MULTI-SUBSPACE MULTI-MODAL MODELING FOR DIFFUSION MODELS: ESTIMATION, CONVERGENCE AND MIXTURE OF EXPERTS

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ABSTRACT

Recently, diffusion models have achieved a great performance with a small dataset of size n and a fast optimization process. Despite the impressive performance, the estimation error suffers from the curse of dimensionality $n^{-1/D}$, where D is the data dimension. Since images are usually a union of low-dimensional manifolds, current works model the data as a union of linear subspaces with Gaussian latent and achieve a $1/\sqrt{n}$ bound. Though this modeling reflects the multi-manifold property of data, the Gaussian latent can not capture the multi-modal property of the latent manifold. To bridge this gap, we propose the mixture subspace of low-rank mixture of Gaussian (MoLR-MoG) modeling, which models the target data as a union of K linear subspaces, and each subspace admits a mixture of Gaussian latent (n_k modals with dimension d_k). With this modeling, the corresponding score function naturally has a mixture of expert (MoE) structure, captures the multi-modal information, and contains nonlinear properties since each expert is a nonlinear latent MoG score. We first conduct real-world experiments to show that the generation results of MoE-latent MoG NN are much better than the results of MoE-latent Gaussian score. Furthermore, MoE-latent MoG NN achieves a comparable performance with MoE-latent Unet with $10\times$ parameters. These results indicate that the MoLR-MoG modeling is reasonable and suitable for real-world data. After that, based on such MoE-latent MoG score, we provide a $R^4\sqrt{\Sigma_{k=1}^K n_k}\sqrt{\Sigma_{k=1}^K n_k d_k}/\sqrt{n}$ estimation error, which escapes the curse of dimensionality by using data structure. Finally, we study the optimization process and prove the convergence guarantee under the MoLR-MoG modeling. Combined with these results, under a setting close to real-world data, this work explains why diffusion models only require a small training sample and enjoy a fast optimization process to achieve a great performance.

1 INTRODUCTION

Recently, diffusion models have achieved impressive performance in many areas, such as 2D, 3D, and video generation (Rombach et al., 2022; Ho et al., 2022; Chen et al., 2023a; Ma et al., 2024; Liu et al., 2024). Due to the score matching technique, diffusion models enjoy a more stable training process and can achieve great performance with a small training dataset.

Despite the empirical success, the theoretical guarantee for the estimation and optimization error of the score matching process is lacking. For estimation error, current results suffer from the curse of dimensionality. More specifically, given training dataset $\{x^i\}_{i=1}^n$ with $x^i \in \mathbb{R}^D$, the estimation error of the score function achieve the minimax $n^{-s'/D}$ results for (conditional) diffusion models with deep ReLU NN and diffusion transformer, where s' is the smoothness parameter of the score function (Oko et al., 2023; Hu et al., 2024b;a; Fu et al., 2024). It is clear that this estimation error is heavily influenced by the external dimension D, which can not explain why diffusion models can generate great images with a small training dataset. Hence, a series of works studies estimation errors under specific target data structures and reduces the curse of dimensionality. There are two notable ways to model the target data: the multi-modal modeling and the low-dimensional modeling. For the multi-modal modeling, as the real-world target data is usually multi-modal, some works study the mixture of Gaussian (MOG) target data and improve the estimation error (Shah et al., 2023; Cui et al.,

2023; Chen et al., 2024). When we delve deeper into the images and text data, a key feature is that the image and text data usually admit a low-dimensional structure (Pope et al., 2021; Brown et al., 2023; Kamkari et al., 2024). Hence, one notable way is to assume the data admits a low-dimensional structure. More specifically, some works assume the data admits a linear subspace $x = Az$, where $A \in \mathbb{R}^{D\times d}$ to convert data to the latent space and $z \in \mathbb{R}^d$ is a bounded support (Chen et al., 2023b; Yuan et al., 2023; Guo et al., 2024). Then, they reduce the estimation error to $n^{-2/d}$, which removes the dependence of D. However, as shown in Brown et al. (2023) and Kamkari et al. (2024), though the image dataset admits low dimension, it is a union of manifolds instead of one manifold. Inspired by this observation, Wang et al. (2024) model the image data as a union of linear subspaces, assume each subspace admits a low-dimensional Gaussian (mixture of low-rank Gaussians (MoLRG)), and achieve a $1/\sqrt{n}$ estimation error. Though the union of the linear subspace is closer to the real-world image dataset, the latent Gaussian assumption is far away from the low-dimensional multi-modal manifold Brown et al. (2023). Hence, the following two natural questions remain open:

Can we propose a modeling that reflects the multi-manifold multi-modal property of real-world data?

Can we escape the curse of dimensionality and enjoy a fast convergence rate based on this modeling?

In this work, for the first time, we propose and analyze the mixture of low-rank mixture of Gaussian (MoLR-MoG) distribution, which is more realistic than MoLRG since it captures the multi-modal property of real-world distribution and has a nonlinear score function. Based on this modeling, we first induce a MoE-latent nonlinear score function and conduct experiments to show that MoLR-MoG modeling is closer to the real-world data. After that, we simultaneously analyze the estimation and optimization error of diffusion models and explain why diffusion models achieve great performance.

1.1 Our Contribution

MoLR-MoG modeling and MoE Structure Nonlinear Score. We propose the MoLR-MoG modeling for the target data, which captures the multi low-dimensional manifold and multi-modal property of real-world data and naturally introduces the MoE-latent MoG score. Through the real-world experiments, we show that with this score, diffusion models can generate images that is comparable with the deep neural network MoE-latent Unet and only has $10\times$ smaller parameters. On the contrary, the MoE-latent Gaussian score induced by previous MoLRG modeling can only generate blurry images, which indicates MoLR-MoG is a suitable modeling for the real-world data.

Take Advantage of MoLR-MoG to Escape the Curse of Dimensionality. For the estimation error, we show that by taking advantage of the union of a low-dimensional linear subspace and the latent MoG property, diffusion models escape the curse of dimensionality. More specifically, we achieve the $R^4\sqrt{\Sigma_{k=1}^K n_k}\sqrt{\Sigma_{k=1}^K n_k d_k}/\sqrt{n}$ estimation error, where R is the diameter of the target data, d_k is the latent dimension and n_k is the number of the modal in the k-the subspace. This result clearly shows the dependence on the number of linear subspaces, modal, and the latent dimensions R, d_k.

Strongly Convex Property and Convergence Guarantee. After directly analyzing the estimation error, we study how to optimize the highly non-convex score-matching objective function. We note that only two works analyze the optimization process under latent space (Yang et al., 2024a; Wang et al., 2024). However, they assume the latent distribution is Gaussian, whose score function is linear. In other words, the minimizer has a closed form. On the contrary, since latent MoG score is nonlinear, we use the gradient descent (GD) algorithm to optimize the objective function, which matches the real-world application. To calculate the Hessian matrix, we take advantage of the closed form of nonlinear MoG score and show that the landscape around the ground truth parameter is strongly convex. Then, with a great initialization area (around the ground-truth parameters), we prove the convergence guarantee when considering MoLR-MoG using the gradient descent algorithm.

Combined with the above results, this work adopts the realistic MoLR-MoG modeling and shows that diffusion models enjoy a small estimation error and a fast convergence rate, which explains the great performance of diffusion models in applications.

2 Related Work

Estimation Error Analysis for Diffusion Models. A series of works analyzes the estimation error of diffusion models. As a start, a series of works Oko et al. (2023) study the general target data

with a deep ReLU and transformer network and achieve the minimax $n^{-s'/D}$ result, where s is the smooth parameter (Oko et al., 2023; Hu et al., 2024b; Fu et al., 2024; Hu et al., 2024a). Then, some works analyze the general target data with a 2-layer wide random feature ReLU NN and achieve $n^{-2/5}$ estimation error with $\exp(n)$ NN size (Li et al., 2023; Han et al., 2024). For the multi-modal modeling, some works study MoG data and improve the estimation error (Shah et al., 2023; Cui et al., 2023; Chen et al., 2024). More specifically, Shah et al. (2023) and Cui et al. (2023) analyze MoG with known variance and achieve a $1/n$ estimation error. Chen et al. (2024) study a general MoG and show that the score matching technique can efficiently reduce the estimation error. Except for the MoG modeling, Cole and Lu (2024) assume the target data is close to the Gaussian distribution and then prove the model escapes the curse of dimensionality. Mei and Wu (2023) analyze Ising models and prove that the term corresponds to n is $1/\sqrt{n}$. For the low-dimensional modeling, some works assume the target data admits a linear subspace (Chen et al., 2023b; Yuan et al., 2023). Chen et al. (2023b) assume the target data admit a linear subspace $x = Az$ with a bounded latent variable $z \in \mathbb{R}^d$ and achieve a $n^{-2/d}$ estimation error. Yuan et al. (2023) analyze data with linear subspace with Gaussian latent and achieve $1/\sqrt{n}$ result. Based on the empirical observation that the image is a union of low-dimensional manifolds, Wang et al. (2024) models the target data as a union of linear subspaces with Gaussian latent and achieve $1/\sqrt{n}$ estimation error for each subspace.

Optimization Analysis for Diffusion Models. Since the score is highly nonlinear (except for Gaussian distribution), the score matching objective function is highly non-convex and non-smooth. Hence, only a few works analyze the optimization process, and most of them focus on the problem in the external dimensional space (Bruno et al., 2023; Cui and Zdeborová, 2023; Shah et al., 2023; Chen et al., 2024; Li et al., 2023; Han et al., 2024). Since the score function of MoG has a nonlinear closed-form, a series of works design algorithms for diffusion models to learn the MoG (Bruno et al., 2023; Cui and Zdeborová, 2023; Shah et al., 2023; Chen et al., 2024). For the general target data, Li et al. (2023) and Han et al. (2024) adopt a wide 2-layer ReLU NN to simplify the problem to a convex optimization. Then, they use the gradient flow algorithm to optimize the objective function and provide a global convergence guarantee. However, as the above discussion, their NN has $\exp(n)$ size, which is not used in the application. For the analysis of the latent space, only two works provide the optimization guarantee under the Gaussian latent (Yang et al., 2024a; Wang et al., 2024). More specifically, Yang et al. (2024a) assume the target data adopts a linear subspace with Gaussian latent and provide the closed-form minimizer of the objective function. Wang et al. (2024) analyze the optimization process of each linear subspace separately, which is also reduced to the optimization problem for the Gaussian distribution.

3 PRELIMINARIES

First, we introduce the basic knowledge and notation of diffusion models. Then, Sec.3.1 introduces our mixture of low-rank mixture of Gaussian (MoLR-MoG) modeling for the target data, which reflects the multi-modal and low-dimensional property of the real-world image and text data. Let p_0 be the data distribution. Given $x_0 \sim p_0 \in \mathbb{R}^D$, the forward process is defined by:

$$\mathrm{d}x_t = f(t)x_t\,\mathrm{d}t + g(t)\,\mathrm{d}B_t,$$

where $\{B_t\}_{t\in[0,T]}$ is a D-dimensional Brownian motion, $f(t)$ is the coefficient of the drift term and $g(t)$ is the coefficient of the diffusion term. Let p_t is the density function of the forward process. After determining the forward process, the conditional distribution $p_t(x_t|x_0)$ has a closed-form

$$p_t\left(x_t|x_0\right) = \mathcal{N}\left(x_t; s_t x_0, s_t^2\sigma_t^2 I_D\right),$$

where $s_t = \exp\left(\int_0^t f(\xi)\mathrm{d}\xi\right), \sigma_t = \sqrt{\int_0^t g^2(\xi)/s^2(\xi)\mathrm{d}\xi}$. To generate samples from p_0, diffusion models reverse the given forward process and obtain the following reverse process (Song et al., 2020):

$$\mathrm{d}y_t = \left[f(t)y_t - g(t)^2\nabla\log p_t(y_t)\right]\mathrm{d}t + g(t)\mathrm{d}\bar{B}_t, \quad y_0 \sim p_0$$

where $\bar{B}_t$ is a reverse-time Brownian motion. A conceptual way to approximate the score function is to minimize the score matching (SM) objective function:

$$\min_{s_\theta\in\mathrm{NN}} \mathcal{L}_{\mathrm{SM}} = \int_\delta^T \mathbb{E}_{x_t\sim q_t}\left\|\nabla\log p_t\left(x_t\right) - s_\theta(x_t,t)\right\|_2^2\mathrm{d}t\,, \tag{1}$$

where NN is a given function class and $\delta > 0$ is the early stopping parameter to avoid a blow-up score. Since the ground truth score $\nabla\log p_t$ is unknown, this objective function can not be calculated. To avoid this problem, Vincent (2011) propose the denoised score matching (DSM) objective function:

$$\min_{s_\theta \in \mathrm{NN}} \mathcal{L}_{\mathrm{DSM}} = \int_\delta^T \mathbb{E}_{x_0 \sim q_0} \mathbb{E}_{x_t|x_0} \left\| \nabla \log p_t\left(x_t|x_0\right) - s_\theta(x_t, t) \right\|_2^2 \mathrm{d}t\,.$$

As shown in Vincent (2011), the DSM and SM objective functions differ up to a constant independent of optimized parameters, which indicates these objective functions have the same landscape.

3.1 Mixture of low-rank mixture of Gaussian (MoLR-MoG) Modeling

In this part, we show our MoLR-MoG modeling, which reflects the low-dimensional (Gong et al., 2019) and multi-modal property (Brown et al., 2023; Kamkari et al., 2024) of real-world data. More specifically, we assume the data distribution lives near a union of K linear subspaces rather than arbitrary manifolds. Concretely, for the k-th subspace of dimension d_k (represented by a matrix $A_k^* \in \mathbb{R}^{D \times d_k}$ with orthonormal columns), we place a n_k-modal MoG within that subspace:

$$w_k(x) = \sum_{l=1}^{n_k} \pi_{k,l}\, \mathcal{N}\big(x; A_k^* \mu_{k,l}^*,\ A_k^* \Sigma_{k,l}^* A_k^{*\top}\big),$$

where covariance $\Sigma_{k,l}^* = U_{k,l}^* U_{k,l}^{*\top}, l = 1, \ldots, n_k$ with $U_{k,l}^* \in \mathbb{R}^{d_k \times d_{k,l}}$ ($d_{k,l} \le d_k$) and $\mu_{k,l}^*$ is the mean of the l-th modal of the k-th subspace. Then, the target distribution has the following form

$$p_0 = \sum_{k=1}^{K} \frac{1}{K} \sum_{l=1}^{n_k} \pi_{k,l}\, \mathcal{N}\big(x; A_k^* \mu_{k,l}^*,\ A_k^* \Sigma_{k,l}^* A_k^{*\top}\big)\,. \tag{2}$$

From the universal approximation perspective, by placing enough components and choosing parameters $\{\pi_{k,l}, \mu_{k,l}^*, \Sigma_{k,l}^*\}$, a MoG can approximate any smooth density arbitrarily well, which is more general than the Gaussian latent of Yang et al. (2024a) and Wang et al. (2024).

Nonlinear Mixture of Experts (MoE)-latent MoG score. Let $\gamma_t = s_t \sigma_t$, $\Sigma_{k,l,t,A} = s_t^2 A_k^* U_{k,l}^* U_{k,l}^{*\top} A_k^{*\top} + \gamma_t^2 I$ and $\delta_{k,l,t,A}(x) = x - s_t \mu_{k,l}^* - \frac{s_t^2}{s_t^2+\gamma_t^2} A_k^* U_{k,l}^* U_{k,l}^{*\top} A_k^{*\top}(x - s_t \mu_{k,l}^* A_k^*)$. Under the MoLR-MoG modeling, the score function has the following form:

$$\nabla \log p_t(x) = -\tfrac{1}{\gamma_t^2} \frac{\displaystyle\sum_{k=1}^{K} \frac{1}{K} \sum_{l=1}^{n_k} \pi_{k,l}\, \mathcal{N}(x; s_t \mu_{k,l}^* A_k^*,\, A_k^* \Sigma_{k,l,t,A}^* A_k^{*\top})\, \delta_{k,l,t,A}(x)}{\displaystyle\sum_{k=1}^{K} \frac{1}{K} \sum_{l=1}^{n_k} \pi_{k,l}\, \mathcal{N}(x; s_t \mu_{k,l}^* A_k^*,\, A_k^* \Sigma_{k,l,t,A} A_k^{*\top})}\,,$$

This score function has a MoE structure, where each expert is the latent nonlinear MoG score. The linear encoder A_k first encodes images to the k-th manifold, and diffusion models run the denoising process. After that, the linear decoder $A_k^\top$ decodes the denoised latent to the full-dimensional images. Since the estimation error introduced by the linear encoder and decoder has the order $Dd_k^3/\sqrt{n}$ (Yang et al., 2024a) and is not the dominant term, we assume the linear encoder and decoder are perfectly learned and focus on the more difficult latent MoG diffusion part in this work. From the empirical part, this operation is similar to using the pretrained stable diffusion VAE and only training the diffusion models in the latent space. For the k-th low-dimensional manifold, the score function is

$$\nabla \log p_{t,k}(x^{\mathrm{LD}}) = -\frac{1}{\gamma_t^2} \frac{\displaystyle\sum_{l=1}^{n_k} \pi_{k,l}\, \mathcal{N}(x^{\mathrm{LD}}; s_t \mu_{k,l}^*, \Sigma_{k,l,t}^*)\, \delta_{k,l,t}(x^{\mathrm{LD}})}{\displaystyle\sum_{l=1}^{n_k} \pi_{k,l}\, \mathcal{N}(x; s_t \mu_{k,l}^*, \Sigma_{k,l,t}^*)}, \tag{3}$$

where $x^{\mathrm{LD}} \in \mathbb{R}^{d_k}$ is a variable in the k-th low-dimensional subspace, $\Sigma_{k,l,t} = s_t^2 U_{k,l}^* U_{k,l}^{*\top} + \gamma_t^2 I$ and $\delta_{k,l,t}(x^{\mathrm{LD}}) = x^{\mathrm{LD}} - s_t \mu_{k,l}^* - \frac{s_t^2}{s_t^2+\gamma_t^2} U_{k,l}^* U_{k,l}^{*\top}(x^{\mathrm{LD}} - s_t \mu_{k,l}^*)$. Let

$$s_k^*(x^{\mathrm{LD}}, t) = \nabla \log p_{t,k}(x^{\mathrm{LD}})\,, s^*(x^{\mathrm{LD}}, t) = (s_1^*(x^{\mathrm{LD}}, t), s_2^*(x^{\mathrm{LD}}, t), \ldots, s_K^*(x^{\mathrm{LD}}, t))\,,$$

where the parameters are $\theta^* = \{\mu_{k,l}^*, U_{k,l}^*\}_{k=1,\ldots,K}$. In this work, we want to learn the parameters of the ground truth score function. Hence, we construct a NN function class $s_\theta = (s_1(\cdot,\cdot), s_2(\cdot,\cdot), ..., s_K(\cdot,\cdot))$ according to the above closed-from of MoE-latent MoG score. Let θ is the union of $\mu_{k,l}$ and $U_{k,l}$. Since we mainly focus on the estimation and optimization in the latent subspace, we omit the superscript LD of the latent subspace when there is no ambiguity.

