A PRticle filter algorithm for nonparametric estimation of multivariate mixing distributions

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Abstract
Predictive recursion (PR) is a fast, recursive algorithm that gives a smooth estimate of the mixing distribution under the general mixture model. However, the PR algorithm requires evaluation of a normalizing constant at each iteration. When the support of the mixing distribution is of relatively low dimension, this is not a problem since quadrature methods can be used and are very efficient. But when the support is of higher dimension, quadrature methods are inefficient and there is no obvious Monte Carlo-based alternative. In this paper, we propose a new strategy, which we refer to as PRticle filter, wherein we augment the basic PR algorithm with a filtering mechanism that adaptively reweights an initial set of particles along the updating sequence which are used to obtain Monte Carlo approximations of the normalizing constants. Convergence properties of the PRticle filter approximation are established and its empirical accuracy is demonstrated with simulation studies and a marked spatial point process data analysis.

Keywords Importance sampling · Marked point process · Mixture model · Monte Carlo · Predictive recursion

1 Introduction
Suppose we have independent and identically distributed (iid) data $X_1, \ldots, X_n$ having common density $m$ supported on $\mathbb{X}$. Furthermore, suppose that we believe this density has the mixture form $m = m_P$, where

$$m_P(x) = \int_{\mathbb{U}} k(x \mid u) P(du), \quad x \in \mathbb{X},$$ \hfill (1)

with $k(x \mid u)$ a known kernel density and $P$ an unknown mixing distribution supported on $\mathbb{U}$. The family in (1) indexed by $P$ is commonly referred to as a mixture model. One interpretation of the mixture model is that there is a set of underlying latent variables driving the data-generating process. That is, suppose the $X_i$'s are obtained through the two-step process:

$$U_1, \ldots, U_n \overset{iid}{\sim} P$$

$$(X_i \mid U_i) \overset{ind}{\sim} k(x \mid U_i), \quad i = 1, \ldots, n.$$

It is easy to check that $X_1, \ldots, X_n$ from this hierarchical model formulation are iid with density $m_P$. This sort of hierarchical, latent variable modeling is common when heterogeneity is present in the observed data. This also covers the class of problems where $U$ represents an unobservable “signal” of interest and $X$ the corresponding noise-corrupted signal, i.e., the “signal plus noise.” One also might adopt (1) simply for the flexibility the mixture model affords (e.g., Das-Gupta 2008, Chapter 33). In any case, the distribution of the latent variables, or signals, may be of some practical interest, in which case the goal becomes estimation of the unknown mixing distribution $P$ based on iid data $X_1, \ldots, X_n$ from the mixture $m_P$ in (1). This is our focus in the present paper.

Estimation of the mixing distribution $P$ is a notoriously difficult problem. Aside from methods tailored to specific mixture model forms, e.g., deconvolution (Fan 1991; Stefanski and Carroll 1990), there are a few general estimation methods available: the two “standard” approaches are nonparametric maximum likelihood and nonparametric Bayes. The former maximizes the likelihood based on observations $X_1, \ldots, X_n$ from $m_P$, with respect to $P$. Given the nonpara-
metric nature of $P$, the resulting estimate is almost surely discrete and the points of support are no greater than $n$ (Lindsay 1983). The latter approach assigns a prior distribution to $P$, typically a Dirichlet process (Ghosh and Ramamoorthi 2003; Ghosal and Van der Vaart 2017; Hjort et al. 2010; Ferguson 1974), and evaluate the corresponding posterior mean, given $(X_1, \ldots, X_n)$. Even though there is no direct imposition of discreteness in the posterior, draws from the posterior distribution of $P$ have atoms (e.g., Blackwell and MacQueen 1973) and the corresponding posterior mean is spiky, “effectively discrete.” Hence, neither the likelihood nor Bayesian approaches give satisfactory solutions to the problem of estimating a mixing distribution $P$ in (1). The point is that, in these traditional approaches, the focus is on identifying candidate $P$ such that resulting mixture density $m_P$ is compatible with the empirical distribution of data, not specifically estimating the mixing distribution.

A third general approach is available, which is the primary focus of this paper, called predictive recursion (PR). Unlike the previous two methods, which are likelihood-based, the PR estimator is based on a stochastic, recursive algorithm that aims specifically to estimating the mixing distribution $P$ based on data from the mixture model (1). This strategy was first proposed in Newton et al. (1998) as a fast and smooth approximation to the posterior mean of $P$ under a Dirichlet process mixture model; see (Martin 2021). The idea behind PR is to start with a initial guess, $P_0$, and then update that guess recursively based on each individual observation $X_i$ for $i = 1, \ldots, n$. PR has a number of desirable computational and statistical properties. First, PR is computationally efficient—its complexity is $O(n)$. Second, the PR estimator, $P_n$, is absolutely continuous with respect to $P_0$, so if $P_0$ has a smooth density, then so does $P_n$. Third, the PR estimator has also been shown to consistently estimate the true mixing distribution $P$ in a series of papers: (Tokdar et al. 2009), Martin and Tokdar (2009), and Dixit and Martin (2021).

Applications of the PR algorithm have appeared in Newton (2002), Martin and Tokdar (2011), Martin and Tokdar (2012), Martin and Han (2016), Tansey et al. (2018), Woody et al. (2022), and Dixit and Martin (2022). In each of these applications, however, the mixing distribution support $\mathbb{U}$ is a relatively low-dimensional space, e.g., one- or two-dimensional. The reason for this constraint is that, while the algorithm itself is completely general, computation of the normalizing constant in Equation (2) below can be a challenge when $\mathbb{U}$ is more than two- or three-dimensional. In particular, the required integration can only be done numerically, but efficient quadrature methods are available only when the domain of integration, in this case $\mathbb{U}$, is low-dimensional. A Monte Carlo-based strategy would be less sensitive to the dimension of $\mathbb{U}$ and, in that sense, would have an advantage. Unfortunately, no such Monte Carlo-based strategy is currently available in the literature, and this paper aims to fill this gap.

