

Appendix:

Optimize to Generalize in Gaussian Processes: An Alternative Objective Based on the Rényi Divergence

Introduction

This appendix contains all technical details in our main paper and some additional empirical results.

A The Variational Rényi Lower Bound

A.1 The Rényi Divergence

The Rényi's α -divergence between p and q is defined as [\[Rényi et al., 1961\]](#)

$$D_\alpha[p||q] = \frac{1}{\alpha - 1} \log \int p(\mathbf{w})^\alpha q(\mathbf{w})^{1-\alpha} d\mathbf{w}, \alpha \in [0, 1),$$

where \mathbf{w} is the parameter for p, q . Let $q := q(\mathbf{f}, \mathbf{U})$ and $p := p(\mathbf{f}, \mathbf{U}, \mathbf{Y})$. In the context of \mathcal{GP} s, we have

$$\begin{aligned} D_\alpha[q(\mathbf{f}, \mathbf{U})||p(\mathbf{f}, \mathbf{U}|\mathbf{Y})] &= \frac{1}{\alpha - 1} \log \int q(\mathbf{f}, \mathbf{U})^\alpha p(\mathbf{f}, \mathbf{U}|\mathbf{Y})^{1-\alpha} d\mathbf{U} d\mathbf{f} \\ &= \frac{1}{1 - \alpha} \log P(\mathbf{Y})^{1-\alpha} - \frac{1}{1 - \alpha} \log \int q(\mathbf{f}, \mathbf{U})^\alpha (p(\mathbf{f}, \mathbf{U}|\mathbf{Y})p(\mathbf{Y}))^{1-\alpha} d\mathbf{U} d\mathbf{f} \\ &= \log p(\mathbf{Y}) - \frac{1}{1 - \alpha} \log \int q(\mathbf{f}, \mathbf{U}) \frac{(p(\mathbf{f}, \mathbf{U}|\mathbf{Y})p(\mathbf{Y}))^{1-\alpha}}{q(\mathbf{f}, \mathbf{U})^{1-\alpha}} d\mathbf{U} d\mathbf{f} \\ &= \log p(\mathbf{Y}) - \frac{1}{1 - \alpha} \log \mathbb{E}_q \left[\left(\frac{p(\mathbf{f}, \mathbf{U}, \mathbf{Y})}{q(\mathbf{f}, \mathbf{U})} \right)^{1-\alpha} \right]. \end{aligned}$$

Therefore, the Rényi variational lower bound can be derived as

$$\mathcal{L}_\alpha(q; \mathbf{Y}) = \frac{1}{1-\alpha} \log \mathbb{E}_q \left[\left(\frac{p(\mathbf{f}, \mathbf{U}, \mathbf{Y})}{q(\mathbf{f}, \mathbf{U})} \right)^{1-\alpha} \right]. \quad (1)$$

A.2 Mean-field Assumption

When we apply the Rényi divergence to \mathcal{GP} and assume that $q(\mathbf{f}, \mathbf{U}) = p(\mathbf{f}|\mathbf{U})q(\mathbf{U})$ (mean-field assumption), we can further obtain

$$\begin{aligned} \mathcal{L}_\alpha(q; \mathbf{Y}) &:= \frac{1}{1-\alpha} \log \mathbb{E}_q \left[\left(\frac{p(\mathbf{f}, \mathbf{U}, \mathbf{Y})}{q(\mathbf{f}, \mathbf{U})} \right)^{1-\alpha} \right] \\ &= \frac{1}{1-\alpha} \log \mathbb{E}_q \left[\left(\frac{p(\mathbf{Y}|\mathbf{f})p(\mathbf{f}|\mathbf{U})p(\mathbf{U})}{p(\mathbf{f}|\mathbf{U})q(\mathbf{U})} \right)^{1-\alpha} \right] \\ &= \frac{1}{1-\alpha} \log \int p(\mathbf{f}|\mathbf{U})q(\mathbf{U}) \left(\frac{p(\mathbf{Y}|\mathbf{f})p(\mathbf{U})}{q(\mathbf{U})} \right)^{1-\alpha} d\mathbf{U} d\mathbf{f} \\ &= \frac{1}{1-\alpha} \log \int p(\mathbf{f}|\mathbf{U})q(\mathbf{U})^\alpha \left(p(\mathbf{Y}|\mathbf{f})p(\mathbf{U}) \right)^{1-\alpha} d\mathbf{U} d\mathbf{f} \\ &= \frac{1}{1-\alpha} \log \int \int p(\mathbf{f}|\mathbf{U})p(\mathbf{Y}|\mathbf{f})^{1-\alpha} d\mathbf{f} q(\mathbf{U})^\alpha p(\mathbf{U})^{1-\alpha} d\mathbf{U}. \end{aligned}$$

