Scalable Bayesian Inference via Particle Mirror Descent

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Abstract

Bayesian methods are appealing in their flexibility in modeling complex data and their ability to capture uncertainty in parameters. However, when Bayes' rule does not result in closed-form, most approximate Bayesian inference algorithms lacks either scalability or rigorous guarantees. To tackle this challenge, we propose a scalable yet simple algorithm, Particle Mirror Descent (PMD), to iteratively approximate the posterior density. PMD is inspired by stochastic functional mirror descent where one descends in the density space using a small batch of data points at each iteration, and by particle filtering where one uses samples to approximate a function. We prove result of the first kind that, after $T$ iterations, PMD provides a posterior density estimator that converges in terms of $KL$-divergence to the true posterior in rate $O(1/\sqrt{T})$. We show that PMD is competitive to several scalable Bayesian algorithms in mixture models, Bayesian logistic regression, sparse Gaussian processes and latent Dirichlet allocation.
1 Introduction

Bayesian methods are attractive because of their ability in modeling complex data and capturing uncertainty in parameters. The crux of Bayesian inference is to compute the posterior distribution, \( p(\theta | X) \) \( \propto p(\theta) \prod_{n=1}^{N} p(x_n | \theta), \) of a parameter \( \theta \in \mathbb{R}^d \) given a set of \( N \) data points \( X = \{x_n\}_{n=1}^{N} \) from \( \mathbb{R}^D \), with a prior distribution \( p(\theta) \) and a model of data likelihood \( p(x|\theta) \). When the prior is not conjugate to the likelihood, the posteriors no longer have a closed-form, and hence a fully-Bayesian inference often results in intractable integration and poses computational challenges. Typically, one resorts to approximate inference such as sampling, e.g., MCMC \[1\], or variational inference \[2, 3\].

Besides the challenges arising from intractability, large scale datasets also pose additional challenges for Bayesian inference. MCMC requires a complete scan of the dataset and evaluating the likelihood of each data point to generate a single sample at every iteration, which is not practical for large scale problem. To address this issue, approximate sampling algorithms have been proposed which uses only a small batch of data points at each iteration \( [e.g. 4, 5, 6] \). For instance, the stochastic Langevin dynamics algorithm \[4\] and its derivatives \[7, 8, 9\] combine ideas from stochastic optimization and Hamiltonian Monte Carlo sampling, and demonstrate that samples from these algorithms are consistent with draws from the posterior. Recently, some convergence results for these algorithms with weak criterion have also been provided, \( [e.g. 10, 11] \), in which the ability of the samples to approximate integrals is analyzed. However, it is unclear whether these dependent samples will lead to the true posterior density. An alternative approximate sampling approach, FireflyMC \[5\], introduces auxiliary variables to switch on and off data points to save computation for likelihood evaluations. However, this algorithm relies on the availability of a lower bound of the likelihood which is model-specific and may be hard to calculate.

Unlike sampling methods, variational inference algorithms attempt to approximate the entire posterior density \[12, 13, 14\]. Although variational inference algorithms can be scaled up using stochastic gradients computed with a small batch of data \[15\], formal analyses of the convergence of such algorithms remain very difficult. This is due largely to the fact that variational inference algorithms typically choose a parametric family to approximate the posterior density, which can be far from the true posterior. More flexible variational family has been explored but largely restricted to mixture models \[12, 13\]. In these cases, it is often difficult to quantify the approximation error at each iteration and analyze how the error accumulates across the iterations. Therefore, a provably convergent algorithm with nonparametric variational family is needed. It remains an open problem how to design a practical and provable nonparametric algorithm.

We present such a scalable, simple and provable algorithm, Particle Mirror Descent (PMD), to iteratively approximate the posterior density \[12, 13, 14\]. Although variational inference algorithms can be scaled up using stochastic gradients computed with a small batch of data \[15\], formal analyses of the convergence of such algorithms remain very difficult. This is due largely to the fact that variational inference algorithms typically choose a parametric family to approximate the posterior density, which can be far from the true posterior. More flexible variational family has been explored but largely restricted to mixture models \[12, 13\]. In these cases, it is often difficult to quantify the approximation error at each iteration and analyze how the error accumulates across the iterations. Therefore, a provably convergent algorithm with nonparametric variational family is needed. It remains an open problem how to design a practical and provable nonparametric algorithm.

We present such a scalable, simple and provable algorithm, Particle Mirror Descent (PMD), to iteratively approximate the posterior density. PMD relies on the connection that Bayes’ rule can be expressed as the solution to a convex optimization problem over the density space \[16\]. However, directly solving the optimization will lead to both computational and representational issues: one scan over the entire dataset at each iteration is needed, and the exact function update has no closed-form. To address these issues, we draw inspiration from two sources:

(i) stochastic mirror descent, where one can instead descend in the density space using a small batch of data points at each iteration; and

(ii) particle filtering and kernel density estimation, where one can maintain a tractable approximate representation of the density using samples.

The correctness and convergence of the algorithm can be understood from the stochastic mirror descent framework \[17\]. Essentially, PMD attempts to optimize the corresponding convex objective by making two stochastic approximations at each iteration, one for the functional gradient, and the other for the solution of the prox-mapping subproblem. PMD works due to

(i) the property of stochastic mirror descent algorithm that as long as the gradient is unbiased, and the prox-mapping can be solved approximately to an error the same order as the variance of the gradient, the convergence of the algorithm is guaranteed; and

PMD connects stochastic optimization, functional analysis, kernel density estimation and Monte Carlo approximation to Bayesian inference, and possesses a number of desiderata:

**Simplicity.** PMD applies to many probabilistic models with continuous variables, even with non-conjugate priors. The algorithm can be summarized in just a few lines of codes, and only requires the value of likelihood and prior, different from other approximate inference techniques [4, 13, 14, 15, e.g.], which typically require their first and/or second-order derivatives.

**Flexibility.** Different from other variational inference algorithms, which sacrifice the model flexibility for tractability, our method approximates the posterior by particles or kernel density estimator. The flexibility of nonparametric model enable PMD to capture multi-modal densities easily.

**Scalability.** The key computation comes from sampling from a kernel density estimator and updating the sample weights. At \( t \)-th iteration, our algorithm only visits a subset of the whole dataset to compute the stochastic functional gradient, and samples \( O(t) \) points from the solution. Therefore, PMD can be applied to large-scale datasets.

**Theoretical guarantees.** We shows the density estimator provided by PMD converges in terms of KL-divergence to the true posterior density in rate \( O(1/T) \) with a larger memory requirement, and in rate \( O(1/\sqrt{T}) \) with a smaller memory requirement. To our best knowledge, these results are the first of the kind in Bayesian inference for approximating the entire posterior density.

In the remainder, we will introduce the optimization view of Bayes’ rule before presenting our algorithm. We will then provide both theoretical and empirical supports. The performance of the proposed inference algorithm in mixture models, Bayesian logistic regression, sparse Gaussian processes (GPs) and latent Dirichlet allocation (LDA) is competitive, sometimes even better, to several existing large-scale Bayesian inference algorithms.

## 2 Optimization View of Bayesian Inference

Our algorithm is rooted in the connection between Bayes’ rule and optimization. Throughout this paper, we denote \( KL \) as the Kullback-Leibler divergence, function \( q(\theta) \) as \( q \), a random sequence as \( \theta[\cdot] := \{\theta_1, \ldots, \theta_t\} \), \( \langle \cdot, \cdot \rangle_{L_2} \) as the \( L_2 \) inner product, and \( || \cdot ||_p \) as the \( L_p \) norm for \( 1 \leq p \leq \infty \). Zellner [16] first showed that Bayes’ rule

\[
p(\theta|X) = \frac{p(\theta) \prod_{n=1}^{N} p(x_n|\theta)}{p(X)} \quad \text{where} \quad p(X) = \int p(\theta) \prod_{n=1}^{N} p(x_n|\theta) d\theta,
\]

can be obtained by solving the optimization problem

\[
\min_{q(\theta) \in \mathcal{P}} L(q) := KL(q(\theta) \parallel p(\theta)) - \sum_{n=1}^{N} \left[ \int q(\theta) \log p(x_n|\theta) d\theta \right],
\]

where \( \mathcal{P} \) is the space of valid density. The objection function, \( L(q) \), is continuously differentiable with respect to \( q \in \mathcal{P} \) and we can further show that (all proofs can be found in the appendix)

**Lemma 1** Objective function \( L(q) \) defined on \( q(\theta) \in \mathcal{P} \) is 1-strongly convex w.r.t. \( KL \)-divergence.

Although we could write down the optimal solution, tractably computing, compactly representing or sampling from the solution can be challenging. Computation of the normalization, \( p(X) = \int p(\theta) \prod_{n=1}^{N} p(x_n|\theta) d\theta \), involves high dimensional integral and typically does not have closed-form. Meanwhile, the product in the numerator could be arbitrary complex which makes its representation and sampling difficult. However, this optimization perspective provides us the basis for large scale Bayesian inference by leveraging recent advances from optimization algorithms.
2.1 Stochastic Mirror Descent in Density Space

To avoid scanning through the entire data in each gradient evaluation, we will resort to stochastic optimization. In particular, the stochastic mirror descent framework [17] expands the usual stochastic gradient descent scheme to problems with non-Euclidean geometries, by applying unbiased stochastic subgradients and Bregman distances as prox-map functions. We now explain details of the stochastic mirror descent algorithm. The classical results regarding the convergence rate in Theorem 2 can also be extended and consider the update \( \hat{q}_{t+1} = \mathbb{P}_q(\gamma_t g_t) \), where \( \gamma_t > 0 \) and

\[
\mathbb{P}_q(g) := \arg\min_{\tilde{q}(\theta) \in \mathcal{P}} \{ \langle \tilde{q}(\theta), g(\theta) \rangle_{L_2} + KL(\tilde{q}(\theta) || q(\theta)) \}.
\]

Since we are descending in the density space, the KL-divergence is a natural choice for the prox-function. For any \( q \in \mathcal{P} \) and \( g \in L_2 \), the prox-mapping therefore leads to the update

\[
q_{t+1}(\theta) = \frac{q_t(\theta) \exp(-\gamma_t g_t(\theta))}{Z} = \frac{q_t(\theta)^{1-\gamma_t} p(\theta)^{\gamma_t} p(x_t|\theta)^{N\gamma_t}}{Z},
\]

where the normalization \( Z := \int q_t(\theta) \exp(-\gamma_t g_t(\theta)) d\theta \). This update resembles to the Bayes’ rule. However, an important difference here is that the posterior is updated using the fractional power of the previous solution, the prior and the likelihood. Furthermore, the stochastic mirror descent can go through the dataset several times to refine the solution.

Given the fact that the objective function, \( L(q) \), is 1-strongly convex w.r.t. the KL-divergence, we can immediately arrive at the following convergence results as appeared in Nemirovski et al. [17], if we are able to compute the prox-mapping in Eq. (3) exactly.

**Theorem 2** One prox-mapping step Eq. (3) reduces the error by

\[
\mathbb{E}[KL(q^*||q_{t+1})] \leq (1 - \gamma_t) \mathbb{E}[KL(q^*||q_t)] + \frac{\gamma_t^2 \mathbb{E}[\|g_t\|_\infty^2]}{2}.
\]

With stepsize \( \gamma_t = \frac{2}{t} \), it implies

\[
\mathbb{E}[KL(q^*||q_T)] \leq \max \left\{ KL(q^*||q_1), \frac{\eta^2 \mathbb{E}[\|g_1\|_\infty^2]}{2\eta - 1} \right\} \frac{1}{T}.
\]

Although stochastic mirror descent avoid the need to scan through the entire dataset in each iteration, it does not address the issue to tractable representation for the posterior. Still \( q_{t+1}(\theta) \) may not have closed-form representation, and we may not be able to compute the normalization \( Z \).

2.2 Error Tolerant Stochastic Mirror Descent

In fact, we can show that stochastic mirror descent can tolerate additional error during each prox-mapping step, which will provide us a provable convergent way for dealing with the particle depletion problem later. Given \( \epsilon \geq 0 \) and \( g \in L_2 \), we define the \( \epsilon \)-prox-mapping of \( q \) as the set

\[
\mathbb{P}_q^\epsilon(g) := \{ \tilde{q} \in \mathcal{P} : KL(\tilde{q}||q) + \langle g, \tilde{q} \rangle_{L_2} \leq \min_{\tilde{q} \in \mathcal{P}} \{ KL(\tilde{q}||q) + \langle g, \tilde{q} \rangle_{L_2} \} + \epsilon \},
\]

and consider the update \( \hat{q}_{t+1}(\theta) \in \mathbb{P}_q^\epsilon(\gamma_t g_t) \). When \( \epsilon_t = 0, \forall t \), this reduces to the usual stochastic mirror descent algorithm. The classical results regarding the convergence rate in Theorem 2 can also be extended

**Theorem 3** Let \( q^* = \arg\min_{q \in \mathcal{P}} L(q) \), stochastic mirror descent with inexact prox-mapping after \( T \) steps gives

(a) the recurrence: 

\[
\mathbb{E}[KL(q^*||\hat{q}_{t+1})] \leq \epsilon_t + (1 - \gamma_t) \mathbb{E}[KL(q^*||\hat{q}_t)] + \frac{\gamma_t^2 \mathbb{E}[\|g_t\|_\infty^2]}{2}.
\]
(b) the sub-optimality:

\[ \mathbb{E}[KL(q^* || \hat{q}_T)] \leq \mathbb{E}[L(\hat{q}_T) - L(q^*)] \leq \frac{M^2}{2} \sum_{t=1}^{T} \frac{1}{2} \sum_{t=1}^{T} \gamma_t^2 + \sum_{t=1}^{T} \epsilon_t + D_1 \]

\[ \sum_{t=1}^{T} \gamma_t \]

where \( \hat{q}_T = \sum_{t=1}^{T} \gamma_t \hat{q}_t / \sum_{t=1}^{T} \gamma_t \) and \( D_1 = KL(q^* || \hat{q}_1) \) and \( M^2 := \max_{1 \leq t \leq T} \mathbb{E}[\|g_t\|_\infty^2] \).