Following a brief review in Sect. 2 of the PR algorithm and importance sampling techniques, we propose in Sect. 3 below the PRTicle filter approximation. As the name suggests, this consists of an augmentation of the original PR algorithm with a filtering step that adaptively reweights an initial set of particles along the PR updating sequence. The idea is that, at the $i^{th}$ step, the weighted set of particles resembles a sample from the PR estimate $P_{i-1}$ based on data $X_1, \ldots, X_{i-1}$. Hence, the $n^{th}$ step gives a particle approximation of the PR estimate $P_n$ and Theorem 1 below establishes that, for fixed data $X_1, \ldots, X_n$, this approximation converges almost surely in total variation distance to $P_n$ as the number of sampled particles approaches infinity.

In Sect. 4, we evaluate performance of the proposed PRTicle filter approximation on both real and simulated data sets. For the simulated data sets, the evaluation is split into two types. First, to judge the accuracy of the proposed PRTicle filter approximation, we compare it to the original PR estimator in cases where a quadrature scheme is feasible. In our comparisons, the PRTicle filter accurately approximates the PR estimate for simulations from mixtures corresponding to univariate and bivariate mixing distributions. Second, when the dimension of the mixing distribution support is too large for a quadrature scheme to be practical, we compare our PRTicle filter approximation to a Dirichlet process mixture model-based estimator. The PRTicle filter approximation is faster to compute and of comparable quality compared to the nonparametric Bayes estimator, which is one of the best known solutions.

For a real data illustration, we consider an application where data consists of a marked spatial point process. That is, the observed data consists of spatial locations at which specific events take place, along with some other relevant feature of the events, called marks. As is common in spatial point process models, the relevant quantity is the intensity function. Here we follow (Taddy and Kottas 2012) and model this intensity function as a mixture, with a multivariate mixing distribution support, and apply the PRTicle filter approximation to estimate the mixing distribution and, in turn, the intensity function. This naturally leads to estimates of other relevant features, including conditional distribution of the marks given the spatial locations. We argue that the results obtained through our use of the PRTicle approximation are consistent with patterns seen in the data and with those presented elsewhere in the literature. This application simply would have been impossible using the basic PR algorithm. Some concluding remarks are given in Sect. 5 and the proof of Theorem 1 is presented in Appendix A.
2 Background

2.1 Predictive recursion

Suppose we have data \( X_1, \ldots, X_n \) from \( \mathcal{M} \) in \((1)\), where the goal is estimation of the mixing distribution \( \mathcal{M} \). With a user-defined initial guess \( \mathcal{M}_0 \) and weight sequence \( \{w_i : i \geq 1\} \subset (0, 1) \), the \( i \)-th step in the PR algorithm is given by,

\[
P_i(du) = (1 - w_i) P_{i-1}(du) + w_i \frac{k(X_i | u) P_{i-1}(du)}{\int k(X_i | u) P_{i-1}(du)},
\]

\( i = 1, \ldots, n \)

(2)

For theoretical reasons, the weights must satisfy \( \sum_{i=1}^{\infty} w_i = \infty \) and \( \sum_{i=1}^{\infty} w_i^2 < \infty \); this can be achieved by taking, e.g., \( w_i = (i + 1)^{-\gamma} \) for some \( \gamma \in (0.5, 1) \). The algorithm processes the \( n \) data points sequentially and returns the final update \( P_n \) as the PR estimator of the mixing distribution. The corresponding PR mixture density estimate is \( m_n = m_{P_n} \), where the mapping \( P \mapsto mP \) is given in \((1)\). It is clear that the PR estimator \( P_n \) depends on the ordering of the observations \( X_1, \ldots, X_n \). If this dependence is undesirable, then it can be removed—or at least mitigated—by calculating \( P_n \) over multiple permutations of the data and averaging over the estimates (Newton 2002; Tokdar et al. 2009). With the superior computational efficiency of PR, this permutation-averaging can still be carried in a fraction of the run-time of its competitors.

Key features of the PR algorithm/estimator include its ability to estimate a mixing density and its computational efficiency. By the former, we mean that if the user-defined initial guess \( \mathcal{M}_0 \) has a smooth density with respect to a particular dominating measure, then the final PR estimator \( P_n \) will too. Compare this to the maximum likelihood and Bayes estimators, which are necessarily (or “effectively”) discrete. By the latter computational efficiency claim, we mean that each PR step requires a fixed number of computations, so the overall computational complexity of PR algorithm is \( O(n) \).

As mentioned in Sect. 1, the key step in each iteration of the PR algorithm is calculation of the normalizing constant \( \int k(x_i | u) P_{i-1}(du) \). Since \( P_{i-1} \) is data-driven and fully nonparametric, we cannot expect there to be a closed-form expression for the normalizing constant. Often it can be approximated numerically using a quadrature scheme; this is especially easy to do so when the mixing distribution support \( \mathcal{U} \) is univariate. However, for as the dimension of \( \mathcal{U} \) increases, computation of the normalizing constant becomes more and more challenging. For example, the number of grid points required for accurate quadrature grows exponentially in the dimension of \( \mathcal{U} \) and becomes infeasible or at least inefficient even for moderate \( \text{dim}(\mathcal{U}) \). This creates a computational bottleneck.

In previous work, this challenge was side-stepped by treating some of the latent variables as mixing variables and the others as non-mixing/structural parameters. For example, instead of mixing the kernel \( k(x | u_1, u_2) \) over both the location \( u_1 \) and scale \( u_2 \), the proposal in Martin and Tokdar (2011) was to treat, say, the scale parameter \( u_2 \) as a fixed unknown, so that mixing is required only over the univariate \( u_1 \)-space. Then they developed a PR-based marginal likelihood for \( u_2 \) that could be used for simultaneous estimation of the scale \( u_2 \) and the corresponding mixing distribution over \( u_1 \). This effectively reduces the dimension of the mixing distribution support, thus making it easy to side-step the challenges in computing the normalizing constant. For various reasons, however, it would be preferable to deal with the computational challenges directly, as opposed to using a “hack” to reduce the dimension artificially. This requires new ideas for evaluating the normalizing constant in \((2)\) and, for this, here we develop a novel strategy based on the same ideas behind sequential importance sampling.

