Bayesian Model Averaging with Exponentiated Least Square Loss

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Abstract

The model averaging problem is to average multiple models to achieve a prediction accuracy not much worse than that of the best single model in terms of mean squared error. It is known that if the models are misspecified, model averaging is superior to model selection. Specifically, let $n$ be the sample size, then the worst case regret of the former decays at a rate of $O(1/n)$ while the worst case regret of the latter decays at a rate of $O(1/\sqrt{n})$. The recently proposed $Q$-aggregation algorithm (Dai et al., 2012) solves the model averaging problem with the optimal regret of $O(1/n)$ both in expectation and in deviation; however it suffers from two limitations: (1) for continuous dictionary, the proposed greedy algorithm for solving $Q$-aggregation is not applicable; (2) the formulation of $Q$-aggregation appears ad hoc without clear intuition. This paper examines a different approach to model averaging by considering a Bayes estimator for deviation optimal model averaging by using exponentiated least squares loss. We establish a primal-dual relationship of this estimator and that of $Q$-aggregation and propose new computational procedures that satisfactorily resolve the above mentioned limitations of $Q$-aggregation.

1 Introduction

This paper considers the model averaging problem, where the goal is to average multiple models in order to achieve improved prediction accuracy.

Let $x_1, \ldots, x_n$ be $n$ given design points in a space $X$, let $\mathcal{H} = \{f_1, \ldots, f_M\}$ be a given dictionary of real valued functions on $X$ and denote $f_j = (f_j(x_1), \ldots, f_j(x_n))^\top \in \mathbb{R}^n$ for each $j$. The goal is to estimate an unknown regression function $\eta : X \to \mathbb{R}$ at the design points based on observations

$$y_i = \eta(x_i) + \xi_i,$$

where $\xi_1, \ldots, \xi_n$ are i.i.d $\mathcal{N}(0, \sigma^2)$.

The performance of an estimator $\hat{\eta}$ is measured by its mean squared error (MSE) defined by

$$\text{MSE}(\hat{\eta}) = \frac{1}{n} \sum_{i=1}^{n} (\hat{\eta}(x_i) - \eta(x_i))^2.$$

We want to find an estimator $\hat{\eta}$ that mimics the function in the dictionary with the smallest MSE. Formally, a good estimator $\hat{\eta}$ should satisfy the following exact oracle inequality in a certain probabilistic sense:

$$\text{MSE}(\hat{\eta}) \leq \min_{j=1, \ldots, M} \text{MSE}(f_j) + \Delta(n, M, \sigma^2), \quad (1)$$

where the remainder term $\Delta > 0$ should be as small as possible.
The problem of model averaging has been well-studied, and it is known (see, e.g., Tsybakov, 2003; Rigollet, 2012) that the smallest possible order for $\Delta(n, M, \sigma^2)$ is $\sigma^2 \log M/n$ for oracle inequalities in expectation, where “smallest possible” is understood in the following minimax sense. There exists a dictionary $\mathcal{H} = \{f_1, \ldots, f_M\}$ such that the following lower bound holds. For any estimator $\hat{\eta}$, there exists a regression function $\eta$ such that

$$\mathbb{E} \text{MSE}(\hat{\eta}) \geq \min_{j=1,\ldots,M} \text{MSE}(f_j) + C\sigma^2 \log M/n$$

for some positive constant $C$. It also implies that the lower bound holds not only in expectation but also with positive probability.

Although our goal is to achieve an MSE as close as that of the best model in $\mathcal{H}$, it is known (see Rigollet and Tsybakov, 2012, Theorem 2.1) that there exists a dictionary $\mathcal{H}$ such that any estimator $\hat{\eta}$ taking values restricted to the elements of $\mathcal{H}$ (such an estimator is referred to as a model selection estimator) cannot achieve an oracle inequality of form (1) with a remainder term of order smaller than $\sigma\sqrt{\log M}/n$; in other words, model selection is suboptimal for the purpose of competing with the best single model from a given family.

Instead of model selection, we can employ model averaging to derive oracle inequalities of form (1) that achieves the optimal regret in expectation (see the references in Rigollet and Tsybakov, 2012). More recently, several work has produced optimal oracle inequalities for model averaging that not only hold in expectation but also in deviation (Audibert, 2008; Lecué and Mendelson, 2009; Gaïffas and Lecué, 2011; Rigollet, 2012; Dai et al., 2012). In particular, the current work is closely related to the $Q$-aggregation estimator investigated in (Dai et al., 2012) which solves the optimal model averaging problem both in expectation and in deviation with a remainder term $\Delta(n, M, \sigma^2)$ of order $O(1/n)$; the authors also proposed a greedy algorithm GMA-0 for $Q$-aggregation which improves the Greedy Model Averaging (GMA) algorithm firstly proposed by Dai and Zhang (2011). Yet there are still two limitations of $Q$-aggregation: (1) $Q$-aggregation can be generalized for continuous candidates dictionary $\mathcal{H}$, but the greedy model averaging method GMA-0 can not be applied in such setting; (2) $Q$-aggregation can be regarded intuitively as regression with variance penalty, but it lacks a good decision theoretical interpretation.

In this paper we introduce a novel method called Bayesian Model Averaging with Exponentiated Least Squares Loss (BMAX). We note that the previously studied exponential weighted model aggregation estimator EWMA (e.g. Rigollet and Tsybakov, 2012) is the Bayes estimator under the least squares loss (posterior mean), which leads to optimal regret in expectation but is suboptimal in deviation. In contrast, the new BMAX model averaging estimator is essentially a Bayes estimator under an appropriately defined exponentiated least squares loss, which as we will show in this paper, naturally leads to optimal regret in deviation. Computationally, the new model aggregation method BMAX can be approximately solved by a greedy algorithm and by a gradient descent algorithm that are applicable to continuous candidates dictionary. Moreover, we will show that the $Q$-aggregation formulation (with KL entropy) in Dai et al. (2012) is essentially a dual representation of the newly introduced BMAX formulation. In summary, this paper establishes a natural Bayesian interpretation of $Q$-aggregation, and provides additional computational procedures that are applicable for the continuous dictionary setting. This relationship provides deeper understanding for modeling averaging procedures, and resolves the above mentioned limitations of the $Q$-aggregation scheme.
2 Notations

This section introduces some notations used in this paper. In the following, we denote by $Y = (y_1, \ldots, y_n)^\top$ the observation vector, $\eta = (\eta(x_1), \ldots, \eta(x_n))^\top$ the model output, and $\xi = (\xi_1, \ldots, \xi_n)^\top$ the noise vector. The underlying statistical model can be expressed as

$$Y = \eta + \xi,$$

with $\xi \sim N(0, \sigma^2 I_n)$. We also denote $\ell_2$ norm as $\|Y\|_2 = (\sum_{i=1}^n y_i^2)^{1/2}$, and the inner product as $\langle \xi, f \rangle_2 = \xi^\top f$.

Let $\Lambda^M$ be the flat simplex in $\mathbb{R}^M$ defined by

$$\Lambda^M = \left\{ \lambda = (\lambda_1, \ldots, \lambda_M)^\top \in \mathbb{R}^M : \lambda_j \geq 0, \sum_{j=1}^M \lambda_j = 1 \right\},$$

and $\pi = (\pi_1, \ldots, \pi_M)^\top \in \Lambda^M$ be a given prior.

Each $\lambda \in \Lambda^M$ yields a model averaging estimator as $f_\lambda = \sum_{j=1}^M \lambda_j f_j$; that is, using the vector notation $f_\lambda = (f_\lambda(x_1), \ldots, f_\lambda(x_n))^\top$ we have $f_\lambda = \sum_{j=1}^M \lambda_j f_j$.

The Kullback-Leibler divergence for $\lambda, \pi \in \Lambda^M$ is defined as

$$K(\lambda, \pi) = \sum_{j=1}^M \lambda_j \log(\lambda_j/\pi_j),$$

and in the definition we use the convention $0 \cdot \log(0) = 0$.

3 Deviation Optimal Bayesian Model Averaging Estimator

The traditional Bayesian model averaging estimator is the exponential weighted model averaging estimator EWMA [[Rigollet and Tsybakov, 2012]], which optimizes the least squares loss. Although the estimator is optimal in expectation, it is suboptimal in deviation [[Dai et al., 2012]]. In this section we introduce a different Bayesian model averaging estimator called BMAX that optimizes an exponentiated least squares loss, and we prove that it is not only optimal in expectation, but also optimal in deviation.

In order to introduce the BMAX estimator, we consider the following Bayesian framework, where we note that the assumptions below are only used to derive BMAX, and these assumptions are not used in our theoretical analysis. $Y$ is a normally distributed observation vector with mean $\mu = (\mu_1, \ldots, \mu_M)^\top$ and covariance matrix $\omega^2 I_n$:

$$Y|\mu \sim N(\mu, \omega^2 I_n),$$

and for $j = 1, \ldots, M$, the prior for each model $f_j$ is

$$\pi(\mu = f_j) = \pi_j.$$

In this setting, the posterior distribution of $\mu$ given $Y$ is

$$p(\mu = f_j|Y) = \frac{p(Y|\mu = f_j)p(\mu = f_j)}{\sum_{j=1}^M p(Y|\mu = f_j)p(\mu = f_j)} = \frac{\exp\left(-\frac{\|f_j - Y\|_2^2}{2\omega^2}\right) \pi_j}{\sum_{j=1}^M \exp\left(-\frac{\|f_j - Y\|_2^2}{2\omega^2}\right) \pi_j}.$$
In the Bayesian decision theoretical framework considered in this paper, the quantity of interest is \( \eta = \mathbb{E} Y \), and we consider a loss function \( L(\psi, \mu) \) which we would like to minimize with respect to the posterior distribution. The corresponding Bayes estimator \( \hat{\psi} \) minimizes the posterior expected loss from \( \mu \) as follows:

\[
\hat{\psi} = \arg\min_{\psi \in \mathbb{R}^n} \mathbb{E} [L(\psi, \mu)|Y].
\] (5)

It is worth pointing out that the above Bayesian framework is only used to obtain decision theoretically motivated model averaging estimators (as such estimators have good theoretical properties such as admissibility, etc). In particularly we do not assume that the model itself is correctly specified. That is, in this paper we allow misspecified models, where the parameters \( \mu \) and \( \omega^2 \) are not necessarily equal to the true mean \( \eta \) and the true variance \( \sigma^2 \) in (2), and \( \eta \) does not necessarily belong to the dictionary \( \{f_1, \ldots, f_M\} \).

The Bayesian estimator of (5) depends on the underlying loss function \( L(\cdot, \cdot) \). For example, under the standard least squares loss \( L(\psi, \mu) = \|\psi - \mu\|_2^2 \), the Bayes estimator is the posterior mean, which leads to the Exponential Weighted Model Aggregation (EWMA) estimator (Rigollet and Tsybakov, 2012):

\[
\psi_{\ell_2}(\omega^2) = \frac{\sum_{j=1}^{M} \exp \left( -\frac{\|f_j - Y\|_2^2}{2\omega^2} \right) \pi_j f_j}{\sum_{j=1}^{M} \exp \left( -\frac{\|f_j - Y\|_2^2}{2\omega^2} \right) \pi_j}.
\] (6)

This estimator is optimal in expectation (Dalalyan and Tsybakov, 2007, 2008), but suboptimal in deviation (Dai et al., 2012).