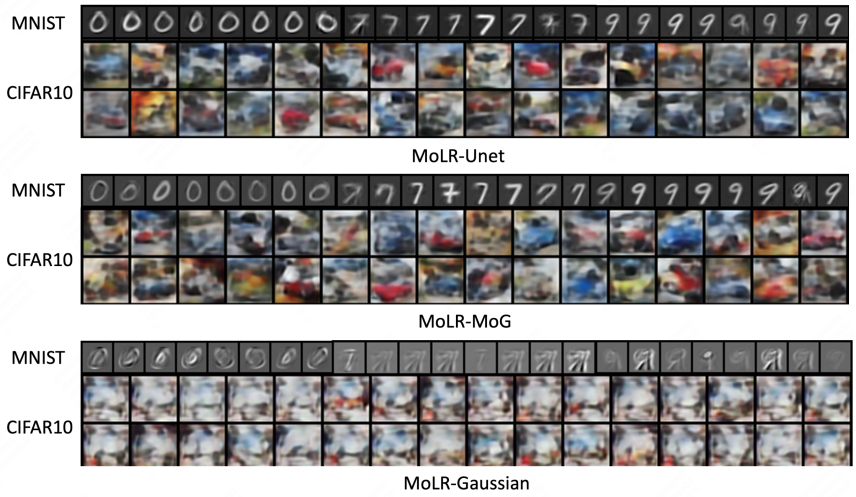
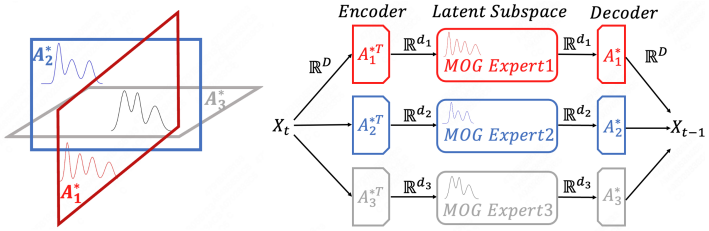


Figure 2: Results of Different Modeling on Real-world Data.

We note that this modeling can capture the information of each low-dimensional manifold and the multi-modal property of each latent distribution. In the next section, through the real-world experiments, we show that the MoE-latent MoG score has a better performance compared with the MoE-latent Gaussian score induced by MoLRG modeling and compatible with the results of the MoE-latent Unet. In Section 5 and 6, we prove that by using the property of MoLR-MoG modeling, diffusion models can escape the curse of dimensionality and enjoy a fast convergence rate.



(a) MoLR-MoG Modeling **(b) MoE-nonlinear MoG Score**

Figure 1: MoLR-MoG Modeling and Corresponding Nonlinear Score

Remark 3.1 (Comparison with MoLRG modeling). Wang et al. (2024) provide the first multi-subspace modeling under diffusion model setting, which is an important and meaningful step. However, they assume a Gaussian latent with 0 mean, which can not capture the multi-modal property of real-world data. We also note that the MoLR-MoG modeling can not be viewed as MoLRG with $\sum_{k=1}^{K} n_k$ subspace since this modeling assumes there are $\sum_{k=1}^{K} n_k$ VAE encoders and decoders, which is not reasonable in the real-world setting. On the contrary, the existing A_k^* of MoLR-MoG completes the clustering for the real-world data, shares information within the cluster, and has K subspaces.

4 Experiments for MoE-latent MoG Score

In this section, we conduct experiments using neural networks based on different modeling approaches (MoLR-MoG, MoLRG) as well as a general U-Net architecture. The goal is to demonstrate that MoLR-MoG provides a suitable modeling for real-world data, and that the MoE-latent MoG score is sufficient to generate images with clear semantic content. Specifically, we first show that training with MoLR-MoG yields significantly better results than the MoLRG model. Then, we show that, with appropriate initialization, the MoE-latent MoG network achieves performance comparable to that of the MoLR-U-Net, while using 10× fewer parameters (Figure 2).

Following Brown et al. (2023), we train 10 VAEs for each number in the MNIST dataset, which represents our K low-dimensional manifold. After obtaining these 10 VAE encoders and decoders, we train diffusion models with different parametrized NNs. We adopt three different parameterizations: latent U-net, latent MoG NN, and latent Gaussian NN. For the latent MoG, we adopt the form of the ground truth score function (Equation (3)) with $n_k = 4$ in MNIST and $n_k = 8$ in CIFAR-10 for $k \in [K]$.We set each mean and covariance metric to be trainable. For the latent Gaussian, we also adopt the form of the closed-form score function (Wang et al., 2024), which leads to a linear NN.

Discussion. As shown in Figure 2, the generation results with MoLRG modeling are difficult to distinguish specific numbers. On the contrary, Moe-latent MoG score can generate clean images comparable with the images generated by MoLR-Unet, which means this modeling captures the multi-modal property of each low-dimensional manifold. Furthermore, the MoLR-MoG NN contains many fewer parameters compared with Unet since it uses the prior of latent MoG. We note that these experiments aim to show that the MoLR-MoG modeling is reasonable instead of achieving the state-of-the-art performance. It is possible to achieve great performance with a small-sized NN using MoLR-MoG modeling in the application. For the large-scale data without labels, we can use the clustering algorithm to divide the datasets into different clusters. Then, we can train a VAE encoder, decoder, and latent MoG score for each cluster. We leave it as an interesting future work.

5 Escape the Curse of Dimensionality With MoLR-MoG Modeling

This section shows that diffusion models can escape the curse of dimensionality by using MoLR-MoG properties. Before introducing our results, we first introduce the assumption on the target data.

Assumption 5.1. For $x \sim p_0$, we have that $\|x\|_2 \leq R$.

The bounded-support assumption is widely used in theoretical works (Chen et al., 2022; Yang et al., 2024a;b) and is naturally satisfied by image datasets. For a latent MoG, each component concentrates almost all mass within a few standard deviations of its mean, so by taking the most component means and variances, one can choose R large enough that $\|x\|_2 \leq R$ holds with high probability.

Since Moe-latent MoG score has a closed-form, we only need to learn the parameters $\mu_{k,l}$ and $U_{k,l}$ at a fixed time t. As a result, we consider the estimation error at a fixed time t. Let $\ell(\theta; x, t) = \left\|s_\theta(x,t) - s^*(x,t)\right\|_2^2$ be the per-sample squared error at time t. In this part, we study the estimation error with a limited training dataset $\{x_i\}_{i=1}^n$:

$$\left|\mathcal{L}(\theta) - \widehat{\mathcal{L}}_n(\theta)\right| \text{, with } \widehat{\mathcal{L}}_n(\theta) = \frac{1}{n}\Sigma_{i=1}^n \ell(\theta; x_i, t)\,.$$

To obtain the estimation error, we first provide the Lipschitz constant for s_θ and the loss function by fully using the property of MoLR-MoG modeling and MoE-latent MoG score.

Lemma 5.2. *[Lipschitz Continuity] Let L_{μ_l} and L_{U_k} be the Lipschitz constant w.r.t. s_θ. With MoLR-MoG modeling and Assumption 5.1, there is a constant*

$$L \leq \sqrt{\Sigma_{i=1}^K n_k (L_{\mu_l}^2 + L_{U_k}^2)} = O\left((\Sigma_{k=1}^K n_k)^{\frac{1}{2}} C_w\right)$$

such that for any θ, θ', $\left\|s_\theta(x,t) - s_{\theta'}(x,t)\right\|_2 \leq L\,\|\theta - \theta'\|_2$, where $C_w = \frac{(R+s_t B_\mu)^3 s_t^2}{\gamma_t^4}$, $B_\mu = \max_{k,l}\|\mu_{k,l}\|_2$. For s_θ and s^*, we have that $2\|s_\theta(x,t) - s^*(x,t)\|_2 \leq 2(R + s_t B_\mu)/\gamma_t^2 := L_l$.

Then, we obtain the Lipschitz constant $L' = L_l L$ for the whole loss function. With this Lipschitz property, the next step is to argue that fitting the network on n samples generalizes to the true population loss. We do so by controlling the Rademacher complexity of the loss class and then using a Bernstein concentration argument to obtain the following theorem.

Theorem 5.3. *Denote by $\widehat{\mathcal{L}}_n(\theta)$ the empirical loss on n i.i.d. samples and by $\mathcal{L}(\theta)$ its population counterpart. Then there exist constants C_1, C_2 such that with probability at least $1-\delta$, for all $\theta \in \Theta$,*

$$\left|\mathcal{L}(\theta) - \widehat{\mathcal{L}}_n(\theta)\right| \;\leq\; O\left(C_1 \frac{(R + s_t B_\mu)^4 s_t^2 \sqrt{\Sigma_{k=1}^K n_k}}{\gamma_t^6} \sqrt{\frac{\Sigma_{k=1}^K n_k d_k}{n}} \;+\; C_2 \sqrt{\frac{\log(1/\delta)}{n}}\right).$$

where $C_1 = \max_{\theta\in\Theta}\|\theta_i - \theta_j\|_2$, $C_2 = \sigma \log 2$, $\sigma^2 = \sup_{\theta\in\Theta} Var[\ell(\theta; X, t)]$.

This result removes the exponential dependence on D with the number of latent subspace K, the latent dimension d_k, and the number of modalities n_k at each linear subspace, which reflects the key feature of the real-world data and escape the curse of dimensionality. The remaining question is why diffusion models enjoy a fast and stable optimization process. In the next part, we show that with MoLR-MoG modeling, the objective function is locally strongly convex and answer this question.

6 STRONGLY CONVEX PROPERTY AND CONVERGENCE GUARANTEE

In this part, by using the property of MoLR-MoG modeling, we derive explicit expressions for the *Jacobian* and *Hessian* of the objective function for 2-modal MoG latent and general MoG latent. Then, we establish conditions under which the resulting score-matching loss is locally strongly convex for each setting. Finally, we provide the convergence guarantee for the optimization.

6.1 2-MODAL LATENT MOG HESSIAN ANALYSIS AND OPTIMIZATION

In this section, we show that, under sufficient cluster separation, the Hessian matrix near θ^* simplifies to a block-diagonal form, yielding local strong convexity, which derives a linear convergence rate. As discussed in Section 3.1, following the real-world setting, we consider the optimization dynamic in the k-th latent subspace. While our modeling contains K encoders and decoders, facing an input image x, we can first determine which cluster image x belongs to, and then use the corresponding A_k to encode it into the corresponding latent space. Then, we only use data belonging to k clustering to train the k-th latent MoG score. This operation matches our experimental settings, and Wang et al. (2024) also adopts this operation. When considering the optimization problem, to simplify the calculation of the Hessian matrix, we set $d_{k,l} = 1$.

Similar to Shah et al. (2023), we start from a latent 2-modal MoG with the same covariance matrix Σ_k^* and $\mu_{k,1}^* = \mu_k^*, \mu_{k,2}^* = -\mu_k^*$, which leads to the following score:

$$\nabla \log p_{t,k}(x) = -\frac{1}{\gamma_t^2} \frac{\frac{1}{2}\mathcal{N}(x; s_t\mu_k^*, \Sigma_k^*)\, \delta_k'(x) + \frac{1}{2}\mathcal{N}(x; -s_t\mu_k^*, \Sigma_k^*)\, \epsilon_k(x)}{\frac{1}{2}\mathcal{N}(x; s_t\mu_k^*, \Sigma_k^*) + \frac{1}{2}(x; -s_t\mu_k^*, \Sigma_k^*)}, \tag{4}$$

where $\epsilon_k(x) = x - s_t\mu_k^* - \frac{s_t^2}{s_t^2+\gamma_t^2} U_k^* U_k^{*\top}(x - s_t\mu_k^*)$, and $\delta_k'(x) = x + s_t\mu_k^* - \frac{s_t^2}{s_t^2+\gamma_t^2} U_k^* U_k^{*\top}(x + s_t\mu_k^*)$. Before providing the convergence guarantee, we make an assumption on the 2-MoG latent distribution.

Assumption 6.1. [Separation within a cluster] Within each cluster k, the two symmetric peaks are well separated in the sense that $\|s_t\mu_k^* - (-s_t\mu_k^*)\| \geq \Delta_{\text{intra}}$, for some $\Delta_{\text{intra}} \gg \gamma_t$. Consequently, if a sample x is drawn from the "+" peak then its responsibility under the "−" peak satisfies

$$r_k^-(x) \;=\; \frac{\frac{1}{2}\,\mathcal{N}(x; -s_t\mu_k^*, \Sigma_k^*)}{\frac{1}{2}\,\mathcal{N}(x; s_t\mu_k^*, \Sigma_k^*) + \frac{1}{2}\,\mathcal{N}(x; -s_t\mu_k^*, \Sigma_k^*)} \;=\; O\big(e^{-\Delta_{\text{intra}}^2/(2\gamma_t^2)}\big) \;\ll\; 1,$$

and symmetrically $r_k^+(x) \ll 1$ when x is drawn from the "−" peak.

The above assumption means that the separation of the two modals is sufficient. For each symmetric sub-peak, if the distance between them is relatively small, we can view them as having a mean of 0. Since they are the same distribution ($\mu = 0$ and $\Sigma = U_k U_k^\top + \gamma_t^2 I$), they are the same regardless of how they mix, which indicates that we can assume $r_k^+ \approx 1$ or $r_k^- \approx 1$. Moreover, in practice, if raw data do not exhibit such clear gaps, one can always apply a simple linear embedding to magnify inter-mean distances relative to noise, thereby enforcing the same hard-assignment regime.

Lemma 6.2. *[Jacobian Simplification] Under Assumption 6.1, in a neighborhood of θ^* the first derivatives simplify to their "self-cluster" terms: $J_k^\mu(x) \;=\; \partial_{\mu_k} s_\theta \;\approx\; s_t(I - \alpha P_k)/\gamma_t^2$, and*

$$J_k^U(x) \approx \frac{2s_t^2}{\gamma_t^2(s_t^2+\gamma_t^2)}\big(r_k^-(x)(U_k^\top(x+s_t\mu_k)I + (x+s_t\mu_k)U_k^\top) + r_k^+(x)(U_k^\top(x-s_t\mu_k)I + U_k(x-s_t\mu_k)^\top)\big)\,.$$

Lemma 6.3. *[Eigenvalues of the Hessian blocks] Under the same conditions, H is convex. If $\forall x \in \mathbb{R}^{d_k}, r_k^+(x) = 1$ or $r_k^-(x) = 1$ are strictly satisfied, the eigenvalues of the Hessian at θ^* are*

$$\lambda_{\min}(H_{\mu_k\mu_k}) = \frac{s_t^2}{(s_t^2+\gamma_t^2)^2}\,, \textit{and}$$

$$\lambda_{\min}(H_{U_kU_k}) = \frac{4(U_k^\top\mu_k))^2 + \|U_k\|_2^2\|\mu_k\|_2^2 - \|U_k\|_2\|\mu_k\|_2\sqrt{8(U_k^\top\mu_k))^2 + \|U_k\|_2^2\|\mu_k\|_2^2}}{2}.$$

Since the ground truth score function has a closed-form under the MoLR-MoG modeling, we focus on the score matching objective function $\mathcal{L}_{\text{SM}}(\theta)$ instead of $\mathcal{L}_{\text{DSM}}(\theta)$ and abbreviate $\mathcal{L}_{\text{SM}}(\theta)$ as

$\mathcal{L}(\theta)$. We note that $\mathcal{L}_{\mathrm{SM}}(\theta)$ and $\mathcal{L}_{\mathrm{DSM}}(\theta)$ are equivalent up to a constant independent of θ, which indicates the optimization landscape is the same. Furthermore, when considering the convergence guarantee under a 2-layer wide ReLU NN, Li et al. (2023) also adopt score matching objective $\mathcal{L}_{\mathrm{SM}}$ instead of $\mathcal{L}_{\mathrm{DSM}}$. Then, we provide the local strongly convexity parameters for the objective function.