2.2 Importance sampling and filtering

The approximation we propose in Sect. 3 uses the principles behind importance sampling and particle filters in general. Before stating our algorithm, we first review these basic principles. Consider the general problem of integrating a function \( h \) with respect to a probability density \( p \), where \( U \in \mathcal{U} \subset \mathbb{R}^d \), for \( d \geq 1 \). In cases where numerical integration is infeasible, e.g., if \( d \) is too large or if either \( h \) or \( p \) is too rough, it is common to use a Monte Carlo approximation by averaging over a random set of observations from probability density \( p \). However, a problem arises if \( p \) cannot be efficiently sampled from. In such cases, an importance sampling approach can be employed. This amounts to generating samples from a different distribution, say with density \( q \), and then reweighting those samples so that they resemble samples from \( p \). In particular, the expected value of \( h \) with respect to \( p \) can be written as

\[
\int_{\mathcal{U}} h(u) p(u) du = \int_{\mathcal{U}} h(u) \frac{p(u)}{q(u)} q(u) du,
\]

and this immediately suggests the Monte Carlo approximation

\[
\frac{1}{T} \sum_{t=1}^{T} \alpha_t h(U_t),
\]

where \( \{U_t : t = 1, \ldots, T\} \) are iid samples from \( q \) and \( \alpha_t = p(U_t)/q(U_t) \) are the weight adjustment factors. If the normalizing constant for \( p \) is unknown, then the \( T^{-1} \) factor can be replaced by \( (\sum_{t=1}^{T} \alpha_t)^{-1} \).
The ratio $\alpha_t = p(U_t)/q(U_t)$ helps to effectively filter out points in low $p$-density regions while increasing the weight put on particles in high $p$-density regions. Agapiou et al. (2017) unify the existing literature on importance sampling with a special focus on determining the size of $T$ such that error in approximation is minimized. The choice of $T$, the Monte Carlo sample size, is important, both in terms of accuracy and efficiency. A practical measure of efficiency used for importance sampling is the effective sample size (ESS), i.e., the effective number of particles. Following (Kong 1992), a commonly used expression for ESS is

$$\text{ESS} = \frac{\left( \sum_{t=1}^{T} \alpha_t \right)^2}{\sum_{t=1}^{T} \alpha_t^2}, \quad (3)$$

where $\alpha_t = p(U_t)/q(U_t)$ as before. By Cauchy–Schwartz, ESS is bounded above by $T$, and the closer it is to $T$ the more efficient the importance sampler. So the goal is to choose the proposal density $q$ such that ESS is as close to $T$ as possible.

These basics behind importance sampling can be connected to more sophisticated Monte Carlo methods with the following interpretation. The procedure above essentially starts with a collection of tentative sample points from $p$, which are commonly referred to as particles. Particles which have small importance ratios, $p/q$, are given small weight, and effectively filtered out. In this sense, importance sampling is a (basic) form of particle filtering. This idea can then be extended in different directions. In particular, it would be possible for the target distribution, $p$, to be changing over some “time” index. In hidden Markov models, for example, the dimension of the target distribution’s support is increasing with time; also, in Bayesian inference, the target $p$ is the posterior distribution which is evolving with the sample size $n$. Sequential Monte Carlo methods have proved useful in these problems (e.g., Doucet et al. 2001; Doucet and Johansen 2011; Del Moral et al. 2006). Sequential importance sampling, in particular, is a powerful tool for particle filtering (Agapiou et al. 2017; Tokdar and Kass 2010). In the context of mixture models, sequential importance sampling (eg. MacEachern et al. 1999) and particle learning algorithms (eg. Carvalho et al. 2010) have been suggested for analyzing mixture models in the Bayesian setting. In our present case, sequential updating is required because we need particles that represent the PR estimate $P_i$ as $i = 1, 2, \ldots, n$. This problem is due to the unique recursive structure inherent in the PR sequence of target distributions and, therefore, calls for different or at least more specialized techniques compared to what is currently available in the sequential Monte Carlo literature.

### 3 PRticle filter approximation

#### 3.1 Algorithm

In this section we propose a particle filter algorithm designed specifically to approximation the PR estimator. For simplicity, and without any real loss of generality, assume that $P_0$ has a density with respect to Lebesgue measure on $\mathbb{R}^d$, denote by $p_0$. Then all the subsequent PR updates $P_i$ have such a density, denoted by $p_i$. At each iteration of PR, one needs to calculate a normalizing constant

$$m_{i-1}(X_i) = \int_{\mathbb{R}^d} k(X_i \mid u) p_{i-1}(u) \, du, \quad i = 1, \ldots, n.$$ 

The analytical form of $p_{i-1}$ is unknown so clearly we cannot evaluate this in closed form. Likewise, we cannot directly generate observations from it to get a Monte Carlo approximation. However, we know that it is a function of the previous updates $p_0, \ldots, p_{i-2}$, so the idea is to leverage the PR algorithm’s recursive formulation and those core importance sampling principles to design an efficient Monte Carlo/particle filter approximation.

Recall that $p_0$ is a user-specified density on $\mathbb{R}$ and we will assume that sampling from $p_0$ is feasible. Generate an iid sample $U_1, \ldots, U_T$ of size $T \gg 1$ from $p_0$. Then, a simple Monte Carlo average gives us an approximation of the first normalizing constant,

$$\hat{m}_0(X_1) = \frac{1}{T} \sum_{i=1}^{T} k(X_1 \mid U_i)$$

where each point $U_i$ is equally weighted by $T^{-1}$. Next, we do not know the form of $p_1$ but we know that it can be expressed in terms of $p_0$ and the data point $X_1$ as

$$p_1(u) = (1 - w_1) p_0(u) + w_1 \frac{k(X_1 \mid u) p_0(u)}{\hat{m}_0(X_1)}$$

$$= \left\{ 1 + w_1 \left( \frac{k(X_1 \mid u)}{\hat{m}_0(X_1)} - 1 \right) \right\} p_0(u).$$

This implies the ratio of consecutive PR density estimates is

$$\frac{p_1(u)}{p_0(u)} = \delta_0(u) := \left\{ 1 + w_1 \left( \frac{k(X_1 \mid u)}{\hat{m}_0(X_1)} - 1 \right) \right\}.$$