Remark. Same as the classical analysis of SA algorithms, using averaging schemes, e.g., simple average \( \hat{q}_T \) here or suffix average are necessary for proving a nonasymptotic convergence rate in terms of objective error. However, in practice, many experimental results suggest similar nonasymptotic behavior for the last iterate as well.

Allowing error in each prox-mapping step gives us rooms to design more flexible approximation algorithms. Essentially, this implies that we can approximate the intermediate density by some tractable representation. As long as the approximation error is not too large, the algorithm will still converge; and if the approximation does not involve costly computation, the overall algorithm will still be efficient. Next, we will introduce the importance weighted particles and kernel density estimator as two efficient ways to represent the intermediate density.

## 3 Particle Mirror Descent Algorithm

We will introduce two algorithms for scalable Bayesian inference, one based on weighted particles and the other based on weighted kernel density estimator. The first algorithm works when we already have a good guess of the true posterior, while the second algorithm aims to deal with the case where initialization is far away from the true posterior. Interestingly, these two methods resemble particle reweighting and rejuvenation respectively in sequential Monte Carlo yet with important differences.

### 3.1 Posterior Approximation with Weighted Particle

When we have a good guess \( \pi(\theta) \) covering the support \( \Omega \) of the true posterior \( p(\theta | X) \), we will simply draw a set of samples (or particles) from \( \pi(\theta) \), and approximate the intermediate posterior using these particles. More specifically, let \( \pi(\theta) \) be such that \( 0 \leq \frac{p(\theta | X)}{\pi(\theta)} < \infty \) and \( q_t(\theta) \in \mathcal{F} := \{ q(\theta) = \frac{\alpha(\theta) \pi(\theta)}{f(\theta) \pi(\theta)} \text{ s.t. } f(\theta) \pi(\theta) = 1, 0 \leq \alpha(\theta) \leq C \} \). We will first sample a set of locations, \( \{ \theta_i \}_{i=1}^m \) i.i.d. from \( \pi(\theta) \) and fix them across iterations. Then given \( \alpha_{t-1}(\theta_i) \) from previous iteration, we will approximate \( q_t(\theta) \) as a set of weighted particles

\[ \hat{q}_t(\theta) = \sum_{i=1}^m \alpha_i \delta(\theta_i), \text{ where } \alpha_i := \frac{\alpha_{t-1}(\theta_i) \exp(-\gamma t g_t(\theta_i))}{\sum_{i=1}^m \alpha_{t-1}(\theta_i) \exp(-\gamma t g_t(\theta_i))}. \]

The update is derived from the closed-form solution to the exact prox-mapping step \( \left[ 3 \right] \), i.e., \( \alpha_{t+1}(\theta) = \alpha_t(\theta) \exp(-\gamma_t g_t(\theta)) / Z \). Since \( Z \) is constant common to all \( \alpha_t(\theta_i) \), and \( \alpha_i \) is a ratio, \( Z \) can be ignored. One can simply update an unnormalized version of \( \alpha_t(\theta_i) \), and then use them to compute \( \alpha_i \). In summary, we can simply update the set of working variable \( \alpha_i \) as

\[ \alpha_i \leftarrow \alpha_i^{1-\gamma t} p(\theta_i) p(x_i | \theta_i)^N, \forall i \] and then \( \alpha_i \leftarrow \frac{\alpha_i}{\sum_{i=1}^m \alpha_i} \).

We can also formally show that this approximation incurs a small and dimension independent error in terms of how well it can approximate integral

**Theorem 4** With the assumption about \( \pi(\theta) \), for \( f \) bounded and integrable,

\[ \mathbb{E} \left[ \int \hat{q}_t(\theta) f(\theta) d\theta - \int q_t(\theta) f(\theta) d\theta \right] \leq \frac{2C \|f\|_\infty}{\sqrt{m}}. \]
Moreover, when the model has several latent variables \( \theta = (\xi, \zeta) \) and part of the variables has closed-form update in \( [3] \), e.g., sparse GPs and LDA (refer to the Appendix \( [5] \), we could incorporate such structure information into algorithm by decomposing the posterior \( q(\theta) = q(\xi)q(\zeta | \xi) \). With the good guess \( \pi(\xi) \), we could sample \( \{\xi_i\}^m \sim \pi(\xi) \) and approximate the posterior with summation of several functions, \( p(\zeta | \xi_i) \), in the form of \( q(\theta) \approx \sum \alpha_i q(\zeta | \xi_i) \).

### 3.2 Posterior Approximation with Weighted Kernel Density Estimator

In general, a good \( \pi(\theta) \) may be difficult to obtain, and a \( \pi(\theta) \) far way from the true posterior will leads to particle depletion and inaccurate estimation of the posterior. To deal with this issue, we will develop an algorithm based on weighted kernel density estimator. The algorithm will leverage the error tolerate stochastic mirror descent, and alternate between sampling from weighted density estimators, and updating the kernel density estimator.

More specifically, given \( \tilde{q}_{t-1}(\theta) \) from previous iteration which is supposed to be easy to sample from, we will approximate \( q_t(\theta) \) as a weighted kernel density estimator

\[
\tilde{q}_t(\theta) = \sum_{i=1}^{m} \alpha_i K_h(\theta - \theta_i), \quad \text{where} \quad \alpha_i := \frac{\exp(-\gamma_i g_t(\theta_i)) \sum_{i=1}^{m} \exp(-\gamma_i g_t(\theta_i))}{\sum_{i=1}^{m} \exp(-\gamma_i g_t(\theta_i))} \quad \text{and} \quad \{\theta_i\}_{i=1}^{m} \overset{i.i.d.}{\sim} \tilde{q}_{t-1}(\theta),
\]

where \( h > 0 \) is the bandwidth parameter and \( K_h(\theta) := \frac{1}{h^d}K(\theta/h) \) is a smoothing kernel. The update is again derived based on the closed-form solution to the exact prox-mapping step \( [3] \). However, the particle location in this case is sampled from the previous solution \( \tilde{q}_{t-1}(\theta) \). The idea here is that \( q_t(\theta) = \tilde{q}_{t-1}(\theta) \exp(-\gamma_t g_t(\theta))/Z \) can be viewed as an importance weighted version of \( \tilde{q}_{t-1}(\theta) \) with weights equal to \( \exp(-\gamma_t g_t(\theta))/Z \). If we want to approximate \( q_t(\theta) \), we can sample \( m \) locations from \( \tilde{q}_{t-1}(\theta) \) and associate each location the normalization weight \( \alpha_i \). To obtain a density for re-sampling in the next iteration, we place a kernel function \( K_h(\theta) \) on each sampled location. Since \( \alpha_i \) is a ratio, we can avoid evaluating the normalization factor \( Z \). In summary, we can simply update the set of working variable \( \alpha_i \) as

\[
\alpha_i \leftarrow \tilde{q}_{t-1}(\theta_i)^{-\gamma}p(\theta_i)^{\gamma}p(x_t | \theta_i)^{N\gamma_i}, \forall i \quad \text{and then} \quad \alpha_i \leftarrow \frac{\alpha_i}{\sum_{i=1}^{m} \alpha_i}.
\]

We can also formally show that the estimator in \( [5] \) possesses similar estimation properties to the standard KDE for densities (for details and formal definitions, refer to the appendix)

**Theorem 5** Let \( \tilde{q}_t \) be a \( (\beta; \mathcal{L}) \)-Hölder density function, and \( K \) be a \( \beta \)-valid density kernel, and the kernel bandwidth chosen as \( h = O(m^{-\frac{1}{d+2}}) \). Then with other mild conditions, \( \mathbb{E} \| \tilde{q}_t(\theta) - q_t(\theta) \|_1 = O(m^{-\frac{\beta}{d+2}}) \).

**Remark.** A kernel function \( K(\cdot) \) is called \( \beta \)-valid, if \( \int z^s K(z)dz = 0 \) holds true for any \( s = (s_1, \ldots, s_d) \in \mathbb{N}^d \) with \( |s| \leq |\beta| \). Notice that all spherically symmetric and product kernels satisfy the condition. For instance, the kernel \( K(\theta) = (2\pi)^{-d/2} \exp(-\|\theta\|^2/2) \) satisfies the condition with \( \beta = \infty \), and it is used through out our experiments. Theorem \( [5] \) implies that the weighted KDE achieves the minmax rate for density estimation in \( (\beta; \mathcal{L}) \)-Hölder function class \( [15] \), where \( \beta \) stands for the smoothness parameter and \( \mathcal{L} \) is the Lipschitz constant up to that level. With further assumption on the smoothness of the density, the weighted KDE can achieve even better rate. For instance, if \( \beta \) scales linearly with dimension, the error of weighted KDE can achieve a rate independent of the dimension.

This weighted kernel density estimation step is equivalent to approximately solving the prox-mapping step \( \mathbf{P}_{\tilde{q}_t}^\theta(\gamma_t g_t) \) as we discussed in Section \( [4] \). Due to the error tolerance of stochastic mirror descent, we will control the weighted kernel density estimation error within certain \( \epsilon \) by sampling an appropriate number, \( m \), of particle locations. In section \( [4] \) we show that with the weighted kernel density estimator, our algorithm actually converges to the true posterior in terms of \( KL \)-divergence.
Algorithm 1: Particle Mirror Descent Algorithm

1: **Input**: Data set $X = \{x_n\}_{n=1}^N$, prior $p(\theta)$
2: **Output**: posterior density estimator $\tilde{q}_T(\theta)$
3: Initialize $\tilde{q}_1(\theta) = p(\theta)$
4: for $t = 1, 2, \ldots, T - 1$ do
5: Sample $x_t \sim u[n] \sim X$
6: if Good $\pi(\theta)$ is provided then
7: \( \{\theta_i\}_{i=1}^{m_t} \sim i.i.d. \pi(\theta) \) when $t = 1$
8: $\alpha_t \leftarrow \alpha_t^{1-\gamma_t} \gamma_t p(\theta_1)^{\gamma_t} p(x_t | \theta_1)^N, \forall i$, and then, $\alpha_t \leftarrow \sum_{i=1}^{m_t} \alpha_i, \forall i$
9: $\tilde{q}_{t+1}(\theta) = \sum_{i=1}^{m_t} \alpha_i \delta(\theta_i)$
10: else
11: \( \{\theta_i\}_{i=1}^{m_t} \sim i.i.d. \tilde{q}_t(\theta) \)
12: $\alpha_t \leftarrow \tilde{q}_t(\theta_i)^{-\gamma_t} \gamma_t p(\theta_1)^{\gamma_t} p(x_t | \theta_1)^N, \forall i$, and then, $\alpha_t \leftarrow \sum_{i=1}^{m_t} \alpha_i, \forall i$
13: $\tilde{q}_{t+1}(\theta) = \sum_{i=1}^{m_t} \alpha_i K_{h_t} (\theta - \theta_i)$
14: end if
15: end for

3.3 Overall Algorithm

We present the overall algorithm, Particle Mirror Descent (PMD), in Algorithm 1 incorporating the two strategies from sections 3.1 and 3.2. PMD takes as input $N$ samples $X = \{x_n\}_{n=1}^N$, a prior $p(\theta)$ over the model parameter and the likelihood $p(x | \theta)$, and outputs the posterior density estimator $\tilde{q}_T(\theta)$ after $T$ iterations. At each iteration, PMD will maintain an approximate $\tilde{q}_t(\theta)$ of the posterior $p(\theta | X)$. In both cases, we exploit randomization for computational benefits. Specifically, we approximate the solution of prox-mapping with either weighted particles or weighted kernel density estimator. Therefore, our method, as a nonparametric variational inference method, also connects to Monte Carlo methods. The weighted particles could be used for integral approximation, while the weighted kernel density estimator returns density approaching to the posterior. In Section 3.4 we will show that, with proper setting of stepsize $\gamma$, number of samples $m_t$, the Algorithm 1 converges in rate $O(1/\sqrt{T})$, in terms of both integral approximation and KL-divergence, to the true posterior.

3.4 Comparison to Sequential Monte Carlo and Annealed Importance Sampling

The proposed algorithm bears some resemblances to the particle filtering/sequential Monte Carlo (SMC) algorithm [20][21][8], both of which rely on importance sampling. The key differences from our algorithm are (i) SMC re-weights the particles with likelihood while our algorithm re-weights based on functional gradient, which can be fractional power of the likelihood, and (ii) The SMC only utilized each datum once while our algorithm can visit each data point multiple time, and keep on refining the solution using the same dataset to approach the posterior.

Our algorithm also shares some similarities to annealed importance sampling (AIS) [22] in the sense that both algorithms are sampling from a series of densities and reweighting the samples to approximate the target distribution. However, we have significant differences. (i) In AIS, the density at each iteration is a weighted product of the joint distribution of all the data and a fixed proposal distribution, while we construct the densities as a weighted product of previous step solution and the functional stochastic gradient with particle data. (ii) The AIS might need MCMC to generate samples from the intermediate densities, while we only samples from a KDE which is more efficient. These differences make our method could handle large-scale dataset while AIS cannot.
4 Theoretical Guarantees

In this section, we show that (i) with assumptions about \( \pi(\theta) \) in Section 3 the convergence rate of the proposed algorithm in terms of integral approximation w.r.t. the true posterior is sublinear; and (ii) in general cases, the sequence \( \{q_t\} \), provided by PMD algorithm, converges in expectation with sublinear rates to the true posterior density in terms of \( KL \)-divergence (convergence in high probability is also provided in the appendix).

4.1 Convergence Analysis for Integral Approximation

The weighted particles approximation, \( \tilde{q}_t(\theta) = \sum_{i=1}^{m} \alpha_i \delta(\theta_i) \), returned by Algorithm 1 can be used directly for Bayesian inference. That is, given a function \( f \), \( \int q^*(\theta) f(\theta)d\theta \) can be approximated as \( \sum_{i=1}^{m} \alpha_i f(\theta_i) \). We will analyze their expected difference, which is commonly used in sequential Monte Carlo [24] and stochastic Langevin dynamics [11]. For simplicity of notation, we may write \( \sum_{i=1}^{m} \alpha_i f(\theta_i) = \int \tilde{q}_t(\theta) f(\theta)d\theta \), although \( \tilde{q}_t(\theta) \) is not a density. With the assumption on \( \pi(\theta) \), we can obtain a rate of convergence independent of the dimension.