Lemma 6.4. *[Local Strong Convexity] Combining Lemma 6.3 with continuity of $\nabla^2\mathcal{L}$, there exist $\alpha > 0$ and neighborhood U of θ^* such that $\nabla^2\mathcal{L}(\theta) \succeq \alpha I, \forall\theta \in \Theta$.If $\forall x \in \mathbb{R}^{d_k}, r_k^+(x) = 1$ or $r_k^-(x) = 1$ are strictly satisfied,*

$$\alpha = \min\left\{\frac{s_t^2}{(s_t^2+\gamma_t^2)^2}, \frac{4(U_k^\top\mu_k))^2 + \|U_k\|_2^2\|\mu_k\|_2^2 - \|U_k\|_2\|\mu_k\|_2\sqrt{8(U_k^\top\mu_k))^2 + \|U_k\|_2^2\|\mu_k\|_2^2}}{2}\right\}.$$

Theorem 6.5. *[Local Linear Convergence] Under Assumptions 5.1 and 6.1, if we take $\eta_m = \eta = 2/(\eta + L')$, and $\kappa = L'/\alpha$, then there exists a neighborhood U of θ^* such that*

$$\|\theta^{(m)} - \theta^\star\|_2 \leq \left(\tfrac{\kappa-1}{\kappa+1}\right)^t \|\theta^{(0)} - \theta^\star\|_2 ,$$

where m is the number of gradient descent iteration.

This result gives a lower bound on the convergence rate near $\theta^\star$. Due to its strongly convex property, the convergence rate is fast, which explains the fast and stable optimization process.

Proof Overview. Assumption 6.1 justifies the Jacobian simplification (Lemma 6.2), which in turn yields the Hessian block structure (Lemma 6.3). By Schur complement, this result gives local strong convexity (Lemma 6.4). Combining with the Lipschitz constant, we finish the proof.

6.2 General MoG Latent Hessian Analysis and Optimization

We now extend our analysis to the case where each subspace k carries an *asymmetric* Gaussian mixture (Equation 3). As before, we first state the key separation assumption and show that on each subspace, the individual Gaussian distributions in the mixture of Gaussian are highly separated from each other. Then, we simplify the Hessian and prove local convexity. Finally, we conclude a linear convergence rate based on the strongly convex and smooth property.

Assumption 6.6. [Highly separated Gaussian] Consider the Gaussian mixture

$$p_k(x) = \sum_{l=1}^{n_k} \pi_{k,l}\,\mathcal{N}(x;\mu_{k,l},\Sigma_{k,l}), \qquad r_{k,l}(x) := \frac{\pi_{k,l}\,\mathcal{N}(x;\mu_{k,l},\Sigma_{k,l})}{\sum_{i=1}^{n_k}\pi_{k,i}\,\mathcal{N}(x;\mu_{k,i},\Sigma_{k,i})}.$$

There exist constants $\varepsilon \ll 1$ and $\delta \ll 1$ such that when $x \sim p_k$ we have

$$\Pr_{x\sim p_k}\Big(\exists\, l \in \{1,\dots,n_k\} \text{ with } r_{k,l}(x) \geq 1-\varepsilon\Big) \;\geq\; 1-\delta.$$

Justification. With MoLR-MoG modeling, after adding diffusion noise of scale γ_t, each point x remains within $O(\gamma_t)$ of the subspace's moment-matched center $\bar{\mu}_k$. Concretely, the subspace structure (or a preliminary projection onto principal components) ensures $\|x - \bar{\mu}_k\|_2 \leq \Delta = C\gamma_t$ with high probability, for some moderate constant C. Hence, any third-order Taylor term $\propto \|x-\bar{\mu}_k\|^3$ is $O(\gamma_t^3)$, which vanishes compared to the leading Hessian scale $O(\gamma_t^2)$. In the following corollary, we further show the approximation effect of equivalent Gaussians.

Corollary 6.7. *Assume that $\|\mu^*_{k,i} - \mu^*_{k,j}\|_2 \leq \delta$, $\|U^*_{k,i} - U^*_{k,j}\|_2 \leq \epsilon$ and $\|x - \bar{\mu}^*_k\|_2 \leq \Delta$. We have*

$$\|\log p(x) - \log\bar{p}(x)\|_2 = O(\epsilon + \delta\Delta + \Delta^3)$$

Remark 6.8 (Separated Gaussian simplification). For simplicity of description, we assume the individual Gaussian distributions in the mixture of Gaussians are highly separated. Actually, if there are n'_k Gaussians that are not separated from each other, we can employ clustering techniques to transform them into n_k mutually independent Gaussian distributions. The error caused by such an operation can be calculated using corollary 6.7. The core intuition is that the modals should not have much influence on each other. Hence, we can also use the idea of recursion to first cluster the general MoG into a 2-modal MoG latent. Then, we can use the analysis of Section 6.1 with Assumption 6.1.

Then, similar to the above section, we also calculate the Hessian matrix and show the local strong convex parameters. Finally, we provide the convergence guarantee for general MoLR-MoG modeling.

Lemma 6.9. *[Eigenvalues of the Hessian] Assume Assumption 6.6, the Hessian at the k-th subspace is convex on a neighborhood of θ^*. If $\forall x \in \mathbb{R}^{d_k}$, $r_k^+(x) = 1$ or 1 are strictly satisfied, we have*

$$\lambda_{\min}(H_{\mu_{k,l}\mu_{k,l}}) = \frac{\pi_{k,l} s_t^2}{(s_t^2+\gamma_t^2)^2},$$

and $\lambda_{\min}(H_{U_{k,l}U_{k,l}})$ has the following form:

$$\left(\pi_{k,l} 4(U_{k,l}^\top \mu_{k,l}))^2 + \|U_{k,l}\|_2^2\|\mu_{k,l}\|_2^2 - \|U_{k,l}\|_2\|\mu_{k,l}\|_2\sqrt{8(U_{k,l}^\top\mu_{k,l}))^2 + \|U_{k,l}\|_2^2\|\mu_{k,l}\|_2^2}\right)/2.$$

Lemma 6.10. *[Local Strong Convexity] Assume Assumption 6.6, in a neighborhood of θ^*, $\nabla^2\mathcal{L}(\theta) \succeq \alpha' I, \alpha' > 0, \forall \theta \in \Theta$. If $\forall x \in \mathbb{R}^{d_k}$, $\exists l \in [n_k], r_{k,l}(x) = 1$ are strictly satisfied, $\alpha' = \min\{\lambda_1, \lambda_2\}$, where $\lambda_1 = \min_{l=1\dots,n_k} \frac{c_{k,l}\gamma_t^4}{(s_t^2+\gamma_t^2)^2}$, $\lambda_2 = \min_{l=1,2,\dots,n_k} = \lambda_{\min}(H_{U_{k,l}U_{k,l}})$.*

Thus, even without symmetry, equivalent Gaussians and sufficient subspace separation recover the same local convexity and linear convergence guarantees as in the asymmetric case. Similar to Theorem 6.5, under Assumption 6.6, we can obtain a convergence guarantee.

Remark 6.11 (Previous MoG Learning through Score Matching). Shah et al. (2023) and Chen et al. (2024) consider MoG data and analyze the optimization process of diffusion models at the full space. However, these works aim to design a specific algorithm to learn the MoG distribution instead of using a standard optimization algorithm. On the contrary, by using the MoLR-MoG property to calculate the Hessian matrix, we adopt the GD algorithm and obtain the convergence guarantee.

Remark 6.12 (Initialization). Since the multi-modal GMM latent leads to a highly non-convex landscape, Theorem 6.5 and the corresponding asymmetric variant require the initialization to be around θ^* to guarantee local strong convexity and obtain a local convergence guarantee. As the MoLR-MoG is the first step to model the multi low-dimensional and multi-modal property, we leave the analysis of the global convergence guarantee as an interesting future work.

7 Conclusion

In this work, we provide a mixture of low-rank mixture of Gaussian (MoLR-MoG) modeling for target data, which reflects the low-dimensional and multi-modal property of real-world data. Through the real-world experiments, we first show that the MoLR-MoG is a suitable modeling for the real-world data. Then, we analyze the estimation error and optimization process under the MoLR-MoG modeling and explain why diffusion models can achieve great performance with a small training dataset and a fast optimization process.

For the estimation error, we show that with the MoLR-MoG modeling, the estimation error is $R^4\sqrt{\Sigma_{k=1}^K n_k}\sqrt{\Sigma_{k=1}^K n_k d_k}/\sqrt{n}$, which means diffusion models can take fully use of the multi subspace, low-dimensional and multi-modal information to escape the curse of dimensionality. For the optimization process, we conducted a detailed analysis of the score-matching loss landscape. By formulating the exact score in both symmetric and asymmetric mixture settings, we derived explicit expressions for the parameter Jacobians and identified the dominant components under standard separation assumptions. Then, we prove that the population loss becomes strongly convex in a neighborhood of the ground truth score function, by estimating the Hessian and presenting lower bounds on both its minimal eigenvalue and the convergence rate. Then, we provide the local convergence guarantee for the score matching objective function, which explains the fast and stable training process of diffusion models.

Future work and limitation. Though we have extended the situation to multi-manifold MoG, how to extend the analysis to more general non-Gaussian sub-manifolds (e.g. heavy-tailed or multi-modal beyond second moments) by higher-order moment matching is still unknown. Meanwhile, we wish to design optimization algorithms or network architectures that explicitly leverage the block-diagonal Hessian structure for faster training. For example, we can perform a natural-gradient step separately in each block with a block-diagonal Hessian with decomposed data, which will accelerate the optimization process.

Ethics statement. Our work aims to deepen the understanding of the modeling of diffusion models and explain the success of diffusion models from a theoretical perspective. The MoLR-MoG modeling has the potential to achieve a great performance with fewer parameters. Hence, this work can be viewed as an important step in understanding diffusion models, and the societal impact is similar to general generative models (Mirsky and Lee, 2021).

Reproducibility statement. The detail and description of the real-world experiments are provided in Appendix E. We detail the model, hyperparameters and data.

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APPENDIX

A THE USE OF LARGE LANGUAGE MODELS (LLMS)

As this work mainly focus on the new modeling of diffusion models from a theoretical perspective, large language models were only used for minor language editing to check grammar. All ideas, new modelings, experiments, theoretical guarantee, discussion and writing decisions were made entirely by the authors.

B SCORE FUNCTION ERROR ESTIMATION

B.1 CALCULATE $\nabla \log p_t(x)$ AND DECOMPOSITION

Consider the k-th subspace

$$p_{t,k}(x) = \sum_{l=1}^{n_k} \pi_{k,l} \mathcal{N}\left(\mu_{k,l}, \Sigma_{k,l}\right)$$

where $\Sigma_{k,l} = s_t^2 U_{k,l} U_{k,l}^\top + \gamma_t^2 I$.

We know that

$$\Sigma_{k,l}^{-1} = \frac{1}{\gamma_t^2}\left(I - \frac{s_t^2}{s_t^2+\gamma_t^2} U_{k,l} U_{k,l}^\top\right),$$
$$\nabla p_{t,k}(x) = \frac{1}{\gamma_t^2} \sum_{l=1}^{n_k} \pi_{k,l} \mathcal{N}(\mu_{k,l}, \Sigma_{k,l}) \left(I - \frac{s_t^2}{s_t^2+\gamma_t^2} U_{k,l} U_{k,l}^\top\right)(x - \mu_{k,l}),$$

which indicates

$$\nabla \log p_{t,k}(x) = \frac{\nabla p_{t,k}(x)}{p_{t,k}(x)} = \frac{1}{\gamma_t^2} \frac{\sum_{l=1}^{n_k} \pi_{k,l} \mathcal{N}(\mu_{k,l}, \Sigma_{k,l}) \left(I - \frac{s_t^2}{s_t^2+\gamma_t^2} U_{k,l} U_{k,l}^\top)(x - \mu_{k,l}\right)}{\sum_{l=1}^{n_k} \pi_{k,l} \mathcal{N}(\mu_{k,l}, \Sigma_{k,l})}.$$

We want to learn the parameters of the score function:

$$s_k^*(x,t) = \nabla \log p_{t,k}(x),$$

where the parameters are $\{\mu_{k,l}^*, U_{k,l}^*\}, k = 1, ..., K$.

And

$$s^*(x,t) = (s_1^*(x,t), s_2^*(x,t), \ldots, s_K^*(x,t))$$

Define

$$R(s_k) = \mathbb{E}\left[\|s_k(x,t) - s_k^*(x,t)\|^2\right], \quad \hat{R}_n(s_k) = \frac{1}{n}\sum_{i=1}^{n} \|s_k(x_i,t_i) - s_k^*(x_i,t_i)\|^2$$

We have the following decomposition:

$$R(\hat{s}_{k,\hat{\theta}_n}) - \hat{R}_n(s_{k,\hat{\theta}_n}) = \underbrace{R(\hat{s}_{k,\hat{\theta}_n}) - \hat{R}(s_k^*)}_{\text{Estimation}} + \underbrace{\hat{R}(s_k^*) - \hat{R}(s_{k,\theta^*})}_{\text{Approximation}} + \underbrace{\hat{R}_n(s_{k,\theta^*}) - \hat{R}_n(\hat{s}_{k,\hat{\theta}_n})}_{\text{optimization}}$$

We can also obtain that

$$R(s) = \sum_{k=1}^{K} R(s_k)$$

Since *Estimation* and *Approximation* reflect the fitting ability of the network, we analyze the first term first. Then, in the next section, we analyze the optimization dynamic.

B.2 ESTIMATION

First, we show that f and loss function are Lipschitz. We will first prove that s_k is Lipschitz for $\forall k$, then we can know that s is Lipschitz.

Lemma B.1. *[Lipschitz Continuity] Let L_{μ_l} and L_{U_k} be the Lipschitz constant w.r.t. s_θ. With MoLR-MoG modeling and Assumption 5.1, there is a constant*

$$L \leq \sqrt{\Sigma_{i=1}^{K} n_k (L_{\mu_l}^2 + L_{U_k}^2)} = O\left((\Sigma_{k=1}^{K} n_k)^{\frac{1}{2}} C_w\right)$$

such that for any θ, θ', $\left\|s_\theta(x,t) - s_{\theta'}(x,t)\right\|_2 \leq L\left\|\theta - \theta'\right\|_2$, where $C_w = \frac{(R+s_t B_\mu)^3 s_t^2}{\gamma_t^4}$, $B_\mu = \max_{k,l} \|\mu_{k,l}\|_2$. For s_θ and s^*, we have that $2\|s_\theta(x,t) - s^*(x,t)\|_2 \leq 2(R + s_t B_\mu)/\gamma_t^2 := L_l$.

Proof. Since we analyze the estimation error at a fixed time t, we ignore subscript t for $\Sigma_{k,l,t}$, $w_{k,t}$, $w_{l,k,t}$ and $\delta_{k,l,t}$ and define by

$$\begin{aligned}
\Sigma_{k,l} &= s_t^2 U_{k,l} U_{k,l}^\top + \gamma_t^2 I \\
w_k(x) &= \Sigma_{l=1}^{n_k} \pi_{k,l} \mathcal{N}(x; s_t \mu_{k,l}, \Sigma_{k,l}) \\
w_{k,l} &= \frac{1}{M} \pi_{k,l} \mathcal{N}(x; s_t \mu_{k,l}, \Sigma_{k,l}) \\
\delta_{k,l}(x) &= x + s_t \mu_{k,l} - \frac{s_t^2}{s_t^2 + \gamma_t^2} U_{k,l} U_{k,l}^\top (x + s_t \mu_{k,l}) \,.
\end{aligned}$$

Assume that $\|U_{k,l}\|_2 \leq B_U, \|\mu_{k,l}\|_2 \leq B_\mu, \max\{B_U, B_\mu\} = C$, and $\|x\|_2 \leq R$ for $\forall x \in X$.

For $\Sigma_{k,l}$, we know that

$$\Sigma_{k,l} = U_{k,l} U_{k,l}^\top + \gamma_t^2 I \succ \gamma_t^2 I \Rightarrow \lambda_{min}(\Sigma_{k,l}) \geq \gamma_t^2 \Rightarrow \|\Sigma_{k,l}^{-1}\|_2 \leq \frac{1}{\gamma_t^2} \,.$$

To obtain the first L in this lemma, we need to bound $\left\|\frac{\partial s_{k,\theta}(x,t)}{\partial \mu_{k,l}}\right\|_2$ and $\left\|\frac{\partial s_{k,\theta}(x,t)}{\partial U_{k,l}}\right\|_2$.

The bound of $\left\|\frac{\partial s_{k,\theta}(x,t)}{\partial \mu_{k,l}}\right\|_2$. For the latent score of the k-th subspace, we have that

$$\begin{aligned}
&s_{k,\theta}(x,t) = -\frac{1}{\gamma_t^2} \frac{\Sigma_{l=1}^{n_k} w_{k,l}(x) \delta_{k,l}(x)}{w_k(x)} \,, \\
&\frac{\partial s_{k,\theta}(x,t)}{\partial \mu_{k,l}} = -\frac{1}{\gamma_t^2} \frac{\Sigma_{l=1}^{n_k} (\frac{\partial w_{k,l}(x)}{\partial \mu_{k,l}} \delta_{k,l}(x) + \frac{\partial \delta_{k,l}(x)}{\partial \mu_{k,l}} w_{k,l}(x)) w_k(x) - \frac{\partial w_k(x)}{\partial \mu_{k,l}} (\Sigma_{l=1}^{n_k} w_{k,l}(x) \delta_{k,l}(x))}{w_k^2(x)} \,, \\
&\left\|\frac{\partial s_{k,\theta}(x,t)}{\partial \mu_{k,l}}\right\|_2 \leq \frac{1}{\gamma_t^2} \left(\left\| \frac{\Sigma_{l=1}^{n_k} (\frac{\partial w_{k,l}(x)}{\partial \mu_{k,l}} \delta_{k,l}(x) + \frac{\partial \delta_{k,l}(x)}{\partial \mu_{k,l}} w_{k,l}(x))}{w_k(x)} \right\|_2 + \left\| \frac{\frac{\partial w_k(x)}{\partial \mu_{k,l}} (\Sigma_{l=1}^{n_k} w_{k,l}(x) \delta_{k,l}(x))}{w_k^2(x)} \right\|_2 \right) .
\end{aligned}$$

To bound this term, we separately show that

$(1) w_k(x)$ has a lower bound.