Now, since

$$m_1(X_2) = \int k(X_2 \mid u) p_1(u) \, du = \int k(X_2 \mid u) \delta_0(u) p_0(u) \, du,$$
we have a very natural Monte Carlo approximation of $\hat{m}_1(X_2)$, namely,

$$\hat{m}_1(X_2) = \frac{1}{T} \sum_{i=1}^{T} k(X_2 | U_i) \delta_0(U_i),$$

where $\delta_0(u)$ is based on plugging in $\hat{m}_0(X_1)$ for $m_0(X_1)$ in the definition of $\delta_0$ above. Here $\delta_0(\cdot)$ acts as a mesh that effectively filters out those particles that are not compatible with the updated distribution $p_1$. Continuing with the same logic, for the $i$th iteration, we get

$$\hat{m}_{i-1}(X_i) = \frac{1}{T} \sum_{i=1}^{T} k(X_i | U_i) \hat{\Delta}_i(U_i), \quad i \geq 1,$$

where $\hat{\Delta}_i(u) \equiv 1$ and

$$\hat{\Delta}_i(u) = \frac{\hat{\Delta}_{i-1}(u) \delta_{i-2}(u)}{\sum_{j=2}^{i} \left( 1 + w_{j-1} \left( \frac{k(X_{j-1} | U_j)}{m_{j-2}(X_{j-1})} - 1 \right) \right)}, \quad i \geq 2.$$

The above steps make up the PRticle filter approximation and these are summarized in Algorithm 1. In the end, the algorithm returns the pairs $\{(U_i, \Delta_n(U_i)) : t = 1, \ldots, T\}$ that collectively represent an approximate sample from the PR estimator $P_n$. From this sample, any features of $P_n$ can be approximated as usual. If an estimate of the density $p_n$ were required, then the weighted collection of particles can be smoothed using, e.g., a kernel density estimator. Just like the PR estimator, the PRticle filter approximation depends on the ordering of observations, and same permutation-averaging can be used here to mitigate the order-dependence, if desired.

Algorithm 1: PRticle filter approximation

| Initialize: Data $X_1, \ldots, X_n$, initial guess $p_0$, random sample $U_1, \ldots, U_T$ from $p_0$, and weight sequence $\{w_i : i \geq 1\} \subset (0, 1)$; |  
| Set $\Delta_i = 1$ for $t = 1, \ldots, T$; |  
| for $i = 1, \ldots, n$ do |  
| set $N_{i,t} = k(X_i | U_t) p_{i-1}(U_t)$ for each $t$, and |  
| $D_t = T^{-1} \sum_{i=1}^{T} k(X_i | U_t) \Delta_i$; |  
| update $p_i(U_t) = (1 - w_t) p_{i-1}(U_t) + w_t N_{i,t}/D_t$ for each $t$; |  
| evaluate $\hat{\Delta}_i = \hat{\Delta}_i[(1 + w_i k(X_i | U_t)/D_t - 1)]$ for each $t$; |  
| end |  
| return $U_t$ and weights $\hat{\Delta}_i$, for $t = 1, \ldots, T$. |  

Theorem 1 For a fixed data set $X_1, \ldots, X_n$, let $p_n$ and $\hat{p}_{n,T}$ denote the PR estimator and its PRticle filter approximation, respectively, both based on the same initial guess with distribution $P_0$. If the kernel is such that

$$\int_{U} \left( \prod_{i \in S} k(X_i | u) \right) P_0(du) < \infty, \quad \text{for all } S \subseteq \{1, \ldots, n\},$$

then

$$\int_{U} |\hat{p}_{n,T}(u) - p_n(u)| du \to 0, \quad \text{with } P_0\text{-probability 1 as } T \to \infty.$$  

Proof See Appendix A.

Theorem 1 establishes that, with a sufficiently large Monte Carlo sample size $T$, the PRticle filter approximation, $\hat{p}_{n,T}$, of the PR mixing density estimator $p_n$ will be quite accurate. Note that $L_1$/total variation convergence implies weak convergence, so virtually any relevant functional of $p_n$ can be accurately approximated by the corresponding functional of $\hat{p}_{n,T}$. The condition (4) on the kernel is rather mild, e.g., it is satisfied if $u \mapsto k(X | u)$ is bounded for almost all $x$. Beyond the fixed-data approximation, the result in Theorem 1, together with the general results in Martin and Tokdar (2009) and Duxit and Martin (2021) on the consistency properties of $p_n$ as $n \to \infty$, suggests that $\hat{p}_{n,T}$ would also be a good estimator of $p$ when both $n$ and $T$ are large.

3.3 Adaptation to handle attrition

The final estimate $p_n$ will depend on the initial $p_0$, not just through the default PR mechanism but also through the dependence on the choice of particles $U_1, \ldots, U_T$ from $p_0$. To ensure that $p_n$ captures the true mixing density $p$, it is generally recommended to choose a relatively diffuse $p_0$ in the PR algorithm. However, the true $p$ is likely to be more concentrated in certain regions of $U$ than in others. So those chosen particles $U_1, \ldots, U_T$ from $p_0$ that happen to fall in those $p$-low-density regions of $U$ should be assigned relatively low weights. The concern is that too many of the particles end up in these low-density regions, hence affecting the effective number of particles. Recall that, an efficiency
measure of the particle filter is given by the effective sample size (ESS) in (3). For our case this can be calculated as,

\[
\text{ESS} = \frac{\left(\sum_{t=1}^{T} \Delta_n(U_t)\right)^2}{\sum_{t=1}^{T} \Delta_n(U_t)^2}.
\]

If too many particles end up with negligible weights, i.e., if \(\Delta_n(U_t) \approx 0\) for \(t'\), then ESS becomes significantly smaller than \(T\). This loss-of-information, called attrition, is a common problem in importance sampling or particle filtering (e.g., Doucet and Johansen 2011); and it cannot be ignored because the effective sample size is what controls the accuracy of the Monte Carlo approximations. To account for this, the general strategy is to resample points from the region of importance such that ESS does not reduce tragically (e.g., Carvalho et al. 2010). Any of the approaches suggested above would be useful in reducing attrition of particles, but more deliberation is needed to conclude which of these strategies would be most efficient. For our purposes here, we use the strategy mentioned before and our simulation results in Sect. 4 show that this is effective in reducing attrition.