In this paper, we introduce the following exponentiated least squares loss motivated from the exponential moment technique for proving large deviation tail bounds for sums of random variables:

\[
L(\psi, \mu) = \exp \left( \frac{1 - \nu^2}{2\omega^2} \|\psi - \mu\|_2^2 \right),
\] (7)

where the parameter \( \nu \in (0, 1) \). It is easy to verify that the Bayes estimator defined by (5) with the loss function defined in (7) can be written as

\[
\psi_X(\omega^2, \nu) = \arg\min_{\psi \in \mathbb{R}^n} J(\psi),
\] (8)

where

\[
J(\psi) = \sum_{j=1}^{M} \pi_j \exp \left( -\frac{1}{2\omega^2} \|f_j - Y\|_2^2 + \frac{1 - \nu}{2\omega^2} \|\psi - f_j\|_2^2 \right).
\] (9)

The estimator \( \psi_X(\omega^2, \nu) \) will be referred to as the Bayesian model aggregation estimator with exponentiated least squares loss (BMAX).

Our main theoretical result concerning this estimator is given by the following theorem, which shows that \( \psi_X(\omega^2, \nu) \) is optimal both in expectation and in deviation when models are misspecified.

**Theorem 1.** Assume that \( \nu \in (0, 1) \) and \( \omega^2 \geq \frac{\sigma^2}{\min(\nu, 1 - \nu)} \). For any \( \lambda \in \Lambda^M \), the following oracle inequality holds

\[
\|\psi_X(\omega^2, \nu) - \eta\|_2^2 \leq \nu \sum_{j=1}^{M} \lambda_j \|f_j - \eta\|_2^2 + (1 - \nu) \|f_\lambda - \eta\|_2^2 + 2\omega^2 K(\lambda, \pi \delta),
\] (10)
with probability at least \(1 - \delta\). Moreover,

\[
\mathbb{E}\|\psi_X(\omega^2, \nu) - \eta\|_2^2 \leq \nu \sum_{j=1}^{M} \lambda_j \|f_j - \eta\|_2^2 + (1 - \nu) \|f_\lambda - \eta\|_2^2 + 2\omega^2 K(\lambda, \pi) .
\]

Since \(\nu \sum_{j=1}^{M} \lambda_j \|f_j - \eta\|_2^2 = \nu \sum_{j=1}^{M} \lambda_j \|f_j - f_\lambda\|_2^2 + \nu \|f_\lambda - \eta\|_2^2\), our theorem implies that \(\psi_X(\omega^2, \nu)\) can compete with an arbitrary \(f_\lambda\) in the convex hull with \(\lambda \in \Lambda^M\) as long as the variance term \(\nu \sum_{j=1}^{M} \lambda_j \|f_j - f_\lambda\|_2^2\) and the divergence term \(K(\lambda, \pi)\) are small.

Although for notation simplicity, the result is stated for finite dictionary \(\mathcal{H}\), the analysis of the paper directly applies to infinite dictionaries where \(M = \infty\) as well as continuous dictionaries. For example, given a matrix \(X \in \mathbb{R}^{n \times d}\), we may consider a continuous dictionary indexed by vector \(w\) as \(\mathcal{H} = \{f_w \in \mathbb{R}^n : f_w = Xw \quad (w \in \mathbb{R}^d ; \|w\|_2 \leq 1)\}\). We may consider the uniform prior \(\pi\) on \(w\), and the theorem is well-defined as long as a distribution \(\lambda\) on \(w \in \mathbb{R}^d\) is concentrated around a single model (so that the variance term corresponding to \(\int \lambda_w \|f_w - f_\lambda\|_2^2 dw\) is small) with finite KL divergence with respect to \(\pi\). For example, \(\lambda\) can be chosen as the uniform distribution on a small ball \(\{w : \|w - w_0\|_2 \leq r\}\). In such case, \(f_\lambda = f_{w_0}\) and the variance term is small when \(r\) is small. Theorem 1 can be applied to derive an oracle inequality that competes with any single model \(f_{w_0}\).

In the case that \(M\) is finite, we can more directly obtain an oracle inequality that competes with the best single model, which is the situation that \(\lambda\) is at a vertex of the simplex \(\Lambda^M\). With \(\nu \in (0, 1)\), the theorem implies that \(\psi_X(\omega^2, \nu)\) is deviation optimal, which is explicitly stated in the following corollary.

**Corollary 1.** Under the assumptions of Theorem 1, \(\psi_X(\omega^2, \nu)\) satisfies

\[
\|\psi_X(\omega^2, \nu) - \eta\|_2^2 \leq \min_{j=1, \ldots, M} \left\{ \|f_j - \eta\|_2^2 + 2\omega^2 \log \left( \frac{1}{\pi_j \delta} \right) \right\} ,
\]

with probability at least \(1 - \delta\). Moreover,

\[
\mathbb{E}\|\psi_X(\omega^2, \nu) - \eta\|_2^2 \leq \min_{j=1, \ldots, M} \left\{ \|f_j - \eta\|_2^2 + 2\omega^2 \log \left( \frac{1}{\pi_j} \right) \right\} .
\]

It is also worth pointing out that the condition \(\omega^2 \geq \frac{\sigma^2}{\min(\nu, 1-\nu)}\) implies that \(\omega^2\) is at least greater than \(2\sigma^2\) (when \(\nu = 1/2\)), and intuitively this inflation of noise allows the Bayes estimator to handle misspecification of the true mean \(\eta\), which is not necessarily included in the candidate dictionary \(\mathcal{H}\).

Finally we note that in the Bayesian framework stated in this section, when we change the underlying loss function \(L(\psi, \mu)\) from the standard least squares loss to the exponentiated least squares loss \(\mathcal{L}\), Bayes estimator changes from EWMA which is optimal only in expectation to BMAX which is optimal both in expectation and in deviation. The difference is that the least squares loss only controls the bias, while the exponentiated least squares loss controls both bias and variance (as well as high order moments) simultaneously. This can be seen by using Taylor expansion

\[
\exp \left( \frac{1 - \nu}{2\omega^2} \|\psi - \mu\|_2^2 \right) = 1 + \frac{1 - \nu}{2\omega^2} \|\psi - \mu\|_2^2 + (1/2) \left( \frac{1 - \nu}{2\omega^2} \|\psi - \mu\|_2^2 \right)^2 + \cdots .
\]

Since deviation bounds require us to control high order moments, the exponentiated least squares loss is naturally suited for obtaining deviation bounds.
4 Numerical Algorithms for BMAX

We have introduced and analyzed the BMAX estimator $\psi_X(\omega^2, \nu)$, which is optimal both in expectation and in deviation for the model averaging problem. In this section, we provide two numerical algorithms to approximate the minimizer $\psi_X(\omega^2, \nu)$ of $\log J(\psi)$. The first algorithm is referred to as Greedy Model Averaging (GMA-BMAX), and the second algorithm is referred to as Gradient Descent (GD-BMAX). The convergence rates of both algorithms will be established. Specifically, denote by $k$ as the number of iterations in the algorithms, GMA-BMAX algorithm has a converge rate of $O(1/k^2)$, and GD-BMAX algorithm converges with a geometric rate of $O(q^k)$ for some $q \in (0, 1)$. Oracle inequalities will be obtained for both methods using the approximate solutions obtained after running the algorithms for $k$-steps.

In the following, we assume that the $\ell_2$-norm of every $f_j$ is bounded by a constant $L \in \mathbb{R}$:

$$\|f_j\|_2 \leq L, \quad \forall j = 1, \ldots, M.$$  \hspace{1cm} (14)

Given $\nu \in (0, 1)$ and $\omega > 0$, and $L$ in (14), we define

$$A_1 = \frac{1 - \nu}{\omega^2},$$  \hspace{1cm} (15)

$$A_2 = \frac{1 - \nu}{\omega^2} + \left(\frac{1 - \nu}{\omega^2}\right)^2 L^2,$$  \hspace{1cm} (16)

$$D = \left(\frac{1 - \nu}{\omega^2}\right) L^2 + \left(\frac{1 - \nu}{\omega^2}\right)^2 L^4.$$  \hspace{1cm} (17)

Using the above notations, we establish Lemma 1 below that shows the smoothness and strong convexity of $\log J(\psi)$. Smoothness and strong convexity are important quantities for analyzing convergence rates of numerical procedures (e.g., Boyd and Vandenberghe, 2004, Section 9.1.2).

Lemma 1. For any $\psi \in \mathbb{R}^n$, define the Hessian matrix of $\log J(\psi)$ as $\nabla^2 \log J(\psi) = \frac{\partial^2 \log J(\psi)}{\partial \psi \partial \psi^\top}$, then we have

$$\nabla^2 \log J(\psi) \geq A_1 I_n.$$  \hspace{1cm} (18)

If $\{f_1, \ldots, f_M\}$ satisfies condition (14), then

$$\nabla^2 \log J(\psi) \leq A_2 I_n,$$  \hspace{1cm} (19)

where $A_1$ and $A_2$ are defined in (15) and (16).

Strong convexity of $\log J(\psi)$ directly implies that the minimizer $\psi_X(\omega^2, \nu)$ is unique. Moreover, it implies the following result which means that an estimator that approximately minimizes $\log J(\psi)$ satisfies an oracle inequality slightly worse than that of $\psi_X(\omega^2, \nu)$ in Theorem 1. This result suggests that we can employ appropriate numerical procedures to approximately solve (8), and Theorem 1 implies an oracle inequality for such approximate solutions.

Proposition 1. Let $\hat{\psi}$ be an $\epsilon$-approximate minimizer of $\log J(\psi)$ for some $\epsilon > 0$:

$$\log J(\hat{\psi}) \leq \min_{\psi} \log J(\psi) + \epsilon.$$  

Then we have

$$\|\hat{\psi} - \eta\|_2^2 \leq \|\psi_X(\omega^2, \nu) - \eta\|_2^2 + 2\sqrt{2\epsilon/A_1}\|\psi_X(\omega^2, \nu) - \eta\|_2 + \frac{2\epsilon}{A_1}.$$  

6
Proof. The strong convexity of $\log J(\cdot)$ in (18) implies that

$$\|\psi - \psi X(\omega^2, \nu)\|_2^2 \leq \frac{2}{A_1} \left( \log J(\psi) - \log J(\psi X(\omega^2, \nu)) \right) \leq 2\epsilon/A_1.$$  

Now plug the above inequality to the following equation

$$\|\psi - \eta\|_2^2 = \|\psi X(\omega^2, \nu) - \eta\|_2^2 + 2\|\psi - \psi X(\omega^2, \nu)\|_2 \|\psi X(\omega^2, \nu) - \eta\|_2 + \|\psi - \psi X(\omega^2, \nu)\|_2^2,$$

we obtain the desired bound. \qed

4.1 Greedy Model Averaging Algorithm (GMA-BMAX)

The GMA-BMAX algorithm given in Algorithm 1 is a greedy algorithm that adds at most one function from the dictionary $\mathcal{H}$ at each iteration. This feature is attractive as it outputs a $k$-sparse solution that depends on at most $k$ functions from the dictionary after $k$ iterations. Similar algorithms for model averaging have appeared in Dai and Zhang (2011) and Dai et al. (2012).