**Theorem 6** Assume the particle proposal distribution \( \pi(\theta) \) has the same support as the true posterior \( q^*(\theta) \), and \( 0 \leq q_t(\theta)/\pi(\theta) \leq C \). Then \( \forall f(\theta) : \mathbb{R}^d \rightarrow \mathbb{R} \) bounded and integrable, with stepsize \( \gamma_t = \frac{\eta}{T} \), the PMD algorithm return \( m \) weighted particles after \( T \) iteration such that

\[
E \left[ \left| \int \tilde{q}_t(\theta) f(\theta)d\theta - \int q^*(\theta) f(\theta)d\theta \right| \right] \leq \frac{2C \|f\|_{\infty}}{\sqrt{m}} + \max \{ \sqrt{KL(q^*||\pi)}, \frac{\eta E\|g\|_{\infty}}{2\eta - 1} \} \|f\|_{\infty}\sqrt{T}.
\]

The proof of theorem leverages the approximation error results of the weighted particles for integration (Theorem 4), and the convergence analysis of mirror descent (Theorem 2). One can see that the error consists of two terms, one due to integration approximation and the other due to optimization error. To achieve the best rate of convergence, we need to balance the two terms. That is when the number particles, \( m \), scales linearly with the number of stochastic mirror descent iterations, we obtain an overall convergence rate of \( O(\frac{1}{\sqrt{T}}) \).

4.2 Convergence Analysis for Density Approximation

The weighted kernel density approximation can not only be used for integral approximation, but it can also be compared directly to the true posterior density. To provide the rate of convergence of densities generated by PMD in terms of \( KL \)-divergence directly in general case, we make the following assumptions ahead for later references:

A. Kernel \( K(\cdot) \) is a \( \beta \)-valid density kernel and there exists \( \mu, \nu > 0 \) such that \( \int K(z)^2dz \leq \mu^2 \) and \( \int \|z\|^\beta |K(z)|dz \leq \nu \).

B. For each \( t \), the function \( \tilde{q}_t \) belongs to a \( (\beta; L) \)-Hölder density class almost surely with bounded support \( \Omega \) and are bounded away from zero by \( \Delta^{-1} > 0 \).

C. For all mini-batch of examples, \( \|g_t\|_{\infty} \leq M \) almost surely for any \( t \);

The second assumption on lower boundedness of densities is pretty standard in the analysis of \( KL \)-divergence [23], although one should note that in principle this bound \( \Delta \) might depend on the problem size. The last assumption is also very common especially when mini-batch samples are used [10] [11]. These assumptions automatically validate all the conditions required to apply Theorem 5 and the corresponding high probability bounds (stated in Corollary 17 in the appendix). Immediately, we have that with high probability,

\[
\|\tilde{q}_{t+1} - P_{\tilde{q}_t}(\gamma_t g_t)\|_1 \leq O(m_t^{-\beta/(d+2\beta)}).
\]

Invoking the convergence analysis about the inexact prox-mapping in stochastic mirror descent with further analysis, we establish the main result as stated below.
Theorem 7 Let the stepsize $\gamma_t$, the number of locations $m_t$ and kernel bandwidth $h_t$ satisfy

$$m_t^{-\beta/(d+2\beta)} = B\gamma_t, \quad h_t = m_t^{-\frac{1}{2+d+2\beta}}, \quad \forall t = 1, \ldots, T.$$ 

Then we have

- Consider $\gamma_t = \frac{\eta}{\sqrt{t}}$ and $m_t = (\frac{\eta}{\sqrt{t}})^{1+\frac{d}{2\beta}}$, one can show that
  $$E_{x,\theta}[KL(q^*||\hat{q}_T)] \leq C_0(r) \frac{C_1\eta + D_1/\eta}{\sqrt{T}},$$

  where $\hat{q}_T = \sum_{i=i-r}^{i=r} \gamma_t \hat{q}_t / \sum_{i=i-r}^{i=r} \gamma_t$ and $C_0(r)$ is a small constant for any $0 < r < 1$.

- Consider $\gamma_t = \frac{\eta}{t}$ with $c > 1$ and $m_t = (\frac{\eta}{t})^{2+\frac{d}{\beta}}$, one can also show that
  $$E_{x,\theta}[KL(q^*||\hat{q}_T)] \leq \max \left\{ \frac{D_1}{2\eta - 1}, \frac{\eta^2 C_1}{2\eta - 1} \right\} \cdot \frac{1}{T},$$

where $\hat{q}_T$ is the solution produced after $T$ steps.

With the above choice of $m_t$, one can easily show that $E[x|x_{t-1}, \theta_{t-1}] \leq O(\sqrt{t})$, which is essentially $O((m_t^{-2\beta/(d+2\beta)})^2)$. Such choice will balance the error from weighted kernel density estimator and the variance from stochastic gradient in each step. Directly applying Theorem 3 (a) and (b), and solving the recursion following [17], we arrive at the two convergence rates under different choices of stepsize. For the sake of space, the corresponding high probability bound is presented in the Appendix E. One can immediately observe that there is twofold trade-off between the overall rate and the number of samples used at each iteration: (i) the convergence rate improves from $O(1/\sqrt{t})$ to $O(1/t)$ when the sample size increases from $O(t^{1+d/2\beta})$ to $O(t^{2+d/\beta})$; (ii) when ratio $B$ increases, the number of samples decrease but the constant $C$ grows.

We conclude that the expected error in terms of the $KL$ divergence of the solution (or averaged solution) after $T$ steps is of order $O(1/\sqrt{T})$ by choosing $O(1/\sqrt{t})$-decaying stepizes and $O(t^{1+\beta})$-growing samples, and of order $O(1/T)$ by choosing $O(1/t)$-decaying stepizes and $O(t^{2+\beta})$-growing samples. These results are the first of the kind for estimating posterior densities directly. The rate in terms of $KL$-divergence achieves the optimal and the dependence to dimension is unavoidable without further assumption.

5 Experiments

We conduct experiments on mixture models, Bayesian logistic regression, sparse Gaussian processes and latent Dirichlet allocation to demonstrate the advantages of the proposed algorithm in capturing multiple modes, dealing with non-conjugate models and incorporate special structures, respectively.

For the mixture model and logistic regression, we compare our algorithm with five general large-scale approximate Bayesian inference methods, including three sampling algorithms, i.e., one-pass sequential Monte Carlo (one-pass SMC) [6] which is an improved version of the SMC for Bayesian inference [21], stochastic gradient Langevin dynamics (SGD Langevin) [14] and Gibbs sampling, and two variational inference methods, i.e., stochastic variational inference (SVI) [15] and the stochastic variant of nonparametric variational inference (SGD NPV) [13]. For sparse GP and LDA, we compare with the existing large-scale inference algorithms designed specifically for the models. For the details of the PMD algorithm derivations for sparse GP and LDA, please refer to the Appendix [F].

5.1 Mixture Models

We conduct comparison on a simple yet interesting mixture model [4], the observations $x_l \sim p N(\theta_1, \sigma_1^2) + (1-p) N(\theta_2, \sigma_2^2)$ and $\theta_1 \sim N(0, \sigma_1^2), \theta_2 \sim N(0, \sigma_2^2)$, where $(\sigma_1, \sigma_2) = (1, 1), \sigma_x = 2.5$ and $p = 0.5$. The means of two Gaussians are tied together which makes $\theta_1$ and $\theta_2$ correlated in the posterior. We generate 1000 data
from the model with \((\theta_1, \theta_2) = (1, -2)\). This is one mode of the posterior, there is another equivalent mode at \((\theta_1, \theta_2) = (-1, 2)\).

For one-pass SMC, we use the suggested kernel bandwidth in [6]. For our method, since we increase the samples, the kernel bandwidth is shrunk in rate of \(O(m^{-\frac{1}{2}})\) as the theorem suggested. The batch size for stochastic algorithms and one-pass SMC is set to be 10. The burn-in period for Gibbs sampling and stochastic Langevin dynamics are 50 and 1000 respectively. We initialize all the inference algorithms with prior on \((\theta_1, \theta_2)\).

We repeat the experiments 10 times and report the average results. The actual recovered posterior distribution of our method and the competitors are illustrated in Figure 1(1)-(7) as a concrete example. PMD fits both modes well and recovers nicely the posterior while other algorithms either miss a mode or fail to fit the multimodal density. To compare these different kinds of algorithms in a quantitative way, we evaluate their performances using total variation and cross entropy of the solution against the true potential functions versus the number of observations visited in Figure 1(8)(9). From these figures, we could have
a direct understand about the behaviors of each competitor. The one-pass SMC performs similar to our algorithm at beginning. However, it cannot utilize the dataset effectively, therefore, it stopped with high error. It should be noticed that the one-pass SMC starts with more particles while our algorithm only requires the same number of particles at final stage according to the analysis. The reason that Gibbs sampling and the SGD Langevin dynamics perform worse is that they stuck in one mode. It is reasonable that Gibbs sampling fits the single mode better than SGD Langevin since it generates one new sample by scanning the whole dataset. We reported the average solution, the two contours in the result of SGD Langevin dynamics do not mean it finds both modes simultaneously. For the SGD NPV, it could locate both modes, however, it optimizes a non-convex objective which is highly costly and makes variance estimation inaccurate. The SVI totally fails because of the highly dependent variables and multimodality in posterior.

5.2 Bayesian Logistic Regression

We test our algorithm on logistic regression with non-conjugate prior for handwritten digits classification on the MNIST8M 8 vs. 6 dataset. The likelihood function for logistic regression is

$$p(y|x, w) = \frac{1}{1+\exp(-yw^\top x)}$$

with $w$ as the latent variables. We use Gaussian prior for $w$ with identity covariance matrix.

The dataset contains about 1.6M training samples and 1932 testing samples. We first reduce the dimension to 50 by PCA. The batch size is set to be 100 and the step size is set to be $\frac{1}{100+\sqrt{t}}$. The burn-in period for SGD Langevin is set to be 1000. We initialize all the inference algorithms with prior distribution and stop the stochastic algorithms after they pass through the whole dataset 5 times. We repeat the experiments 10 times and the results are reported in Figure 2(1).

Obviously, Gibbs sampling [28], which needs scan the whole set, is not suitable to large-scale problem. In this experiment, the SVI performs best at the beginning stage. This is expectable because searching in the Gaussian family is simpler comparing to nonparametric density family. However, it is should be noticed that our algorithm achieves comparable performance with the general nonparametric form when feeding enough data, 98.8%, to SVI which use carefully designed lower bound of the log-likelihood [27]. SGD NPV is flexible with mixture models family, however, its speed becomes the bottleneck. In SGD NPV, the gain from using stochastic gradient is dragged down by using L-BFGS to optimize the second-order approximation of the evidence lower bound.

5.3 Sparse Gaussian Processes

Music Year Prediction. We conduct the comparison on sparse GPs for the task to predict the year of songs [29]. In this task, we compare with SVI for sparse GPs [26], one-pass SMC and subset of data approximation (SoD) [25]. The data contains about 0.5M songs, each of which represented by 90-dimension features. We randomly selected 463,715 songs to train the model and test on 5,163 songs. As in [29], the year values are linearly mapped into $[0,1]$. The data is standardized before regression. Gaussian RBF
kernel is used in the model. The number of inducing inputs in sparse GP is set to be $2^{10}$, and all the other hyperparameters of sparse GP are fixed for all the inference methods, i.e., the kernel bandwidth is set to be the median of pairwise distances between data points (median trick) and the observations precision $\beta^{-1} = 0.01$. We stop the stochastic algorithms after they pass through the whole dataset 2 times. We use 16 particles in both SMC and PMD. The stepsize for both PMD and SVI are in the form of $\eta = \eta_0 + \sqrt{t}$, and the batch size is set to be 512. To demonstrate the advantages of PMD comparing to SMC, we initialize PMD with prior while initialize SMC with the SoD solution. We rerun experiments 10 times and the results are reported in Figure. (2). Our algorithm achieves the best RMSE 0.027, significant better than one-pass SMC, SVI and the baseline SoD.

**Synthetic Dataset.** To demonstrate the behavior of the PMD in sparse Gaussian processes, we also conduct experiments on 1D synthetic set. We generate 2048 data by

$$y = 3x^2 + (\sin(3.53\pi x) + \cos(7.7\pi x)) \exp(-1.6\pi|x|) + 0.1e$$

where $x \in [-0.5, 0.5]$ and $e \sim \mathcal{N}(0, 1)$. We use Gaussian RBF kernel in sparse GP and set the kernel bandwidth $\sigma$ to be 0.1 times the median of pairwise distances between data points, and $\beta^{-1} = 0.001$. We set the batch size to be 128 and the stepsize in the form of $\eta = \eta_0 + \sqrt{t}$ for PMD. We initial the $u = 0$ and random sample $Z$ from training set in PMD. Figure. (1)-(7) illustrates the evolving of the posterior provided by PMD with 16 particles and 128 inducing variables when the algorithm visits more and more data. As we can see, the posterior mean of sparse GP fits the ground truth better with more data. The convergence of the posterior mean of sparse GP provided by PMD is also illustrated in Figure. (8).

![Figure 3](image)

Figure 3: Visualization of posterior prediction distribution. The red curve is the mean function and the pale red region is the variance of the posterior. The cyan curve is the ground truth. The last one shows convergence of the posterior mean of sparse GP provided by PMD.