### 4 Numerical results

#### 4.1 Density estimation

Here we show three density estimation examples. Examples 1–2, involving Euclidean data and data on a sphere, respectively, compare the PRTicle filter approximation to the original PR estimator in low-dimensional cases where the latter can be computed efficiently. Example 3 considers cases where the mixing distribution support is too high-dimensional to compute the original PR estimator, so we compare the PRTicle filter approximation results to those of the Dirichlet process mixture model fit.

**Example 1** For \(d\)-dimensional data \(X\), consider a normal mixture model of the form (1) with \(k(x | u) = N_d(x | u, \sigma^2 I_d)\) the multivariate normal density with mean vector \(u\), where \(I_d\) is the \(d\)-dimensional identity matrix. Throughout, \(\sigma^2 = 0.5\) will be taken as fixed. So that we can compare the PRTicle filter approximation directly to the original PR estimator, we consider only the cases \(d = 1\) and \(d = 2\) here. For the \(d = 1\) case, we take the true mixing distribution to be \(P = \text{Beta}(10, 5)\), a beta distribution scaled to \([0, 10]\); for the \(d = 2\) case, we take \(P = \text{Beta}(10, 5) \times \text{Beta}(5, 10)\), a joint distribution supported on \([0, 10]^2\) corresponding to independent scaled beta marginals. In both cases, samples of size \(n = 500\) are generated and we compare the PRTicle filter approximation to the original PR estimator in terms of the Kullback–Leibler divergence \(K(m_n, \hat{m}_n)\), where \(m_n\) is the PR estimator of
the mixture density and \(\hat{m}_n\) is the corresponding PRticle filter approximation. Both are based on weight sequence \(w_i = (i + 1)^{-1}\) and initial guess \(P_0 = \text{Unif}(U)\). The PRticle filter approximation relies on samples \(U_1, \ldots, U_T\) taken from \(P_0\) and here we consider four samples sizes, \(T \in \{100, 300, 500, 1000\}\). Table 1 summarizes both the Kullback–Leibler divergence and the ESS for both the \(d = 1\) and \(d = 2\) cases. As expected, the ESS tends to be smaller for \(d = 2\) than for \(d = 1\), with the former retaining about 15% of the original sample while the latter retains about 33%. However, the Kullback–Leibler divergence tends to be small across the board and does not vary much as a function of \(T\) for both cases.

Example 2

Next, following (Dixit and Martin 2022), we compare the PRticle filter approximation to the original PR estimate for mixture models on the unit sphere \(S \subset \mathbb{R}^3\) commonly used for directional data. The particular mixture model we consider is one with a so-called angular Gaussian distribution (Tyler 1987) kernel

\[
k(x \mid \mu, \beta) \propto |\Sigma_{\mu, \beta}|^{-1/2} (x^\top \Sigma_{\mu, \beta}^{-1} x)^{-3/2}, \quad x \in S,
\]

\((\mu, \beta) \in S \times (0, \infty),\)

where \(\Sigma_{\mu, \beta} = Q_\mu^\top D_\beta Q_\mu\), with \(D_\beta = \text{diag}(1, 1, \beta^{-2})\) and \(Q_\mu\) is the rotation matrix mapping \((0, 0, 1)^\top\) onto the unit vector \(\mu \in S\), given by

\[
Q_\mu = \begin{pmatrix}
\cos \theta_\mu & \cos \phi_\mu - \sin \phi_\mu \sin \theta_\mu & \sin \phi_\mu \\
-\sin \theta_\mu & \cos \phi_\mu & \sin \phi_\mu \\
0 & 0 & \cos \theta_\mu
\end{pmatrix}
\]

and \((\theta_\mu, \phi_\mu)\) is the spherical coordinate representation of \(\mu\). For the original PR estimator, Dixit and Martin (2022) treated \(\beta\) as a fixed unknown structural parameter, not a latent variable being mixed over. That is, they treated the kernel as \(k_\beta(x \mid u)\), depending on the unknown \(\beta\), where \(u = \mu\) is the only latent variable mixed over. Then they employed the PR marginal likelihood strategy to estimate the fixed unknown \(\beta\). Here, using the added flexibility of the PRticle filter approximation, we fit the model that mixes over latent variable \(u = (\mu, \beta)\), so that there are no unknown structural parameters to be estimated separately. Here we generate \(n = 2000\) samples from the above mixture model where the true mixing distribution \(P\) has a smooth bimodal density in \(\mu\) and a point mass at \(\beta = 0.1\)—this means that PR’s mixture model, that takes \(\beta\) fixed and unknown, is correctly specified while the PRticle filter’s mixture model is misspecified. For the PR estimator, we take \(w_i = (i + 1)^{-1}\) and \(P_0\) to be uniform on \(S\). For the PRticle filter approximation, which mixes over both \(\mu\) and \(\beta\), the initial guess \(P_0\) is a product of uniform distributions on \(S\) and a uniform distribution on \(0, 0.5\). Plots of the PR estimate \(m_n\) and PRticle approximation \(\hat{m}_n\), based on \(T = 1000\) initial particles, are provided in Fig. 1. The approximation based on PRticle filter clearly captures all the relevant features of the PR estimate, and in much less time thanks to not needing to employ the marginal likelihood strategy to estimate a fixed \(\beta\).

Example 3

For the third part of the simulation study, we mix a bivariate normal kernel over all mean \((\mu_1, \mu_2)\) and covariance \((\sigma_1^2, \sigma_2^2, \rho)\) parameters. This means that the mixing distribution \(P\) is defined over five variables. Using PR with numerical integration is not possible in this situation as a quadrature scheme is infeasible. The PRticle filter approximation can instead be used to fit this mixture density. For comparison, we consider a Dirichlet process mixture model fit, where the prior for the mixing distribution is \(P \sim \text{DP}(\alpha, P_0)\), a Dirichlet process with precision parameter \(\alpha > 0\) and base measure \(P_0\), which we take to be the same as PR’s initialization (see below). The Dirichlet process mixture model estimate of the mixture density is the corresponding posterior mean, which is calculated using the DirichletProcessMvnormal function in the R package dirichletprocess (Ross and Markwick 2019) with 1000 iterations. To compare the two approaches we take \(U = (\mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \rho)\) with the true mixing distribution \(P\) corresponding to independent \(\mu_1 \sim N(5, 3^2), \mu_2 \sim N(10, 3^2), \sigma_1^2 \sim \text{Gamma}(1, 1), \sigma_2 \sim \text{Gamma}(5, 1)\), and \(\rho \sim \text{Beta}(10, 5)\). In this, we generate \(n = 500\) observations from the true mixture density and fit a multivariate normal mixture density using the PRticle filter approximation and the Dirichlet process mixture model machinery. As before we initialize the PRticle filter with a uniform distribution \(P_0\) over all parameters and a weight sequence \(w_i = (i + 1)^{-1}\). However, to avoid possible attrition we improve the filter by using the strategy proposed in Sect. 3.3 and rerun the algorithm with an updated \(P_0\). Contour plots of the estimated mixture densities are given in Fig. 2. The PRticle filter approximation plots are able to capture the structure of the true mixture density, \(m\), just like the Dirichlet process mixture model fit. For a numerical comparison we calculate the Monte Carlo approximation of the Kullback–Leibler divergence between the true mixture density and the esti-
Fig. 1 Estimated mixture density on the sphere based on the PR algorithm and the PRticle filter approximation for bimodal continuous mixing distribution, views from north and south poles.