**Algorithm 1** Greedy Model Averaging Algorithm (GMA-BMAX)

**Input:** Noisy observation $Y$, dictionary $\mathcal{H} = \{f_1, \ldots, f_M\}$, prior $\pi \in \Lambda^M$, parameters $\nu, \omega$.

**Output:** Aggregate estimator $\psi^{(k)}$.

Let $\psi^{(0)} = 0$.

for $k = 1, 2, \ldots$ do

Set $\alpha_k = \frac{2}{k+1}$

$J^{(k)} = \arg\min_j \log J(\psi^{(k-1)} + \alpha_k(f_j - \psi^{(k-1)}))$

$\psi^{(k)} = \psi^{(k-1)} + \alpha_k(f_j^{(k)} - \psi^{(k-1)})$

end for

The following proposition follows from the standard analysis in Frank and Wolfe (1956); Jones (1992); Barron (1993). It shows that the estimator $\psi^{(k)}$ from Algorithm 1 converges to $\psi X(\omega^2, \nu)$.

**Proposition 2.** For $\psi^{(k)}$ as defined in Algorithm 1 (GMA-BMAX), if $\{f_1, \ldots, f_M\}$ satisfies condition (14), then

$$\log J(\psi^{(k)}) \leq \log J(\psi X(\omega^2, \nu)) + \frac{8D}{k+3}.$$  

Proposition 2 states that, after running Algorithm GMA-BMAX for $k$ steps to obtain $\psi^{(k)}$, the corresponding objective value $\log J(\psi^{(k)})$ converges to the optimal objective value $\log J(\psi X(\omega^2, \nu))$ at a rate $O(1/k)$. Combine this result with Proposition 1 we obtain the following oracle inequality, which shows that the regret of the estimator $\psi^{(k)}$ after running $k$ steps of GMA-BMAX converges to that of $\psi X(\omega^2, \nu)$ in Theorem 1 at a rate $O(1/\sqrt{k})$.

**Theorem 2.** Assume $\nu \in (0, 1)$ and $\omega^2 \geq \frac{\sigma^2}{\min(\nu, 1-\nu)}$. Consider $\psi^{(k)}$ as in Algorithm 1 (GMA-BMAX). For any $\lambda \in \Lambda^M$, the following oracle inequality holds

$$\|\psi^{(k)} - \eta\|_2^2 \leq \nu \sum_{j=1}^M \lambda_j \|f_j - \eta\|_2^2 + (1 - \nu) \|f_\lambda - \eta\|_2^2 + 2\omega^2 \mathcal{K}(\lambda, \pi \delta)$$

$$+ 2 \sqrt{\frac{16D}{A_1(k+3)}} \|\psi X(\omega^2, \nu) - \eta\|_2 + \frac{16D}{A_1(k+3)}.$$  

7
with probability at least $1 - \delta$. Moreover,

$$
\mathbb{E}\|\psi^{(k)} - \eta\|^2_2 \leq \nu \sum_{j=1}^{M} \lambda_j \|f_j - \eta\|^2_2 + (1 - \nu) \|f_\lambda - \eta\|^2 + 2\omega^2 K(\lambda, \pi)
$$

$$
+ 2\sqrt{\frac{16D}{A_1(k + 3)}} \mathbb{E}\|\psi_X(\omega^2, \nu) - \eta\|_2 + \frac{16D}{A_1(k + 3)}.
$$

(22)

From Theorem 2, if $\omega^2 \geq \frac{\sigma^2_{\min(\nu, 1 - \nu)}}{\min(\nu, 1 - \nu)}$, for any $j = 1, \ldots, M$ we have

$$
\text{MSE}(\psi^{(k)}) \leq \text{MSE}(f_j) + 2\omega^2 \log \left(\frac{1}{\pi_j^\delta}\right) + O(1/\sqrt{k})
$$

with probability at least $1 - \delta$, and

$$
\mathbb{E}\text{MSE}(\psi^{(k)}) \leq \text{MSE}(f_j) + 2\omega^2 \log \left(\frac{1}{\pi_j^\delta}\right) + O(1/\sqrt{k}).
$$

When $k \to \infty$, $\psi^{(k)}$ achieves the optimal deviation bound. However, it does not imply optimal deviation bound for $\psi^{(k)}$ with small $k$, while the greedy algorithms described in [Dai and Zhang (2011)] (GMA) and [Dai et al. (2012)] (GMA-0 and GMA-0+) achieve optimal deviation bounds for small $k$ when $k \geq 2$. The advantage of GMA-BMAX is that the resulting estimator $\psi^{(k)}$ competes with any $f_\lambda$ with $\lambda \in \Lambda^M$ under the KL entropy, and such a result can be applied even for infinite dictionaries containing functions indexed by continuous parameters, as long as the KL divergence $K(\lambda, \pi)$ is well-defined (see relevant discussions in Section 3). On the other hand, the greedy estimators of [Dai et al. (2012)] for the $Q$-aggregation scheme can only deal with an upper bound of KL divergence referred to as linear entropy (see Section 5) that is not well-defined for continuous dictionaries. This means that GMA-BMAX is more generally applicable than the corresponding greedy procedures in [Dai et al. (2012)].

4.2 Gradient Descent Algorithm (GD-BMAX)

We may also employ gradient descent to approximate the BMAX estimator $\psi_X(\omega^2, \nu)$, and the resulting algorithm is referred to as GD-BMAX in Algorithm 2.

To derive the gradient descent formula, we note that

$$
\nabla \log J(\psi^{(k-1)}) = \nabla J(\psi^{(k-1)}) \frac{1 - \nu}{\omega^2} (\psi^{(k-1)} - f_{\lambda^{(k-1)}}),
$$

where $\lambda^{(k-1)} \in \Lambda^M$ is defined as (23); this implies that the $k$-th step update in Algorithm 2 can be written as

$$
\psi^{(k)} = (1 - t_k \frac{1 - \nu}{\omega^2}) \psi^{(k-1)} + t_k \frac{1 - \nu}{\omega^2} f_{\lambda^{(k-1)}} = \psi^{(k-1)} - t_k \nabla \log J(\psi^{(k-1)}).
$$

Therefore Algorithm 2 is essentially the standard gradient decent algorithm for minimizing $\log J(\psi)$ with step size $t_k$. 

8
Algorithm 2 Gradient Descent Algorithm (GD-BMAX)

Input: Noisy observation $Y$, dictionary $H = \{f_1, \ldots, f_M\}$, prior $\pi \in \Lambda^M$, parameters $\nu, \omega^2$.

Output: Aggregate estimator $\psi(k)$.

Let $\psi^{(0)} = 0$.

for $k = 1, 2, \ldots$ do

Choose fixed step size $t_k = s \in (0, 2/A_2)$ for $k > 0$.

$$f^{(k-1)}_\lambda = \sum_{j=1}^{M} \lambda^{(k-1)}_j f_j$$

where $\lambda^{(k-1)} \in \Lambda^M$ and

$$\lambda^{(k-1)}_j \propto \pi_j \exp \left( -\frac{1}{2\omega^2} \|f_j - Y\|^2 + \frac{1 - \nu}{2\omega^2} \|\psi^{(k-1)} - f_j\|^2 \right)$$ (23)

and $f^{(k-1)}_\lambda$ can be approximated by Algorithm 3 when $M$ is large.

$$\psi^{(k)} = (1 - t_k \frac{1 - \nu}{\omega^2}) \psi^{(k-1)} + t_k \frac{1 - \nu}{\omega^2} f^{(k-1)}$$

end for

Proposition 3. For $\psi^{(k)}$ as defined in Algorithm 2 and choose fixed step size $t_k = s \in (0, 2/A_2)$ for $k > 0$, if $\{f_1, \ldots, f_M\}$ satisfies condition (14), then

$$\log J(\psi^{(k)}) - \log J(\psi_X(\omega^2, \nu)) \leq [1 - 2A_1(s - (A_2/2)s^2)]^k \frac{A_1}{2} L^2.$$ 

Remark 1. For the step size $t_k$, we may choose $t_k = s = 1/A_2$ to minimize the right hand side of (24); it follows that with this choice, we have the following convergence rate

$$\log J(\psi^{(k)}) - \log J(\psi_X(\omega^2, \nu)) \leq (1 - A_1/A_2)^k \frac{A_1}{2} L^2.$$ 

Remark 2. The convergence rate can be improved using accelerated gradient methods (see, e.g., Poljak, 1987; Nesterov and Nesterov, 2004).

Proposition 3 states that after running $k$ steps of GD-BMAX, it produces an estimator $\psi^{(k)}$ so that the objective value $\log J(\psi^{(k)})$ converges geometrically to the optimal value of $\log J(\psi_X(\omega^2, \nu))$. This result together with Proposition 4 imply the following oracle inequalities showing that the regret of the estimator $\psi^{(k)}$ after running $k$ steps of GD-BMAX converges to that of $\psi_X(\omega^2, \nu)$ in Theorem 1 at a geometric rate.

Theorem 3. Assume $\nu \in (0, 1)$ and if $\omega^2 \geq \frac{\sigma^2}{\min(\nu, 1 - \nu)}$. Consider $\psi^{(k)}$ as in Algorithm 2 (GD-
BMXAX). For any $\lambda \in \Lambda^M$, the following oracle inequality holds

$$
\|\psi^{(k)} - \eta\|_2^2 \leq \nu \sum_{j=1}^{M} \lambda_j \|f_j - \eta\|_2^2 + (1 - \nu) \|f_{\lambda} - \eta\|_2^2 + 2\omega^2 \mathcal{K}(\lambda, \pi) + 2\omega^2 \log(1/\delta)
$$

$$
+ 2\sqrt{L^2[1 - 2A_1(s - (A_2/2)s^2)]^k} \|\psi_X(\omega^2, \nu) - \eta\|_2
$$

$$
+ L^2[1 - 2A_1(s - (A_2/2)s^2)]^k
$$

with probability at least $1 - \delta$. Moreover,

$$
\mathbb{E}\|\psi^{(k)} - \eta\|_2^2 \leq \nu \sum_{j=1}^{M} \lambda_j \|f_j - \eta\|_2^2 + (1 - \nu) \|f_{\lambda} - \eta\|_2^2 + 2\omega^2 \mathcal{K}(\lambda, \pi)
$$

$$
+ 2\sqrt{L^2[1 - 2A_1(s - (A_2/2)s^2)]^k} \mathbb{E}\|\psi_X(\omega^2, \nu) - \eta\|_2
$$

$$
+ L^2[1 - 2A_1(s - (A_2/2)s^2)]^k.
$$

(24)

From Theorem 3 if $\omega^2 \geq \frac{s^2}{\min(\nu, 1 - \nu)}$, for any $j = 1, \ldots, M$ we have

$$
\text{MSE}(\psi^{(k)}) \leq \text{MSE}(f_j) + 2\omega^2 \log \left( \frac{1}{\pi_j \delta} \right) + O(q^k),
$$

with probability at least $1 - \delta$ and

$$
\mathbb{E}\text{MSE}(\psi^{(k)}) \leq \text{MSE}(f_j) + 2\omega^2 \log \left( \frac{1}{\pi_j} \right) + O(q^k),
$$

for some constant $q \in (0, 1)$.

