuracy.

4. Sample a new value for $\alpha$ from

$$f(\alpha | \omega, a_0, b_0) \propto f_{\text{Gamma}}(\alpha | a_0, b_0) \times f_{\text{GP}}(\omega | 1, \alpha, 1, \alpha)$$

$$\propto f_{\text{Gamma}}(\alpha | a_0^*, b_0^*),$$

where $a_0^* = a_0 + N - 1$ and $b_0^* = b_0 - \log(\omega_N) = b_0 - \sum_{k=1}^{N-1} \log(1 - V_k)$.

5. Sample a new value for $m$ from (31) with $\{(\zeta_k, \Omega_k)\}_{k=1}^N$ replaced by $\{(\zeta_k, \Omega_k)\}_{k=1}^N$.

6. Sample a new value for $\lambda$ from (32) with $\{(\zeta_k, \Omega_k)\}_{k=1}^N$ replaced by $\{(\zeta_k, \Omega_k)\}_{k=1}^N$ and $K^*$ replaced by $N$.

7. Sample a new value for $\Psi$ from (33) with $\{(\zeta_k, \Omega_k)\}_{k=1}^N$ replaced by $\{(\zeta_k, \Omega_k)\}_{k=1}^N$ and $K^*$ replaced by $N$.

We can see that steps 5-7 are similar to steps 2-4 in Appendix B except that steps 2-4 in Appendix B update hyper-parameters of $G_0$ using $(\zeta_k, \Omega_k)$’s associated with at least one observation while steps 5-7 update hyper-parameters of $G_0$ using all the $(\zeta_k, \Omega_k)$’s. Since some of $\{(\zeta_k, \Omega_k)\}_{k=1}^N$ are not related to any observations, the Markov chain of hyper-parameters will mix slowly if the blocked Gibbs sampler is used.

**D. Density Estimation Based on Pólya Urn Gibbs Sampler**

In this section, we describe the density estimation approach of Müller et al. (1996) using Algorithm 8 of Neal (2000).

The predictive density $f(z_{n+1} | \{z_i\}_{i=1}^n)$ can be expressed as follows

$$f(z_{n+1} | \{z_i\}_{i=1}^n) = \int \int f(z_{n+1}, \Sigma_{n+1} | \mu_{n+1}, \Sigma_{n+1}) f(\mu_{n+1}, \Sigma_{n+1} | \{(\zeta_k, \Omega_k)\}_{k=1}^N) d(\mu_{n+1}, \Sigma_{n+1})$$

$$dF(\{(\zeta_k, \Omega_k)\}_{k=1}^N | \{z_i\}_{i=1}^n),$$

(34)
where $f(z_{n+1} | \mu_{n+1}, \Sigma_{n+1})$ is the normal likelihood, $F(\{\zeta_k, \Omega_k\}_{k \in \{\kappa_i\}_{i=1}^n} \mid \{z_i\}_{i=1}^n)$ is the posterior distribution, and $f(\mu_{n+1}, \Sigma_{n+1} \mid \{\zeta_k, \Omega_k\}_{k \in \{\kappa_i\}_{i=1}^n})$ can be obtained from (8) with $G$ integrated out and can be represented using the following Polya Urn scheme:

$$
\begin{align*}
    f(\mu_{n+1}, \Sigma_{n+1} \mid \{\zeta_k, \Omega_k\}_{k \in \{\kappa_i\}_{i=1}^n}) &= \frac{\alpha}{\alpha + n} G_0(\mu_{n+1}, \Sigma_{n+1}) \\
    &+ \sum_{k \in \{\kappa_i\}_{i=1}^n} \frac{n_k}{\alpha + n} \delta(\zeta_k, \Omega_k)(\mu_{n+1}, \Sigma_{n+1}).
\end{align*}
$$