### 5.4 Latent Dirichlet Allocation

We compare with SVI [15], stochastic gradient Riemannian Langevin dynamic (SGRLD) [30], and SMC specially designed for LDA [31] on Wikipedia dataset [30]. The dataset contains 150,000 documents, about 2M words, and the vocabulary size is approximately 8000. The perplexity was estimated using the method discussed in [30] on a separate holdout set with 1000 documents. Since we evaluate the performance of algorithms in terms of perplexity rather than recovering the true posterior, we follow the same setting
in [32, 33] in which one particle is used in SMC and PMD to save computation and memory cost. Still, we set the number of topic 100 and fix the hyperparameters, $\alpha = 0.1$, $\beta = 0.01$, to solely compare the inference algorithms. We stop the stochastic algorithms after they pass through the whole dataset 5 times. The batch size is set to be 100. We use stepsizes $\eta_n = \eta_0 + t$ for PMD, SVI and SGRLD. We use the default burn-in period in SGRLD provided by [30]. For each algorithm a grid-search was run on step-size parameters and the best performance is reported. The results are reported in Figure 2(3). The top words from several topics found by our algorithm are illustrated in Figure 4.

Our algorithm achieves the best perplexity, significantly improves the performances of SGRLD and SVI. In this experiment, the SMC performs well at the beginning stage since it treats each document equally and updates with full likelihood. However, it only uses each datum once, while the stochastic algorithms, e.g., SGRLD, SVI and our algorithm, could further refine the solution with the same set several passes.

6 Conclusion

We propose a scalable, provable yet simple algorithm, Particle Mirror Descent, for large-scale Bayesian inference. Our algorithm is rooted in the connection between optimization and Bayesian inference. By introducing tolerate error in stochastic optimization, our algorithm maintains a tractable representation of the approximate posterior and keeps on refining it iteratively using a small batch of the data in each step. We provide strong empirical supports on several popular models for large-scale problems. We also prove the first kind result that our algorithm converges in rate $O(1/\sqrt{t})$ in terms of $KL$-divergence to the true posterior. Most importantly, the Particle Mirror Descent algorithm opens the door to a new research direction, i.e., connecting function analysis and optimization with Monte Carlo to Bayesian inference, which could be promising.

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References


Appendix

A Strong convexity

As we discussed, the posterior from Bayes’s rule could be viewed as the optimal of an optimization problem in Eq (1). We will show that the objective function is strongly convex w.r.t $KL$-divergence.

**Proof for Lemma**[7] The lemma directly results from the generalized Pythagoras theorem for Bregman divergence. Particularly, for $KL$-divergence, we have

$$KL(q_1||q) = KL(q_1||q_2) + KL(q_2||q) - \langle q_1 - q_2, \nabla \phi(q) - \nabla \phi(q_2) \rangle_2$$

where $\phi(q)$ is the entropy of $q$.

Notice that $L(q) = KL(q||q^*) - \log Z$, where $q^* = \frac{\theta^N_p(x_i|\theta)}{\int \theta^N_p(x_i|\theta)}$, we have

$$KL(q_1||q^*) - KL(q_2||q^*) - \langle q_1 - q_2, \nabla \phi(q_2) - \nabla \phi(q^*) \rangle_2 = KL(q_1||q_2)$$

$KL(q_1||q^*) - KL(q_2||q^*) - \langle q_1 - q_2, \log q_2 - \log q^* \rangle_2 = KL(q_1||q_2)$

$KL(q_1||q^*) - KL(q_2||q^*) - \langle q_1 - q_2, \log q_2 - \log \theta \Pi_i^N p(x_i|\theta) \rangle_2 + \langle q_1 - q_2, \log Z \rangle_2 = KL(q_1||q_2)$

$\Rightarrow L(q_1) - L(q_2) - \langle q_1 - q_2, \nabla L(q_2) \rangle_2 = KL(q_1||q_2)$

### B Finite Convergence of Stochastic Mirror Descent with Inexact Prox-Mapping in Density Space

Since the prox-mapping of stochastic mirror descent is intractable when directly being applied to the optimization problem (1), we propose the $\epsilon$-inexact prox-mapping within the stochastic mirror descent framework in Section 3. Instead of solving the prox-mapping exactly, we approximate the solution with $\epsilon$ error. In this section, we will show as long as the approximation error is tolerable, the stochastic mirror descent algorithm still converges.

**Theorem**[3] Denote $q^* = \arg\min_{q \in \mathcal{P}} L(q)$, the stochastic mirror descent with inexact prox-mapping after $T$ steps gives

(a) the recurrence:

$$\forall t \leq T, \mathbb{E}[KL(q^*||\tilde{q}_{t+1})] \leq \epsilon_t + (1 - \gamma_t)\mathbb{E}[KL(q^*||\tilde{q}_t)] + \frac{\gamma_t^2 \mathbb{E}[\|g_t\|^2_2]}{2}$$

(b) the sub-optimality:

$$\mathbb{E}[KL(q^*||\tilde{q}_T)] \leq \mathbb{E}[L(\tilde{q}_T) - L(q^*)] \leq \frac{M^2}{2} \sum_{t=1}^T \gamma_t^2 + \sum_{t=1}^T \epsilon_t + D_1 \sum_{t=1}^T \gamma_t$$

where $\tilde{q}_T = \sum_{t=1}^T \gamma_t q_t / \sum_{t=1}^T \gamma_t$ and $D_1 = KL(q^*||\tilde{q}_1)$ and $M^2 := \max_{1 \leq t \leq T} \mathbb{E}[\|g_t\|^2_2]$.

**Remark.** Based on [17], one can immediately see that, to guarantee the usual rate of convergence, the error $\epsilon_t$ can be of order $O(\sqrt{T})$. The first recurrence implies an overall $O(T)$ rate of convergence for the $KL$-divergence when the stepsize $\gamma_t$ is as small as $O(1/t)$ and error $\epsilon_t$ is as small as $O(1/t^2)$. The second result implies an overall $O(1/T)$ rate of convergence for objective function when larger stepsize $\gamma_t = O(1/\sqrt{T})$ and larger error $\epsilon_t = O(1/t)$ are adopted.

**Proof for Theorem**[3] (a) By first-order optimality condition, $\tilde{q}_{t+1} \in \mathcal{P}_{\tilde{q}_t}^{\epsilon} (\gamma_t g_t)$ is equivalent as

$$\langle g_t + \log(\tilde{q}_{t+1}) - \log(\tilde{q}_t), \tilde{q}_{t+1} - q \rangle_{L_2} \leq \epsilon_t, \forall q \in \mathcal{P},$$
which implies that
\[
\langle \gamma_t g_t, \tilde{q}_{t+1} - q \rangle_2 \leq (\log(\tilde{q}_t) - \log(\tilde{q}_{t+1}), \tilde{q}_{t+1} - q)_2 + \epsilon_t \leq KL(q||\tilde{q}_t) - KL(q||\tilde{q}_{t+1}) - KL(\tilde{q}_{t+1}||\tilde{q}_t) + \epsilon_t
\]

Hence,
\[
\langle \gamma_t g_t, \tilde{q}_t - q \rangle_2 \leq KL(q||\tilde{q}_t) - KL(q||\tilde{q}_{t+1}) - KL(\tilde{q}_{t+1}||\tilde{q}_t) + \langle \gamma_t g_t, \tilde{q}_t - \tilde{q}_{t+1} \rangle_2.
\]

By Young’s inequality, we have
\[
\langle \gamma_t g_t, \tilde{q}_t - q \rangle_2 \leq \frac{1}{2} \|\tilde{q}_t - \tilde{q}_{t+1}\|_1^2 + \frac{\gamma_t^2}{2} \|g_t\|_\infty^2.
\]

Also, from Pinsker’s inequality, we have
\[
KL(\tilde{q}_{t+1}||\tilde{q}_t) \geq \frac{1}{2} \|\tilde{q}_t - \tilde{q}_{t+1}\|_1^2.
\]

Therefore, combining (7), (8), and (9), we have \(\forall q \in \mathcal{P}\)
\[
\langle \gamma_t g_t, \tilde{q}_t - q \rangle_2 \leq \epsilon_t + KL(q||\tilde{q}_t) - KL(q||\tilde{q}_{t+1}) + \frac{\gamma_t^2}{2} \|g_t\|_\infty^2.
\]

Plugging \(q^*\) and taking expectation on both sides, the LHS becomes
\[
\mathbb{E}_x \left[ \langle \tilde{q}_t - q^*, \gamma_t g_t \rangle \right] = \mathbb{E}_x \left[ \langle \tilde{q}_t - q^*, \gamma_t \mathbb{E}[g_t] \rangle \bigg| x_{t-1} \right] = \mathbb{E}_x \left[ \langle \tilde{q}_t - q^*, \gamma_t \nabla L(\tilde{q}_t) \rangle \right],
\]

Therefore, we have
\[
\mathbb{E}_x \left[ \langle \tilde{q}_t - q^*, \gamma_t \nabla L(\tilde{q}_t) \rangle \right] \leq \epsilon_t + \mathbb{E}_x \left[ KL(q^*||\tilde{q}_t) \right] - \mathbb{E}_x \left[ KL(q^*||\tilde{q}_{t+1}) \right] + \frac{\gamma_t^2}{2} \mathbb{E}_x \|g_t\|_\infty^2
\]

Because the objective function is 1-strongly convex w.r.t. KL-divergence,
\[
\langle q^* - q, \nabla L(q^*) - \nabla L(q) \rangle = KL(q^*||q) + KL(q||q'),
\]

and the optimality condition, we have
\[
\langle \tilde{q}_t - q^*, \nabla L(\tilde{q}_t) \rangle \geq KL(q^*||\tilde{q}_t)
\]

we obtain the recursion with inexact prox-mapping,
\[
\mathbb{E}_x[KL(q^*||\tilde{q}_{t+1})] \leq \epsilon_t + (1 - \gamma_t)\mathbb{E}_x[KL(q^*||\tilde{q}_t)] + \frac{\gamma_t^2}{2} M^2
\]

(b) Summing over \(t = 1, \ldots, T\) of equation (11), we get
\[
\sum_{t=1}^{T} \mathbb{E}_x[\langle \tilde{q}_t - q^*, \gamma_t \nabla L(\tilde{q}_t) \rangle] \leq \sum_{t=1}^{T} \epsilon_t + KL(q^*||\tilde{q}_t) + \sum_{t=1}^{T} \frac{\gamma_t^2}{2} M^2
\]

By convexity and optimality condition, this leads to
\[
\left( \sum_{t=1}^{T} \gamma_t \right) \mathbb{E}_x[L(\tilde{q}_T) - L(q^*)] \leq \mathbb{E}_x \left[ \sum_{t=1}^{T} \gamma_t (L(\tilde{q}_t) - L(q^*)) \right] \leq \sum_{t=1}^{T} \epsilon_t + KL(q^*||\tilde{q}_1) + \sum_{t=1}^{T} \frac{\gamma_t^2}{2} M^2
\]

Furthermore, combined with the 1-strongly-convexity, it immediately follows that
\[
\mathbb{E}_x[KL(q^*||\tilde{q}_T)] \leq \mathbb{E}_x[L(\tilde{q}_T) - L(q^*)] \leq \frac{1}{2} \sum_{t=1}^{T} \gamma_t^2 M^2 + \sum_{t=1}^{T} \epsilon_t + D_1.
\]
C Convergence Analysis for Integral Approximation

In this section, we provide the details of the convergence analysis of the proposed algorithm in terms of integral approximation w.r.t. the true posterior using a good initialization.

Assume that we have some good guess covering the support \( \Omega \) of true posterior distribution \( p(\theta | X) \) such that \( 0 \leq \frac{p(\theta | X)}{\pi(\theta)} \leq C^* < \infty \), then, we define

\[
\mathcal{F} = \left\{ q(\theta) = \alpha(\theta) \pi(\theta), \int \alpha(\theta) \pi(\theta) d\theta = 1, 0 \leq \alpha(\theta) \leq C \right\}
\]

and one can show

**Lemma 8** \( \forall q \in \mathcal{F}, \) let \( \{\theta_i\}_{i=1}^m \) is i.i.d. sampled from \( \pi(\theta) \), we could construct \( \tilde{q}(\theta) = \sum_{i=1}^m \frac{\alpha(\theta_i) \delta(\theta_i)}{\sum_{i=1}^m \alpha(\theta_i)} \), such that \( \forall f(\theta) : \mathbb{R}^d \rightarrow \mathbb{R} \) bounded and integrable,

\[
\mathbb{E} \left[ \left| \int \tilde{q}(\theta) f(\theta) d\theta - \int q(\theta) f(\theta) d\theta \right| \right] \leq \frac{2C \|f\|_\infty}{\sqrt{m}}.
\]

**Proof**

Given \( q(\theta) \), we sample i.i.d. \( \{\theta_i\}_{i=1}^m \) from \( \pi(\theta) \), and construct a function

\[
\tilde{q}(\theta) = \frac{1}{m} \sum_{i=1}^m \alpha(\theta_i).
\]

It is obviously that

\[
\mathbb{E}_\theta[\tilde{q}(\theta)] = \mathbb{E}_\theta \left[ \frac{1}{m} \sum_{i=1}^m \alpha(\theta_i) \right] = \frac{1}{m} \sum_{i=1}^m \mathbb{E}_\theta[\alpha(\theta_i)] = q(\theta)
\]

and

\[
\mathbb{E}_\theta \left[ \int \tilde{q}(\theta) f(\theta) d\theta \right] = \mathbb{E}_\theta \left[ \frac{1}{m} \sum_{i=1}^m \alpha(\theta_i) f(\theta_i) \right] = \frac{1}{m} \sum_{i=1}^m \mathbb{E}_\theta[\alpha(\theta_i) f(\theta_i)] = \int q(\theta) f(\theta) d\theta
\]

Then,

\[
\mathbb{E}_\theta \left[ \left| \int \tilde{q}(\theta) f(\theta) d\theta - \int q(\theta) f(\theta) d\theta \right|^2 \right] = \mathbb{E}_\theta \left[ \left| \int \tilde{q}(\theta) f(\theta) d\theta - \mathbb{E}_\theta \left[ \int \tilde{q}(\theta) f(\theta) d\theta \right] \right|^2 \right]
\]

\[
= \frac{1}{m} \left( \mathbb{E}_\theta \|\alpha(\theta_i) f(\theta_i)\|_2^2 - \|\mathbb{E}_\theta[\alpha(\theta_i) f(\theta_i)]\|_2^2 \right) \leq \frac{1}{m} \mathbb{E}_\theta \|\alpha(\theta_i) f(\theta_i)\|_2^2 \leq \frac{C^2}{m} \|f(\theta)\|_\infty^2
\]