Although the GD-BMAX algorithm does not produce a sparse output as GMA-BMAX algorithm does, it has a faster geometric convergence rate than the $O(1/k)$ rate of GMA-BMAX. When $M$ is large, it is not practical to directly calculate $f_{\lambda^{(k-1)}} \in \mathbb{R}^n$ in the GD-BMAX algorithm with

$$
\lambda^{(k-1)} \propto \pi_j \exp \left( -\frac{1}{2\omega^2} \|f_j - Y\|_2^2 + \frac{1 - \nu}{2\omega^2} \|\psi^{(k-1)} - f_j\|_2^2 \right).
$$

In practice, we can also apply the Metropolis-Hastings (MH) method to approximate $f_{\lambda^{(k-1)}}$ for the $k$-th iteration of Algorithm 2.

The MH algorithm described in Algorithm 3 can be used to approximate $f_{\lambda^{(k-1)}}$ with $u^{(k-1)}_T$, and the resulting sequence $\{\psi^{(k)}\}$ are only approximations of the gradient descent algorithm in GD-BMAX. In the following, we present a simple proposition describing how the error of approximating $f_{\lambda^{(k-1)}}$ influences the convergence of $\{\log J(\psi^{(k)})\}$ to $\log J(\psi_X(\omega^2, \nu))$.

**Proposition 4.** Given $Y \in \mathbb{R}^n$, for all $k > 0$, we assume $u^{(k-1)}_T$ from Algorithm 3 satisfying the following:

$$
\mathbb{E}[u^{(k-1)}_T|\psi^{(k-1)}] = f_{\lambda^{(k-1)}}
$$

$$
\|\text{COV}[u^{(k-1)}_T|\psi^{(k-1)}]\|_{op} \leq s^2
$$

(26) (27)
Algorithm 3 Metropolis-Hastings (MH) Sampler for estimating $f_{\lambda(k-1)}$ at $k$-th step in Algorithm 2

**Input:** Noisy observation $Y$, dictionary $\mathcal{H} = \{f_1, \ldots, f_M\}$, prior $\pi \in \Lambda M$, parameters $\nu, \omega^2$, $(k-1)$-th step estimator $\psi^{(k-1)}$.

**Output:** $u_{(k-1)}$ as estimator of $f_{\lambda(k-1)} = \sum_{j=1}^{M} \lambda^{(k-1)}_j f_j$.

Initialize $j(0) = 0$.

for $t = 1, \ldots, T_0 + T$ do
  Generate $\tilde{j} \sim q(\cdot|j(t - 1))$.
  Compute
  \[
  \rho(j(t - 1), \tilde{j}) = \min \left( \frac{q(\tilde{j}|j(t - 1))\theta(\tilde{j})}{q(j(t - 1)|\tilde{j})\theta(j(t - 1))}, 1 \right),
  \]
  where
  \[
  \theta(j) = \pi_j \exp \left( -\frac{1}{2\omega^2} \| f_j - Y \|^2_2 + \frac{1}{2\omega^2} \| \psi^{(k-1)} - f_j \|^2_2 \right).
  \]
  Generate a random variable
  \[
  j(t) = \begin{cases} 
  \tilde{j}, & \text{with probability } \rho(j(t - 1), \tilde{j}) \\
  j(t - 1), & \text{with probability } 1 - \rho(j(t - 1), \tilde{j})
  \end{cases}
  \]
end for

Calculate
\[
\mathbf{u}_{(k-1)} = \frac{1}{T} \sum_{t=T_0+1}^{T_0+T} f_j(t).
\]
where \( \| \cdot \|_{op} \) is matrix spectral norm. Then we have

\[
\mathbb{E} \left( \log J(\psi^{(k)}) - \log J(\psi_X(\omega^2, \nu)) \right) \leq [1 - 2A_1(s - (A_2/2)s^2)]^k A_1^2 L^2 + A_1ns^2/2 ,
\]

where the expectation is with respect to the randomness of the algorithm.

This result can be combined with a slight extension of Proposition 1 (to handle randomization) to obtain an oracle inequality similar to those of Theorem 3.

5 Dual Representation and \( Q \)-aggregation

In this section, we will show that the \( Q \)-aggregation scheme of Dai et al. (2012) with the standard Kullback-Leibler entropy solves a dual representation of the BMAX formulation defined by (8) and (9).

Given \( Y \) and \( \{f_1, \ldots, f_M\} \), \( Q \)-aggregation \( f_{\lambda Q} \) is defined as following:

\[
f_{\lambda Q} = \sum_{j=1}^{M} \lambda^Q_j f_j , \tag{28}
\]

where \( \lambda^Q = (\lambda_1^Q, \ldots, \lambda_M^Q)^T \in \Lambda^M \) such that

\[
\lambda^Q \in \arg\min_{\lambda \in \Lambda^M} Q(\lambda) , \tag{29}
\]

\[
Q(\lambda) = \|f_\lambda - Y\|^2_2 + \nu \sum_{j=1}^{M} \lambda_j \|f_j - f_\lambda\|^2_2 + 2\omega^2 \mathcal{K}_\rho(\lambda, \pi) , \tag{30}
\]

for some \( \nu \in (0, 1) \), where the \( \rho \)-entropy \( \mathcal{K}_\rho(\lambda, \pi) \) is defined as

\[
\mathcal{K}_\rho(\lambda, \pi) = \sum_{j=1}^{M} \lambda_j \log \left( \frac{\rho(\lambda_j)}{\pi_j} \right) , \tag{31}
\]

where \( \rho \) is a real valued function on \([0, 1]\) satisfying

\[
\rho(t) \geq t , \quad t \log \rho(t) \text{ is convex} . \tag{32}
\]

When \( \rho(t) = t \), \( \mathcal{K}_\rho(\lambda, \pi) \) becomes \( K(\lambda, \pi) \), the Kullback-Leibler entropy. When \( \rho(t) = 1 \), \( \mathcal{K}_\rho(\lambda, \pi) = \sum_{j=1}^{M} \lambda_j \log(1/\pi_j) \), a linear entropy in \( \Lambda^M \), and in particular the penalty \( \mathcal{K}_\rho(\lambda, \pi) \) in (30) becomes a constant when \( \pi \) is a flat prior.

To illustrate duality, we shall first introduce a function \( T : \mathbb{R}^n \rightarrow \mathbb{R} \) as

\[
T(h) = -\frac{\nu}{1-\nu} \|h - Y\|^2_2 - 2\omega^2 \log \left( \sum_{j=1}^{M} \pi_j \exp \left( -\frac{\nu}{2\omega^2} \|f_j - h\|^2_2 \right) \right) , \tag{33}
\]

and denote the maximizer of \( T(h) \) as

\[
\hat{h} = \arg\max_{h \in \mathbb{R}^n} T(h) . \tag{34}
\]
Define function \( S : \Lambda^M \times \mathbb{R}^n \to \mathbb{R} \) as

\[
S(\lambda, h) = -\frac{\nu}{1-\nu} \| h - Y \|_2^2 + \nu \sum_{j=1}^{M} \lambda_j \| f_j - h \|_2^2 + 2\omega^2 K(\lambda, \pi). \tag{35}
\]

Define two hyper-surfaces \( A \) and \( B \) in \( \Lambda^M \times \mathbb{R}^n \) as

\[
A = \left\{ (\lambda, h) \in \Lambda^M \times \mathbb{R}^n : h = \frac{1}{\nu} Y - \frac{1-\nu}{\nu} f_\lambda \right\},
\]

\[
B = \left\{ (\lambda, h) \in \Lambda^M \times \mathbb{R}^n : \lambda_j = \frac{\exp \left( -\frac{\nu}{2\omega^2} \| f_j - h \|_2^2 \right) \pi_j}{\sum_{i=1}^{M} \exp \left( -\frac{\nu}{2\omega^2} \| f_i - h \|_2^2 \right) \pi_i} \right\}. \tag{36}
\]

The following duality lemma states the relationship between \( \hat{h} \) and \( f_\lambda \psi \).

**Lemma 2.** When \( \rho(t) = t \), we have the following result

\[
\min_{\lambda \in \Lambda^M} Q(\lambda) = \min_{\lambda \in \Lambda^M} \max_{h \in \mathbb{R}^n} S(\lambda, h) = \max_{h \in \mathbb{R}^n} \min_{\lambda \in \Lambda^M} S(\lambda, h) = \max_{h \in \mathbb{R}^n} T(h).
\]

Moreover, \( A \cap B = \left\{ (\lambda^Q, \hat{h}) \right\} \).

Lemma 2 states that, \( (\lambda^Q, \hat{h}) \) is the joint of hyper-surfaces \( A \) and \( B \), and the saddle point of function \( S(\lambda, h) \) over space \( \Lambda^M \times \mathbb{R}^n \).

With \( T(h) \) defined as in (33), we can employ the transformation \( h = \frac{1}{\nu} Y - \frac{1-\nu}{\nu} \psi \), and it is easy to verify that

\[
T(h) = -2\omega^2 \log \left( J(\psi) \right), \tag{37}
\]

where \( J(\psi) \) is defined in (29).

It follows that maximizing \( T(h) \) is equivalent to minimizing \( J(\psi) \), and thus

\[
\hat{h} = \frac{1}{\nu} Y - \frac{1-\nu}{\nu} \psi_X(\omega^2, \nu).
\]

We can combine this representation with

\[
\hat{h} = \frac{1}{\nu} Y - \frac{1-\nu}{\nu} f_\lambda \psi
\]

from Lemma 2 to obtain \( \psi_X(\omega^2, \nu) = f_\lambda \psi \). Therefore we have the following relationship:

**Theorem 4.** When \( \rho(t) = t \),

\[ \psi_X(\omega^2, \nu) = f_\lambda \psi, \]

where \( \psi_X(\omega^2, \nu) \) is defined by (8) and (9), and \( f_\lambda \psi \) is defined by (28), (29) and (30).

Theorem 4 states that, when \( \rho(t) = t \), \( K_\rho(\lambda, \pi) \) becomes the Kullback-Leibler entropy, and Q-aggregation with the Kullback-Leibler entropy leads to an estimator \( f_\lambda \psi \) that is essentially a dual representation of the BMAX estimator \( \psi_X(\omega^2, \nu) \). It follows that, \( f_\lambda \psi \) shares the same expectation and deviation optimality as \( \psi_X(\omega^2, \nu) \) in solving the model averaging problem, and this matches
the results in Theorem 3.1 of Dai et al. (2012), which showed optimality of $f_{\lambda Q}$ with more general $K_{\rho}(\lambda, \pi)$ where $\rho(t)$ only needs to satisfy the condition (32).