$(2) w_{k,l}(x)$, $\delta_{k,l}(x)$, $\frac{\partial w_{k,l}(x)}{\partial \mu_k}$, $\frac{\partial \delta_{k,l}(x)}{\partial \mu_k}$ have upper bounds.

$(3) \left\| \frac{\frac{\partial w_k(x)}{\partial \mu_{k,l}} \delta_{k,l}(x)}{w_k} \right\|_2$, $\left\| \frac{\Sigma_{l=1}^{n_k} \frac{\partial \delta_{k,l}(x)}{\partial \mu_{k,l}} w_{k,l}(x)}{w_k(x)} \right\|_2$, $\left\| \frac{\frac{\partial w_k(x)}{\partial \mu_{k,l}} \Sigma_{l=1}^{n_k} w_{k,l}(x) \delta_{k,l}(x)}{w_k^2(x)} \right\|_2$ have upper bounds.

(1) $w_k(x)$ has a lower bound.

$$w_k(x) = \Sigma_{l=1}^{n_k} \pi_{k,l} \mathcal{N}(x; s_t \mu_{k,l}, \Sigma_{k,l}), \text{which is continuous.}$$

Since continuous function has maximum and minimum in a closed internal and $\|x\|_2 \leq R$, we can assume that $w_k(x) \geq m_w$. And for any x, $w_k(x) > 0$, so $m_w > 0$ holds.

(2) $w_{k,l}(x)$, $\delta_{k,l}(x)$, $\frac{\partial \delta_{k,l}(x)}{\partial \mu_k}$, $\frac{\partial w_{k,l}(x)}{\partial \mu_k}$ have upper bounds.

We already know that continuous function has maximum and minimum in a closed internal and $\|x\|_2 \leq R$. Thus, we can assume that $w_k(x) \leq M_{w_k}$. We also have that

$$w_k(x) \leq M_{w_k} \leq \Sigma_{l=1}^{n_k} \pi_{k,l} (2\pi)^{-\frac{n}{2}} |\Sigma_{k,l}|^{-\frac{1}{2}} .$$

For the second term, we have that

$$\delta_{k,l}(x) = x - s_t \mu_{k,l} - \frac{s_t^2}{s_t^2 + \gamma_t^2} U_{k,l} U_{k,l}^\top (x - s_t \mu_{k,l}) = \left(I - \frac{s_t^2}{s_t^2 + \gamma_t^2} U_{k,l} U_{k,l}^\top \right) (x - s_t \mu_{k,l}) ,$$

whose L_2 norm is bounded by

$$\left\| \left(I - \frac{s_t^2}{s_t^2 + \gamma_t^2} U_{k,l} U_{k,l}^\top \right) (x - s_t \mu_{k,l}) \right\|_2 \leq \|x - s_t \mu_{k,l}\|_2 \leq \|x\|_2 + \|s_t \mu_{k,l}\|_2 \leq R + s_t B_\mu .$$

Then, for the third term, we know that

$$\frac{\partial \delta_{k,l}(x)}{\partial \mu_{k,l}} = -s_t + \frac{s_t^3}{s_t^2 + \gamma_t^2} U_{k,l} U_{k,l}^\top = -s_t \left(I - \frac{s_t^2}{s_t^2 + \gamma_t^2} U_{k,l} U_{k,l}^\top \right) .$$

For the last term, we have we have the following expression

$$\frac{\partial w_{k,l}(x)}{\partial \mu_{k,l}} = -\frac{s_t}{2} \mathcal{N}(x; s_t \mu_{k,l}, \Sigma_{k,l}) \Sigma_{k,l}^{-1} (x - s_t \mu_{k,l}) .$$

For term $\|\Sigma_{k,l}^{-1}(x - s_t \mu_{k,l})\|_2$, we have that

$$\|\Sigma_{k,l}^{-1}(x - s_t \mu_{k,l})\|_2 \leq \|\Sigma_{k,l}^{-1}\|_2 \|x - s_t \mu_{k,l}\|_2 = \frac{1}{\gamma_t^2} \|x - s_t \mu_{k,l}\|_2 \leq \frac{1}{\gamma_t^2} (R + \|s_t \mu_{k,l}\|_2) ,$$

which indicates

$$\left\| \frac{\partial w_{k,l}(x)}{\partial \mu_{k,l}} \right\|_2 \leq s_t \mathcal{N}(x; s_t \mu_{k,l}, \Sigma_{k,l}) \frac{1}{\gamma_t^2} (R + \|s_t \mu_{k,l}\|_2) \leq s_t \mathcal{N}(x; s_t \mu_{k,l}, \Sigma_{k,l}) \frac{1}{\gamma_t^2} (R + s_t B_\mu)$$

$$\left\| \frac{\partial w_k(x)}{\partial \mu_{k,l}} \right\|_2 \leq \Sigma_{l=1}^{n_k} s_t \mathcal{N}(x; s_t \mu_{k,l}, \Sigma_{k,l}) \frac{1}{\gamma_t^2} (R + s_t B_\mu).$$

(3) $\left\| \frac{\frac{\partial w_k(x)}{\partial \mu_{k,l}} \delta_{k,l}(x)}{w_k} \right\|_2$, $\left\| \frac{\Sigma_{l=1}^{n_k} \frac{\partial \delta_{k,l}(x)}{\partial \mu_{k,l}} w_{k,l}(x)}{w_k(x)} \right\|_2$, $\left\| \frac{\frac{\partial w_k(x)}{\partial \mu_{k,l}} \Sigma_{l=1}^{n_k} w_{k,l}(x) \delta_{k,l}(x)}{w_k^2(x)} \right\|_2$ have upper bounds.

For the first two term,

$$\left\| \frac{\frac{\partial w_k(x)}{\partial \mu_{k,l}} \delta_{k,l}(x)}{w_k} \right\|_2 \leq \frac{s_t}{\gamma_t^2} (R + s_t B_\mu)^2 ,$$

and

$$\left\| \frac{\partial \delta_{k,l}(x)}{\partial \mu_{k,l}} \right\|_2 = \text{Constant} \leq s_t , \left\| \frac{\Sigma_{l=1}^{n_k} \frac{\partial \delta_{k,l}(x)}{\partial \mu_{k,l}} w_{k,l}(x)}{w_k(x)} \right\|_2 \leq s_t .$$

For the third term, we know that

$$\left\| \frac{\frac{\partial w_k(x)}{\partial \mu_{k,l}} \Sigma_{l=1}^{n_k} w_{k,l}(x) \delta_{k,l}(x)}{w_k^2(x)} \right\|_2 \leq \left\| \frac{s_t w_k^2(x) \frac{s_t}{\gamma_t^2} (R + s_t B_\mu)}{w_k^2(x)} \right\|_2 = \frac{s_t^2}{\gamma_t^2} (R + s_t B_\mu) .$$

Combined with the above three, we obtain the bound for $\left\| \frac{\partial s_{k,\theta}(x,t)}{\partial \mu_{k,l}} \right\|_2$:

$$\left\| \frac{\partial s_{k,\theta}(x,t)}{\partial \mu_{k,l}} \right\|_2 \leq \frac{1}{\gamma_t^2} \left(\left\| \frac{\Sigma_{l=1}^{n_k} (\frac{\partial w_{k,l}(x)}{\partial \mu_{k,l}} + \frac{\partial \delta_{k,l}(x)}{\partial \mu_{k,l}}) \delta_{k,l}(x)}{w_k(x)} \right\|_2 + \left\| \frac{\frac{\partial w_k(x)}{\partial \mu_{k,l}} (\Sigma_{l=1}^{n_k} w_{k,l}(x) \delta_{k,l}(x))}{w_k^2(x)} \right\|_2 \right)$$

$$\leq \frac{s_t^2}{\gamma_t^2} (R + s_t B_\mu)^2 + s_t + \frac{s_t}{\gamma_t^2} (R + s_t B_\mu) = O\left(\frac{s_t^2 (R + s_t B_\mu)^2}{\gamma_t^2} \right) .$$

The bound of $\left\|\frac{\partial s_{k,\theta}(x,t)}{\partial U_{k,l}}\right\|_2$. Now we compute the part about $U_{k,l}$. Through some simple algebra, we know that

$$\frac{\partial s_{k,\theta}(x,t)}{\partial U_{k,l}} = -\frac{1}{\gamma_t^2}\frac{\Sigma_{l=1}^{n_k}(\frac{\partial w_{k,l}(x)}{\partial U_{k,l}}\delta_{k,l}(x) + \frac{\partial \delta_{k,l}(x)}{\partial U_{k,l}}w_{k,l}(x))w_k(x) - \frac{\partial w_k(x)}{\partial U_{k,l}}(\Sigma_{l=1}^{n_k}w_{k,l}(x)\delta_{k,l}(x))}{w_k^2(x)}\,.$$

Then, we have the following inequality

$$\frac{\partial s_{k,\theta}(x,t)}{\partial U_{k,l}} = -\frac{1}{\gamma_t^2}\frac{\Sigma_{l=1}^{n_k}(\frac{\partial w_{k,l}(x)}{\partial U_{k,l}}\delta_{k,l}(x) + \frac{\partial \delta_{k,l}(x)}{\partial U_{k,l}}w_{k,l}(x))w_k(x) - \frac{\partial w_k(x)}{\partial U_{k,l}}(\Sigma_{l=1}^{n_k}w_{k,l}(x)\delta_{k,l}(x))}{w_k^2(x)}$$

$$\left\|\frac{\partial s_{k,\theta}(x,t)}{\partial U_{k,l}}\right\|_2 \le \frac{1}{\gamma_t^2}\left(\left\|\frac{\Sigma_{l=1}^{n_k}(\frac{\partial w_{k,l}(x)}{\partial U_{k,l}}\delta_{k,l}(x) + \frac{\partial \delta_{k,l}(x)}{\partial U_{k,l}}w_{k,l}(x))}{w_k(x)}\right\|_2 + \left\|\frac{\frac{\partial w_k(x)}{\partial U_{k,l}} * (\Sigma_{l=1}^{n_k}w_{k,l}(x)\delta_{k,l}(x))}{w_k^2(x)}\right\|_2\right)\,.$$

Similar with $\left\|\frac{\partial s_{k,\theta}(x,t)}{\partial \mu_{k,l}}\right\|_2$, we need to provide:

(1) The upper bound of $\frac{\partial w_{k,l}}{\partial U_{k,l}}$ and $\frac{\partial \delta_{k,l}}{\partial U_{k,l}}$,

(2) The upper bound of $\left\|\frac{\Sigma_{l=1}^{n_k}(\frac{\partial w_{k,l}(x)}{\partial U_{k,l}}\delta_{k,l}(x)+\frac{\partial \delta_{k,l}(x)}{\partial U_{k,l}}w_{k,l}(x))}{w_k(x)}\right\|_2$ and $\left\|\frac{\frac{\partial w_k(x)}{\partial U_{k,l}}*(\Sigma_{l=1}^{n_k}w_{k,l}(x)\delta_{k,l}(x))}{w_k^2(x)}\right\|_2$.

(1) The upper bound of $\frac{\partial w_{k,l}}{\partial U_{k,l}}$ and $\frac{\partial \delta_{k,l}}{\partial U_{k,l}}$.

For the first term, we have the following form

$$\begin{aligned}\frac{\partial w_{k,l}}{\partial U_{k,l}} &= \pi_{k,l}\frac{\partial \mathcal{N}(x; s_t\mu_{k,l}, \Sigma_{k,l})}{\partial U_k} \\ &= 2\pi_{k,l}s_t^2[\mathcal{N}(x; s_t\mu_{k,l}, \Sigma_{k,l})(\Sigma_k^{l^{-1}}(x - s_t\mu_{k,l})(x - s_t\mu_{k,l})^\top\Sigma_{k,l}^{-1} - \Sigma_{k,l}^{-1})]U_{k,l}\,.\end{aligned}$$

Then, we know that

$$\begin{aligned}\left\|\frac{\partial w_{k,l}}{\partial U_{k,l}}\right\|_2 &\le 2\pi_{k,l}\mathcal{N}(x; s_t\mu_{k,l}, \Sigma_{k,l})s_t^2(\frac{(R + s_t\|\mu_{k,l}\|_2)^2}{\gamma_t^4} + \frac{1}{\gamma_t^2}) \\ &\le 2\pi_{k,l}\mathcal{N}(x; s_t\mu_{k,l}, \Sigma_{k,l})s_t^2(\frac{(R + s_tB_\mu)^2}{\gamma_t^4} + \frac{1}{\gamma_t^2})\,.\end{aligned}$$

For the second term, we have that

$$\frac{\partial \delta_{k,l}(x)}{\partial U_{k,l}} = -2\frac{s_t^2}{s_t^2 + \gamma_t^2}(U_{k,l}^\top(x - s_t\mu_{k,l})I + U_{k,l}(x - s_t\mu_{k,l})^\top)\,,$$

which indicates

$$\begin{aligned}\left\|\frac{\partial \delta_{k,l}(x)}{\partial U_{k,l}}\right\|_2 &\le 2\frac{s_t^2}{s_t^2 + \gamma_t^2}(R + \|s_t\mu_{k,l}\|_2) \le 2(R + \|s_t\mu_{k,l}\|_2) \\ &\le 2(R + s_tB_\mu)\,.\end{aligned}$$

(2) The upper bound of $\left\|\frac{\Sigma_{l=1}^{n_k}(\frac{\partial w_{k,l}(x)}{\partial U_{k,l}}\delta_{k,l}(x)+\frac{\partial \delta_{k,l}(x)}{\partial U_{k,l}}w_{k,l}(x))}{w_k(x)}\right\|_2$ and $\left\|\frac{\frac{\partial w_k(x)}{\partial U_{k,l}}*(\Sigma_{l=1}^{n_k}w_{k,l}(x)\delta_{k,l}(x))}{w_j^2(x)}\right\|_2$.

$$\left\|\frac{\Sigma_{l=1}^{n_k}(\frac{\partial w_{k,l}(x)}{\partial U_{k,l}}\delta_{k,l}(x) + \frac{\partial \delta_{k,l}(x)}{\partial U_{k,l}}w_{k,l}(x))}{w_k(x)}\right\|_2 \le s_t^2(\frac{(R + s_tB_\mu)^3}{\gamma_t^4} + \frac{1}{\gamma_t^2}) + 2(R + s_tB_\mu)$$

We also have

$$\left\|\frac{\frac{\partial w_k(x)}{\partial U_{k,l}}(\Sigma_{l=1}^{n_k}w_{k,l}(x)\delta_{k,l}(x))}{w_k^2(x)}\right\|_2 \le s_t^2(\frac{(R + s_tB_\mu)^2}{\gamma_t^4} + \frac{1}{\gamma_t^2})(R + s_tB_\mu)$$

$$\left\|\frac{\partial s_{k,\theta}(x,t)}{\partial U_{k,l}}\right\|_2 \le s_t^2\left(\frac{(R+s_tB_\mu)^2}{\gamma_t^4}+\frac{1}{\gamma_t^2}\right)+2(R+s_tB_\mu)+s_t^2\left(\frac{(R+s_tB_\mu)^2}{\gamma_t^4}+\frac{1}{\gamma_t^2}\right)(R+s_tB_\mu)$$
$$= O\left(\frac{(R+s_tB_\mu)^3 s_t^2}{\gamma_t^4}\right).$$

Therefore, $s_{\theta,k}$ is L_k-lipshiz, where

$$L_k \le \sqrt{n_k(L_{\mu_{k,l}}^2+L_{U_{k,l}}^2)} = O\left(n_k^{\frac{1}{2}}\frac{(R+s_tB_\mu)^3 s_t^2}{\gamma_t^4}\right).$$

Furthermore, we know that

$$\|s_\theta(x)-s_\theta(y)\|_2 = \left(\sum_{i=1}^K \left\|s_{\theta,i}(x^{(i)})-s_{\theta,i}(y^{(i)}))\right\|^2\right)^{\frac{1}{2}} \le (\sum_{i=1}^K L_i\|(x^{(i)}-y^{(i)}\|_2^2)^{\frac{1}{2}} \le \sqrt{\sum_{i=1}^k L_i^2}\|x-y\|_2.$$

Thus,

$$L = \sqrt{\sum_{i=1}^k L_i^2} = O\left(\sqrt{\sum_{i=1}^k n_i^{\frac{1}{2}}}\frac{(R+s_tB_\mu)^3 s_t^2}{\gamma_t^4}\right).$$

After obtaining the Lipschitz constant for s_θ, we bound the gap between s_θ and s^*:

$$\nabla \log p_{t,k}(x) = -\frac{1}{\gamma_t^2}\frac{\Sigma_{l=1}^{n_k}\pi_{k,l}\mathcal{N}(x;s_t\mu_{k,l},s_t^2U_{k,l}^\star U_{k,l}^{\star\top}+\gamma_t^2 I)\left(x-s_t\mu_{k,l}-\frac{s_t^2}{s_t^2+\gamma_t^2}U_{k,l}^\star U_{k,l}^{\star\top}(x-s_t\mu_{k,l})\right)}{\Sigma_{l=1}^{n_k}\pi_{k,l}\mathcal{N}(x;s_t\mu_{k,l},s_t^2U_{k,l}^\star U_{k,l}^{\star\top}+\gamma_t^2 I)}.$$