4.2 Marked point process modeling

Here we showcase an interesting application of multivariate mixture modeling using PR, which is made possible by the PRticle filter approximation. Suppose our data consists of spatial locations \( s \) of an interesting occurrence possibly accompanied by some attributes \( x \) at those locations. Typically, when only location observations \( s_1, \ldots, s_n \) are available, there is interest in the intensity of the incident occurrence. These are typically modeled as realizations from a non-homogeneous Poisson process with intensity function \( \lambda(s), s \in \mathbb{S} \subseteq \mathbb{R}^d \) (e.g., Liang et al. 2008). For example, in an epidemiological study, \( s_i \) might be the geographic location of the \( i \)th individual showing symptoms of a particular disease and hence there is interest in modeling the intensity of the disease occurrences. For such a non-homogeneous Poisson process, a likelihood function can be written as,
Fig. 2  Mixture density estimates for a multivariate normal mixture with the observed data overlaid

(a) DP mixture estimate  
(b) PRticle estimate with only one run

(c) PRticle estimate with updated $p_0$

Fig. 2  Mixture density estimates for a multivariate normal mixture with the observed data overlaid

Fig. 3  Quantile-quantile plots for each component of $U = (\mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \rho)$ of the mixing distribution corresponding to the multivariate normal mixture. Black line corresponds to quantiles from the PRticle filter estimate, while the red line corresponds to quantiles from the Dirichlet process-based Bayes estimate

(a) $\mu_1$  
(b) $\mu_2$

(c) $\sigma_1^2$  
(d) $\rho$

(e) $\sigma_2^2$
Figs. 4. Tree locations on a 200 × 200 grid (longleaf dataset), where the size of each point is proportional to the respective tree diameter; gray coloring is to make different points easier to distinguish. Yellow triangles indicate locations at which the conditional mark density is estimated in Fig. 5.

\[
L(\lambda | s_1, \ldots, s_n) = \Lambda^n \exp\{-\Lambda\} \prod_{i=1}^{n} m(s_i)
\]

where \( m \) is the normalized intensity function, i.e., \( m(s) = \lambda(s)/\Lambda \), and \( \Lambda = \int \lambda(t) \, dt \). Given the separable nature of the likelihood above, \( \Lambda \) and \( m \) can be estimated separately. A regression approach is to model \( \lambda \) by a log Gaussian Cox process (e.g., Liang et al. 2008). However, given the nonparametric nature of the problem it is desirable to use a robust model for \( \lambda \) to capture all the shape/scale features of the function. Mixture models offer this flexibility and an approach to modeling \( \lambda \) or \( m \) by a Dirichlet process mixture was proposed in Kottas and Sansó (2007).

Additionally, there could be other attributes \( X_1, \ldots, X_n \) present with the location data, for example, indicator variable for type of disease, when there is interest in the association between disease locations. Then to account for this association and its effect on the model, a joint intensity function \( \psi(s, x) \) can be defined. The resulting process is known as the marked point process, where the attributes are called marks. The nonparametric mixture density in (1) offers the required flexibility to model a fully nonparametric function \( \psi(s, x) \). Taddy and Kottas (2012) propose mixture models for such marked point processes using conditionally conjugate Dirichlet process mixture models. The idea is to model the joint intensity \( \psi(s, x) \) of the locations \( s \) and marks \( x \) as,

\[
\psi(s, x) = \lambda(s) g(x | s) = \Lambda m(s) g(x | s) = \Lambda m(s, x),
\]

where \( g(x | s) \) represents the conditional density of mark \( X \), given location \( s \). Features of this joint intensity can be identified by modeling \( m(s, x) \) with a mixture model. The flexibility and computational efficiency offered by PR means that it is tailor-made to fit such a mixture model. However, given the multivariate nature of the problem we need the PRticle filter approximation to actually implement PR.

We illustrate the above on a real dataset as suggested in Example 5.3 of Taddy and Kottas (2012). The suggested dataset, longleaf is part of the R package spatstat (Baddeley and Turner 2005) and a detailed space-time survival analysis based on this was developed in Rathbun and Cressie (1994). The observations are locations of 584 pine trees in a 200 × 200 square and the marks are diameters of the trees at breast height (only for trees having this diameter greater than 2 cm). A scatter plot of the data is given in Fig. 4. One can clearly see that the distribution of trees is not uniform, i.e., mature (larger diameter) trees are more evenly distributed than younger (smaller diameter) trees, which appear in clusters. Hence, the goal is to model the joint intensity of the locations and marks of these trees. Taddy and Kottas (2012) model \( m(s, x) \) as a mixture model with a trivariate normal kernel and a mixing distribution defined over all the parameters of this multivariate normal distribution, i.e.,

\[
m(s, x) = \int P(d\mu, d\Sigma) \left[ \frac{\text{N}_3\left((\logit \left( \frac{s_1}{200}, \frac{s_2}{200}, \frac{s_3}{200}\right), \log(x - 2) | \mu, \Sigma\right))}{(x - 2) \prod_{i=1}^{3} \left( \frac{\mu_i}{200}\right) \left(1 - \frac{\mu_i}{200}\right)} \right]
\]

(6)