However, unlike the primal objective function $J(\psi)$ which is defined on $\mathbb{R}^n$, the dual objective function $Q(\lambda)$ is defined on $\mathbb{R}^M$. When $M$ is large or infinity, the optimization of $Q(\lambda)$ is non-trivial. Although greedy algorithms are proposed in (Dai et al., 2012), they cannot handle the standard KL-divergence; instead they can only work with the linear entropy where $\rho(t) = 1$; it gives a larger penalty than the standard KL-divergence (and thus worse resulting oracle inequality), and it cannot be generalized to handle continuous dictionaries (because in such case, the linear entropy with $\rho(t) = 1$ will always be $+\infty$). Therefore the numerical greedy procedures of Dai et al. (2012) converges to a solution with a worse oracle bound than that of the solution for the primal formulation considered in this paper. For comparison purpose, we list the GMA-0 algorithm in Dai et al. (2012) below which tries to optimize $Q(\lambda)$ with linear entropy.

### Algorithm 4 GMA-0 Algorithm

**Input:** Noisy observation $Y$, dictionary $H = \{f_1, \ldots, f_M\}$, prior $\pi \in \Lambda^M$, parameters $\nu, \beta$.

**Output:** Aggregate estimator $f_{\lambda^{(k)}}$.

Let $\lambda^{(0)} = 0$, $f_{\lambda^{(0)}} = 0$.

for $k = 1, 2, \ldots$ do

Set $\alpha_k = \frac{2}{k+1}$

$J^{(k)} = \arg\min_j Q(\lambda^{(k-1)} + \alpha_k (e^{(j)} - \lambda^{(k-1)}))$ with linear entropy $\rho(t) = 1$

$\lambda^{(k)} = \lambda^{(k-1)} + \alpha_k (e^{(J^{(k)})} - \lambda^{(k-1)})$

end for

In GMA-0 algorithm, $e^{(j)}$ denotes the $j$th vector of the canonical basis of $\mathbb{R}^M$. Similar to GMA-BMAX, it is a greedy algorithm that add at most one function from the dictionary at each iteration. It outputs a $k$-sparse solution that depends on at most $k$ functions from the dictionary after $k$ iterations. One interesting feature of GMA-0 is that it produces sparse estimators that achieve the optimal deviation bounds for small $k \geq 2$ (proved in Theorem 4.1 and 4.2 in Dai et al. (2012)), while the estimators from GMA-BMAX (sparse) and GD-BMAX (dense) only have such bounds when $k \to \infty$. However, the procedure does not work with the standard KL entropy where $\rho(t) = t$. The best way to work with the KL entropy is via the primal formulation which we propose in this paper. As we have shown, the primal objective function is both smooth and strongly convex, allowing efficient numerical procedures to solve it.

## 6 Experiments

Although the contribution of this work is mainly theoretical, we include some simulations to illustrate the performance of the two numerical procedures proposed for the BMAX formulation. We focus on the average performance of different algorithms and configurations.

### 6.1 Model Setup

We identify a function $f$ with a vector $(f(x_1), \ldots, f(x_n))^T \in \mathbb{R}^n$. Define $f_1, \ldots, f_M$ so that the $n \times M$ design matrix $X = \{f_1, \ldots, f_M\}$ has i.i.d standard Gaussian entries. Let $I_n$ denote the identity matrix of $\mathbb{R}^n$ and let $\Delta \sim \mathcal{N}(0, I_n)$ be a random vector. The regression function is defined
by $\eta = f_1 + 0.5\Delta$. Note that typically $f_1$ will be the closest function to $\eta$ but not necessarily. The noise vector $\xi \sim N(0, \sigma^2 I_n)$ is drawn independently of $X$ where $\sigma = 2$.

We define the oracle model (OM) $f_{k^*}$, where $k^* = \arg\min_j \text{MSE}(f_j)$. The model $f_{k^*}$ is clearly not a valid estimator because it depends on the unobserved $\eta$, however it can be used as a performance benchmark. The performance difference between an estimator $\hat{\eta}$ and the oracle model $f_{k^*}$ is measured by the regret defined as:

$$R(\hat{\eta}) = \text{MSE}(\hat{\eta}) - \text{MSE}(f_{k^*}) .$$  \hspace{1cm} (38)

Since the target is $\eta = f_1 + 0.5\Delta$, and $f_1$ and $\Delta$ are random Gaussian vectors, the oracle model is likely $f_1$ (but it may not be $f_1$ due to the misspecification vector $\Delta$). The noise $\sigma = 2$ is relatively large, which implies a situation where the best convex aggregation does not outperform the oracle model. This is the scenario we considered here. For simplicity, all algorithms use a flat prior $\pi_j = 1/M$ for all $j$.

The experiment is performed with the parameters $n = 50$, $M = 200$, and $\sigma = 2$, and repeated for 500 replications.

One method we compare to is the STAR algorithm of Audibert (2008) which is optimal both in expectation and in deviation under the uniform prior. Mathematically, suppose $f_{k_1}$ is the empirical risk minimizer among functions in $\mathcal{H}$, where

$$k_1 = \arg\min_j \hat{\text{MSE}}(f_j) ,$$  \hspace{1cm} (39)

the STAR estimator $f^*$ is defined as

$$f^* = (1 - \alpha^*)f_{k_1} + \alpha^*f_{k_2} ,$$  \hspace{1cm} (40)

where

$$(\alpha^*, k_2) = \arg\min_{\alpha \in (0,1), j} \hat{\text{MSE}}((1 - \alpha)f_{k_1} + \alpha f_j) .$$  \hspace{1cm} (41)

Another natural solution to solve the model averaging problem is to take the vector of weights $\lambda^{\text{PROJ}}$ defined by

$$\lambda^{\text{PROJ}} \in \arg\min_{\lambda \in \Lambda^M} \hat{\text{MSE}}(f_{\lambda}) ,$$  \hspace{1cm} (42)

which minimizes the empirical risk. We call $\lambda^{\text{PROJ}}$ the vector of projection weights since the aggregate estimator $f_{\lambda^{\text{PROJ}}}$ is the projection of $Y$ onto the convex hull of the $f_j$s.

GMA-BMAX and GD-BMAX algorithms are provided to solve BMAX. Q-aggregation (with Kullback-Leibler entropy) is a dual representation of BMAX , which can be solved using the GMA-0 algorithm (with linear entropy); therefore GMA-0 is also included for comparison purpose. From the definition of $Q(\lambda)$ \cite{30}, it is easy to see that, the minimizer of $Q(\lambda)$ (when $\rho(t) = 1$ with flat prior) becomes $\lambda^{\text{PROJ}}$ in \cite{12} by setting $\nu = 0$, so $\lambda^{\text{PROJ}}$ is approximated by GMA-0 with $\nu = 0$ by running 200 iterations, and the projection algorithm is denoted by “PROJ”.

GMA-BMAX, GD-BMAX and GMA-0 are run for $K$ iterations up to $K = 150$, with $\nu = 1/2$ (this choice theoretically optimize upper bound of the oracle inequality \cite{10},\cite{11}), parameter $\omega$ for GMA-BMAX, GD-BMAX is chosen as $\omega^2 = \sigma^2/5$, and parameter $\omega$ for exponential weighted model averaging (denoted by “EWMA”) is tuned by ten fold cross validation. STAR estimator is also included. Regrets of all algorithms defined in \cite{38} are reported for comparisons.
Table 1: Performance Comparison

|       | STAR   | EWMA   | PROJ   |
|-------|--------|--------|--------|
|       | 0.458 ± 0.44 | 0.435 ± 0.5 | 0.425 ± 0.3 |

|       | k = 1 | k = 5 | k = 15 | k = 60 | k = 100 | k = 150 |
|-------|-------|-------|--------|--------|---------|---------|
| GMA-BMAX | 0.687 ± 0.72 | 0.493 ± 0.43 | 0.417 ± 0.38 | 0.376 ± 0.37 | 0.37 ± 0.37 | 0.368 ± 0.38 |
| GD-BMAX | 0.974 ± 0.23 | 0.873 ± 0.21 | 0.69 ± 0.2 | 0.415 ± 0.33 | 0.376 ± 0.36 | 0.368 ± 0.38 |
| GMA-0  | 0.549 ± 0.78 | 0.395 ± 0.45 | 0.373 ± 0.41 | 0.368 ± 0.4 | 0.369 ± 0.41 | 0.368 ± 0.4 |

Table 1 is a comparison of commonly used estimators (STAR, EWMA and PROJ) with GMA-BMAX, GD-BMAX, GMA-0. The regrets are reported using the “mean ± standard deviation” format.

The results in Table 1 indicate that GMA-BMAX, GD-BMAX and GMA-0 perform better as iteration $k$ increases, and all three algorithms beat STAR, EWMA and PROJ when $k$ is large enough. GMA-0 outperforms STAR, EWMA and PROJ after as small as $k = 5$ iterations, which still gives a relatively sparse averaged model. This is consistent with Theorem 4.1 and 4.2 in Dai et al. (2012) which states that GMA-0 has optimal bounds for small $k$ ($k \geq 2$).

Figure 1: Regrets $R(\psi^{(k)})$ versus iterations $k$.

Figure 1 compares the MSE performance of GMA-BMAX, GD-BMAX and GMA-0 with $\nu = 1/2$. Note that GMA-BMAX and GD-BMAX initialize both with $\psi^{(0)} = 0$, but they produce difference estimators after the first iteration ($k = 1$). GMA-BMAX selects $j \in \{1, \ldots, M\}$ that minimizes $\log J(f_j)$ and GD-BMAX outputs a dense estimator, whiles GMA-0 selects $j \in \{1, \ldots, M\}$ that minimizes $Q(f_j)$ and the first stage output is actually the empirical risk minimizer $f_{k_1}$ where $k_1 = \arg\min_j \overline{\text{MSE}}(f_j)$. For this experiments, the two algorithms for the BMAX formulation (GMA-
BMAX and GD-BMAX) requires more iterations to converge. Although the potential theoretical advantage of the two BMAX algorithms (with KL entropy) over that of GMA-0 (with linear entropy) is not shown in these experiments, they nevertheless show that the two algorithms work in practice.

7 Conclusion

This paper introduces a new formulation for deviation optimal model averaging which we refer to as BMAX. It is motivated by Bayesian theoretical considerations with an appropriately defined exponentiated least squares loss. Moreover we established a primal-dual relationship of this estimator and the \( Q \)-aggregation scheme (with KL entropy) by Dai et al. (2012). This relationship not only establishes a natural Bayesian interpretation for \( Q \)-aggregation but also leads to new numerical algorithms for model aggregation that are suitable for the continuous dictionary setting. The new formulation and its relationship to \( Q \)-aggregation provides deeper understanding of deviation optimal model averaging procedures.