By Jensen’s inequality, we have

\[
\mathbb{E}_\theta \left[ \left| \int \tilde{q}(\theta) f(\theta) d\theta - \int q(\theta) f(\theta) d\theta \right| \right] \leq \sqrt{\mathbb{E}_\theta \left[ \left| \int \tilde{q}(\theta) f(\theta) d\theta - \int q(\theta) f(\theta) d\theta \right|^2 \right]} \leq \frac{C \|f(\theta)\|_\infty}{\sqrt{m}}
\]

Apply the above conclusion to \( f(\theta) = 1 \), we have

\[
\mathbb{E} \left[ \frac{1}{m} \sum_{i=1}^m \alpha_i - 1 \right] \leq \frac{C}{\sqrt{m}}
\]
Let \( \tilde{q}(\theta) = \sum_{i}^{m} \frac{\alpha(\theta_i) \delta(\theta_i)}{\sum_{i}^{m} \alpha(\theta_i)} \), then \( \sum_{i}^{m} \frac{\alpha_i}{\sum_{i}^{m} \alpha_i} = 1 \), and

\[
E_\theta \left[ \int \tilde{q}(\theta) f(\theta) d\theta - \int \hat{q}(\theta) f(\theta) d\theta \right] = E_\theta \left[ \int \frac{1}{\sum_{i}^{m} \alpha(\theta_i)} \sum_{i}^{m} \alpha(\theta_i) f(\theta_i) \right] - \frac{1}{m} \sum_{i}^{m} \alpha(\theta_i) f(\theta_i) \]

\[
= E_\theta \left[ \int \frac{1}{\sum_{i}^{m} \alpha(\theta_i)} \sum_{i}^{m} \alpha(\theta_i) f(\theta_i) \right] - \frac{1}{m} \sum_{i}^{m} \alpha(\theta_i) f(\theta_i) \]

Then, we have achieved our conclusion that

\[
\mathbb{E}_\theta \left[ \int \tilde{q}(\theta) f(\theta) d\theta - \int q(\theta) f(\theta) d\theta \right] \leq \frac{2C\|f\|_\infty}{\sqrt{m}}
\]

With the knowledge of \( \pi(\theta) \) and \( p(\theta|X) \), we set \( q_i(\theta) = \alpha_i(\theta) \pi(\theta) \), the PMD algorithm will reduce to adjust \( \alpha(\theta_i) \) for samples \( \{\theta_i\}_{i=1}^{m} \sim \pi(\theta) \) according to the stochastic gradient. Plug the gradient formula into the exact update rule and the constrains on \( \alpha_{t+1}(\theta) \), we have

\[
q_{t+1}(\theta) = \frac{q_t(\theta) \exp(-\gamma_t g_t(\theta))}{Z} = \frac{\alpha_t(\theta) \exp(-\gamma_t g_t(\theta)) \pi(\theta)}{Z} = \alpha_{t+1}(\theta) \pi(\theta)
\]

where \( \alpha_{t+1}(\theta) = \alpha_t(\theta) \exp(-\gamma_t g_t(\theta)) \). Since \( Z \) is constant, ignoring it will not affect the multiplicative update. Therefore, we have the fact from Lemma 8 that

**Theorem 4** \( \forall t = 1, \ldots, T \) and \( \forall f \) bounded and integrable, the PMD algorithm generates in weighted particles such that

\[
\mathbb{E} \left[ \int \tilde{q}_t(\theta) f(\theta) d\theta - \int q_t(\theta) f(\theta) d\theta \right] \leq \frac{2C\|f\|_\infty}{\sqrt{m}}.
\]

**Lemma 9** Let \( q_t \) is the exact solution of the prox-mapping at \( t \)-step, then \( \forall f(\theta) : \mathbb{R}^d \rightarrow \mathbb{R} \), which is bounded and integrable, we have

\[
\mathbb{E} \left[ \int q_t(\theta) f(\theta) d\theta - \int q(\theta) f(\theta) d\theta \right] \leq \max \left\{ \sqrt{\text{KL}(q^*||q_t)}, \frac{\eta \mathbb{E} \|g\|_\infty}{\sqrt{2\eta - 1}} \right\} \|f\|_\infty \sqrt{t}.
\]

**Proof**

\[
\mathbb{E} \left[ \int q_t(\theta) f(\theta) d\theta - \int q^*(\theta) f(\theta) d\theta \right] = \mathbb{E} \|q_t(\theta) - q^*(\theta) f(\theta)\|_2 \leq \mathbb{E} \|q_t(\theta) - q^*(\theta)\|_1 \leq \mathbb{E} \|f\|_\infty \mathbb{E} \left\{ \frac{1}{2} \text{KL}(q^*||q_t) \right\} \leq \max \left\{ \sqrt{\text{KL}(q^*||q_t)}, \frac{\eta \mathbb{E} \|g\|_\infty}{\sqrt{2\eta - 1}} \right\} \|f\|_\infty \sqrt{t}
\]

The second last inequality comes from Pinsker’s inequality and the last inequality comes from Theorem 2.
Proof for Theorem 6. We set the $C = C_t$ so that $q_t(\theta) \in \mathcal{F}$, this conclusion directly comes from Theorem 4 and Lemma 9.

D Error Bound of Weighted Kernel Density Estimator

Before we start to prove the finite convergence in general case, we need to characterize the error induced by weighted kernel density estimator. In this section, we analyze the error in terms of both $L_1$ and $L_2$ norm, which are used for convergence analysis measured by KL-divergence in the Appendix E.

D.1 $L_1$-Error Bound of Weighted Kernel Density Estimator

We approximate the density function $q(\theta) = \omega(\theta)p(\theta)$ using the weighted kernel density estimator $\tilde{q}(\theta) = \sum_{i=1}^{m} \omega(\theta_i)K_h(\theta - \theta_i)$ and would like to bound the $L_1$ error, i.e. $\|\tilde{q}(\theta) - q(\theta)\|_1$ both in expectation and with high probability. Particularly, in our case in $t$-step, the $\omega(\theta) = \exp(-\gamma t g_k(\theta)) / Z$ and $p(\theta) = q_t(\theta)$.

We consider an unnormalized kernel density estimator as the intermediate quantity

$$q_m(\theta) = \frac{1}{m} \sum_{i=1}^{m} \omega(\theta_i)K_h(\theta, \theta_i)$$

Note that $E[q_m(\theta)] = E_\theta[\omega(\theta_i)K_h(\theta, \theta_i)] = q \ast K_h$. Then the error can be decomposed into three terms as

$$\epsilon := E\|\tilde{q}(\theta) - q(\theta)\|_1 \leq E\|\tilde{q}(\theta) - q_m(\theta)\|_1 + E\|q_m(\theta) - E\tilde{q}_m(\theta)\|_1 + \|E\tilde{q}_m(\theta) - q(\theta)\|_1$$

We now present the proof for each of these error bounds.

To formally show that, we begin by giving the definition of a special class of kernels and Hölder classes of densities that we consider.

Definition 10 (($\beta; \mu, \nu$)-valid density kernel) We say a kernel function $K(\cdot)$ is a $(\beta; \mu, \nu)$-valid density kernel, if $K(\theta, \theta) = K(\theta - \theta)$ is a bounded, compactly supported kernel such that

(i) $\int K(z)^r dz \leq \infty$ for any $r \geq 1$, particularly, $\int K(z)^2 dz \leq \mu^2$ for some $\mu > 0$.

(ii) $\int z^s K(z) dz = 0$, for any $s = (s_1, \ldots, s_d) \in \mathbb{N}^d$ such that $1 \leq |s| \leq |\beta|$. In addition, $\int \|z\|^\beta|K(z)|dz \leq \nu$ for some $\nu > 0$.

For simplicity, we sometimes call $K(\cdot)$ as a $\beta$-valid density kernel if the constants $\mu$ and $\nu$ are not specifically given. Notice that all spherically symmetric compactly supported probability density and product kernels based on compactly supported symmetric univariate densities satisfy the conditions. For instance, the kernel $K(\theta) = (2\pi)^{-d/2}\exp(-|\theta|^2/2)$ satisfies the conditions with $\beta = \infty$, and it is used throughout our experiments. Furthermore, we will focus on a class of smooth densities

Definition 11 (($\beta; \mathcal{L}$)-Hölder density function) We say a density function $q(\cdot)$ is a $(\beta; \mathcal{L})$-Hölder density function if function $q(\cdot)$ is $|\beta|$-times continuously differentiable on its support $\Omega$ and satisfies

(i) for any $z_0$, there exists $L(z_0) > 0$ such that

$$|q(z) - q^{(\beta)}_{z_0}(z)| \leq L(z_0)\|z - z_0\|^\beta, \forall z \in \Omega$$

where $q^{(\beta)}_{z_0}$ is the $|\beta|$-order Taylor approximation, i.e.

$$q^{(\beta)}_{z_0}(z) := \sum_{s=(s_1,\ldots,s_d):|s|\leq|\beta|} \frac{(z - z_0)^s}{s!} D^s q(z_0);$$

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(ii) in addition, the integral $\int L(z)dz \leq L$.

Then given the above setting for the kernel function and the smooth densities, we can characterize the error of the weighted kernel density estimator as follows.

### D.1.1 KDE error due to bias

**Lemma 12 (Bias)** If $q(\cdot) \in C^2_{L}(\Omega)$ and $K$ is a $(\beta;\mu,\nu)$-valid density kernel, then

$$\|q(\theta) - \mathbb{E}[q_m(\theta)]\|_1 \leq \nu L h^\beta.$$

**Proof** The proof of this lemma follows directly from Chapter 4.3 in [34].

\[
|\mathbb{E}[q_m(\theta)] - q(\theta)| = |q * K_h(\theta) - q(\theta)| \\
= \int \frac{1}{h^d} K(\frac{z-\theta}{h})q(z)dz - q(\theta) \\
= \int \frac{1}{h^d} K(\frac{z}{h})q(\theta + z) - q(\theta)dz \\
= \int K(z)|q(\theta + hz) - q(\theta)|dz \\
\leq \left| \int K(z)|q(\theta + hz) - q_\theta(\theta + hz)|dz \right| + \int |K(z)q_\theta(\theta + hz) - q(\theta)|dz \\
\leq L(\theta) \int |K(z)||hz|^\beta dz + \int |K(z)q_\theta(\theta + hz) - q(\theta)|dz
\]

Note that $q_\theta(\theta + hz) - q(\theta)$ is a polynomial of degree at most $|\beta|$ with no constant, by the definition of $(\beta;\mu,\nu)$-valid density kernel, the second term is zero. Hence, we have $|\mathbb{E}[q_m(\theta)] - q(\theta)| \leq \nu L(\theta) h^\beta$, and therefore

$$\|\mathbb{E}[q_m(\theta)] - q(\theta)\|_1 \leq \nu h^\beta \int L(\theta)d\theta \leq \nu L h^\beta.$$

### D.1.2 KDE error due to variance

The variance term can be bounded using similar techniques as in [35].

**Lemma 13 (Variance)** Assume $\omega\sqrt{p} \in L_1$ with bounded support, then

$$\mathbb{E}\|q_m(\theta) - \mathbb{E}[q_m(\theta)]\|_1 \leq \frac{\mu}{\sqrt{m}h^\frac{d}{2}} \int \omega\sqrt{p} d\theta + o((mh^d)^{-\frac{1}{2}}).$$

**Proof** For any $\theta$, we have

\[
\sigma^2(\theta) : = \mathbb{E}\left[\left(q_m(\theta) - \mathbb{E}[q_m(\theta)]\right)^2\right] = \frac{1}{m} \sum_{i=1}^{m} \mathbb{E}\left[\omega^2(\theta_i)K_h^2(\theta,\theta_i)\right] - (q * K_h)^2 \leq \frac{(\omega^2 q) * K_h^2}{m}
\]

Denote $\mu(K) := \sqrt{\int K(\theta)^2 d\theta}$ and kernel $K^+(\theta) = \frac{K(\theta)}{\mu(K)^2}$, then $\mu(K) \leq \mu$, $\int K^+ d\theta = 1$ and

$$K_h^+(\theta) = \frac{1}{h^d} K^+(\theta/d) = \frac{1}{h^d} \frac{K(\theta/h)K(\theta/h)}{\mu^2(K)} = \frac{h^d}{\mu^2(K)} K_h^2(\theta).$$
Hence,
\[
\sigma^2(\theta) \leq \frac{\mu^2(K)(\omega^2 p) \ast K_h^+}{mh^d} \leq \frac{\mu^2(\omega^2 p) \ast K_h^+ - \omega^2 p}{mh^d} + \frac{\mu^2(\omega^2 p)}{mh^d}.
\]

Note that \( \sigma(\theta) = \sqrt{\text{Var}(\theta)} \geq \text{Var}(\theta) \), hence,
\[
\mathbb{E} \|\bar{q}(\theta) - q_m(\theta)\|_1 = \int \mathbb{E}[q_m(\theta)] d\theta \leq \int \sigma(\theta) d\theta.
\]

From Theorem 2.1 in [35], we have \( \int |(\omega^2 p) \ast K_h^+ - \omega^2 p| d\theta = o(1) \). Therefore, we conclude that
\[
\mathbb{E} \|\bar{q}(\theta) - q_m(\theta)\|_1 \leq \frac{\mu}{\sqrt{mh^{d/2}}} \|\omega \sqrt{\mathcal{P}}\|_1 + o((mh^d)^{1/2}).
\]

\[\square\]

D.1.3 KDE error due to normalization

The normalization error term can be easily derived based on the variance.