With the following bound

$$\|x-s_t\mu_{k,l}-\frac{s_t^2}{s_t^2+\gamma_t^2}U_{k,l}^\star U_{k,l}^{\star\top}(x-s_t\mu_{k,l})\|_2 \le R+s_tB_\mu,$$

we have that

$$\|\nabla \log p_{t,k}(x)\|_2 \le \frac{1}{\gamma_t^2}(R+s_tB_\mu), \text{and } \|s_{k,\theta}(x)\|_2 \le \frac{1}{\gamma_t^2}(R+s_tB_\mu),$$

which indicates

$$\|s_{k,\theta}(x)-\nabla\log p_{t,k}(x)\|_2 \le \frac{2}{\gamma_t^2}(R+s_tB_\mu).$$

Hence, we obtain that

$$L_l \le 2\|s_{k,\theta}(x)-\nabla\log p_{t,k}(x)\|_2 = O(R+s_tB_\mu).$$

■

Lemma B.2. *[Rademacher Complexity] Let $\mathcal{F}=\{\ell(\theta;\cdot,\cdot)\colon \theta\in\Theta\}$ and suppose Θ has diameter R_Θ. Then the empirical Rademacher complexity satisfies*

$$\widehat{\mathfrak{R}}_n(\mathcal{F}) \;=\; O\Big(L'\sqrt{\frac{p}{n}}\Big).$$

Proof. Let function class $\mathcal{F} = \{S_\theta(x) : \theta = (\{\{\mu_{k,l},U_{k,l}\}_{l=1}^{n_k}\}_{k=1}^K) \in \Theta\}$, where $\mu_{k,l}\in\mathbb{R}^d, U_{k,l}\in\mathbb{R}^d$

We know that the number of parameters

$$p = \Sigma_{k=1}^K n_k(d+d) = 2\Sigma_{k=1}^K n_k d_k.$$

And the covering number of the parameter space is

$$\mathcal{N}(\epsilon, \Theta, \|\cdot\|_2) \leq (\frac{C}{\epsilon})^p$$

If f is L-lipschitz, we know that

$$\forall \theta_1, \theta_2 \in \Theta, \|f_{\theta_1} - f_{\theta_2}\|_{L_2(p)} \leq L\|\theta_1 - \theta_2\|_2 \qquad and \qquad \forall \theta,\ \exists \theta_j,\ s.t. \|\theta - \theta_j\|_2 \leq \frac{\epsilon}{L}$$
$$\Rightarrow \|f_\theta - f_{\theta_j}\|_{L_2(p)} \leq L\|\theta - \theta_j\|_2 \leq \epsilon.$$

Thus, assume that $\|\theta_i - \theta_j\|_2 \leq C_1$ for any θ_i,$\theta_j \in \Theta$

$$\mathcal{N}(\epsilon, \Theta, \|\cdot\|_2) \leq (\frac{C_1}{\epsilon})^p$$
$$\Rightarrow \mathcal{N}(\frac{\epsilon}{L}, \Theta, \|\cdot\|_2) \leq (\frac{C_1 L}{\epsilon})^p$$
$$\Rightarrow \mathcal{N}(\epsilon, \mathcal{F}, \|\cdot\|_{L_2(p)}) \leq \mathcal{N}(\frac{\epsilon}{L}, \Theta, \|\cdot\|_2) \leq (\frac{C_1 L}{\epsilon})^p \leq (\frac{C_1 L}{\epsilon})^p,\ \ \log \mathcal{N}(\frac{\epsilon}{L}, \mathcal{F}, \|\cdot\|_{L_2(p)}) \leq p \log(\frac{C_1 L}{\epsilon}).$$

We also know that $diam(\mathcal{F}) \leq L\, diam(\Theta) = C_1 L$, with Dudley integral, we have

$$\begin{aligned}
\mathcal{R}_n(\mathcal{F}) &\leq \frac{12}{\sqrt{n}} \int_0^{diam(\mathcal{F})} \sqrt{\log N(\epsilon, \mathcal{F}, \|\cdot\|_{L_2(p)})} d\epsilon \\
&\leq \frac{12}{\sqrt{n}} \int_0^{C_1 L} \sqrt{p \log(\frac{C_1 L}{\epsilon})} d\epsilon \\
&\leq \frac{12}{\sqrt{n}} \int_0^{\infty} pCL\sqrt{t} \exp(-t) dt = \frac{6\sqrt{\pi p}}{\sqrt{n}} C_1 L = O(C_1 L \sqrt{\frac{p}{n}}).
\end{aligned}$$

We take the squared loss function.

$$\mathcal{R}_n(\mathcal{L}) \leq L_l \mathcal{R}_n(\mathcal{F}) = O(C_1 L_l L \sqrt{\frac{p}{n}}).$$

■

Theorem 5.3. *Denote by $\widehat{\mathcal{L}}_n(\theta)$ the empirical loss on n i.i.d. samples and by $\mathcal{L}(\theta)$ its population counterpart. Then there exist constants C_1, C_2 such that with probability at least $1-\delta$, for all $\theta \in \Theta$,*

$$\left|\mathcal{L}(\theta) - \widehat{\mathcal{L}}_n(\theta)\right| \ \leq\ O\left(C_1 \frac{(R + s_t B_\mu)^4 s_t^2 \sqrt{\Sigma_{k=1}^K n_k}}{\gamma_t^6} \sqrt{\frac{\Sigma_{k=1}^K n_k d_k}{n}} \ +\ C_2 \sqrt{\frac{\log(1/\delta)}{n}} \right).$$

where $C_1 = \max_{\theta \in \Theta} \|\theta_i - \theta_j\|_2,\ C_2 = \sigma \log 2,\ \sigma^2 = \sup_{\theta \in \Theta} Var[\ell(\theta; X, t)]$.

Proof. Since

$$L_l \mathcal{R}_n(\mathcal{F}) = O(C_1 L_l L \sqrt{\frac{p}{n}}).$$

We have

$$\Delta = \sup_{\theta \in \Theta} |\hat{L}(\theta) - L(\theta)| = O(C_1 L_l L \sqrt{\frac{p}{n}})$$
$$\Rightarrow \mathbb{E}[\Delta] = O(C_1 L_l L \sqrt{\frac{p}{n}}).$$

By Bernstein inequality,let $\sigma^2 = \sup_{\theta \in \Theta} Var[l(X; \theta)]$,we know that

$$Pr(\sup_{\theta \in \Theta} |\hat{L}(\theta) - L(\theta)| \geq \mathbb{E}[\Delta] + \epsilon) \leq 2\exp(-\frac{n\epsilon^2}{2(\sigma^2 + L_l L C_1 \epsilon/3)}) \leq 2\exp(-\frac{n\epsilon^2}{3\sigma^2}).$$

Let $2\exp(-\frac{n\epsilon^2}{3\sigma^2}) < \delta$, we can obtain that

$$Pr(\sup_{\theta \in \Theta} |\hat{L}(\theta) - L(\theta)| \geq C_1 L L_l \sqrt{\frac{p}{n}} + C_2 \sqrt{\frac{\log(1/\delta)}{n}}) \leq \delta.$$

■

B.3 APPROXIMATION

Since our network can represent $\nabla \log p(x)$ strictly, we have

$$\text{Approximation Error} = 0$$

C 2-MODE MOG OPTIMIZATION

C.1 SETTING

In this section, we analyze

$$\nabla \log p_{t,k}(x) = \frac{\nabla p_{t,k}(x)}{p_{t,k}(x)} = -\frac{1}{\gamma_t^2} \frac{\begin{matrix} \frac{1}{2}\mathcal{N}(x; s_t\mu_k, s_t^2 U_k^\star U_k^{\star\top} + \gamma_t^2 I)\left(x - s_t\mu_k - \frac{s_t^2}{s_t^2+\gamma_t^2} U_k^\star U_k^{\star\top}(x - s_t\mu_k)\right) \\ + \frac{1}{2}\mathcal{N}(x; -s_t\mu_k, s_t^2 U_k^\star U_k^{\star\top} + \gamma_t^2 I)\left(x + s_t\mu_k - \frac{s_t^2}{s_t^2+\gamma_t^2} U_K^\star U_K^{\star\top}(x + s_t\mu_k)\right) \end{matrix}}{\frac{1}{2}\mathcal{N}(x; s_t\mu_k, s_t^2 U_k^\star U_k^{\star\top} + \gamma_t^2 I) + \frac{1}{2}\mathcal{N}(x; -s_t\mu_k, s_t^2 U_k^\star U_k^{\star\top} + \gamma_t^2 I)},$$

which can be reduced to

$$\nabla \log p_{t,k}(x) = -\frac{1}{\gamma_t^2} \frac{\frac{1}{2}\mathcal{N}(x; s_t\mu_k, \Sigma_k)\, \delta_k'(x) + \frac{1}{2}\mathcal{N}(x; -s_t\mu_k, \Sigma_k)\, \epsilon_k(x)}{\frac{1}{2}\mathcal{N}(x; s_t\mu_k, \Sigma_k) + \frac{1}{2}(x; -s_t\mu_k, \Sigma_k)}, \tag{5}$$

where $\epsilon_k(x) = x - s_t\mu_k - \frac{s_t^2}{s_t^2+\gamma_t^2} U_k^* U_k^{*\top}(x - s_t\mu_k)$, and $\delta_k'(x) = x + s_t\mu_k - \frac{s_t^2}{s_t^2+\gamma_t^2} U_k^* U_k^{*\top}(x + s_t\mu_k)$.

C.2 OPTIMIZATION

Assumption C.1. [Separation within a cluster] Within each cluster k, the two symmetric peaks are well separated in the sense that $\|s_t\mu_k^* - (-s_t\mu_k^*)\| \geq \Delta_{\text{intra}}$, for some $\Delta_{\text{intra}} \gg \gamma_t$. Consequently, if a sample x is drawn from the "+" peak then its responsibility under the "−" peak satisfies

$$r_k^-(x) \;=\; \frac{\frac{1}{2}\,\mathcal{N}(x; -s_t\mu_k^*, \Sigma_k^*)}{\frac{1}{2}\,\mathcal{N}(x; s_t\mu_k^*, \Sigma_k^*) + \frac{1}{2}\,\mathcal{N}(x; -s_t\mu_k^*, \Sigma_k^*)} \;=\; O\big(e^{-\Delta_{\text{intra}}^2/(2\gamma_t^2)}\big) \;\ll\; 1,$$

and symmetrically $r_k^+(x) \ll 1$ when x is drawn from the "−" peak.

In the following discussion, we assume that $x \in k$-th manifold, which means that $w_i(x) = 0$ if $i \neq k$.

Lemma C.2. *[Jacobian Simplification] Under Assumption 6.1, in a neighborhood of θ^* the first derivatives simplify to their "self-cluster" terms: $J_k^\mu(x) \;=\; \partial_{\mu_k} s_\theta \;\approx\; s_t(I - \alpha P_k)/\gamma_t^2$, and*

$$J_k^U(x) \approx \frac{2s_t^2}{\gamma_t^2(s_t^2+\gamma_t^2)}(r_k^-(x)(U_k^\top(x+s_t\mu_k)I + (x+s_t\mu_k)U_k^\top) + r_k^+(x)(U_k^\top(x-s_t\mu_k)I + U_k(x-s_t\mu_k)^\top)).$$

Proof.

$$\begin{aligned} J_k^\mu &= -\frac{1}{\gamma_t^2} \frac{\frac{\partial w_k^-(x)}{\partial \mu_k}\delta_k'(x) + \frac{\partial w_k^+(x)}{\partial \mu_k}\epsilon_k(x) + \frac{\partial \delta_k'(x)}{\partial \mu_k} w_k^-(x) + \frac{\partial \epsilon_k(x)}{\partial \mu_k} w_k^+(x)) * \Sigma_{k=1}^K w_k(x) - \Sigma_{k=1}^K \frac{\partial w_k(x)}{\partial \mu_k} * \Sigma_{k=1}^K (w_k^-(x)\delta_k'(x) + w_k^+(x)\epsilon_k(x)}{w_k^2(x)} \\ &= \underbrace{\frac{w_k^-(x)\frac{\partial \delta_k'(x)}{\partial \mu_k} + w_k^+(x)\frac{\partial \epsilon_k(x)}{\partial \mu_k}}{\gamma_t^2 w_k(x)} - \frac{\frac{\partial w_k^-(x)}{\partial \mu_k}\delta_k'(x) + \frac{\partial w_k^+(x)}{\partial \mu_k}\epsilon_k(x)}{\gamma_t^2 w_k(x)}}_{TermA} \\ &\quad + \underbrace{\frac{\frac{\partial w_k(x)}{\partial \mu_k}(w_k^-(x)\delta_k'(x) + w_k^+\epsilon_k(x))}{\gamma_t^2 w_k^2(x)}}_{TermB}. \end{aligned}$$

We will now prove that term B can be ignored compared to term A under our assumptions.

For term B, we have

$$\frac{\frac{\partial w_k(x)}{\partial \mu_k}(w_k^-(x)\delta_k'(x)+w_k^+\epsilon_k(x))}{\gamma_t^2 w_k^2(x)}-\frac{\frac{\partial w_k^-(x)}{\partial \mu_k}\delta_k'(x)+\frac{\partial w_k^+(x)}{\partial \mu_k}\epsilon_k(x)}{\gamma_t^2 w_k(x)}$$
$$=\frac{1}{\gamma_t^2 w_k^2(x)}(\frac{\partial w_k(x)}{\partial \mu_k}(w_k^-(x)\delta_k'(x)+w_k^+(x)\epsilon_k(x))-w_k(x)(\frac{\partial w_k^-(x)}{\partial \mu_k}\delta_k'(x)+\frac{\partial w_k^+(x)}{\partial \mu_k}\epsilon_k(x)))$$
$$=\frac{1}{\gamma_t^2 w_k^2(x)}(\frac{\partial w_k^+(x)}{\partial \mu_k}w_k^-(x)\delta_k'(x)+\frac{\partial w_k^-(x)}{\partial \mu_k}w_k^+(x)\epsilon_k(x)-w_k^+(x)\frac{\partial w_k^-(x)}{\partial \mu_k}\delta_k'(x)-w_k^-(x)\frac{\partial w_k^+(x)}{\partial \mu_k}\epsilon_k(x))$$
$$=\frac{1}{\gamma_t^2 w_k^2(x)}(\frac{\partial w_k^+}{\partial \mu_k}w_k^--\frac{\partial w_k^-}{\partial \mu_k}w_k^+)(\epsilon_k(x)-\delta_k'(x))$$
$$=-\frac{2}{\gamma_t^2 w_k^2(x)}(\frac{\partial w_k^+}{\partial \mu_k}w_k^--\frac{\partial w_k^-}{\partial \mu_k}w_k^+)\left(I+\frac{s_t^2}{s_t^2+\gamma_t^2}U_kU_k^\top\right)s_t\mu_k$$
$$=-\frac{4}{\gamma_t^2 w_k^2(x)}s_t^2 w_k^- w_k^+\Sigma_k^{-1}x\left(I+\frac{s_t^2}{s_t^2+\gamma_t^2}U_kU_k^\top\right)\mu_k=O(\frac{r_k^+r_k^-}{\gamma_t^4}s_t\|\mu_k\|_2\|x\|_2).$$

And for term A, we have

$$\frac{w_k^-(x)\frac{\partial\delta_k'(x)}{\partial\mu_k}+w_k^+(x)\frac{\partial\epsilon_k(x)}{\partial\mu_k}}{\gamma_t^2 w_k(x)}=O\left(\frac{s_t\|\mu_k\|_2}{\gamma_t^2}|w_k^+-w_k^-|\right).$$

Thus,

$$\frac{O\left(\frac{r_k^+r_k^-}{\gamma_t^4}s_t\|\mu_k\|_2\|x\|_2\right)}{O\left(\frac{s_t\|\mu_k\|_2}{\gamma_t^2}|w_k^+-w_k^-|\right)}=O\left(\frac{r_k^+r_k^-w_k\|x\|_2}{\gamma_t^2|r_k^+-r_k^-|}\right)=O\left(\frac{r_k^+r_k^-w_k\|x\|_2}{\gamma_t^2}\right)\to 0.$$

Thus, $J_k^\mu\approx-\frac{1}{\gamma_t^2}(r_k^+(x)\frac{\partial\delta_k'(x)}{\partial\mu_k}+r_k^-(x)\frac{\partial\epsilon_k(x)}{\partial\mu_k})=-\frac{s_t}{\gamma_t^2}(r_k^+(x)-r_k^-(x))\left(I-\frac{s_t^2}{s_t^2+\gamma_t^2}U_kU_k^\top\right).$

We will analyze J_k^U now.

$$J_k^U=-\frac{1}{\gamma_t^2}\frac{(\frac{\partial w_k^-(x)}{\partial U_k}\delta_k'(x)+\frac{\partial\delta_k'(x)}{\partial U_k}w_k^-(x)+\frac{\partial\epsilon_k(x)}{\partial U_k}w_k^+(x)+\frac{\partial w_k^+(x)}{\partial U_k}\epsilon_k(x))*w_k(x)-\frac{\partial w_k(x)}{\partial U_k}*(w_k^-(x)\delta_k'(x)+w_k^+\epsilon_k(x))}{w_k^2(x)}$$
$$=-\frac{1}{\gamma_t^2}(\frac{\frac{\partial\delta_k'(x)}{\partial U_k}w_k^-(x)+\frac{\partial\epsilon_k(x)}{\partial U_k}w_k^+(x)}{w_k(x)}$$
$$+\frac{\frac{\partial w_k^-(x)}{\partial U_k}\delta_k'(x)+\frac{\partial w_k^+(x)}{\partial U_k}\epsilon_k(x)}{w_k(x)}-\frac{\frac{\partial w_k(x)}{\partial U_k}*(w_k^-(x)\delta_k'(x)+w_k^+\epsilon_k(x))}{w_k^2(x)}).$$

By calculating, we have

$$\frac{\frac{\partial w_k^-(x)}{\partial U_k}\delta_k(x)+\frac{\partial w_k^+(x)}{\partial U_k}\epsilon_k(x)}{w_k(x)}-\frac{\frac{\partial w_k(x)}{\partial U_k}*(w_k^-(x)\delta_k'(x)+w_k^+\epsilon_k(x))}{w_k^2(x)}$$
$$=\frac{1}{w_k^2(x)}((w_k(x)(\frac{\partial w_k^-(x)}{\partial U_k}\delta_k'(x)+\frac{\partial w_k^+(x)}{\partial U_k}\epsilon_k(x))-\frac{\partial w_k(x)}{\partial U_k}(w_k^-(x)\delta_k'(x)+w_k^+\epsilon_k(x)))$$
$$=\frac{1}{w_k^2(x)}(w_k(x)(\frac{\partial w_k^-(x)}{\partial U_k}\delta_k'(x)+\frac{\partial w_k^+(x)}{\partial U_k}\epsilon_k(x))-\frac{\partial w_k(x)}{\partial U_k}(w_k^-(x)\delta_k'(x)+w_k^+\epsilon_k(x)))$$
$$=\frac{1}{w_k^2(x)}(\frac{\partial w_k^+}{\partial U_k}w_k^--\frac{\partial w_k^-}{\partial U_k}w_k^+)(\epsilon_k(x)-\delta_k'(x))$$
$$=-\frac{2\,s_t^3}{w_k^2(x)}\Big[\mathcal{N}(x;s_t\mu_k,\Sigma)\,M^+(x)\;-\;\mathcal{N}(x;-s_t\mu_k,\Sigma)\,M^-(x)\Big]\,U_k\,(I-\alpha\,U_kU_k^\top)\,\mu_k$$
$$=O(r_k^+r_k^-\frac{s_t^3}{\gamma_t^2(s_t^2+\gamma_t^2)}).$$

where $M^+(x) = \Sigma^{-1}(x - s_t\mu_k)(x - s_t\mu_k)^\top\Sigma^{-1} - \Sigma^{-1}, M^-(x) = \Sigma^{-1}(x + s_t\mu_k)(x + s_t\mu_k)^\top\Sigma^{-1} - \Sigma^{-1}, \alpha = \frac{s_t^2}{s_t^2+\gamma_t^2}$.