With the model in (6), we can estimate the conditional distribution of the marks at different locations to capture the varying distribution of trees, which in essence is an indication of the survival. We propose using the PR approach to fit this joint intensity function and estimate \( P \). Of course, that this is a mixture of a nine-dimensional latent variable space—three mean parameters and six covariance matrix parameters—makes it impossible to fit with the PR algorithm directly, so the PRticle filter approximation is necessary. Assuming a mixing distribution over all nine dimensions is possible using the PRticle filter approximation, but for model comparison we actually fit two models: the nine-dimensional model above and a reduced model that assumes the covariance terms in \( \Sigma \) are fixed at 0. The mixing distribution is then estimated.
Fig. 5 Conditional density estimates for the marks, i.e., the diameter of trees in the longleaf dataset at four specific locations, $s$, in the $200 \times 200$ grid with full nine-dimensional (black), reduced six-dimensional (red) mixture model overlayed with an empirical distribution of marks in the neighborhood (dashed).

by PR with the PRticle filter approximation. From this fitted mixture model $m(s, x)$ we extract the conditional density $g(x | s)$ at specific locations to see how the diameter distribution varies with $s$ as displayed in Fig. 5. As we can see in the scatter plot, each chosen location has unique characteristics in terms of diameter distribution. Locations $s = (81, 120)$ and $s = (100, 100)$ have higher concentrations of mature, large-diameter trees, which is correctly captured by both models (nine-dimensional and six-dimensional) in Fig. 5. On the other hand, locations $s = (105, 140)$ and $s = (185, 87)$ have clusters of younger, smaller-diameter trees which, again, is correctly captured in Fig. 5. Each plot in Fig. 5 is overlaid with an empirical probability density of marks using the density function in R based on observations that are within a radius of 30 units from the chosen location. The fitted model retains these local features while being globally smoother than the empirical density. In terms of model comparison, both the six and nine-dimensional model reasonably capture the varying diameter distribution at all locations. A difference between the two estimates is that the full model estimate is smoother than the reduced model one. This is because the kernel density in the former inherently contains an average over the covariance parameters, while the latter fixes these at zero. The full model also appears to capture certain features better than the reduced model. For example, consider the locations $s = (105, 140)$ and $s = (185, 87)$, whose conditional mark density is shown in Panels (c) and (d) of Fig. 5, respectively. These two points have relatively high concentration of small-diameter trees, as seen in Fig. 4; but upon closer inspection, the concentration at $s = (105, 140)$ seems higher than at $s = (185, 87)$, and we see that the conditional density estimates based on the full model capture these differing features better than those based on the reduced model. Similar results were obtained in Taddy and Kottas (2012) via their proposed Dirichlet process mixture fit. An interesting difference between our results and those of Taddy and Kottas is that their plot at $s = (100, 100)$ shows a sharp spike in the conditional density near $x = 0$, whereas ours does not. Since there is no evidence in the scatter plot for a high concentration of small-diameter trees, our guess is that their spike is actually a boundary effect, commonly seen in density estimation on bounded domains, and
not an inherent feature in the data. That the PR estimate does not suffer from a boundary effect in this case is another benefit.

5 Conclusion

In this paper we proposed a new filtering mechanism, a PRticle filter, for fitting nonparametric mixture models using the PR algorithm in multivariate problems. This new development is an important addition because, previously, the PR algorithm could only handle mixtures over relatively low-dimensional spaces. This contribution creates new opportunities for PR-based methodology in non-trivial problems like marked spatial point process modelling in Sect. 4.2. Theoretically, we show that the PRticle filter approximation of the mixing distribution converges to the PR estimate in a strong sense as the number of particles $T$ goes to infinity, when the data $X_1, \ldots, X_n$ of size $n$ remains fixed. This holds for the primary PR run only, an analysis of the attrition-handling embellishments in Sect. 3.3 would require more sophisticated techniques. Coupling this with results in literature on consistency (as $n \to \infty$) of the PR estimator strengthens both the theoretical and practical aspects of PR. Our numerical results show that the PRticle filter approximation gives as accurate results as the traditional PR approach for univariate and bivariate mixtures and is also effective in estimating a multivariate mixture density.

One might also be interested in quantifying uncertainty about the mixing distribution and its features, like in Sect. 4.2. Capturing the variability in the PR estimate is a difficult problem, but suggestions have been made in Fortini and Petrone (2020) and Dixit and Martin (2019). The former uses a quasi-Bayes strategy to construct credible intervals for the PR estimate, while in the latter we leverage the order dependence of the PR estimator for uncertainty quantification. This strategy, which constructs multiple PR estimates based on distinct permutation of the data sequence, would be applicable for the PRticle filter approximation. There are some theoretical gaps that need to be filled, however, so remains an ongoing work.

One of our numerical illustrations considered nonparametric estimation of mixing distributions supported on the sphere in three-dimensions. A natural question is if this approach could be extended to other cases involving mixture defined on more general compact manifolds, e.g., higher-dimensional spheres, tori, etc. All that would be needed to extend the proposed strategy in such cases is a map from the surface of the manifold to an underlying Euclidean space where the computations can be carried out. In the special case of the sphere, there is a “global” Euclidean-space representation but, for more general manifolds, the corresponding Euclidean spaces would be “local,” which creates some new and interesting conceptual and computational challenges.

An interesting theoretical question is if consistency of the PRticle filter approximation could be established. That is, if $\hat{P}_{n,T}$ is the PRticle filter approximation of the PR estimator $P_n$, then the goal would be to show that $\hat{P}_{n,T} \to P$ as both $n$ and $T$ go to infinity. Of course, this would require $T = T_n$ to be increasing sufficiently fast with $n$. Direct extension of the argument used in the proof of Theorem 1 may be possible using some naive techniques, e.g., the classical union bound, but, if successful, this would require $T$ to be exponentially large with $n$. Our gut feeling is that such a large number of particles would not be necessary, so some important insights are still missing. We save this as a topic for future work.

A remaining practical challenge is the handling of attrition when the dimension of the mixing distribution support is relatively high. What we proposed in Sect. 3.3 is able to adequately control attrition rates for mixtures over at least nine-dimensional spaces. We have not thoroughly tested the performance of the PRticle filter approximation in dimensions higher than this, but we fully expect that controlling the attrition rate will be more and more difficult as the dimension increases. This is not a limitation of the proposed method, it is a challenge that any importance sampling-based method will face in high-dimensional applications. New insights would be needed to make this leap to high-dimensional mixtures but it may be possible to take advantage of the PR-specific recursive structure that we used to develop the PRticle filter approximation here.