Lemma 14 (Normalization error) Assume \( \omega \sqrt{\mathcal{P}} \in L_2 \)
\[
\mathbb{E} \|\bar{q}(\theta) - q_m(\theta)\|_1 \leq \frac{1}{\sqrt{m}} \left( \int \omega^2(\theta)p(\theta) d\theta \right)^{1/2}.
\]

Proof Denote \( \omega_i := \omega(\theta_i) \), then \( \mathbb{E}[\omega_i] = \int \omega(\theta)p(\theta) d\theta = 1 \) and \( \mathbb{E}[\omega_i^2] = \int \omega^2(\theta)p(\theta) d\theta \), for any \( i = 1, \ldots, m \). Hence,
\[
\mathbb{E}\left[ \frac{1}{m} \sum_{i=1}^{m} \omega_i - 1 \right]^2 = \frac{1}{m} \int \omega^2(\theta)p(\theta) d\theta.
\]

Recall that \( \bar{q}(\theta) = \sum_{i=1}^{m} \omega_i K_h(\theta, \theta_i) \) and \( q_m(\theta) = \frac{1}{m} \sum_{i=1}^{m} \omega_i K_h(\theta, \theta_i) \).
\[
\mathbb{E} \|\bar{q}(\theta) - q_m(\theta)\|_1 \leq \mathbb{E} \left\| \frac{1}{m} \sum_{i=1}^{m} \omega_i K_h(\theta, \theta_i) - \frac{1}{m} \sum_{i=1}^{m} \omega_i K_h(\theta, \theta_i) \right\|_1
\]
\[
\leq \mathbb{E} \left\| \frac{1}{m} \sum_{i=1}^{m} \omega_i K_h(\theta, \theta_i) - \frac{1}{m} \sum_{i=1}^{m} \omega_i K_h(\theta, \theta_i) \right\|_1
\]
\[
\leq \mathbb{E} \left\| \frac{1}{m} \sum_{i=1}^{m} \omega_i K_h(\theta, \theta_i) \right\|_1
\]

Since \( \|K_h\|_1 = \int \frac{1}{m} K(\theta/h) d\theta = \int K(\theta) d\theta = 1 \), we have
\[
\mathbb{E} \|\bar{q}(\theta) - q_m(\theta)\|_1 \leq \frac{1}{1/m} \sqrt{\int \omega^2(\theta)p(\theta) d\theta} = \frac{1}{\sqrt{m}} \|\omega \sqrt{\mathcal{P}}\|_2.
\]

\[\square\]
D.1.4 KDE error in expectation and with high probability

Based on the above there lemmas, namely, Lemma 12-14 we can immediately arrive at the bound of the $L_1$ error in expectation as stated in Theorem 5. We now provide the proof for the high probability bound as stated below.

\textbf{Corollary 15 (Overall error in high probability)} Besides the above assumption, let us also assume that $\omega(\theta)$ is bounded, i.e. there exists $0 < B_1 \leq B_2 < \infty$ such that $B_1 \leq \omega(\theta) \leq B_2, \forall \theta$. Then, with probability at least $1 - \delta$,

$$\|\hat{q}(\theta) - q(\theta)\|_1 \leq \nu L h^2 + \frac{\mu}{\nu m h^2} \|\omega\|_1 + \frac{1}{\sqrt{m}} \|\omega\|_2 + \frac{1}{\sqrt{m}} \sqrt{8B_1 B_2 \log(1/\delta) + o((mh^d)^{-\frac{1}{2}})}.$$ 

\textbf{Proof} We use McDiarmid’s inequality to show that the function $f(\Theta) = \|\hat{q}(\Theta) - q(\Theta)\|_1$, defined on the random data $\Theta = (\theta_1, \ldots, \theta_m)$, is concentrated on the mean. Let $\bar{\Theta} = (\bar{\theta}_1, \ldots, \bar{\theta}_j, \ldots, \bar{\theta}_m)$. We denote $\omega = (\omega(\theta_1), \ldots, \omega(\theta_m))$ and $\tilde{\omega} = (\omega(\bar{\theta}_1), \ldots, \omega(\bar{\theta}_j), \ldots, \omega(\theta_m))$. Denote $k = (K_h(\bar{\theta}_1), \ldots, K_h(\theta_j), \ldots, K_h(\theta_m))$. We first show that $|f(\Theta) - f(\Theta')|$ is bounded.

$$|f(\Theta) - f(\Theta')| = \left| \|\hat{q}_\Theta(\theta) - q(\theta)\|_1 - \|\hat{q}_{\Theta'}(\theta) - q(\theta)\|_1 \right| \leq \|\hat{q}_\Theta(\theta) - \hat{q}_{\Theta'}(\theta)\|_1$$

$$= \frac{\sum_{i=1}^{m} \omega_i k_i}{\sum_{i=1}^{m} \omega_i} - \frac{\sum_{i=1}^{m} \tilde{\omega}_i k_i}{\sum_{i=1}^{m} \tilde{\omega}_i} \leq \frac{\|\sum_{i=1}^{m} \omega_i k_i - \sum_{i=1}^{m} \tilde{\omega}_i k_i\|_1}{\sum_{i=1}^{m} \omega_i} \leq \frac{2B_1 B_2}{m} + \frac{2B_1 B_2}{m} \leq \frac{4B_1 B_2}{m}$$

Invoking the McDiarmid’s inequality, we have

$$\Pr(f(\Theta) - \mathbb{E}_{\Theta}[f(\Theta)] \geq \epsilon) \leq \exp \left\{ - \frac{m \epsilon^2}{8B_1^2 B_2^2} \right\}, \forall \epsilon > 0$$

which implies the corollary.

\section*{D.2 $L_2$-Error Bound of Weighted Kernel Density Estimator}

Following same argument yields also similar $L_2$-error bound of the weighted kernel density estimator, i.e. $\|\hat{q}(\theta) - q(\theta)\|_2$. For completeness and also for future reference, we provide the exact statement of the bound below in line with Theorem 5 and Corollary 15.

\textbf{Theorem 16 (L2-error in expectation)} Let $q = \omega p \in C_b^\beta(\Omega)$ and $K$ be a $(\beta; \mu, \nu)$-valid density kernel. Assume that $\omega^2 p \in L_2$ and has bounded support. Then

$$\mathbb{E} \|\hat{q}(\theta) - q(\theta)\|_2^2 \leq 2(\nu h^d L^2) + \frac{8\mu^2}{mh^d} \|\omega\|_2^2 + o((mh^d)^{-1}).$$
Proof for Theorem 16. The square L₂-error can also be decomposed into three terms.

\[ E \| \hat{q}(\theta) - q(\theta) \|_2^2 \leq 4 E \| \hat{q}(\theta) - \hat{q}_m(\theta) \|_2^2 + 4 E \| \hat{q}_m(\theta) - E q_m(\theta) \|_2^2 + 2 \| E q_m(\theta) - q(\theta) \|_2^2 \]

(normalization error) (sampling error (variance)) (approximation error (bias))

This uses the inequality \((a + b + c)^2 \leq 2a^2 + 4b^2 + 4c^2\) for any \(a, b, c\). From Lemma 12 we already have \(|E[q_m(\theta)] - q(\theta)| \leq L(\theta) \int |K(z)||h_2||^2 dz, \forall \theta\). Hence,

\[ \|E[q_m(\theta)] - q(\theta)\|_2^2 \leq \mu^2 h^2 \beta \int L^2(\theta) d\theta \leq (\nu h^2 \beta L)^2. \tag{12} \]

From proof for Lemma 13 we have

\[ E \| \hat{q}_m(\theta) - E \hat{q}_m(\theta) \|_2^2 = \int E[\hat{q}_m(\theta) - E \hat{q}_m(\theta)]^2 d\theta \leq \int \sigma^2(\theta) d\theta \leq \int \frac{\mu^2}{m^2 h^4} \|\omega \sqrt{p}\|_2^2 + o(m^{-1}) \tag{13} \]

In addition, we have for the normalization error term,

\[ E \| \hat{q}(\theta) - q_m(\theta) \|_2^2 \leq E \| \left(1 - \frac{\sum_{i=1}^m \omega_i}{m}\right) \sum_{i=1}^m \omega_i K_h(\theta,\theta_i) \|_2^2 \tag{15} \]

Combining equation 12, 13 and 15, it follows that

\[ E \| \hat{q}(\theta) - q(\theta) \|_2^2 \leq 2(\nu h^2 L)^2 + \frac{8 \mu^2}{m^2 h^4} \|\omega \sqrt{p}\|_2^2 + o(m^{-1}). \]

\[ \square \]

Corollary 17 \((L₂-error in high probability)\. Besides the above assumption, let us also assume that \(\omega(\theta)\) is bounded, i.e. there exists \(0 < B_1 \leq B_2 < \infty\) such that \(B_1 \leq \omega(\theta) \leq B_2, \forall \theta\). Then, with probability at least \(1 - \delta\),

\[ \| \hat{q}(\theta) - q(\theta) \|_2^2 \leq 2(\nu h^2 L)^2 + \frac{8 \mu^2}{m^2 h^4} \|\omega \sqrt{p}\|_2^2 + o(m^{-1}) \]

\[ \varepsilon \leq \frac{16 B_1 B_2 \mu^2}{m} \sqrt{\log(1/\delta)}. \]

Proof for Theorem 17. Use McDiarmid’s inequality similar as proof for Corollary 15. \[ \square \]

E Convergence Analysis for Density Approximation

In this section, we consider the rate of convergence for the entire density measured by KL-divergence. We start with the following lemmas that show the importance weight \(\omega_t(\theta) = \frac{\exp(-\gamma_t g_t(\theta))}{q_t(\theta)}\) at each step are bounded under proper assumptions. Moreover, the error of the prox-mapping at each step incurred by the weighted density kernel density estimation is bounded.

Lemma 18 Assume for all mini-batch of examples \(\| g_t(\theta) \|_\infty^2 \leq M^2\), then we have

(a) \(\exp(-2\gamma_t M) \leq \omega_t(\theta) = \frac{\hat{q}_t(\theta)}{q_t(\theta)} \leq \exp(2\gamma_t M)\),

(b) \(\| \nabla F_t(\hat{q}_t^+) \|_\infty \leq 3\gamma_t M\).
Proof for Lemma 18. Let $Z := \int q_t(\theta) \exp(-\gamma_t g_t(\theta)) d\theta$. We have $\exp(-\gamma_t M) \leq Z \leq \exp(\gamma_t M)$.

(a) Since $\|g_t(\theta)\|_\infty^2 \leq M^2$, we have

$$\exp(-2\gamma_t M) \leq \omega_t(\theta) = \frac{\tilde{q}_t^+(\theta)}{q_t(\theta)} \leq \exp(2\gamma_t M).$$

(b) Also, because $\nabla F_t(q_t^+) = \gamma_t g_t + \log \frac{\tilde{q}_t^+}{q_t} = \gamma_t g_t + \log(\omega_t)$, it immediately follows

$$\|\nabla F_t(q_t^+)\|_\infty = \|\gamma_t g_t + \log(\omega_t)\|_\infty \leq \gamma_t \|g_t\|_\infty + \|\log(\omega_t)\|_\infty \leq \gamma_t M + (2\gamma_t M) = 3\gamma_t M.$$  

Lemma 19 Let $\epsilon_t := F_t(\tilde{q}_{t+1}^+) - F_t(\tilde{q}_t^+)$, which implies $\tilde{q}_{t+1} \in P^{\epsilon_t}_{\tilde{q}_t}(\gamma_t g_t)$. Assume also that for all $t$, the density function $\tilde{q}_t \in C^2(\Omega)$ have bounded support $\Omega$ and are bounded away from zero by $\Delta^{-1} > 0$. Let the bandwidth at step $t$ satisfies

$$h_t = O(1)m_t^{-1/(d+2\beta)},$$

one can guarantee that

$$\mathbb{E}_\theta[\epsilon_t | x_{[t-1]}, \theta_{[t-1]}] \leq O(1)(\mu^2 + \nu^2 L^2)\Delta m_t^{-\frac{2\beta}{d+2\beta}} + O(1)M(\mu + \nu L)\gamma_t m_t^{-\frac{\beta}{d+2\beta}}$$

In addition, with probability at least $1 - 2\delta$ in $\theta_t | x_{[t-1]}, \theta_{[t-1]}$, we have

$$\epsilon_t \leq O(1)(\mu^2 \sqrt{\log(1/\delta)} + \nu^2 L^2)\Delta m_t^{-\frac{2\beta}{d+2\beta}} + O(1)M(\mu + \nu L + \sqrt{\log(1/\delta)})\gamma_t m_t^{-\frac{\beta}{d+2\beta}}$$

where $O(1)$ is some constant.