We also know that

$$\frac{\Sigma_{k=1}^K(\frac{\partial\delta_k(x)}{\partial U_k}w_k^-(x) + \frac{\partial\epsilon_k(x)}{\partial U_k}w_k^+(x))}{\Sigma_{k=1}^K w_k(x)} = O\left(\frac{s_t^2\|x\|_2}{s_t^2+\gamma_t^2}\right) = O\left(\frac{s_t^3\|\mu_k\|_2}{s_t^2+\gamma_t^2}\right)$$

$$\frac{O(r_k^+ r_k^- \frac{s_t^3}{\gamma_t^2(s_t^2+\gamma_t^2)})}{O(\frac{s_t^3\|\mu_k\|_2}{s_t^2+\gamma_t^2})} \to 0.$$

Thus,

$$J_k^U \approx \frac{2s_t^2}{\gamma_t^2(s_t^2+\gamma_t^2)}(r_k^-(x)(U_k^\top(x+s_t\mu_k)I + (x+s_t\mu_k)U_k^\top) + r_k^+(x)(U_k^\top(x-s_t\mu_k)I + U_k(x-s_t\mu_k)^\top)).$$

■

Before we provide the simplification of Hessian, we first prove that for $a, b \in \mathbb{R}^n$ $M = a^\top bI_n + ba^\top$,$MM^\top$ is positive-definite if and only if $b^\top a \neq 0$. At the same time, we provide the minimum eigenvalue of $MM^\top$, which will be used later.

Lemma C.3. *Let $a, b \in \mathbb{R}^n$ and $M = a^\top bI_n + ba^\top$. $MM^\top$ is positive-definite if and only if $b^\top a \neq 0$.*

Moreover,

$$\lambda_{min}(MM^\top) = \mu_2 = \frac{4(a^\top b)^2 + \|a\|_2^2\|b\|_2^2 - \|a\|_2\|b\|_2\sqrt{8(a^\top b)^2 + \|a\|_2^2\|b\|_2^2}}{2}.$$

Proof. Let $M = a^\top bI_n + ba^\top$, $c = a^\top b$. We know that $\forall x \in \mathbb{R}^n$,

$$\begin{aligned} x^\top MM^\top x &= (M^\top x)^\top(M^\top x) \\ &= \|M^\top x\|_2^2 \geq 0. \end{aligned}$$

Thus, $MM^\top$ is semi-positive definite.

We can also have that

$$|M| = |a^\top bI_n + ba^\top| = c^n|I_n + \frac{1}{c}ba^\top| = 2c^n \geq 0,$$

where $c^n = 0$ if and only if $b^\top a = 0$.

The last equation holds because

$$|I_n + uv^\top| = 1 + v^\top u$$

Thus, $|MM^\top| > 0$, $MM^\top$ is positive definite.

We can further get the eigenvalues of $MM^\top$.

Expanding gives the convenient representation

$$MM^\top = (a^\top b)^2 I_n + a^\top b\big(ba^\top + ab^\top\big) + a^\top abb^\top. \tag{6}$$

$\forall x \in \mathbb{R}^n$, if $x^\top a = 0$ and $x^\top b = 0$, we have:

$$MM^\top x = (a^\top b)^2 x.$$

Thus, $(a^\top b)^2$ is an eigenvalue of M, and its eigenspace contains the orthogonal complement of $\mathrm{span}\{a, b\}$.If a and b are linearly independent then $\dim(\mathrm{span}\{a, b\}) = 2$, so the multiplicity of the eigenvalue α^2 is at least $n - 2$.

To find the remaining eigenvalues we restrict M to the subspace $\mathcal{S} := \text{span}\{a, b\}$. Assume first that a and b are linearly independent so that $\mathcal{S}$ is two-dimensional.

Using equation 6, we can compute $tr(MM^\top)$, which is

$$\begin{aligned} tr(MM^\top) &= tr((a^\top b)^2 I_n + a^\top b\big(ba^\top + ab^\top\big) + a^\top abb^\top) \\ &= n(a^\top b)^2 + 2(a^\top b)^2 + \|a\|_2^2\|b\|_2^2 \\ &= (n+2)(a^\top b)^2 + \|a\|_2^2\|b\|_2^2. \end{aligned}$$

The second equation holds because of $tr(xy^\top) = tr(y^\top x) = y^\top x$.

We set the other two eigenvalues are μ_1 and μ_2.Thus

$$\begin{aligned} tr(MM^\top) &= \Sigma_{i=1}^n \lambda_i \\ &= (n-2)(a^\top b)^2 + \mu_1 + \mu_2 \\ &= (n+2)(a^\top b)^2 + \|a\|_2^2\|b\|_2^2, \end{aligned}$$

and

$$\begin{aligned} |MM^\top| &= \Pi_{i=1}^n \lambda_i \\ &= (a^\top b)^{2(n-2)}\mu_1\mu_2 \\ &= 4(a^\top b)^{2n}. \end{aligned}$$

So μ_1 and μ_2 are the two solutions of

$$x^2 - \big(4(a^\top b)^2 + \|a\|_2^2\|b\|_2^2\big)\, x + 4(a^\top b)^4 = 0. \tag{7}$$

Solving equation 7, we have

$$\mu_1, \mu_2 = \frac{4(a^\top b)^2 + \|a\|_2^2\|b\|_2^2 \pm \|a\|_2\|b\|_2\sqrt{8(a^\top b)^2 + \|a\|_2^2\|b\|_2^2}}{2}.$$

Now we obtain all eigenvalues.Moreover, we can calculate the minimum of eigenvalues.

$$\lambda_{min}(MM^\top) = \mu_2 = \frac{4(a^\top b)^2 + \|a\|_2^2\|b\|_2^2 - \|a\|_2\|b\|_2\sqrt{8(a^\top b)^2 + \|a\|_2^2\|b\|_2^2}}{2}.$$

■

Lemma C.4. *[Eigenvalues of the Hessian blocks] Under the same conditions, H is convex. If $\forall x \in \mathbb{R}^{d_k}$,$r_k^+(x) = 1$ or $r_k^-(x) = 1$ are strictly satisfied, the eigenvalues of the Hessian at θ^* are*

$$\lambda_{\min}(H_{\mu_k\mu_k}) = \frac{s_t^2}{(s_t^2+\gamma_t^2)^2}\,, \textit{and}$$

$$\lambda_{\min}(H_{U_kU_k}) = \frac{4(U_k^\top\mu_k))^2 + \|U_k\|_2^2\|\mu_k\|_2^2 - \|U_k\|_2\|\mu_k\|_2\sqrt{8(U_k^\top\mu_k))^2 + \|U_k\|_2^2\|\mu_k\|_2^2}}{2}.$$

Proof. We first state the convexity of the loss function near the true value $\theta^\star$.

Let $\theta = \theta^\star + \Delta\theta$

$$s_\theta(x,t) = S_{\theta^\star}(x,t) + (\nabla_\theta S_\theta(x,t)|_{\theta^\star})^\top[\Delta\theta] + O(\|\Delta\theta\|_2^2).$$

$$\begin{aligned} L(\theta) &= \mathbb{E}_{x\sim p_t(x)}[(s_\theta(x,t) - \nabla\log p_t(x))^\top(s_\theta(x,t) - \nabla\log p_t(x))] \\ &= \mathbb{E}_{x\sim p_t(x)}[(S_{\theta^\star}(x,t) + (\nabla_\theta S_\theta(x,t)|_{\theta^\star})^\top[\Delta\theta] + O(\|\Delta\theta\|_2^2) - \nabla\log p_t(x))^\top \\ &\quad (S_{\theta^\star}(x,t) + (\nabla_\theta S_\theta(x,t)|_{\theta^\star})^\top[\Delta\theta] + O(\|\Delta\theta\|_2^2) - \nabla\log p_t(x))] \\ &= \mathbb{E}_{x\sim p_t(x)}[((\nabla_\theta S_\theta(x,t)|_{\theta^\star})^\top[\Delta\theta])^\top(\nabla_\theta S_\theta(x,t)|_{\theta^\star}[\Delta\theta])] + O(\|\Delta\theta\|_2^3) \\ &= (\Delta\theta)^\top\mathbb{E}_{x\sim p_t(x)}[(\nabla_\theta S_\theta(x,t)|_{\theta^\star})(\nabla_\theta S_\theta(x,t)|_{\theta^\star})^\top]\Delta\theta \\ &\triangleq (\Delta\theta)^\top H\Delta\theta. \end{aligned}$$

$$\frac{\partial^2 L(\theta)}{\partial \theta^2} = 2H.$$

We then analyze the convexity of $\mathbb{E}_{x\sim p_t(x)}[(\nabla_\theta S_\theta(x,t)|_{\theta^\star})(\nabla_\theta S_\theta(x,t)|_{\theta^\star})^\top] \triangleq H$. We can divide H into 4 parts:$H_{\mu\mu}, H_{UU}, H_{\mu U}$ and $H_{U\mu}$, where $H_{U\mu} = (H_{\mu U})^\top$.

Let $J_k^\mu|_\theta = \frac{\partial s_\theta}{\partial \mu_k}|_\theta$.

$$\begin{aligned} H &= \mathbb{E}_{x\sim p_t(x)}[(\nabla_\theta S_\theta(x,t)|_{\theta^\star})(\nabla_\theta S_\theta(x,t)|_{\theta^\star})^\top] \\ &= \mathbb{E}_{x\sim p_t(x)}[J_{\theta^\star}(x,t) J_{\theta^\star}(x,t)^\top. \end{aligned}$$

Term $H_{\mu\mu}$

We will show that $H_{\mu_k\mu_k}$ is α-convex, where $\alpha > 0$.

$$H_{\mu_k\mu_k} = \mathbb{E}_{x\sim p_t(x)}[J_k^\mu J_k^{\mu\top}]$$

$$H_{\mu_k\mu_k} \approx \mathbb{E}_{x\sim p_t(x)}[J_\mu^k J_\mu^{k\top}] \approx \frac{s_t^2}{\gamma_t^4}\mathbb{E}_{x\sim p_t(x)}[(r_k^+(x) - r_k^-(x))^2](I - \frac{s_t^2}{s_t^2+\gamma_t^2}U_k U_k^\top)^2.$$

Let $P_k = U_k U_k^\top$, $\alpha = \frac{s_t^2}{s_t^2+\gamma_t^2}$,

$$(I-\alpha P_k)(I-\alpha P_k)^\top = (I-\alpha P_k)^2 = I - 2\alpha P_k + \alpha^2 P_k^2 = (I-\alpha P_k)^2.$$

We then prove that $\lambda_{min}((I-\alpha P_k)^2) = (\frac{\gamma_t^2}{s_t^2+\gamma_t^2})^2$.

First, we calculate the eigenvalue of P.

$$P^2 = P \Rightarrow \lambda_1 = 1,\ \lambda_2 = 0.$$

Then we take subspace $Col(P) = \{v\ ; v = Px,\ x \in \mathcal{R}^D\}$ corresponding to λ_1, and subspace $Ker(P) = \{v\ ; Pv = 0,\ x \in \mathcal{R}^D\}$ corresponding to λ_2.

If $w \in Col(P)$, $Pw = w$:

$$\begin{aligned} &(I-\alpha P)w = (1-\alpha)w \\ &(I-\alpha P)^2 w = (1-\alpha)^2 w \\ &\Rightarrow \lambda_1' = (1-\alpha)^2. \end{aligned}$$

If $w \in Ker(P)$, $Pw = 0$:

$$\begin{aligned} &(I-\alpha P)w = w \\ &(I-\alpha P)^2 w = w \\ &\Rightarrow \lambda_2' = 1. \end{aligned}$$

$$\begin{aligned} &H_{\mu\mu} = \mathbb{E}[J_k^\mu (J_k^\mu)^\top] \\ &\lambda_{min}(H_{\mu\mu}) \approx \frac{s_t^2}{(s_t^2+\gamma_t^2)^2}. \end{aligned}$$

Therefore, $\lambda_{min}((I-\alpha P_k)^2) = \left(\frac{\gamma_t^2}{s_t^2+\gamma_t^2}\right)^2$.Hence, we have

$$\lambda_{min}(H_{\mu_k\mu_k}) \geq \frac{c_k s_t^2}{(s_t^2+\gamma_t^2)^2} \approx \frac{s_t^2}{(s_t^2+\gamma_t^2)^2},$$

where $c_k = \mathbb{E}_{x\sim p_t(x)}[(r_k^+(x) - r_k^-(x))^2] \approx 1$.

Term $H_{U_kU_k}$

$$
\begin{aligned}
H_{U_kU_k} &\approx \mathbb{E}_{x\sim p_t(x)}[J_U^k J_U^{k\top}] \\
&\approx \frac{4s_t^4}{\gamma_t^4(s_t^2+\gamma_t^2)^2}\mathbb{E}_{x\sim p_t(x)}[(U_k^\top(x+s_t\mu_k)I+(x+s_t\mu_k)U_k^\top)(U_k^\top(x+s_t\mu_k)I+(x+s_t\mu_k)U_k^\top)^\top] \\
&= \frac{4s_t^4}{\gamma_t^4(s_t^2+\gamma_t^2)^2}(s_t^2U_k^\top\mu_k\mu_k^\top U_kI+s_t^2\mu_k^\top U_k(\mu_kU_k^\top+U_k\mu_k^\top)+\mu_kU_k^\top U_k\mu_k^\top+M(x),)
\end{aligned}
$$

where $M(x)$ is semi-positive for $\mathbb{E}_{x\sim p_t(x)}[x]=0$.

Using lemma C.3, we can take $a=U_k$ and $b=\mu_k$ and obtain that

$H_{U_kU_k}$ is positive definite and

$$
\lambda_{min}(H_{U_kU_k}) = \frac{4(U_k^\top\mu_k))^2+\|U_k\|_2^2\|\mu_k\|_2^2-\|U_k\|_2\|\mu_k\|_2\sqrt{8(U_k^\top\mu_k))^2+\|U_k\|_2^2\|\mu_k\|_2^2}}{2}.
$$

Term $H_{\mu_kU_k}$ and Term $H_{U_k\mu_k}$

Since $H_{U_k\mu_k}=H_{\mu_kU_k}^\top$, we just analyze $H_{\mu_kU_k}$. We want to analyze the Hessian block

$$
H_{\mu_kU_k}=\mathbb{E}_{x\sim p_t}\left[J_k^U(x)\left(J_k^\mu(x)\right)^\top\right],
$$

and show that under symmetric assumptions, this cross-term is zero.