A Proofs

A.1 Proof of Theorem 1

Proposition 5. For any \( \lambda \in \Lambda^M \), real numbers \( \{x_j\}_{j=1}^M \), and a constant \( a > 0 \), we have

\[
\sum_{j=1}^M \lambda_j x_j - aK(\lambda, \pi) \leq a \log \left( \sum_{j=1}^M \pi_j e^{x_j/a} \right).
\]

Proof. The result follows directly from Jensen’s Inequality as

\[
\exp \left( \sum_{j=1}^M \lambda_j (x_j/a - \log(\lambda_j/\pi_j)) \right) \leq \sum_{j=1}^M \lambda_j \exp \left( (x_j/a) - \log(\lambda_j/\pi_j) \right) = \sum_{j=1}^M \pi_j e^{x_j/a}.
\]

We also need the following lemma to prove the theorem.

Lemma 3. For any \( \psi \in \mathbb{R}^n \), let \( \lambda \in \Lambda^M \) defined as

\[
\lambda_j \propto \pi_j \exp \left( -\frac{1}{2\omega^2} \|f_j - Y\|_2^2 + \frac{1}{2\omega^2} \|\psi - f_j\|_2^2 \right)
\]

Then we have the following equation

\[
\frac{\nabla J(\psi)}{J(\psi)} = \frac{1-\nu}{\omega^2} (\psi - f_\lambda),
\]
\[ \|f_\lambda - \eta\|^2 - \left( \nu \sum_{j=1}^{M} \theta_j \|f_j - \eta\|^2 + (1 - \nu)\|f_\theta - \eta\|^2 \right) \]

\[ = -\nu \sum_{j=1}^{M} \lambda_j \|f_j - f_\lambda\|^2 - (1 - \nu)\|f_\theta - f_\lambda\|^2 + 2\xi^\top (f_\lambda - f_\theta) - 2\omega^2 K(\lambda, \pi) + 2\omega^2 K(\theta, \pi) - 2\omega^2 K(\theta, \lambda) - 2(1 - \nu)(f_\theta - f_\lambda)^\top (f_\lambda - \psi). \]

**Proof.** Since

\[ J(\psi) = \sum_{j=1}^{M} \pi_j \exp \left( -\frac{1}{2\omega^2} \|f_j - Y\|^2 + \frac{1 - \nu}{2\omega^2} \|\psi - f_j\|^2 \right), \]

and

\[ \nabla J(\psi) = \sum_{j=1}^{M} \pi_j \exp \left( -\frac{1}{2\omega^2} \|f_j - Y\|^2 + \frac{1 - \nu}{2\omega^2} \|\psi - f_j\|^2 \right) \frac{1 - \nu}{\omega^2} (\psi - f_j), \]

Then we have

\[ \frac{\nabla J(\psi)}{J(\psi)} = \frac{1 - \nu}{\omega^2} (\psi - f_\lambda). \]

From the definition of \( \lambda \) we have,

\[ \lambda_j = \frac{\pi_i}{\pi_j} \exp \left( -\frac{1}{2\omega^2} \|f_i - Y\|^2 + \frac{1 - \nu}{2\omega^2} \|\psi - f_i\|^2 \right). \]

It follows that there exists a constant \( c_0 \) such that

\[ 2\omega^2 \log(\lambda_i/\pi_i) + \|f_i - Y\|^2 + (1 - \nu)\|\psi - f_i\|^2 \]

\[ = 2\omega^2 \log(\lambda_j/\pi_j) + \|f_j - Y\|^2 + (1 - \nu)\|\psi - f_j\|^2 = c_0. \]

Taking weighted sum with respect to \( \lambda \in \Lambda^M \) and any chosen \( \theta \in \Lambda^M \), we obtain

\[ \sum_{j=1}^{M} \lambda_j \|f_j - Y\|^2 - (1 - \nu) \sum_{j=1}^{M} \lambda_j \|f_j - \psi\|^2 + 2\omega^2 \sum_{j=1}^{M} \lambda_j \log(\lambda_j/\pi_j) \]

\[ = \sum_{j=1}^{M} \lambda_j c_0 = c_0 = \sum_{j=1}^{M} \theta_j c_0 \]

\[ = \sum_{j=1}^{M} \theta_j \|f_j - Y\|^2 - (1 - \nu) \sum_{j=1}^{M} \theta_j \|f_j - \psi\|^2 + 2\omega^2 \sum_{j=1}^{M} \theta_j \log(\lambda_j/\pi_j). \]
Combine the above equation and the following two facts:

$$\sum_{j=1}^{M} \lambda_j \|f_j - \psi\|_2^2 = \|f_\lambda - \psi\|_2^2 + \sum_{j=1}^{M} \lambda_j \|f_j - f_\lambda\|_2^2,$$

and

$$\sum_{j=1}^{M} \theta_j \|f_j - \psi\|_2^2 = \|f_\theta - \psi\|_2^2 + \sum_{j=1}^{M} \theta_j \|f_j - f_\theta\|_2^2 = \|f_\theta - f_\lambda\|_2^2 + \|f_\lambda - \psi\|_2^2 + 2(f_\theta - f_\lambda)^T (f_\lambda - \psi) + \sum_{j=1}^{M} \theta_j \|f_j - f_\theta\|_2^2,$$

we have

$$\sum_{j=1}^{M} \lambda_j \|f_j - Y\|_2^2 - (1 - \nu) \sum_{j=1}^{M} \lambda_j \|f_j - f_\lambda\|_2^2 + 2\omega^2 \mathcal{K}(\lambda, \pi)$$

$$= \sum_{j=1}^{M} \theta_j \|f_j - Y\|_2^2 - (1 - \nu) \sum_{j=1}^{M} \theta_j \|f_j - f_\theta\|_2^2 + 2\omega^2 \mathcal{K}(\theta, \pi) - 2\omega^2 \mathcal{K}(\theta, \lambda)$$

$$- (1 - \nu)\|f_\theta - f_\lambda\|_2^2 - 2(1 - \nu)(f_\theta - f_\lambda)^T (f_\lambda - \psi). \quad (43)$$

Plug the following two equations to each side of (43)

$$\sum_{j=1}^{M} \lambda_j \|f_j - Y\|_2^2 - (1 - \nu) \sum_{j=1}^{M} \lambda_j \|f_j - f_\lambda\|_2^2 = \|f_\lambda - Y\|_2^2 + \nu \sum_{j=1}^{M} \lambda_j \|f_j - f_\lambda\|_2^2,$$

$$\sum_{j=1}^{M} \theta_j \|f_j - Y\|_2^2 - (1 - \nu) \sum_{j=1}^{M} \theta_j \|f_j - f_\theta\|_2^2 = \nu \sum_{j=1}^{M} \theta_j \|f_j - Y\|_2^2 + (1 - \nu)\|f_\theta - Y\|_2^2,$$

and rearrange the terms we obtain

$$\|f_\lambda - Y\|_2^2 - \left( \nu \sum_{j=1}^{M} \theta_j \|f_j - Y\|_2^2 + (1 - \nu)\|f_\theta - Y\|_2^2 \right)$$

$$= -\nu \sum_{j=1}^{M} \lambda_j \|f_j - f_\lambda\|_2^2 - (1 - \nu)\|f_\theta - f_\lambda\|_2^2 - 2\omega^2 \mathcal{K}(\lambda, \pi) + 2\omega^2 \mathcal{K}(\theta, \pi)$$

$$- 2\omega^2 \mathcal{K}(\theta, \lambda) - 2(1 - \nu)(f_\theta - f_\lambda)^T (f_\lambda - \psi).$$

Now by combining the above equation with $Y = \eta + \xi$ it follows that

$$\|f_\lambda - \eta\|_2^2 - \left( \nu \sum_{j=1}^{M} \theta_j \|f_j - \eta\|_2^2 + (1 - \nu)\|f_\theta - \eta\|_2^2 \right)$$

$$= -\nu \sum_{j=1}^{M} \lambda_j \|f_j - f_\lambda\|_2^2 - (1 - \nu)\|f_\theta - f_\lambda\|_2^2 + 2\xi^T (f_\lambda - f_\theta) - 2\omega^2 \mathcal{K}(\lambda, \pi)$$

$$+ 2\omega^2 \mathcal{K}(\theta, \pi) - 2\omega^2 \mathcal{K}(\theta, \lambda) - 2(1 - \nu)(f_\theta - f_\lambda)^T (f_\lambda - \psi).$$

19
This proves the lemma.

Now we are ready to prove Theorem 1.
From the definition of $\psi_X(\omega^2, \nu)$ in (8), $\psi_X(\omega^2, \nu)$ is the minimizer of $J(\psi)$; thus we have $\nabla J(\psi_X(\omega^2, \nu)) = 0$. From the first part of Lemma 3 we know that $\psi_X(\omega^2, \nu) = f_\lambda$ with $\lambda \in \Lambda^M$ given by

$$\lambda_j \propto \pi_j \exp \left( -\frac{1}{2\omega^2} \|f_j - Y\|_2^2 + \frac{1 - \nu}{2\omega^2} \|\psi_X(\omega^2, \nu) - f_j\|_2^2 \right).$$

Now by applying the second part of Lemma 3 with $\psi = \psi_X(\omega^2, \nu) = f_\lambda$, we have

$$\|f_\lambda - \eta\|_2^2 - \left( \nu \sum_{j=1}^M \theta_j \|f_j - \eta\|_2^2 + (1 - \nu)\|f_\theta - \eta\|_2^2 \right)$$

$$= -\nu \sum_{j=1}^M \lambda_j \|f_j - f_\lambda\|_2^2 - (1 - \nu)\|f_\theta - f_\lambda\|_2^2 + 2\xi^T (f_\lambda - f_\theta) - 2\omega^2 \mathcal{K}(\lambda, \pi) + 2\omega^2 \mathcal{K}(\theta, \pi) - 2\omega^2 \mathcal{K}(\theta, \lambda).$$

It is also easy to verify that the following inequality holds:

$$-\nu \sum_{j=1}^M \lambda_j \|f_j - f_\lambda\|_2^2 - (1 - \nu)\|f_\theta - f_\lambda\|_2^2 \leq -\nu_1 \sum_{j=1}^M \lambda_j \|f_j - f_\theta\|_2^2,$$

where $\nu_1 = \min(\nu, 1 - \nu)$.