Thus, with each posterior sample $\{\{\kappa^{(i)}_1\}_{i=1}^n, \{\zeta^{(i)}_k, \Omega^{(i)}_k\}_{k \in \{\kappa^{(i)}_i\}_{i=1}^n}\}$ from the Polya urn Gibbs sampler, the inside integral of (34) can be estimated by

$$
\frac{\alpha}{\alpha + n} f(z_{n+1} | \zeta^*, \Omega^*) + \sum_{k \in \{\kappa^{(i)}_1\}_{i=1}^n} \frac{n_k}{\alpha + n} f(z_{n+1} \mid \zeta^{(i)}_k, \Omega^{(i)}_k),
$$

where $(\zeta^*, \Omega^*)$ is sampled from the base distribution $G_0$. The predictive density (34) can be estimated by taking the average of (35) across all the MCMC samples. The derivation above assumes that $\alpha$ and hyper-parameters of $G_0$ are fixed. If the hierarchical model (10) is assumed, the estimator in (35) can be adjusted by using the latest update of $\alpha$ and the hyper-parameters.

When the Polya urn Gibbs sampler is used, we use the DPdensity() function in DPpackage to estimate the predictive conditional density $f(Y_{n+1} \mid x_{n+1}, \{z_i\}_{i=1}^n)$ using an extension of the approach of Müller et al. (1996). They first fit a DPM of multivariate normals model on the joint data $\{z_i\}_{i=1}^n$ and get a sequence of posterior samples. Then a weight dependent mixture model is induced from the joint DPM model. Based on the stick-breaking representation of DP in (13), the weight dependent mixture model has the following form

$$
f(Y_{n+1} \mid x_{n+1}, \{z_i\}_{i=1}^n) = \int \left( \sum_{j=1}^\infty \omega_j(x_{n+1}) f_{\text{Normal}}(Y_{n+1} \mid \beta_0 + x_{n+1}^\top \beta_j, \sigma_j^2) \right) dF(\mathcal{P}_\infty \mid \{z_i\}_{i=1}^n),
$$

where $\omega_j(x_{n+1}), \beta_0, \beta_j$ and $\sigma_j^2$ are functions of the components of $\mathcal{P}_\infty$, i.e., $\{\omega_j\}_{j=1}^\infty, \{\kappa_i\}_{i=1}^n$ and $\{\zeta_k, \Omega_k\}_{k \in \{\kappa_i\}_{i=1}^n}$. Finally, the $\epsilon$-DP approximation proposed by Muliere and Tardella (1998) with $\epsilon = 0.01$ is used for the inference of (36). The detailed procedure of estimating the summation in (36) is summarized in Algorithm 4.

The estimation of a predictive conditional density in (36) based on the Polya urn sampler has similar construction of that in (19) based on the blocked Gibbs sampler. However, it is important to note that the one based on the Polya urn sampler is much more complicated and computationally intensive, because it does not have the direct access to the mixing weights. To estimate a predictive conditional density, Algorithm 4 has to repeatedly generate stick-breaking weights to satisfy the conditions of $\epsilon$-DP approximation, after each MCMC iteration of the DPM model. This typically involves thousands of stick-breaking weights, which implies that it takes thousands of basic operations to evaluate the density for only one data point.

E. Marginal Partition Posterior and Likelihood for DPM Models
Algorithm 4 Weight Dependent DPMM for Conditional Predictive Density

1. **procedure** ESTIMATE THE SUM IN (36) GIVEN A POSTERIOR SAMPLE \( \{ \kappa_i, \zeta_{k_i}, \Omega_{k_i} \}_{i=1}^n \) FROM THE JOINT DPM MODEL WITH \( \epsilon = 0.01 \)

2. Label \( \{ \kappa_1, \cdots, \kappa_n \} \) with \( \{ 1, \cdots, K^* \} \)

3. **for** \( k \in \{ 1, \cdots, K^* \} \) **do**

4. Calculate \( \tilde{\beta}_{0k}, \tilde{\beta}_k \) and \( \tilde{\sigma}_k^2 \) as follows:

\[
\begin{align*}
\tilde{\beta}_k &= \Omega_{12k} \Omega_{22k}^{-1}, \\
\tilde{\beta}_{0k} &= \zeta_{1k} - \tilde{\beta}_k \zeta_{2k}, \\
\tilde{\sigma}_k^2 &= \Omega_{11k} - \tilde{\beta}_k \Omega_{21k}, \\
\zeta_k &= \begin{pmatrix} \zeta_{1k} \\ \zeta_{2k} \end{pmatrix} \\
\Omega_k &= \begin{pmatrix} \Omega_{11k} & \Omega_{12k} \\ \Omega_{21k} & \Omega_{22k} \end{pmatrix}
\end{align*}
\]