The first-order derivative with respect to μ_k is approximately:

$$
J_k^\mu(x)\approx-\frac{s_t}{\gamma_t^2}\left(r_k^+(x)-r_k^-(x)\right)\left(I-\alpha\,U_kU_k^\top\right),\qquad \alpha=\frac{s_t^2}{s_t^2+\gamma_t^2}.
$$

The first-order derivative with respect to U_k is approximately:

$$
J_k^U(x)\approx-\frac{1}{\gamma_t^2}\left[r_k^-(x)\frac{\partial\delta_k(x)}{\partial U_k}+r_k^+(x)\frac{\partial\epsilon_k(x)}{\partial U_k}\right],
$$

with

$$
\frac{\partial\delta_k(x)}{\partial U_k}=-2\frac{s_t^2}{s_t^2+\gamma_t^2}U_k(x+s_t\mu_k),\qquad \frac{\partial\epsilon_k(x)}{\partial U_k}=-2\frac{s_t^2}{s_t^2+\gamma_t^2}U_k(x-s_t\mu_k).
$$

combining terms:

$$
J_k^U(x)=C\cdot U_k\left[r_k^-(x)(x+s_t\mu_k)+r_k^+(x)(x-s_t\mu_k)\right],
$$

where $C=\frac{2s_t^2}{\gamma_t^2(s_t^2+\gamma_t^2)}$. Assume that the underlying component distribution $p_k(x)$ is symmetric:

$$
p_k(x)=p_k(-x),
$$

and the weights satisfy:

$$
r_k^+(-x)=r_k^-(x),\qquad r_k^-(-x)=r_k^+(x).
$$

Then we have:

(a) $J_k^\mu(x)$ is an odd function:

$$
\begin{aligned}
J_k^\mu(-x) &= -\frac{s_t}{\gamma_t^2}(r_k^+(-x)-r_k^-(-x))(I-\alpha U_kU_k^\top) \\
&= -\frac{s_t}{\gamma_t^2}(r_k^-(x)-r_k^+(x))(I-\alpha U_kU_k^\top) \\
&= -J_k^\mu(x).
\end{aligned}
$$

(b) $J_k^U(x)$ is an odd function:

$$\begin{aligned} J_k^U(-x) &= C\,U_k\left[r_k^-(-x)(-x+s_t\mu_k)+r_k^+(-x)(-x-s_t\mu_k)\right] \\ &= C\,U_k\left[r_k^+(x)(-x+s_t\mu_k)+r_k^-(x)(-x-s_t\mu_k)\right] \\ &= -C\,U_k\left[r_k^-(x)(x+s_t\mu_k)+r_k^+(x)(x-s_t\mu_k)\right] \\ &= -J_k^U(x). \end{aligned}$$

Now compute:

$$H_{\mu_k U_k} = \int J_k^U(x)\,(J_k^\mu(x))^\top\, p_k(x)\,dx.$$

Using symmetry:

$$= \int J_k^U(-x)\,(J_k^\mu(-x))^\top\, p_k(-x)\,dx = \int (-J_k^U(x))\,(-J_k^\mu(x))^\top\, p_k(x)\,dx = H_{\mu_k U_k}.$$

Thus,

$$H_{\mu_k U_k} = \mathbb{E}_{x\sim p_{data}}[J_k^\mu (J_k^U)^\top] = \mathbb{E}_{x\sim p_{data}}[\frac{2s_t^3}{\gamma_t^4(s_t^2+\gamma_t^2)}(r_k^+(x)-r_k^-(x))(1-\frac{s_t^2}{s_t^2+\gamma_t^2}U_kU_k^\top)$$
$$(r_k^-(x)(U_k^\top(x+s_t\mu_k)I+U_k(x+s_t\mu_k)^\top)+r_k^+(x)(U_k^\top(x-s_t\mu_k)I+U_k(x-s_t\mu_k)^\top))].$$

$$\begin{aligned} \lambda_{H_{\mu\mu}} &= \mathbb{E}_{x\sim p_{data}}[(u^\top J_\mu^k)^2] \\ \lambda_{H_{UU}} &= \mathbb{E}_{x\sim p_{data}}[(u^\top J_U^k)^2] \\ \lambda_{H_{\mu U}} &= \mathbb{E}_{x\sim p_{data}}[(u^\top J_\mu^k)(u^\top J_U^k)] \le \sqrt{\lambda_{H_{\mu\mu}}\lambda_{H_{\mu U}}}. \end{aligned}$$

■

Analyze H

$$H = \begin{pmatrix} H_{\mu_k\mu_k} & H_{\mu_k U_k} \\ H_{\mu_k U_k} & H_{U_k U_k} \end{pmatrix}$$

. If we can prove that $H_{\mu_k\mu_k} - H_{U_k\mu_k}H_{U_kU_k}^{-1}H_{U_k\mu_k}^\top$ is positive-definite, then H is positive-definite for Schur's Theorem.

$$\lambda_H \ge \lambda_S \ge \lambda_{H_{\mu_k\mu_k}} - \frac{r^2\lambda_{H_{\mu_k\mu_k}}\lambda_{H_{U_kU_k}}}{\lambda_{H_{U_kU_k}}} = (1-r^2)\lambda_{H_{\mu_k\mu_k}} \ge (1-r^2)\frac{s_t^2}{(s_t^2+\gamma_t^2)^2} > 0.$$

$$r \;=\; \max_{\|u\|=1,\|v=1\|} \frac{u^\top H_{\mu_k U_k} v}{\sqrt{u^\top H_{\mu_k\mu_k} u \cdot v^\top H_{U_kU_k} v]}} \le 1.$$

$r=1$ if and only if $u^\top J_\mu^k = cv^\top J_U^k$, $c\neq 0$, which is almost impossible to happen.

More specially, if we assume that $\forall x\in\mathbb{R}^{d_k}$,$r_k^+=1$ or $r_k^-=1$, for

$$H_{\mu_k U_k} = \mathbb{E}_{x\sim p_{data}}[J_k^\mu (J_k^U)^\top] = \mathbb{E}_{x\sim p_{data}}[\frac{2s_t^3}{\gamma_t^4(s_t^2+\gamma_t^2)}(r_k^+(x)-r_k^-(x))(1-\frac{s_t^2}{s_t^2+\gamma_t^2}U_kU_k^\top)$$
$$(r_k^-(x)(U_k^\top(x+s_t\mu_k)I+U_k(x+s_t\mu_k)^\top)+r_k^+(x)(U_k^\top(x-s_t\mu_k)I+U_k(x-s_t\mu_k)^\top))]$$
$$= \mathbb{E}_{x\sim\mathcal{N}(s_t\mu_k,\Sigma_k)}[\frac{2s_t^3}{\gamma_t^4(s_t^2+\gamma_t^2)}(r_k^+(x)-r_k^-(x))\left(1-\frac{s_t^2}{s_t^2+\gamma_t^2}U_kU_k^\top\right)$$
$$(r_k^-(x)(U_k^\top(x+s_t\mu_k)I+U_k(x+s_t\mu_k)^\top)+r_k^+(x)(U_k^\top(x-s_t\mu_k)I+U_k(x-s_t\mu_k)^\top))]$$
$$= \mathbb{E}_{x\sim\mathcal{N}(s_t\mu_k,\Sigma_k)}[\frac{2s_t^3}{\gamma_t^4(s_t^2+\gamma_t^2)}\left(1-\frac{s_t^2}{s_t^2+\gamma_t^2}U_kU_k^\top\right)+(U_k^\top(x-s_t\mu_k)I+U_k(x-s_t\mu_k)^\top))]$$
$$= 0.$$

We have $r = 0$,

$$\alpha = \min\{\frac{s_t^2}{(s_t^2+\gamma_t^2)^2}, \frac{4(U_k^\top \mu_k))^2 + \|U_k\|_2^2\|\mu_k\|_2^2 - \|U_k\|_2\|\mu_k\|_2\sqrt{8(U_k^\top \mu_k))^2 + \|U_k\|_2^2\|\mu_k\|_2^2}}{2}\}.$$

Utill now, We have shown that H is α-convex and L-lipschiz, where $\alpha = (1-r^2)\lambda_{H_{\mu_k\mu_k}}$. And we can know that $L(\theta)$ is exponentially convergent.

Theorem C.5. *If we take $\eta_t = \eta = \frac{2}{\eta+L}$, and $\kappa = \frac{L}{\alpha}$, then*

$$\|\theta^t - \theta^\star\|_2 \le \left(\frac{\kappa-1}{\kappa+1}\right)^t \|\theta^{(0)} - \theta^\star\|_2.$$

D K-MODE MOG OPTIMIZATION

D.1 SETTING

In this section, we analyze

$$\begin{aligned}\nabla \log p_{t,k}(x) &= \frac{\nabla p_{t,k}(x)}{p_{t,k}(x)} \\ &= -\frac{1}{\gamma_t^2}\frac{\Sigma_{l=1}^{n_k}\pi_{k,l}\mathcal{N}(x; s_t\mu_{k,l}, s_t^2 U_{k,l}^\star U_{k,l}^{\star\top} + \gamma_t^2 I)\left(x - s_t\mu_{k,l} - \frac{s_t^2}{s_t^2+\gamma_t^2}U_{k,l}^\star U_{k,l}^{\star\top}(x - s_t\mu_{k,l})\right)}{\Sigma_{l=1}^{n_k}\pi_{k,l}\mathcal{N}(x; s_t\mu_{k,l}, s_t^2 U_{k,l}^\star U_{k,l}^{\star\top} + \gamma_t^2 I)}.\end{aligned}$$

D.2 OPTIMIZATION

Assumption D.1. [Highly separated Gaussian] Consider the Gaussian mixture

$$p_k(x) = \sum_{l=1}^{n_k}\pi_{k,l}\,\mathcal{N}(x;\mu_{k,l},\Sigma_{k,l}), \qquad r_{k,l}(x) := \frac{\pi_{k,l}\,\mathcal{N}(x;\mu_{k,l},\Sigma_{k,l})}{\sum_{i=1}^{n_k}\pi_{k,i}\,\mathcal{N}(x;\mu_{k,i},\Sigma_{k,i})}.$$

There exist constants $\varepsilon \ll 1$ and $\delta \ll 1$ such that when $x \sim p_k$ we have

$$\Pr_{x\sim p_k}\Big(\exists\, l \in \{1,\dots,n_k\} \text{ with } r_{k,l}(x) \ge 1-\varepsilon\Big) \;\ge\; 1-\delta.$$

We assume that the gap between the subspaces is large, and the gap within the subspace is relatively small, and the equivalent Gaussian is used to replace the whole subspace.

Corollary D.2. *Assume that $\|\mu_{k,i}^* - \mu_{k,j}^*\|_2 \le \delta$, $\|U_{k,i}^* - U_{k,j}^*\|_2 \le \epsilon$ and $\|x - \bar{\mu}_k^*\|_2 \le \Delta$. We have*

$$\|\log p(x) - \log \bar{p}(x)\|_2 = O(\epsilon + \delta\Delta + \Delta^3)$$

Proof. For k-th subspace, $w_k(x) = \Sigma_{l=1}^{n_k}\pi_{k,l}\mathcal{N}(x; s_t\mu_{k,l}, \Sigma_{k,l})$, we take

$$\widetilde{w}_k(x) = \mathcal{N}\big(x;\, \bar{\mu}_k, \bar{\Sigma}_k\big).$$

where

$$\begin{aligned}&\mathbb{E}_{\widetilde{w}_k}[x] = \bar{\mu}_k = \mathbb{E}_{w_k}[x] = \Sigma_{l=1}^{n_k}\pi_{k,l}s_t\mu_{k,l} \\ &Cov_{\widetilde{w}_k}(x) = Cov_{w_k}(x) = \mathbb{E}[(x-\bar{\mu}_k)(x-\bar{\mu}_k)^\top] = \Sigma_{l=1}^{n_k}\pi_{k,l}(\Sigma_{k,l} + s_t^2\mu_{k,l}\mu_{k,l}^\top - s_t^2\bar{\mu}_{k,l}\bar{\mu}_{k,l}^\top) \\ &\Rightarrow \bar{\Sigma}_k = \Sigma_{l=1}^{n_k}(\Sigma_{k,l} + s_t^2\mu_{k,l}\mu_{k,l}^\top - s_t^2\bar{\mu}_{k,l}\bar{\mu}_{k,l}^\top).\end{aligned}$$

We next show the order of the estimation under the condition that $\|\mu_{k,i} - \mu_{k,j}\|_2 \le \delta$, $\|U_{k,i} - U_{k,j}\|_2 \le \epsilon$ and $\|x - \bar{\mu}_k\|_2 \le \Delta$.Using Taylor's Theorem and take $x_0 = \bar{\mu}_k$, we can obtain that

$$\log p(x) = \log p(x_0) + (x-x_0)^\top\nabla\log p(x_0) + \frac{1}{2}(x-x_0)^\top\nabla^2\log p(x_0)(x-x_0) + O(\|x-x_0\|^3)$$

$$\log \tilde{p}(x) = \log \tilde{p}(x_0) + (x-x_0)^\top\nabla\log \tilde{p}(x_0) + \frac{1}{2}(x-x_0)^\top\nabla^2\log \tilde{p}(x_0)(x-x_0) + O(\|x-x_0\|^3).$$

$$\begin{aligned}\log p(x_0) - \log \tilde{p}(x_0) &= \log \frac{\Sigma_{l=1}^{n_k} \pi_{k,l} \mathcal{N}(x_0; \mu_{k,l}, \Sigma_{k,l})}{\mathcal{N}(x_0; \bar{\mu}_k, \bar{\Sigma}_k)} \\ &= \log \left(\Sigma_{l=1}^{n_k} \pi_{k,l} \frac{1}{|\Sigma_{k,l}|^{\frac{1}{2}}} \exp(-\frac{1}{2}(\bar{\mu} - \mu_{k,l})^\top \Sigma_{k,l}^{-1}(\bar{\mu} - \mu_{k,l})) \right) + \frac{1}{2} \log |\bar{\Sigma}_k| \\ &= \log \left(\Sigma_{l=1}^{n_k} \pi_{k,l} \frac{1}{|\Sigma_{k,l}|^{\frac{1}{2}}} (1 + O(\delta^2)) \right) + \frac{1}{2} \log |\bar{\Sigma}_k| \\ &= \log \left(\Sigma_{l=1}^{n_k} \pi_{k,l} \frac{|\bar{\Sigma}_k|^{\frac{1}{2}}}{|\Sigma_{k,l}|^{\frac{1}{2}}} + O(\delta^2) \right) \\ &= O \left(\Sigma_{l=1}^{n_k} \pi_{k,l} (\frac{|\bar{\Sigma}_k|^{\frac{1}{2}}}{|\Sigma_{k,l}|^{\frac{1}{2}}} - 1 \right) + O(\delta^2).\end{aligned}$$

$$\| \log p(x_0) - \log \tilde{p}(x_0) \|_2 = O(\epsilon + \delta^2).$$

$$\begin{aligned}\nabla \log p(x_0) - \nabla \log \tilde{p}(x_0) &= \nabla \log \Sigma_{l=1}^{n_k} \pi_{k,l} \mathcal{N}(x; \mu_{k,l}, \Sigma_{k,l})|_{x_0} \\ &= \frac{\Sigma_{l=1}^{n_k} \pi_{k,l} \mathcal{N}(x_0; \mu_{k,l}, \Sigma_{k,l})(-\Sigma_{k,l}^{-1}(\bar{\mu} - \mu_{k,l})))}{p(x_0)}.\end{aligned}$$

$$\|\nabla \log p(x_0) - \nabla \log \tilde{p}(x_0)\|_2 = O(\delta).$$

$$\begin{aligned}\nabla^2 \log p(x_0) - \nabla^2 \log \tilde{p}(x_0) &= \frac{\nabla^2 p(x_0)}{p(x_0)} - (\frac{\nabla p(x_0)}{p(x_0)})(\frac{\nabla p(x_0)}{p(x_0)})^\top - \frac{\nabla^2 \tilde{p}(x_0)}{\tilde{p}(x_0)} \\ &= (\frac{\nabla^2 p(x_0)}{p(x_0)} - \frac{\nabla^2 \tilde{p}(x_0)}{\tilde{p}(x_0)}) - (\frac{\nabla p(x_0)}{p(x_0)})(\frac{\nabla p(x_0)}{p(x_0)})^\top.\end{aligned}$$

$$\|\nabla^2 \log p(x_0) - \nabla^2 \log \tilde{p}(x_0)\|_2 = O(\epsilon^2 + \delta^2).$$

Thus, $\| \log p(x) - \log \tilde{p}(x) \|_2 = O(\epsilon + \delta\Delta + \Delta^3)$. ■

Lemma D.3. *[Eigenvalues of the Hessian] Assume Assumption 6.6, the Hessian at the k-th subspace is convex on a neighborhood of θ^*. If $\forall x \in \mathbb{R}^{d_k}$, $r_k^+(x) = 1$ or 1 are strictly satisfied, we have*

$$\lambda_{\min}(H_{\mu_{k,l}\mu_{k,l}}) = \frac{\pi_{k,l} s_t^2}{(s_t^2 + \gamma_t^2)^2},$$

and $\lambda_{\min}(H_{U_{k,l}U_{k,l}})$ has the following form:

$$\left(\pi_{k,l} 4(U_{k,l}^\top \mu_{k,l}))^2 + \|U_{k,l}\|_2^2 \|\mu_{k,l}\|_2^2 - \|U_{k,l}\|_2 \|\mu_{k,l}\|_2 \sqrt{8(U_{k,l}^\top \mu_{k,l}))^2 + \|U_{k,l}\|_2^2 \|\mu_{k,l}\|_2^2} \right) / 2.$$

Proof. According to the previous conclusion, we only need to calculate J_μ and J_U.With these assumptions and simplifications, similar to the symmetry case, we will prove that $J_{k,l}^\mu$ and $J_{k,l}^U$ have

dominant terms.

$$
\begin{aligned}
&J^{\mu}_{k,l}(x) \\
&= -\frac{1}{\gamma_t^2}\frac{\partial s_\theta(x,t)}{\partial \mu_{k,l}} \\
&= -\frac{1}{\gamma_t^2}\frac{\Sigma_{l=1}^{n_k}\left(\frac{\partial w_{k,l}(x)}{\partial \mu_{k,l}}\delta_{k,l}(x)+\frac{\partial \delta_{k,l}(x)}{\partial \mu_{k,l}}w_{k,l}(x)\right)w_k(x)-\frac{\partial w_k(x)}{\partial \mu_{k,l}}\Sigma_{l=1}^{n_k}w_{k,l}(x)\delta_{k,l}(x)}{w_k^2(x)} \\
&= -\frac{1}{\gamma_t^2}\left(\frac{\Sigma_{l=1}^{n_k}\frac{\partial w_{k,l}(x)}{\partial \mu_{k,l}}\delta_{k,l}(x)}{w_k(x)}+\frac{\Sigma_{l=1}^{n_k}\frac{\partial \delta_{k,l}(x)}{\partial \mu_{k,l}}w_{k,l}(x)}{w_k(x)}-\frac{\frac{\partial w_k(x)}{\partial \mu_{k,l}}\Sigma_{l=1}^{n_k}w_{k,l}(x)\delta_{k,l}(x)}{w_k^2(x)}\right).
\end{aligned}
$$

Let's go ahead and do the calculation.

$$
\begin{aligned}
&\frac{\Sigma_{l=1}^{n_k}\frac{\partial w_{k,l}(x)}{\partial \mu_{k,l}}\delta_{k,l}(x)}{w_k(x)}-\frac{(\frac{\partial w_k(x)}{\partial \mu_{k,l}})\Sigma_{l=1}^{n_k}w_{k,l}(x)\delta_{k,l}(x)}{w_k^2(x)}=\frac{\frac{\partial w_{k,l}(x)}{\partial \mu_{k,l}}}{w_k(x)}(\delta_{k,l}(x)-\bar{\delta}_k(x)) \\
&\frac{\Sigma_{l=1}^{n_k}\frac{\partial \delta_{k,l}(x)}{\partial \mu_{k,l}}w_{k,l}(x)}{w_k(x)}\approx\frac{s_t}{\gamma_t^2}\Sigma_{l=1}^{n_k}r_{k,l}(x)\left(I-\frac{s_t^2}{s_t^2+\gamma_t^2}U_{k,l}U_{k,l}^{\top}\right).
\end{aligned}
$$

where $r_{k,l}(x)=\frac{\pi_{k,l}\mathcal{N}\left(x;\bar{\mu}_k,\bar{\Sigma}_k\right)}{\Sigma_{j=1}^{K}\mathcal{N}\left(x;\bar{\mu}_j,\bar{\Sigma}_j\right)}$.