Combining the above two inequalities with $-2\omega^2 \mathcal{K}(\theta, \lambda) \leq 0$ we obtain

$$\|f_\lambda - \eta\|_2^2 - \left( \nu \sum_{j=1}^M \theta_j \|f_j - \eta\|_2^2 + (1 - \nu)\|f_\theta - \eta\|_2^2 \right)$$

$$\leq -\nu_1 \sum_{j=1}^M \lambda_j \|f_j - f_\theta\|_2^2 + 2\xi^T (f_\lambda - f_\theta) - 2\omega^2 \mathcal{K}(\lambda, \pi) + 2\omega^2 \mathcal{K}(\theta, \pi)$$

$$= \sum_{j=1}^M \lambda_j \left( -\nu_1 \|f_j - f_\theta\|_2^2 + 2\xi^T (f_j - f_\theta) \right) - 2\omega^2 \mathcal{K}(\lambda, \pi) + 2\omega^2 \mathcal{K}(\theta, \pi)$$

$$\leq 2\omega^2 \log \left( \sum_{j=1}^M \pi_j \exp \left\{ -\nu_1 \|f_j - f_\theta\|_2^2 + 2\xi^T (f_j - f_\theta) \right\} \right) + 2\omega^2 \mathcal{K}(\theta, \pi),$$

where the last inequality is from Proposition 3 with $x_j = -\nu_1 \|f_j - f_\theta\|_2^2 + 2\xi^T (f_j - f_\theta)$ and $a = 2\omega^2$. 
Taking exponential and then taking expectation with respect to $\xi$, we have
\[
\mathbb{E} \exp \left[ \frac{1}{2\omega^2} \|f_\lambda - \eta\|_2^2 - \frac{1}{2\omega^2} \left( \nu \sum_{j=1}^M \theta_j \|f_j - \eta\|_2^2 + (1 - \nu)\|\theta - \eta\|_2^2 \right) \right]
\leq \mathbb{E} \exp \left[ \log \left( \sum_{j=1}^M \pi_j \exp \left\{ -\nu \|f_j - \theta\|_2^2 + 2\xi^\top (f_j - \theta) \right\} \right) + \mathcal{K}(\theta, \pi) \right]
= \sum_{j=1}^M \pi_j \mathbb{E} \exp \left\{ -\nu \|f_j - \theta\|_2^2 + 2\xi^\top (f_j - \theta) \right\} + \mathcal{K}(\theta, \pi)
\leq \sum_{j=1}^M \pi_j \exp \left\{ (-\nu + \sigma^2/\omega^2) \|f_j - \theta\|_2^2 + \mathcal{K}(\theta, \pi) \right\}
\leq \exp \{\mathcal{K}(\theta, \pi)\},
\]
where the second inequality comes from the Gaussian assumption which implies that $\mathbb{E} \exp(\xi^\top f) \leq \exp(\sigma^2\|f\|_2^2/2)$ for all $f \in \mathbb{R}^n$, and the last inequality is because of the assumption that $\omega^2 \geq \sigma^2/\nu = \min(\sigma^2/1-\nu)$. 

Now define the random variable
\[
u_\theta(Y) = \frac{1}{2\omega^2} \left[ \|f_\lambda - \eta\|_2^2 - \left( \nu \sum_{j=1}^M \theta_j \|f_j - \eta\|_2^2 + (1 - \nu)\|\theta - \eta\|_2^2 \right) \right] - \mathcal{K}(\theta, \pi),
\]
we can rewrite the previously displayed inequality as
\[
\mathbb{E}_Y \exp[\nu_\theta(Y)] \leq 1.
\]
It follows from the Chernoff bound that with probability at least $1 - \delta$, $\nu_\theta(Y) \leq \log(1/\delta)$, and from the convexity of the function $\exp(\cdot)$ that $\nu_\theta(Y) \leq 0$. These bounds lead to the claims of the theorem.

A.2 Proof of Lemma 1

Define $\lambda \in \Lambda^M$ as
\[
\lambda_j \propto \pi_j \exp \left( -\frac{1}{2\omega^2} \|f_j - Y\|_2^2 + \frac{1 - \nu}{2\omega^2} \|\psi - f_j\|_2^2 \right)
\]
It follows that
\[
\nabla J(\psi) = \frac{1 - \nu}{\omega^2} (\psi - f_\lambda)
\]
and
\[
\nabla^2 J(\psi) = \frac{\lambda}{J(\psi)} = \sum_{j=1}^M \lambda_j \left( \left( \frac{1 - \nu}{\omega^2} \right)^2 (\psi - f_j)(\psi - f_j) + \left( \frac{1 - \nu}{\omega^2} \right) I_n \right) .
\]
Then we have

$$
\nabla^2 \log J(\psi) = \frac{(\nabla^2 J(\psi))J(\psi) - (\nabla J(\psi)) (\nabla J(\psi))^\top}{J^2(\psi)}
$$

$$
= \sum_{j=1}^{M} \lambda_j \left( \left( \frac{1-\nu}{\omega^2} \right)^2 (\psi - f_j)(\psi - f_j)^\top + \left( \frac{1-\nu}{\omega^2} \right) I_n \right) - \left( \frac{1-\nu}{\omega^2} \right)^2 (\psi - f_\lambda)(\psi - f_\lambda)^\top
$$

$$
= \left( \frac{1-\nu}{\omega^2} \right) I_n + \sum_{j=1}^{M} \lambda_j \left( \frac{1-\nu}{\omega^2} \right)^2 (f_\lambda - f_j)(f_\lambda - f_j)^\top.
$$

Therefore \( \nabla^2 \log J(\psi) \geq \left( \frac{1-\nu}{\omega^2} \right) I_n \). With the assumption that \( \|f_j\|_2 \leq L \) for all \( j \), we have

$$
\sum_{j=1}^{M} \lambda_j (f_\lambda - f_j)(f_\lambda - f_j)^\top = \sum_{j=1}^{M} \lambda_j f_j f_j^\top - f_\lambda f_\lambda^\top
$$

$$
\leq \sum_{j=1}^{M} \lambda_j f_j f_j^\top \leq \sum_{j=1}^{M} \lambda_j L^2 I_n = L^2 I_n.
$$

It follows that \( \nabla^2 \log J(\psi) \leq \left( \frac{1-\nu}{\omega^2} \right) + \left( \frac{1-\nu}{\omega^2} \right)^2 L^2 \right) I_n. \]

### A.3 Proof of Proposition 2

As in the proof of Theorem 1, \( \psi_X(\omega, \nu) = f_\lambda \) with \( \lambda \in \Lambda^M \) defined as

$$
\lambda_j \propto \pi_j \exp \left( -\frac{1}{2\omega^2} \|f_j - Y\|_2^2 + \frac{1-\nu}{2\omega^2} \|\psi_X(\omega, \nu) - f_j\|_2^2 \right).
$$

For any \( j = 1, \ldots, M \),

$$
\log J(\psi^{(k)}) = \log J \left( \psi^{(k-1)} + \alpha_k (f_j - \psi^{(k-1)}) \right)
$$

$$
\leq \log J \left( \psi^{(k-1)} + \alpha_k (f_j - \psi^{(k-1)}) \right)
$$

$$
\leq \log J(\psi^{(k-1)}) + \alpha_k (f_j - \psi^{(k-1)})^\top \frac{\nabla J(\psi^{(k-1)})}{J(\psi^{(k-1)})} + 2\alpha_k^2 D,
$$

where the first inequality comes from definition, the second inequality is from Taylor expansion at \( \psi^{(k-1)} \) and \( \|f_j - \psi^{(k-1)}\|_2^2 \leq 4L^2 \).
We multiply the above inequality by $\lambda_j$ and sum over $j$ to obtain

$$
\log J(\psi^{(k)}) \leq \log J(\psi^{(k-1)}) + \alpha_k \sum_{j=1}^{M} \lambda_j (f_j - \psi^{(k-1)})^\top \frac{\nabla J(\psi^{(k-1)})}{J(\psi^{(k-1)})} + 2\alpha_k^2 D
$$

$$
= \log J(\psi^{(k-1)}) + \alpha_k (\psi_X(\omega^2, \nu) - \psi^{(k-1)})^\top \frac{\nabla J(\psi^{(k-1)})}{J(\psi^{(k-1)})} + 2\alpha_k^2 D
$$

$$
\leq \log J(\psi^{(k-1)}) + \alpha_k (\log J(\psi_X(\omega^2, \nu)) - \log J(\psi^{(k-1)})) + 2\alpha_k^2 D,
$$

where the last inequality follows from the convexity of $\log J(\psi)$.

Denote by $\delta_k = \log J(\psi^{(k)}) - \log J(\psi_X(\omega^2, \nu))$, it follows that

$$
\delta_k \leq (1 - \alpha_k)\delta_{k-1} + 2\alpha_k^2 D.
$$

We now bound $\delta_0$. Note that if we let $\mu_j \propto \pi_j \exp \left(-\frac{1}{2\omega^2}||f_j - Y||_2^2\right)$ such that $\sum_{j=1}^{M} \mu_j = 1$, then

$$
\delta_0 = \log J(\psi^{(0)}) - \log J(\psi_X(\omega^2, \nu))
$$

$$
= \log \sum_{j} \mu_j \exp \left(\frac{1 - \nu}{2\omega^2}||\psi^{(0)} - f_j||_2^2\right) - \log \sum_{j} \mu_j \exp \left(\frac{1 - \nu}{2\omega^2}||\psi_X(\omega^2, \nu) - f_j||_2^2\right)
$$

$$
\leq \log \left(\sum_{j=1}^{M} \mu_j \exp \left(\frac{1 - \nu}{2\omega^2}||\psi^{(0)} - f_j||_2^2\right)\right)
$$

$$
\leq \frac{1 - \nu}{2\omega^2}L^2 \leq 2D.
$$

(44)

The claim thus hold for $\delta_0$. By mathematical induction, if $\delta_{k-1} \leq \frac{8D}{k+2}$ then

$$
\delta_k \leq (1 - \alpha_k)\delta_{k-1} + 2\alpha_k^2 D
$$

$$
\leq (1 - 2/(k + 1))\frac{8D}{k + 2} + 2(2/(k + 1))^2 D \leq \frac{8D}{k + 3}.
$$

This proves the desired bound.

\[\blacksquare\]

### A.4 Proof of Proposition 3

We will first prove the following result.

**Lemma 4.** For any $\psi \in \mathbb{R}^n$ we have the following inequalities

$$
\log J(\psi) - \log J(\psi_X(\omega^2, \nu)) \leq \frac{1}{2A_1}||\nabla \log J(\psi)||_2^2,
$$

(45)

where $A_1$ is defined in (15).

**Proof.** From inequality (15), for any $\psi_1 \in \mathbb{R}^n$ we have

$$
\log J(\psi_1) \geq \log J(\psi_2) + (\psi_1 - \psi_2)^\top \frac{\nabla J(\psi_2)}{J(\psi_2)} + (A_1/2)||\psi_1 - \psi_2||_2^2
$$
The right hand side of the above inequality is a convex quadratic function of \( \psi_1 \) (for fixed \( \psi_2 \)). Setting its gradient with respect to \( \psi_1 \) to zero, we find that 
\[
\hat{\psi}_1 = \psi_2 - \left(1 / A_1 \right) \frac{\nabla J(\psi_2)}{J(\psi_2)}
\]
minimizes the right hand side. Therefore we have
\[
\log J(\psi_1) \geq \log J(\psi_2) + (\psi_1 - \psi_2)^\top \frac{\nabla J(\psi_2)}{J(\psi_2)} + (A_1/2)\|\psi_1 - \psi_2\|^2_2
\]
\[
\geq \log J(\psi_2) + (\hat{\psi}_1 - \psi_2)^\top \frac{\nabla J(\psi_2)}{J(\psi_2)} + (A_1/2)\|\hat{\psi}_1 - \psi_2\|^2_2
\]
\[
= \log J(\psi_2) - \frac{1}{2A_1} \left\| \nabla J(\psi_2) \right\|^2_2
\]
Since this holds for any \( \psi_1 \in \mathbb{R}^n \), we have
\[
\log J(\psi_X(\omega^2, \nu)) \geq \log J(\psi_2) - \frac{1}{2A_1} \left\| \nabla J(\psi_2) \right\|^2_2.
\]

From the gradient update rule
\[
\psi^{(k)} = \psi^{(k-1)} - t_k \nabla \log J(\psi^{(k-1)}),
\]
we obtain
\[
\log J(\psi^{(k)}) = \log J(\psi^{(k-1)} - t_k \nabla \log J(\psi^{(k-1)}))
\leq \log J(\psi^{(k-1)}) - t_k \| \nabla \log J(\psi^{(k-1)}) \|^2 + (A_2/2)t_k^2 \left\| \nabla \log J(\psi^{(k-1)}) \right\|^2_2
\]
\[
= \log J(\psi^{(k-1)}) - (t_k - (A_2/2)t_k^2) \| \nabla \log J(\psi^{(k-1)}) \|^2_2,
\]
where the inequality is from (47).