Proof for Lemma 19. Invoking the definition of function $F_t(\cdot)$, we have

$$F_t(\tilde{q}_{t+1}^+) - F_t(\tilde{q}_t^+) = KL(\tilde{q}_{t+1}^+ || \tilde{q}_t^+) + \langle \nabla F_t(\tilde{q}_t^+) , \tilde{q}_{t+1}^+ - \tilde{q}_t^+ \rangle_{L^2}$$

$$\leq KL(\tilde{q}_{t+1}^+ || \tilde{q}_t^+) + 3\gamma_t M \| \tilde{q}_{t+1}^+ - \tilde{q}_t^+ \|_1$$

$$\leq \int \frac{(\tilde{q}_{t+1}^+ - \tilde{q}_t^+)^2}{2\tilde{q}_{t+1}^+} d\theta + 3\gamma_t M \| \tilde{q}_{t+1}^+ - \tilde{q}_t^+ \|_1$$

$$\leq \frac{1}{2} \| \tilde{q}_{t+1}^+ - \tilde{q}_t^+ \|_2^2 + 3\gamma_t M \| \tilde{q}_{t+1}^+ - \tilde{q}_t^+ \|_1$$

Applying the result of Theorem 5 and 16 for $\tilde{q}_{t+1}^+$ and $\tilde{q}_t^+$, we have

$$\mathbb{E}_\theta[\epsilon_t | x_{[t-1]}, \theta_{[t-1]}] \leq \frac{\Delta}{2} \left[ (\nu \beta h_t^2 \mathcal{L})^2 + \frac{8\mu^2}{m_t h_t^2} \| \omega_t \sqrt{\tilde{q}_t} \|_2^2 + o((m_t h_t^{-d-1})) \right]$$

$$+ 3\gamma_t M \left[ \nu \mathcal{L} \beta + \frac{\mu}{\sqrt{m_t h_t^{-d-1}}} \| \omega_t \sqrt{\tilde{q}_t} \|_1 + \frac{1}{\sqrt{m_t}} \| \omega_t \sqrt{\tilde{q}_t} \|_2 + o((m_t h_t^{-d-1})) \right]$$

Under the Assumption C, we already proved that $\| \omega_t \|_\infty \leq \exp(2\gamma_t M)$, hence, $\| \omega_t \sqrt{\tilde{q}_t} \|_2^2 \leq \exp(4\gamma_t M)$. Without loss of generality, we can assume $\int \sqrt{\tilde{q}_t(\theta)} d\theta = O(1)$ and $\gamma_t M \leq O(1)$ for all $t$, then we can simply write $\| \omega_t \sqrt{\tilde{q}_t} \|_1 \leq O(1)$ and $\| \omega_t \sqrt{\tilde{q}_t} \|_2^2 \leq O(1)$. When $h_t = O(1)m_t^{-1/(d+2\beta)}$, the above result can be simplified as

$$\mathbb{E}_\theta[\epsilon_t | x_{[t-1]}, \theta_{[t-1]}] \leq O(1)(\mu^2 + \nu^2 L^2)\Delta m_t^{-\frac{2\beta}{d+2\beta}} + O(1)M(\mu + \nu L)\gamma_t m_t^{-\frac{\beta}{d+2\beta}}$$
Similarly, combining the results of Corollary 15 and 17, we have with probability at least $1 - 2\delta$,

$$
\epsilon_t \leq \frac{\Delta}{2} \left[ 2(\nu h^2 L)^2 + \frac{8\mu^2}{m_t h_t^2} \|\omega_t \sqrt{q_t^2} \|_2^2 + o \left( \frac{m_t h_t^d}{m_t} \right) - 1 \right] + \frac{16B_1B_2\mu^2}{m_t} \sqrt{\log(1/\delta)}
+ 3\gamma_t M \left[ \nu L h^2 + \frac{\mu}{\sqrt{m_t h_t^2}} \|\omega_t \sqrt{q_t^2} \|_2 + \frac{1}{\sqrt{m_t}} \sqrt{8B_1B_2 \log(1/\delta) + o \left( \frac{m_t h_t^d}{m_t} \right)^{-\frac{1}{2}}} \right]
$$

which leads to the lemma.

Our main Theorem [7] follows immediately by applying the results in the above lemma to Theorem [3].

Proof of Theorem [7] Given that

$$m_t^{-\beta/(d+2\beta)} = B\gamma_t, \forall t = 1, \ldots, T,$$

invoking the above lemma, we have

$$\mathbb{E}_q[\epsilon_t | x_{[t-1]}, \theta_{[t-1]}] \leq O(1)(\mu^2 + \nu^2 L^2)\Delta B^2 \gamma_t^2 + O(1)(\mu + \nu L)B\gamma_t^2.$$

Expanding the result from Theorem [3], it follows that

$$\mathbb{E}_{x, \theta}[KL(q^* || \hat{q}_{t+1})] \leq (1 - \gamma_t)\mathbb{E}_{x, \theta}[KL(q^* || \hat{q}_t)] + C_1(\mu, \nu, L, \Delta, B)\gamma_t^2$$

where the constant $C_1(\mu, \nu, L, \Delta, B) = O(1)(\mu^2 + \nu^2 L^2)\Delta B^2 \gamma_t^2 + O(1)(\mu + \nu L)B\gamma_t^2 + M^2/2$, which can be further simplified as $O(1)(\mu + \Delta^{1/2} B(\mu + \nu L))^2$. Similarly, we also have

$$\mathbb{E}[KL(q^* || \hat{q}_T)] \leq \frac{M^2}{2} \sum_{t=1}^T \gamma_t^2 + \sum_{t=1}^T C_1(\mu, \nu, L, \Delta, B)\gamma_t^2 + D_1,$$

Based on [17], these will lead to the conclusion.

Remark. The convergence in terms of KL-divergence is measuring the entire density and much more stringent compared to integral approximation. Similar to Lemma [2] with Pinsker’s inequality, we could easily obtain the the rate of convergence in terms of integral approximation from Theorem [7]. After $T$ steps, in general cases, the PMD algorithm converges in terms of integral approximation in rate $O(T^{-1/4})$ by choosing $O(1/\sqrt{T})$-decaying stepsizes and $O(t^{1/2})$-growing samples, and of order $O(1/\sqrt{T})$ by choosing $O(1/t)$-decaying stepsizes and $O(t^{1/2})$-growing samples.

The high probability bound can be therefore derived in similar fashion based on the high probability bound for $\epsilon_t$. We provide the proof for Theorem 20 in below.

Theorem 20 (High probability bound) Under same condition, we have with probability at least $1 - 3\delta$,

$$KL(q^* || \hat{q}_T) \leq \frac{(C_2 \sqrt{\log(T/\delta)} + C_1)\sum_{t=1}^T \gamma_t^2 + D_1}{\sum_{t=1}^T \gamma_t}$$

where $C_2 = C_2(\mu, \Delta, B) = O(1)(\mu^2 B^2 \Delta + BM)$ that depends only linearly on $\Delta$ and $M$.

Proof for Theorem 20 Let us denote $d_t = \nabla L(\hat{q}_t) - g_t$. Revisiting (10) in the proof of Theorem 3, we have

$$\langle \gamma_t \nabla L(\hat{q}_t), \hat{q}_t - q^* \rangle \leq \epsilon_t + KL(q^* || \hat{q}_t) - KL(q^* || \hat{q}_{t+1}) + \frac{\gamma_t^2}{2} \|g_t\|_\infty^2 + \langle \gamma_t d_t, \hat{q}_t - q^* \rangle$$
Summing over $t$ and invoking the convexity, this leads to
\[
\sum_{t=1}^{T} \gamma_t [L(\tilde{q}_t) - L(q^*)] \leq \sum_{t=1}^{T} \epsilon_t + D_1 + \frac{\gamma_t^2}{2} M^2 + \sum_{t=1}^{T} \langle \gamma_t d_t, \tilde{q}_t - q^* \rangle
\]
where $\tilde{q}_t = (\sum_{t=1}^{T} \gamma_t)^{-1} \sum_{t=1}^{T} \gamma_t \tilde{q}_t$ and $D_1 = KL(q^* || \tilde{q}_1)$. By the definition of $d_t$, we have $\mathbb{E}_x[d_t | x_{[t-1]}, \theta_{[t-1]}] = 0$, implying that the sequence $z_t = \langle \gamma_t d_t, \tilde{q}_t - q^* \rangle$ is a sequence of martingale difference. Also, we have $|z_t| \leq \gamma_t \| d_t \|_\infty \cdot \| \tilde{q}_t - q^* \|_1 \leq 4 \gamma_t M$ since $\| d_t \|_\infty \leq \| \mathbb{E}_x[g_t | x_{[t-1]}, \theta_{[t-1]}] \|_\infty + \| g_t \|_\infty \leq 2 M$. By Azuma’s inequality, we have
\[
P_{x,\theta} \left( \sum_{t=1}^{T} z_t \geq \epsilon \right) \leq \exp \left\{ - \frac{\epsilon^2}{32 M^2 \sum_{t=1}^{T} \gamma_t} \right\}, \forall \epsilon > 0
\]
which implies that
\[
P_{x,\theta} \left( \sum_{t=1}^{T} z_t \geq 4 \sqrt{2} M \sum_{t=1}^{T} \gamma_t^2 \sqrt{\log(1/\delta)} \right) \leq \delta, \forall \delta > 0
\]
From lemma [19] and with the choice of $m_t^{-\beta/(d+2\beta)} = B\gamma_t$, we have with probability at least $1 - 2\delta'$ over $\theta, x,$
\[
\epsilon_t \leq O(1)(\mu^2 \sqrt{\log(1/\delta')} + \nu^2 \mathcal{L}^2) B^2 \gamma_t^2 + O(1)M(\mu + \nu \mathcal{L} + \sqrt{\log(1/\delta')}) B \gamma_t^2
\]
which implies
\[
\sum_{t=1}^{T} \epsilon_t \leq O(1)(\mu^2 \sqrt{\log(T/\delta')} + \nu^2 \mathcal{L}^2) B^2 \gamma_t^2 + O(1)M(\mu + \nu \mathcal{L} + \sqrt{\log(T/\delta')}) B \gamma_t^2
\]
with probability at least $1 - 2\delta$. Hence, with probability at least $1 - 3\delta$,
\[
L(\tilde{q}_T) - L(q^*) \leq \frac{(C_2 \sqrt{\log(T/\delta')} + C_1) \sum_{t=1}^{T} \gamma_t^2 + D_1}{\sum_{t=1}^{T} \gamma_t}.
\]
where $C_2 = O(1)(\mu^2 B^2 \Delta + BM)$.

\section{Derivation Details for Sparse Gaussian Processes and Latent Dirichlet Allocation}

We apply the Particle Mirror Descent algorithm to sparse Gaussian processes and latent Dirichlet allocation. For these two models, we decompose the latent variables and incorporate the structure of posterior into the algorithm. The derivation details are presented below.

\subsection{Sparse Gaussian Processes}

Given data $X = \{x_i\}_{i=1}^{n}, \quad x_i \in \mathbb{R}^{d \times 1}$ and $y = \{y_i\}_{i=1}^{n}$. The sparse GP introduce a set of inducing variables, $Z = \{z_i\}_{i=1}^{m}, \quad z_i \in \mathbb{R}^{d \times 1}$ and the model is specified as
\[
p(y_n | u, Z) = \mathcal{N}(y_n | K_{nn}K_{mm}^{-1}u, \tilde{K})
p(u | Z) = \mathcal{N}(u | 0, K_{mm}).
\]
where $K_{mm} = [k(z_i, z_j)]_{i,j=1,...,m}$, $K_{nm} = [k(x_i, z_j)]_{i=1,...,n,j=1,...,m}$. For different $\tilde{K}$, there are different sparse approximations for GPs. Please refer [23] for details. In [20], the authors essentially conduct the
stochastic variational inference on the model with $\tilde{K} = \beta^{-1}I$. For fairness, we also apply our algorithm on the same model. However, it should be noticed that our algorithm could be easily extended to other sparse approximations [25].

We treat the inducing variables as the latent variables with uniform prior in sparse Gaussian processes. Then, the posterior of $Z, u$ could be thought as the solution to the optimization problem

$$
\min_{q(Z, u)} \int q(Z, u) \log \frac{q(Z, u)}{p(Z)p(u)} \, du \, dZ - \sum_{i=1}^{n} \int q(Z, u) \log p(y_i|x_i, u, Z) \, du \, dZ
$$

(16)

The stochastic gradient of Eq. (16) w.r.t. $q(Z, u)$ will be

$$
g(q(Z, u)) = \frac{1}{n} \log q(Z, u) - \frac{1}{n} \log p(Z)p(u) - \log p(y_i|x_i, u, Z)
$$

and therefore, the prox-mapping in $t$-step is

$$
\min_{q(Z, u)} \int q(Z, u) \log \frac{q(Z, u)}{q_t(Z, u)1-\gamma_t/n p(Z, u)^{\gamma_t/n}} \, du \, dZ
$$

which could be re-written as

$$
\int \frac{\log q(Z)}{q_t(Z)^{1-\gamma_t/n} p(Z)^{\gamma_t/n}} - \gamma_t \log p(y_i|x_i, u, Z) \, du \, dZ
$$

$L(q(u|Z))$

We update $q_{t+1}(u|Z)$ to be the optimal of $L(q(u|Z))$ as

$$
q_{t+1}(u|Z) \propto q_t(u|Z)^{1-\gamma_t/n} p(u|Z)^{\gamma_t/n} p(y_i|x_i, u, Z)^{\gamma_t/n}
$$

$$
= \mathcal{N}(u|m_t, \Lambda_t^{-1})^{1-\gamma_t/n} \mathcal{N}(u|0, K_{mm})^{\gamma_t/n} \mathcal{N}(y_i|K_{im}, K_{mm}^{-1} u, \Gamma)^{\gamma_t/n}
$$

$$
= \mathcal{N}(u|m_{t+1}, \Lambda_{t+1}^{-1})
$$

where $\Gamma = \text{diag}(\tilde{K}_{ii} - Q_{ii}) + \beta^{-1}I$, $Q_{ii} = K_{im} K_{mm}^{-1} K_{mi}$,

$$
\Lambda_{t+1} = (1 - \gamma_t/n) \Lambda_t + \gamma_t/n K_{mm}^{-1} + \gamma_t K_{im} K_{mm}^{-1} \Gamma^{-1} K_{mm} K_{mi}
$$

$$
m_{t+1} = \Lambda_{t+1}^{-1} \left( (1 - \gamma_t/n) \Lambda_t^{-1} m_t + \gamma_t/n K_{mm}^{-1} m_0 + \gamma_t K_{mm}^{-1} \Gamma^{-1} y \right)
$$