(37)

5. Calculate \( f_{\text{Normal}}(x_{n+1} | \zeta_{2k}, \Omega_{22k}) \) and \( f_{\text{Normal}}(Y_{n+1} | \tilde{\beta}_{0k} + x_{n+1}^T \tilde{\beta}_k, \tilde{\sigma}_k^2) \)

6. **end for**

7. Set \( \omega_0 = 0 \) and \( j = J = 0 \)

8. **while** \( 1 - \sum_{j=0}^{J} \omega_j > \epsilon \) **do**

9. Update \( j = j + 1 \) and \( J = J + 1 \)

10. Sample \( V_j \) from Beta\((1, \alpha + n)\), and compute \( \omega_j = V_j \prod_{x=0}^{j-1} (1 - V_{x-1}) \)

11. Sample \( k_j \) from \( \{ 1, \cdots, K^* + 1 \} \) with probabilities \( \{ \frac{\omega_1}{\alpha + n}, \cdots, \frac{\omega_{K^*}}{\alpha + n} \} \)

12. **if** \( k_j \leq K^* \) **then**

13. Set \( \beta_{0j} = \tilde{\beta}_{0k_j}, \beta_j = \tilde{\beta}_k \) and \( \sigma_j^2 = \tilde{\sigma}_k^2 \)

14. Use \( f_{\text{Normal}}(x_{n+1} | \zeta_{2k_j}, \Omega_{22k_j}) \) in step 5 to calculate \( \tilde{\omega}_j(x_{n+1}) \) as follows:

\[
\tilde{\omega}_j(x_{n+1}) = \omega_j f_{\text{Normal}}(x_{n+1} | \zeta_{2k_j}, \Omega_{22k_j})
\]

(38)

15. **else**

16. Sample \( (\zeta^*, \Omega^*) \) from the base distribution \( G_0 \)

17. Calculate \( \beta_{0j}, \beta_j, \sigma_j^2 \) and \( \tilde{\omega}_j(x_{n+1}) \) using (37) and (38), respectively, with \( (\zeta_k, \Omega_k) \) replaced by \( (\zeta^*, \Omega^*) \)

18. **end if**

19. **end while**

20. The sum in (36) is estimated by

\[
\frac{\sum_{j=1}^{J} \tilde{\omega}_j(x_{n+1}) f_{\text{Normal}}(Y_{n+1} | \beta_{0j} + x_{n+1}^T \beta_j, \sigma_j^2)}{\sum_{j=1}^{J} \tilde{\omega}_j(x_{n+1})}
\]

(39)

and notice that for those \( j \) such that \( k_j \leq K^* \), the conditional density \( f_{\text{Normal}}(Y_{n+1} | \beta_{0j} + x_{n+1}^T \beta_j, \sigma_j^2) \) is computed in step 5

21. **end procedure**
The likelihood functions given the data \( \{ \mathbf{z}_i \}_{i=1}^n \) under the DPM of multivariate normals model fitted by the Pólya urn Gibbs sampler (Algorithm 1) and the blocked Gibbs sampler (Algorithm 2) have the same form as follows,

\[
L \left( \{ \kappa_i \}_{i=1}^n, \{ \mathbf{z}_i \}_{i=1}^n \right) = \int \prod_{k=1}^{K^*} \left[ f_{\text{NIW}}(\mathbf{z}_{i,k}^*, \mathbf{z}_{i,k}^* \mid \mathbf{m}, \lambda, \nu, \Psi) \prod_{\kappa_i = \kappa_j^*} f_{\text{Normal}}(\mathbf{z}_i \mid \mathbf{z}_{i,k}^*, \mathbf{z}_{i,k}^*) \right] \\
\times \frac{d\kappa_i^*}{\pi^{d/2}} \prod_{j=1}^{K^*} \Gamma \left( \frac{\nu + n_j}{2} \right) \prod_{j=1}^{K^*} \frac{1}{\| \Psi_j^* \|^{n_j + \nu_j/2}}
\]

where \( N^* \) is the pre-specified number of clusters \( N \) if the blocked Gibbs sampler is used and is the number of non-empty clusters \( K^* \) if the Pólya urn Gibbs sampler is used, and \( \kappa^* = \{ \kappa_j^* \}_{j=1}^{K^*} \) are the unique values in \( \{ \kappa_i \}_{i=1}^n \).