Then by subtracting \( \log J(\psi_X(\omega^2, \nu)) \) from each side, we have
\[
\log J(\psi^{(k)}) - \log J(\psi_X(\omega^2, \nu)) \leq \log J(\psi^{(k-1)}) - \log J(\psi_X(\omega^2, \nu)) - (t_k - (A_2/2)t_k^2) \| \nabla \log J(\psi^{(k-1)}) \|^2_2. \tag{46}
\]

Also from (45) we have
\[
\| \nabla \log J(\psi^{(k-1)}) \|^2_2 \geq 2A_1 \left( \log J(\psi^{(k-1)}) - \log J(\psi_X(\omega^2, \nu)) \right). \tag{47}
\]

Therefore by choosing fixed step size \( t_k = s \in (0, 2/A_2) \) for any \( k > 0 \), we obtain from (46) and (47) that
\[
\log J(\psi^{(k)}) - \log J(\psi_X(\omega^2, \nu)) \leq [1 - 2A_1(s - (A_2/2)s^2)] \left( \log J(\psi^{(k-1)}) - \log J(\psi_X(\omega^2, \nu)) \right).
\]

It follows that
\[
\log J(\psi^{(k)}) - \log J(\psi_X(\omega^2, \nu)) \leq [1 - 2A_1(s - (A_2/2)s^2)]^k \left( \log J(\psi^{(0)}) - \log J(\psi_X(\omega^2, \nu)) \right).
\]

Using (44) we obtain the desired inequality. \qed
A.5 Proof of Proposition 4

We fix $Y$, and the following expectation is respect to the randomness from the MH algorithm. For $k > 0$, $u_T^{(k-1)}$ from Algorithm 3 is an estimator of $f_{\lambda^{(k-1)}} = \sum_{j=1}^{M} \lambda^{(k-1)}_j f_\nu$. Then in Algorithm 2 we update $\psi^{(k)}$ by

$$
\psi^{(k)} = \psi^{(k-1)} - t_k \frac{1 - \nu}{\omega^2}(\psi^{(k-1)} - u_T^{(k-1)}).
$$

Let $v^{(k-1)} = \frac{1 - \nu}{\omega^2}(\psi^{(k-1)} - u_T^{(k-1)})$, then we have

$$
E[v^{(k-1)}|\psi^{(k-1)}] = \frac{1 - \nu}{\omega^2}(\psi^{(k-1)} - f_{\lambda^{(k-1)}}) = \nabla \log J(\psi^{(k-1)})
$$

and

$$
\|\text{COV}[v^{(k-1)}|\psi^{(k-1)}]\|_{op} = \left(\frac{1 - \nu}{\omega^2}\right)^2 \|\text{COV} [u_T^{(k-1)}|\psi^{(k-1)}]\|_{op} \leq \left(\frac{1 - \nu}{\omega^2}\right)^2 s^2.
$$

It follows that

$$
\log J(\psi^{(k)}) = \log J(\psi^{(k-1)} - t_k v^{(k-1)}) \leq \log J(\psi^{(k-1)}) - t_k \nabla \log J(\psi^{(k-1)})^T v^{(k-1)} + \frac{A_2}{2} t_k^2 \|v^{(k-1)}\|_2^2,
$$

where the inequality is from (19).

Let $\delta_k = \log J(\psi^{(k)}) - \log J(\psi_{\lambda}(\omega^2, \nu))$. By subtracting $\log J(\psi_{\lambda}(\omega^2, \nu))$ from each side and take expectation conditioned on $\psi^{(k-1)}$, we have

$$
E[\delta_k|\psi^{(k-1)}] \leq \delta_{k-1} - t_k \nabla \log J(\psi^{(k-1)})^T E[v^{(k-1)}|\psi^{(k-1)}] + \frac{A_2}{2} t_k^2 E[\|v^{(k-1)}\|_2^2|\psi^{(k-1)}] - t_k \nabla \log J(\psi^{(k-1)})^T v^{(k-1)}
$$

$$
\leq \delta_{k-1} - t_k \|\nabla \log J(\psi^{(k-1)})\|_2^2 + \frac{A_2}{2} t_k^2 \left(\|\nabla \log J(\psi^{(k-1)})\|_2^2 + n \left(\frac{1 - \nu}{\omega^2}\right)^2 s^2\right)
$$

$$
= \delta_{k-1} - \frac{1}{2 A_2} \|\nabla \log J(\psi^{(k-1)})\|_2^2 + \frac{A_2}{2} \left(\frac{1 - \nu}{\omega^2}\right)^2 n s^2.
$$

Combine the above inequality with (15), we obtain

$$
E[\delta_k|\psi^{(k-1)}] \leq \delta_{k-1}(1 - A_1/A_2) + \frac{A_2^2}{2 A_2} n s^2.
$$

It follows that

$$
E[\delta_k] \leq E[\delta_{k-1}](1 - A_1/A_2) + \frac{A_2^2}{2 A_2} n s^2,
$$

which implies that

$$
E[\delta_k] \leq E[\delta_0](1 - A_1/A_2)^k + \frac{A_1}{2} n s^2.
$$

The desired bound follows from (44).
A.6 Proof of Lemma 2

Note that let $\hat{h}$ be the maximizer of $T(h)$ in (33), then by setting the derivative of (33) to zero, it is easy to observe that there exists a corresponding $\hat{\lambda}$ so that $(\lambda, \hat{h}) \in A \cap B$. This means that $A \cap B \neq \emptyset$.

Now consider any $(\lambda^0, h^0) \in A \cap B$. We have

$$Q(\lambda^0) \geq \min_{\lambda \in \Lambda^M} Q(\lambda) = \min_{\lambda \in \Lambda^M} \max_{h \in \mathbb{R}^n} S(\lambda, h) \geq \max_{h \in \mathbb{R}^n} \min_{\lambda \in \Lambda^M} S(\lambda, h).$$

The second equality is from simple algebra and the third inequality is from Lemma 36.1 in Rockafellar (1997).

Also we have

$$\max_{h \in \mathbb{R}^n} \min_{\lambda \in \Lambda^M} S(\lambda, h) = \max_{h \in \mathbb{R}^n} T(h) = T(\hat{h}) \geq T(h^0).$$

We thus have

$$Q(\lambda^0) \geq \min_{\lambda \in \Lambda^M} Q(\lambda) = \min_{\lambda \in \Lambda^M} \max_{h \in \mathbb{R}^n} S(\lambda, h) \geq \max_{h \in \mathbb{R}^n} \min_{\lambda \in \Lambda^M} S(\lambda, h) = \max_{h \in \mathbb{R}^n} T(h) \geq T(h^0).$$

Our target is now to prove $Q(\lambda^0) = T(h^0)$. Since $(\lambda^0, h^0) \in A \cap B$ we have

$$\begin{cases}
h^0 = \frac{1}{\nu} Y - \frac{1 - \eta}{\nu} f_{\lambda^0}, \\
\lambda^0_j = \frac{\exp \left( \frac{\nu}{2\omega^2} \| f_j - h^0 \|_2^2 \right) \pi_j}{\sum_{i=1}^M \exp \left( \frac{\nu}{2\omega^2} \| f_i - h^0 \|_2^2 \right) \pi_i}.
\end{cases}$$

It follows that for all $j$

$$\sum_{i=1}^M \exp \left( -\frac{\nu}{2\omega^2} \| f_i - h^0 \|_2^2 \right) \pi_i = \frac{\exp \left( -\frac{\nu}{2\omega^2} \| f_j - h^0 \|_2^2 \right) \pi_j}{\lambda^0_j},$$

which implies that

$$\log \left( \sum_{i=1}^M \exp \left( -\frac{\nu}{2\omega^2} \| f_i - h^0 \|_2^2 \right) \pi_i \right) = -\frac{\nu}{2\omega^2} \| f_j - h^0 \|_2^2 - \log(\lambda^0_j / \pi_j) = \sum_{i=1}^M \lambda^0_i \left( -\frac{\nu}{2\omega^2} \| f_i - h^0 \|_2^2 - \log(\lambda^0_i / \pi_i) \right).$$
Plug back into \( T(h^0) \),

\[
T(h^0) = -\frac{\nu}{1-\nu}\|h^0 - Y\|_2^2 - 2\omega^2 \left[ \sum_{i=1}^{M} \lambda_i^0 \left( -\frac{\nu}{2\omega^2}\|f_i - h^0\|_2^2 - \log(\lambda_i^0/\pi_i) \right) \right]
\]

\[
= -\frac{\nu}{1-\nu}\|h^0 - Y\|_2^2 + \nu \sum_{i=1}^{M} \lambda_i^0\|f_i - h^0\|_2^2 + 2\omega^2 \mathcal{K}(\lambda^0, \pi)
\]

\[
= \|f_{\lambda^0} - Y\|_2^2 + \nu \sum_{i=1}^{M} \lambda_i^0\|f_i - f_{\lambda^0}\|_2^2 + 2\omega^2 \mathcal{K}(\lambda^0, \pi)
\]

\[
= Q(\lambda^0).
\]

Note that the third equality is obtained by plugging in \( h^0 = \frac{1}{\nu}Y - \frac{1-\nu}{\nu}f_{\lambda^0} \) and simplify.

Therefore

\[
Q(\lambda^0) = \min_{\lambda \in \Lambda^M} Q(\lambda) = \min_{\lambda \in \Lambda^M} \max_{\lambda \in \Lambda^M} \min_{h \in \mathbb{R}^n} S(\lambda, h) = \max_{h \in \mathbb{R}^n} \min_{\lambda \in \Lambda^M} S(\lambda, h) = \max_{h \in \mathbb{R}^n} T(h) = T(h^0).
\]

Since \( Q(\cdot) \) and \( T(\cdot) \) are both strictly convex functions, we have \( \hat{h} = h^0 \) and \( \lambda^Q = \lambda^0 \). Using \( h^0 = \frac{1}{\nu}Y - \frac{1-\nu}{\nu}f_{\lambda^0} \), we have

\[
\hat{h} = \frac{1}{\nu}Y - \frac{1-\nu}{\nu}f_{\lambda^Q}.
\]

This proves that \( A \cap B \) contains the unique point \((\lambda^Q, \hat{h})\).

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