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A Proof of Theorem 1

Recall that,

$$\hat{m}_{i-1}(X_i) = \frac{1}{T} \sum_{t=1}^{T} k(X_i \mid U_t) \hat{A}_i(U_t), \quad i \geq 1,$$

where $\hat{A}_1(u) \equiv 1$ and

$$\hat{A}_i(u) = \hat{A}_{i-1}(u) \hat{A}_{i-2}(u)$$

$$= \prod_{j=2}^{i} \left\{ 1 + \frac{k(X_{j-1} \mid u)}{\hat{m}_{j-2}(X_{j-1})} - 1 \right\}, \quad i \geq 2.$$

By the strong law of large numbers, we have that

$$\hat{m}_{0,T}(X_1) = \frac{1}{T} \sum_{t=1}^{T} k(X_1 \mid U_t) \to m_0(X_1),$$

with $P_0$-probability 1 as $T \to \infty$. 

To prove a similar claim for all \( \hat{m}_{\ell,T}(X_{\ell+1}) \), we proceed by induction. That is, we start by assuming that

\[
\hat{m}_{i-1,T}(X_i) \to m_{i-1}(X_i)
\]

with \( P_0 \)-probability 1, for all \( i \leq \ell \),

and then use that assumption, along with the structure of the algorithm, to prove

\[
\hat{m}_{\ell,T}(X_{\ell+1}) \to m_\ell(X_{\ell+1}),
\]

with \( P_0 \)-probability 1, as \( T \to \infty \).

Towards this, we have

\[
\hat{m}_{\ell,T}(X_{\ell+1}) = \frac{1}{T} \sum_{t=1}^{T} k(X_{\ell+1} \mid U_t) \tilde{\Delta}_{\ell+1}(U_t)
\]

\[
= \frac{1}{T} \sum_{t=1}^{T} k(X_{\ell+1} \mid U_t) \prod_{i=1}^{\ell} \left\{ (1 - w_i) + w_i \frac{k(X_i \mid U_i)}{\hat{m}_{i-1,T}(X_i)} \right\}.
\]

The product above can be expanded as

\[
\prod_{i=1}^{\ell} \left\{ (1 - w_i) + w_i \frac{k(X_i \mid U_i)}{\hat{m}_{i-1,T}(X_i)} \right\}
\]

\[
= \sum_{S(\ell)} \prod_{j \in S(\ell)} (1 - w_j) \prod_{i \notin S(\ell)} w_i \frac{k(X_i \mid U_i)}{\hat{m}_{i-1,T}(X_i)},
\]

where \( S(\ell) \) is a generic subset of \( \{1, \ldots, \ell\} \) and the sums and products are over all \( 2^\ell \) such subsets. Going back the formula for \( \hat{m}_{\ell,T}(X_{\ell+1}) \), we can distribute the average over \( t \) through the product, which gives

\[
\hat{m}_{\ell,T}(X_{\ell+1}) = \sum_{S(\ell)} \frac{\prod_{j \in S(\ell)} (1 - w_j) \prod_{i \notin S(\ell)} w_i}{\prod_{i \notin S(\ell)} \hat{m}_{i-1,T}(X_i)} \left\{ \frac{1}{T} \sum_{t=1}^{T} k(X_{\ell+1} \mid U_t) \prod_{i \notin S(\ell)} k(X_i \mid U_i) \right\}.
\]

By the induction hypothesis (7), we have that

\[
\prod_{i \notin S(\ell)} \hat{m}_{i-1,T}(X_i) \to \prod_{i \notin S(\ell)} m_{i-1}(X_i),
\]

with \( P_0 \)-probability 1, uniformly in \( S(\ell) \).

Moreover, by the assumption (4), the strong law of large numbers gives

\[
\frac{1}{T} \sum_{t=1}^{T} k(X_{\ell+1} \mid U_t) \prod_{i \notin S(\ell)} k(X_i \mid U_i) \to \int k(X_{\ell+1} \mid u) \prod_{i \notin S(\ell)} k(X_i \mid u) P_0(du),
\]

with \( P_0 \)-probability 1, as \( T \to \infty \), again uniformly in \( S(\ell) \). The two ‘uniformly in \( S(\ell) \)’ claims above follow because there are only finitely many such \( S(\ell) \). Putting everything together, we have that \( \hat{m}_{\ell,T}(X_{\ell+1}) \) converges with \( P_0 \)-probability 1, as \( T \to \infty \), to

\[
\sum_{S(\ell)} \frac{\prod_{j \in S(\ell)} (1 - w_j) \prod_{i \notin S(\ell)} w_i}{\prod_{i \notin S(\ell)} \hat{m}_{i-1,T}(X_i)} \left\{ \int k(X_{\ell+1} \mid u) \prod_{i \notin S(\ell)} k(X_i \mid u) P_0(du) \right\}.
\]

Moving the integration over \( u \) to the outside of the sum over \( S(\ell) \) and undoing the product expansion above eventually leads to \( \hat{m}_{\ell,T}(X_{\ell+1}) \to m_\ell(X_{\ell+1}) \) with \( P_0 \)-probability 1. We showed above that

\[
\hat{m}_{i-1,T}(X_i) \to m_{i-1}(X_i) \quad \text{with} \quad P_0 \text{-probability 1 as} \quad T \to \infty,
\]

uniformly in \( i = 1, \ldots, n \) without any assumptions on the convergence of the mixing distribution approximation. Since the final mixing density estimator \( \hat{p}_{n,T} \) is a continuous function of \( \{\hat{m}_{i-1,T}(X_i) : i = 1, \ldots, n\} \), it follows that

\[
\hat{p}_{n,T}(u) \to p_n(u),
\]

with \( P_0 \)-probability 1, as \( T \to \infty \), for all \( u \).

Since these are density functions, it follows from Scheffé’s theorem that \( \hat{p}_{n,T} \) converges in \( L_1(du) \) to \( p_n \), with \( P_0 \)-probability 1, as \( T \to \infty \).

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