Therefore, we can obtain that

$$
\begin{aligned}
&\|\frac{\Sigma_{l=1}^{n_k}\frac{\partial w_{k,l}(x)}{\partial \mu_{k,l}}\delta_{k,l}(x)}{w_k(x)}-\frac{\frac{\partial w_k(x)}{\partial \mu_{k,l}}\Sigma_{l=1}^{n_k}(w_{k,l}(x)\delta_{k,l}(x))}{w_k^2(x)}\|_2=O(\delta(R+s_tB_\mu)\frac{s_t^2}{\gamma_t^2}) \\
&\|\frac{\Sigma_{l=1}^{n_k}\frac{\partial \delta_{k,l}(x)}{\partial \mu_{k,l}}w_{k,l}(x)}{w_k(x)}\|_2=O(s_t).
\end{aligned}
$$

where $\delta\le\|\mu_{k,i}-\mu_{k,j}\|_2\ll 1$.

Thus, we have

$$
J^{\mu}_{k,l}(x)=\frac{\partial s_\theta}{\partial \mu_{k,l}}\approx\frac{s_t}{\gamma_t^2}r_{k,l}(x)\left(I-\frac{s_t^2}{s_t^2+\gamma_t^2}U_{k,l}U_{k,l}^{\top}\right).
$$

$$
\begin{aligned}
H_{\mu_{k,l}\mu_{k,l}}&=\mathbb{E}_{x\sim p_t}\left[J^{\mu}_{k,l}(x)\,J^{\mu}_{k,l}(x)^{\top}\right] \\
&=\frac{s_t^2}{\gamma_t^4}\,\mathbb{E}\left[r_{k,l}(x)^2\right]\,\left(I-\frac{s_t^2}{s_t^2+\gamma_t^2}\,U_{k,l}U_{k,l}^{\top}\right)\left(I-\frac{s_t^2}{s_t^2+\gamma_t^2}\,U_{k,l}U_{k,l}^{\top}\right)^{\top}.
\end{aligned}
$$

For a given x, since we focus on the equivalent Gaussian distribution for each cluster,we have

$$
H_{\mu_k\mu_k}\approx diag(\mathbb{E}[r_{k,1}^2]H_{\mu_{k,1}\mu_{k,1}},\,\mathbb{E}[r_{k,2}^2]H_{\mu_{k,2}\mu_{k,2}},\,\ldots,\,\mathbb{E}[r_{k,n_k}^2]H_{\mu_{k,n_k}\mu_{k,n_k}}).
$$

We first show that $\mathbb{E}[r_{k,l}^2]H_{\mu_{k,l}\mu_{k,l}}$ is positive-definite, then we will further show that $H_{\mu_k\mu_k}$ is positive-definite.

For $H_{\mu_{k,l}\mu_{k,l}}$, we know that

$$
\begin{aligned}
\lambda_{min}(H_{\mu_{k,l}\mu_{k,l}})&=c_{k,l}\lambda_{min}(J^{\mu}_{k,l}(J^{\mu}_{k,l})^{\top}) \\
&=c_{k,l}\lambda_{min}((I-\alpha P_k)^2) \\
&=\frac{c_{k,l}\gamma_t^4}{(s_t^2+\gamma_t^2)^2},
\end{aligned}
$$

where

$$c_{k,l} = \frac{s_t^2}{\gamma_t^4}\mathbb{E}[r_{k,l}^2] \approx \pi_{k,l}\frac{s_t^2}{\gamma_t^4}\,.$$

We know that for a block matrix $A = diag(A_1, A_2, \ldots, A_k)$,

$$\lambda(A) = \cup_{i=1}^{k}\lambda(A_i).$$

Therefore,

$$\lambda_{min}(H_{\mu_k\mu_k}) = \min_{l=1\ldots,n_k} \frac{c_{k,l}\gamma_t^4}{(s_t^2+\gamma_t^2)^2}.$$

Thus, we take

$$\lambda_{H_{\mu_k\mu_k}} = \frac{c_{k,n_k}\gamma_t^4}{(s_t^2+\gamma_t^2)^2}.$$

Similar to previous situation ,because

$$\frac{\|\frac{\Sigma_{l=1}^{n_k}(\frac{\partial\delta_{k,l}(x)}{\partial U_{k,l}}w_{k,l}(x))(w_k(x))-(\frac{\partial w_k(x)}{\partial U_{k,l}})\Sigma_{l=1}^{n_k}w_{k,l}(x)\delta_{k,l}(x)}{w_k^2(x)}\|_2}{\|\frac{\Sigma_{l=1}^{n_k}\frac{\partial\delta_{k,l}(x)}{\partial U_{k,l}}w_{k,l}(x)}{w_k(x)}\|_2} \to 0.$$

we can obtain that

$$\begin{aligned}
J_{k,l}^U(x) &= -\frac{1}{\gamma_t^2}\frac{\Sigma_{l=1}^{n_k}(\frac{\partial w_{k,l}(x)}{\partial U_{k,l}}\delta_{k,l}(x) + w_{k,l}(x)\frac{\partial\delta_{k,l}(x)}{\partial U_{k,l}})w_k(x) - (\frac{\partial w_k(x)}{\partial U_{k,l}})\Sigma_{l=1}^{n_k}w_{k,l}(x)\delta_{k,l}(x)}{w_k^2(x)} \\
&= -\frac{1}{\gamma_t^2}\frac{\Sigma_{l=1}^{n_k}w_{k,l}(x)\frac{\partial\delta_{k,l}(x)}{\partial U_{k,l}}}{w_k(x)} \\
&\approx \frac{1}{\gamma_t^2}\frac{s_t^2}{s_t^2+\gamma_t^2}\, r_{k,l}(x)\, \Big[U_{k,l}(x-\mu_{k,l})^\top \;+\; (x-\mu_{k,l})^\top U_{k,l} I\Big].
\end{aligned}$$

$$H_{U_kU_k} \approx diag(\mathbb{E}[r_{k,1}^2]H_{U_{k,1}U_{k,1}},\, \mathbb{E}[r_{k,2}^2]H_{U_{k,2}U_{k,2}},\, \ldots,\, \mathbb{E}[r_{k,n_k}^2]H_{U_{k,n_k}U_{k,n_k}}).$$

$$\begin{aligned}
H_{U_{k,l}U_{k,l}} &= \mathbb{E}[J_{k,l}^U(x)(J_{k,l}^U(x))^\top] \\
&= \mathbb{E}[(\frac{\alpha}{\gamma_t^2})^2\left(U_{k,l}(x-\mu_{k,l})^\top(x-\mu_{k,l})U_{k,l}^\top + U_{k,l}^\top(x-\mu_{k,l})U_{k,l}(x-\mu_{k,l})^\top\right)] \\
&+ \mathbb{E}[(\frac{\alpha}{\gamma_t^2})^2\left(U_{k,l}^\top(x-\mu_{k,l})(x-\mu_{k,l})U_{k,l}^\top + (U_{k,l}^\top(x-\mu_{k,l}))^2\right)].
\end{aligned}$$

Similar to our calculation in 6.3, we can use C.3 to calculate the minimum eigenvalue of $H_{U_{k,l}U_{k,l}}$. $H_{U_{k,l}U_{k,l}}$ is positive definite and

$$\lambda_{\min}(H_{U_{k,l}U_{k,l}}) = \frac{4(U_{k,l}^\top\mu_{k,l}))^2 + \|U_{k,l}\|_2^2\|\mu_{k,l}\|_2^2 - \|U_{k,l}\|_2\|\mu_{k,l}\|_2\sqrt{8(U_{k,l}^\top\mu_{k,l}))^2 + \|U_{k,l}\|_2^2\|\mu_{k,l}\|_2^2}}{2}.$$

Recall that

$$H_{U_kU_k} \approx diag(\mathbb{E}[r_{k,1}^2]H_{U_{k,1}U_{k,1}},\, \mathbb{E}[r_{k,2}^2]H_{U_{k,2}U_{k,2}},\, \ldots,\, \mathbb{E}[r_{k,n_k}^2]H_{U_{k,n_k}U_{k,n_k}}).$$

and $\mathbb{E}[r_{k,l}^2] \approx \pi_{k,l}$, we can obtain the minimum eigenvalue of $H_{U_kU_k}$, which is

$$\min_{l=1,2,\ldots,n_k} \pi_{k,l}\frac{4(U_{k,l}^\top\mu_{k,l}))^2 + \|U_{k,l}\|_2^2\|\mu_{k,l}\|_2^2 - \|U_{k,l}\|_2\|\mu_{k,l}\|_2\sqrt{8(U_{k,l}^\top\mu_{k,l}))^2 + \|U_{k,l}\|_2^2\|\mu_{k,l}\|_2^2}}{2}.$$

■

Lemma D.4. *[Local Strong Convexity] Assume Assumption 6.6, in a neighborhood of θ^*, $\nabla^2\mathcal{L}(\theta) \succeq \alpha' I, \alpha' > 0, \forall\theta \in \Theta$. If $\forall x \in \mathbb{R}^{d_k}$, $\exists l \in [n_k], r_{k,l}(x) = 1$ are strictly satisfied, $\alpha' = \min\{\lambda_1, \lambda_2\}$, where $\lambda_1 = \min_{l=1\dots,n_k} \frac{c_{k,l}\gamma_t^4}{(s_t^2+\gamma_t^2)^2}$, $\lambda_2 = \min_{l=1,2,\dots,n_k} = \lambda_{\min}(H_{U_{k,l}U_{k,l}})$.*

Proof.

$$H_{\mu_k U_k} = diag(H_{\mu_{k,1}U_{k,1}}, H_{\mu_{k,2}U_{k,2}}, \dots, H_{\mu_{k,1n_k}U_{k,n_k}}).$$

$$\|H_{\mu_k U_k}\| \le \sqrt{\|H_{\mu_k\mu_k}\|\,\|H_{U_kU_k}\|} = O\Big(\frac{s_t^3}{\gamma_t^2\,(s_t^2+\gamma_t^2)^2}\Big).$$

$$H = \begin{pmatrix} \operatorname{diag}\big(H_{\mu_{k,1}\mu_{k,1}}, \dots, H_{\mu_{k,n_k}\mu_{k,n_k}}\big) & \operatorname{diag}\big(H_{\mu_{k,1}U_{k,1}}, \dots, H_{\mu_{k,n_k}U_{k,n_k}}\big) \\ \operatorname{diag}\big(H_{\mu_{k,1}U_{k,1}}, \dots, H_{\mu_{k,n_k}U_{k,n_k}}\big) & \operatorname{diag}\big(H_{U_{k,1}U_{k,1}}, \dots, H_{U_{k,n_k}U_{k,n_k}}\big) \end{pmatrix}.$$

Let

$$S = H_{\mu\mu} - H_{\mu U}H_{UU}^{-1}H_{U\mu}$$

we have

$$\lambda_H \ge \lambda_S \ge \lambda_{H_{\mu_k\mu_k}} - \frac{r^2\lambda_{H_{\mu_k\mu_k}}\lambda_{H_{U_kU_k}}}{\lambda_{H_{U_kU_k}}} = (1-r^2)\lambda_{H_{\mu_k\mu_k}} \ge (1-r^2)\frac{s_t^2}{(s_t^2+\gamma_t^2)^2} > 0.$$

$$r \;=\; \max_{\|u\|=1,\|v=1\|} \frac{u^\top H_{\mu_k U_k} v}{\sqrt{u^\top H_{\mu_k\mu_k} u \cdot v^\top H_{U_kU_k} v]}} \le 1.$$

$r = 1$ if and only if $u^\top J_\mu^k = cv^\top J_U^k$, $c \neq 0$, which is almost impossible to happen.

More specifically, if we assume that $\forall x \in \mathbb{R}^{d_k}, \exists l \in [n_k], r_{k,l}(x) = 1$, we have

$$\begin{aligned}
&H_{\mu_{k,l}U_{k,l}} = \mathbb{E}_{x\sim p_k}\left[J_{k,l}^U(x)\,(J_{k,l}^\mu(x))^\top\right] \\
&= \frac{1}{\gamma_t^4}\frac{s_t^3}{s_t^2+\gamma_t^2}\,\mathbb{E}_{x\sim p_k}\Big[r_{k,l}(x)^2((x-\mu_{k,l})U_{k,l}^\top \;+\; (x-\mu_{k,l})^\top U_{k,l}I)\Big]\left(I - \frac{s_t^2}{s_t^2+\gamma_t^2}U_{k,l}U_{k,l}^\top\right) \\
&= \frac{1}{\gamma_t^4}\frac{s_t^3}{s_t^2+\gamma_t^2}\,\mathbb{E}_{x\sim \pi_{k,l}\mathcal{N}_{k,l}}\Big[r_{k,l}(x)^2((x-\mu_{k,l})U_{k,l}^\top \;+\; (x-\mu_{k,l})^\top U_{k,l}I)\Big]\left(I - \frac{s_t^2}{s_t^2+\gamma_t^2}U_{k,l}U_{k,l}^\top\right) \\
&\approx 0
\end{aligned}$$

The second equation holds because $\forall x$, if $x \notin \mathcal{N}_{k,l}(\mu_{k,l}, \Sigma_{k,l})$, $r_{k,l}(x) = 0$. And the third equation holds because if $x \sim \mathcal{N}_{k,l}, (\mu_{k,l}, \Sigma_{k,l})$, $\forall$ Const C,

$$\mathbb{E}_{x\sim\pi_{k,l}\mathcal{N}_{k,l}}[C(x-\mu_{k,l})] = 0.$$

.

Thus, let α' be the minimum eigenvalue of H,

$$\alpha' = \min\{\lambda_1, \lambda_2\}, \tag{8}$$

where

$$\lambda_1 = \min_{l=1\dots,n_k} \frac{c_{k,l}\gamma_t^4}{(s_t^2+\gamma_t^2)^2},$$

and

$$\lambda_2 = \min_{l=1,2,\dots,n_k} \pi_{k,l}\frac{4(U_{k,l}^\top\mu_{k,l}))^2 + \|U_{k,l}\|_2^2\|\mu_{k,l}\|_2^2 - \|U_{k,l}\|_2\|\mu_{k,l}\|_2\sqrt{8(U_{k,l}^\top\mu_{k,l}))^2 + \|U_{k,l}\|_2^2\|\mu_{k,l}\|_2^2}}{2}.$$

■

E THE DETAIL OF THE REAL-WORLD EXPERIMENTS

In the part, we provide the detail of the experiments, including dataset and training pipeline. We use MNIST and CIFAR-10 as the datasets, and we adopt the mixture Gaussian distribution as the prior distribution in both cases.

For MNIST, our model consists of MLP-based encoder and decoder networks, each with a single hidden layer of 256 dimensions. The model is trained with the AdamW optimizer at a learning rate of 0.0005. We train 10 VAEs with the numbers 1 to 10 as the ten clusters.

On CIFAR-10, we implement a 3-layer RNN encoder and decoder for CIFAR-10. The encoder hidden dimensions are [64, 128, 256], and the decoder's are [256, 128, 64].And we train 10 VAEs for each of the ten clusters based on the classification by category. Each layer in both networks stacks 3 recurrent blocks.The model is trained with the AdamW optimizer at a learning rate of 0.0001.

Our experiment was conducted on RTX4090.