The marginal partition posterior is only available for the blocked Gibbs sampling. Under Model (16), the marginal partition posterior is defined as follows

\[
f(\kappa_1, \ldots, \kappa_n \mid \{ \mathbf{z}_i \}_{i=1}^n) \propto f(\{ \mathbf{z}_i \}_{i=1}^n \mid \kappa_1, \ldots, \kappa_n) \times f(\kappa_1, \ldots, \kappa_n).
\]

The first term on the right hand side is the marginal likelihood with \( \mathbf{z}_i \)'s and \( \mathbf{z}_k \)'s integrated out, and can be calculated as follows

\[
f(\{ \mathbf{z}_i \}_{i=1}^n \mid \kappa_1, \ldots, \kappa_n) = \int \prod_{j=1}^{K^*} \left[ f_{\text{NIW}}(\mathbf{z}_{i,k}^*, \mathbf{z}_{i,k}^* \mid \mathbf{m}, \lambda, \nu, \Psi) \prod_{\kappa_i = \kappa_j^*} f_{\text{Normal}}(\mathbf{z}_i \mid \mathbf{z}_{i,k}^*, \mathbf{z}_{i,k}^*) \right] \\
\times \frac{d\kappa_i^*}{\pi^{d/2}} \prod_{j=1}^{K^*} \Gamma \left( \frac{\nu + n_j}{2} \right) \prod_{j=1}^{K^*} \frac{1}{\| \Psi_j^* \|^{n_j + \nu_j/2}}
\]

where \( n_j \) and \( \Psi_j^* \) are defined in (30) and \( \Gamma(\cdot) \) is a multivariate gamma function with dimension \( d \). Note that in the first equality above, the second integral is 1, and the first integral is a product of \( K^* \) marginal likelihoods of \( \{ \mathbf{z}_i \}_{i=1}^n \) given \( K^* \) conjugate normal-inverse-Wishart priors, respectively.

The second term on the right hand side of (40) is the marginal prior distribution of \( \{ \kappa_i \}_{i=1}^n \), and it can be computed as follows

\[
f(\kappa_1, \ldots, \kappa_n) = \int \int f(\kappa_1, \ldots, \kappa_n \mid \omega) f(\omega \mid \alpha) f(\alpha \mid a_0, b_0) d\omega d\alpha.
\]

For simplicity, we fix \( \alpha \), for example, at its posterior mean \( \alpha^* \), so the density of interest can be calculated as follows

\[
f(\kappa_1, \ldots, \kappa_n) = \int f(\kappa_1, \ldots, \kappa_n \mid \omega) f(\omega \mid \alpha^*) d\omega
\]

\[
= \int \left( \prod_{j=1}^{K^*} \omega_{\kappa_j^*}^{n_j} \right) \times f_{\text{GD}}(\omega_1, \ldots, \omega_N \mid 1, \alpha^*, \ldots, 1, \alpha^*) d\omega
\]

\[
= \frac{\alpha^*^{N-1} \Gamma(b_{N-1}) \prod_{k=1}^{N-1} \Gamma(a_k)}{\Gamma(n + \alpha^* + 1) \prod_{k=1}^{N-2} b_k}.
\]
where $a_k$ and $b_k$ are defined in the step 2 of Appendix C. The last equality of the equation above is from the conjugacy of the generalized Dirichlet distribution and the multinomial distribution.

F. More Simulation Results

Figure 10: From left to right, subfigures are contours of the difference between the estimated density and the true density, the estimated density, and the true density, for the DPM of multivariate normals model using the Pólya urn Gibbs sampler for the example in (23).

Figure 11: Estimated conditional density for the DPM of multivariate normals model using the Pólya urn Gibbs sampler for the example in (24).
**Figure 12:** Estimated conditional CDF for the DPM of multivariate normals model using the Pólya urn Gibbs sampler for the example in (24).

**Figure 13:** Estimated conditional mean for the DPM of multivariate normals model using the Pólya urn Gibbs sampler for the example in (24).