Plug this into the $L(q(u|Z))$, we have

$$
L(q(u|Z)) = \int q(u|Z) \left[ \log \frac{q(u|Z)}{q_t(u|Z)^{1-\gamma_t/n} p(u|Z)^{\gamma_t/n}} - \gamma_t \log p(y_i|x_i, u, Z) \right] du = -\log \tilde{p}(y_i|x_i, Z)
$$

where

$$
\tilde{p}(y_i|x_i, Z) = \int q_t(u|Z)^{1-\gamma_t/n} p(u|Z)^{\gamma_t/n} p(y_i|x_i, u, Z)^{\gamma_t/n} du
$$

$$
= \mathcal{N}(u|m_t, \Lambda_t^{-1})^{1-\gamma_t/n} \mathcal{N}(u|0, K_{mm})^{\gamma_t/n} \mathcal{N}(y_i|K_{im}, K_{mm}^{-1} u, \Gamma)^{\gamma_t/n} du
$$

$$
= \mathcal{N}(y_i|K_{im} K_{mm}^{-1} c, \Sigma)
$$
where

\[ A_{t+1} = (1 - \gamma_t/n)A_t + \gamma_t/nK_{min}^{-1} \]
\[ c = \bar{A}_{t+1}^{-1}((1 - \gamma_t/n)A_m + \gamma_t/nK_{min}^{-1}m_0) \]
\[ \Sigma = K_{im}K_{mn}^{-1}K_{mn}^{-1}K_{mi} + \frac{1}{\gamma_t} \Gamma \]

Solve

\[ \min_{q(Z)} \int q(Z) \log \frac{q(Z)}{q_t(Z)1-\gamma_t/n} p(Z)\gamma_t/n dZ - \int q(Z) \log \tilde{p}(y_t|x_t, Z) dZ \]

will result the update rule for \( q(Z), \)

\[ q_{t+1}(Z) \propto q_t(Z)^{1-\gamma_t/n} p(Z)\gamma_t/n \tilde{p}(y_t|x_t, Z) \]

We approximate the \( q(Z) \) with particles, i.e., \( q(Z) = \sum_{j=1}^{J} w_j \delta(Z_j) \). The update rule for \( w_j^t \) is

\[ w_j^{t+1} = \frac{w_j^t \exp(-\gamma_t/n \log(w_j^t) + \gamma_t/n \log p(Z_j) + \log \tilde{p}(y_t|x_t, Z_j))}{\sum_{j} w_j^t \exp(-\gamma_t/n \log(w_j^t) + \gamma_t/n \log p(Z_j) + \log \tilde{p}(y_t|x_t, Z_j))} \]

### F.2 Latent Dirichlet Allocations

In LDA, the topics \( \Phi \in \mathbb{R}^{K \times W} \) are \( K \) distributions on the words \( W \) in the text corpora. The text corpora contains \( D \) documents, the length of the \( d \)-th document is \( N_d \). The document is modeled by a mixture of topics, with the mixing proportion \( \theta_d \in \mathbb{R}^{1 \times K} \). The words generating process for \( X_d \) is following: first drawing a topic assignment \( z_{dn} \), which is 1-by-\( K \) indicator vector, i.e. \( \theta_d \) from \( \theta_d \) for word \( x_{dn} \) which is 1-by-\( W \) indicator vector, and then drawing the word \( x_{dn} \) from the corresponding topic \( \Phi_{z_{dn}} \). We denote \( z_d = \{z_{dn}\}_{n=1}^{N_d} \in \mathbb{R}^{N_d \times K}, x_d = \{x_{dn}\}_{n=1}^{N_d} \in \mathbb{R}^{N_d \times W} \) and \( X = \{x_d\}_{d=1}^{D} Z = \{Z_d\}_{d=1}^{D} \). Specifically, the joint probability is

\[ p(x_d, z_d, \theta_d, \Phi) = \prod_{n=1}^{N_d} \prod_{w=1}^{W} \prod_{k=1}^{K} \Phi_{z_{dk}}^{x_{dnw}} \]
\[ p(x_d|z_d, \Phi) = \prod_{n=1}^{N_d} \prod_{w=1}^{W} \prod_{k=1}^{K} \Phi_{z_{dk}}^{x_{dnw}} \]
\[ p(z_d|\theta_d) = \prod_{n=1}^{N_d} \prod_{k=1}^{K} \theta_{z_{nk}}^{\delta_{z_{nk}}} \]

The \( p(\Phi) \) and \( p(\theta) \) are the priors for parameters, \( p(\theta|\alpha) = \frac{\Gamma(K\alpha)}{\Gamma(\alpha)\alpha^K} \prod_{k}^{K} \theta_{\alpha k}^{\alpha-1} \) and \( p(\Phi|\beta_0) = \prod_{k}^{K} \frac{\Gamma(W\beta_k)}{\Gamma(\beta_0)\beta_k^{W\beta_k}} \prod_{w}^{W} \Phi_{w k}^{\beta_0-1} \), both are Dirichlet distributions.

We incorporate the special structure into the proposed algorithm. Instead of modeling the \( p(\Phi) \) solely, we model the \( Z \) \( \{Z_d\}_{d=1}^{D} \) and \( \Phi \) together as \( q(Z, \Phi) \). Based on the model, given \( Z \), the \( q(\Phi|Z) \) will be Dirichlet distribution and could be obtained in closed-form.

The posterior of \( Z, \Phi \) is the solution to

\[ \min_{q(Z, \Phi)} \frac{1}{D} \int q(Z, \Phi) \log \frac{q(Z, \Phi)}{p(Z|\alpha)p(\Phi|\beta)} dZ d\Phi - \frac{1}{D} \sum_{d=1}^{D} \int q(Z, \Phi) \log p(x_d|z_d, \Phi) dZ d\Phi \]

We approximate the finite summation by expectation, then the objective function becomes

\[ \min_{q(Z, \Phi)} \frac{1}{D} \int q(Z, \Phi) \log \frac{q(Z, \Phi)}{p(Z|\alpha)p(\Phi|\beta)} dZ d\Phi - \mathbb{E}_{x} \left[ \int q(Z, \Phi) \log p(x_d|z_d, \Phi) dZ d\Phi \right] \]
We approximate the \( q(Z) \approx \sum_{i=1}^{m} w^i \delta(Z^i) \) by particles, and therefore, \( q(Z, \Phi) \approx \sum_{i=1}^{m} w^i P(\Phi | Z^i) \) where \( P(\Phi | Z^i) \) is the Dirichlet distribution as we discussed. It should be noticed that from the objective function, we do not need to instantiate the \( z_d \) until we visit the \( x_d \). By this property, we could first construct the particles \( \{Z^i\}_{i=1}^{m} \) ‘conceptually’ and assign the value to \( \{z_d\}_{i=1}^{m} \) when we need it. The gradient of Eq. 18 w.r.t. \( q(\Phi, Z) \) is

\[
g(q(Z, \Phi)) = \frac{1}{D} \log q(Z, \Phi) - \frac{1}{D} \log p(\Phi)p(Z) - E_x[\log p(x_d | \Phi, z_d)]
\]

Then, the SGD prox-mapping is

\[
\min_{q(Z, \Phi)} \int q(Z, \Phi) \log \frac{q(Z, \Phi)}{q_t(Z, \Phi)} + \gamma_t \int q(Z, \Phi) \left[ \frac{\log q_t(Z, \Phi)}{D} - \log p(\Phi)p(Z)/D - \log p(x_d | \Phi, z_d) \right] dZ d\Phi
\]

We rearrange the prox-mapping,

\[
\min_{q(Z, \Phi)} \int q(Z) q(\Phi|Z) \log \frac{q(Z) q(\Phi|Z)}{q_t(Z)} \frac{q(Z)}{q_t(Z)^{1-\gamma/D} q_t(\Phi|Z) \gamma/D} - \gamma_t \int q(Z) q(\Phi|Z) \left[ \frac{\log p(\Phi)p(Z)/D + \log p(x_d | \Phi, z_d)}{D} \right] dZ d\Phi
\]

The stochastic functional gradient update for \( q(\Phi|Z^i) \) is

\[
q_{t+1}(\Phi|Z^i) \propto q_t(\Phi|Z^i)^{1-\gamma/D} p(\Phi)^{\gamma/D} p(x_d | \Phi, z_d)^{\gamma/t}
\]

Let \( q_t(\Phi|Z^i) = \text{Dir}(\beta_t^i) \), then, the \( q_{t+1}(\Phi|Z^i) \) is also Dirichlet distribution

\[
q_{t+1}(\Phi|Z^i) \propto \text{Dir}(\beta_t^{i+1}) \text{Dir}(\beta_0)^{\gamma_t} \left( \prod_k \prod_w \Phi_{k,w}^{N_d} \delta(z_{dnk} = 1, x_{dnw} = 1) \right)^{D \gamma_t} = \text{Dir}(\beta_{t+1}^i)
\]

where \( \gamma_t = \gamma_t/D \) and

\[
[\beta_{t+1}^i]_{kw} = (1 - \gamma_t) [\beta_t^i]_{kw} + \gamma_t \beta_0 + D \gamma_t \sum_n \delta(z_{dnk} = 1, x_{dnw} = 1).
\]

In mini-batch setting, the updating will be

\[
[\beta_{t+1}^i]_{kw} = (1 - \gamma_t) [\beta_t^i]_{kw} + \gamma_t \beta_0 + D B \gamma_t \sum_{d=1}^{B} \sum_n \delta(z_{dnk} = 1, x_{dnw} = 1).
\]

Plug the \( q_{t+1}(\Phi|Z^i) \) into prox-mapping, we have

\[
L(q(\Phi|Z)) = \int q(\Phi|Z) \left[ \log \frac{q(\Phi|Z)}{q_t(\Phi|Z)^{1-\gamma/t} p(\Phi)^{\gamma/t}} - D \gamma_t \log p(x_d | \Phi, z_d) \right] d\Phi
\]

\[
= - \log \tilde{p}(x_d | z_d, Z)
\]
where \( \hat{p}(x_d|z_d, Z^i) = \int q_t(\Phi|Z^i)^{-\gamma_t} p(\Phi)^{\gamma_t} p(x_d|\Phi, z_d)^{D\gamma_t} d\Phi \) which have closed-form

\[
\hat{p}(x_d|z_d, Z^i) = \int q_t(\Phi|Z^i)^{-\gamma_t} p(\Phi)^{\gamma_t} p(x_d|\Phi, z_d)^{D\gamma_t} d\Phi \\
= \int \text{Dir}(\beta_t^1)^{-\gamma_t} \text{Dir}(\beta_0) \gamma_t \left( \prod_k \prod_w \Phi_{kw}^{\sum_{d} \delta(z_{dkn} - 1, x_{dnw} - 1)} \right)^{D\gamma_t} d\Phi \\
= \prod_k \left( \Gamma(\sum_w [\beta_t^i]_{kw}) \over \prod_w \Gamma([\beta_t^i]_{kw}) \right)^{-\gamma_t} \left( \Gamma(W \beta_t) \over \Gamma(\beta_0)^W \right) \gamma_t \prod_w \Gamma([\beta_{t+1}^i]_{kw})
\]

and

\[
\log \hat{p}(x_d|z_d, Z^i) \propto \sum_k \left( 1 - \gamma_t \right) \log \Gamma(\sum_w [\beta_t^i]_{kw}) + \sum_w \log \Gamma([\beta_{t+1}^i]_{kw}) \\
\quad - \log \Gamma(\sum_w [\beta_t^i]_{kw}) - (1 - \gamma_t) \sum_w \log \Gamma([\beta_t^i]_{kw})
\]

Then, we could update \( q_t(Z) = \sum_i w^i \delta(Z^i) \) by

\[
q_{t+1}(Z^i) \propto q_t(Z^i) \exp \left( -\frac{\gamma_t}{D} \log q_t(Z^i) + \frac{\gamma_t}{D} \log p(Z^i|\alpha) + \log \hat{p}(x_d|z_d, Z^i) \right)
\]

If we set \( \alpha = 1, p(Z^i) \) will be uniformly distributed which has no effect to the update. For general setting, to compute \( \log p(Z^i|\alpha) \), we need prefix all the \( \{z_{dk}^i\}_{d=1}^D \). However, when \( D \) is huge, the second term will be small and we could ignore it approximately.

Till now, we almost complete the algorithm except the how to assign \( z_d \) when we visit \( x_d \). We could assign the \( z_d \) randomly. However, considering the requirement for the \( z_{dk} \) assignment that the \( q(z_{dk}^i|Z^i_{d-1}) > 0 \), which means the assignment should be consistent, an better way is using the average or sampling proportional to \( \int p(x_d|\Phi, z_d) q_t(\Phi|Z^i) p(z_d|Z^i_{d-1}) d\Phi \) where \( p(z_d|Z^i_{d-1}) = \int p(z_d|\alpha) p(\alpha|Z^i_{d-1}) d\alpha, \) or \( \int p(x_d|\Phi, z_d) q_t(\Phi|Z^i) p(z_d|\alpha) d\Phi \).

**Perplexity Estimation.** We estimate the perplexity following [33]. For a document \( x_d \) in holdout set, the perplexity is computed by

\[
\text{perp}(x_d|X, \alpha, \beta) = \exp \left( -\frac{\sum_{n=1}^{N_d} \log p(x_{dn}|X, \alpha, \beta)}{N_d} \right)
\]

where

\[
p(x_{dn}|X, \alpha, \beta) = E_{\theta_d} q \left[ \theta_d^\top \Phi, x_{dn} \right].
\] (19)

We separate the documents in testing set into two non-overlapped parts, \( x_{d,\text{estimation}} \) and \( x_{d,\text{evaluation}} \). We first evaluate the \( \theta_d \) based on the \( x_{d,\text{estimation}} \). For different inference methods, we use their corresponding strategies in learning algorithm to obtain the distribution of \( \theta_d \) based on \( x_{d,\text{estimation}} \). We evaluate \( p(x_{dn}|X, \alpha, \beta) \) on \( x_{d,\text{evaluation}} \) with the obtained distribution of \( \theta_d \). Specifically,

\[
p(x_{dn}^{\text{evaluation}}|X, \alpha, \beta) = E_{\Phi|X, \beta} E_{\theta_d^{\text{evaluation}}|\Phi, \alpha, x_{d,\text{estimation}}} \left[ \theta_d^\top \Phi, x_{dn} \right]
\]

For PMD, SMC and SGRLD,

\[
\theta_d^{\text{evaluation}} = \sum_{n=1}^{N_{\text{estimation}}} \delta(z_{dnk}^{\text{estimation}} = 1) + \alpha \\
N_{\text{estimation}} + K \alpha
\]

For SVI, \( q(\theta_d) \) is updated as in the learning procedure.