For simplicity, we drop the notation \mathbf{Y} in the $\mathcal{L}_\alpha(q; \mathbf{Y})$. It can be easily shown that $p(\mathbf{f}|\mathbf{U}) = \phi(\mathbf{K}_{f,U} \mathbf{K}_{U,U}^{-1} \mathbf{U}, \mathbf{K}_{f,f} - \mathbf{Q})$, where $\mathbf{Q} = \mathbf{K}_{f,U} \mathbf{K}_{U,U}^{-1} \mathbf{K}_{U,f}$. Besides, we have $p(\mathbf{Y}|\mathbf{f}) = \phi(\mathbf{f}, \sigma_\epsilon^2 I)$. Therefore,

$$\begin{aligned} &\int p(\mathbf{f}|\mathbf{U})p(\mathbf{Y}|\mathbf{f})^{1-\alpha} d\mathbf{f} \\ &= \int p(\mathbf{f}|\mathbf{U}) (|2\pi\sigma_\epsilon^2 I|^{-0.5} e^{-\frac{1}{2}(\mathbf{Y}-\mathbf{f})^T (\sigma_\epsilon^2 I)^{-1} (\mathbf{Y}-\mathbf{f})})^{1-\alpha} d\mathbf{f} \\ &= \frac{|2\pi\sigma_\epsilon^2 I|^{-0.5(1-\alpha)}}{|2\pi\sigma_\epsilon^2 I/(1-\alpha)|^{-0.5}} \int p(\mathbf{f}|\mathbf{U}) \phi(\mathbf{f}, \frac{\sigma_\epsilon^2 I}{1-\alpha}) d\mathbf{f} \\ &= \frac{|2\pi\sigma_\epsilon^2 I|^{-0.5(1-\alpha)}}{|2\pi\sigma_\epsilon^2 I/(1-\alpha)|^{-0.5}} \phi(\mathbf{K}_{f,U} \mathbf{K}_{U,U}^{-1} \mathbf{U}, \frac{\sigma_\epsilon^2}{1-\alpha} I + \mathbf{K}_{f,f} - \mathbf{Q}) \\ &= (2\pi\sigma_\epsilon^2)^{\frac{\alpha N}{2}} \left(\frac{1}{1-\alpha} \right)^{\frac{N}{2}} \phi(\mathbf{K}_{f,U} \mathbf{K}_{U,U}^{-1} \mathbf{U}, \frac{\sigma_\epsilon^2}{1-\alpha} I + \mathbf{K}_{f,f} - \mathbf{Q}) \\ &= p_\alpha(\mathbf{Y}|\mathbf{U}). \end{aligned}$$

A.3 Find the Optimal Member, q , of the Family of Approximate Densities \mathcal{Q}

Instead of treating $q(\mathbf{U})$ as a pool of free parameters, it is desirable to find the optimal $q^*(\mathbf{U})$ to maximize the lower bound. To proceed, we have,

$$\begin{aligned}\mathcal{L}_\alpha(q) &= \frac{1}{1-\alpha} \log \int p_\alpha(\mathbf{Y}|\mathbf{U}) q(\mathbf{U})^\alpha p(\mathbf{U})^{1-\alpha} d\mathbf{U} \\ &= \frac{1}{1-\alpha} \log \int q(\mathbf{U}) \left(\frac{p_\alpha(\mathbf{Y}|\mathbf{U})^{1/(1-\alpha)} p(\mathbf{U})}{q(\mathbf{U})} \right)^{1-\alpha} d\mathbf{U} \\ &= \frac{1}{1-\alpha} \log \mathbb{E}_q \left(\frac{p_\alpha(\mathbf{Y}|\mathbf{U})^{1/(1-\alpha)} p(\mathbf{U})}{q(\mathbf{U})} \right)^{1-\alpha}\end{aligned}$$

By taking derivative of $\mathcal{L}_\alpha(q)$ with respect to $q(\mathbf{U})$ and set it to 0, we can obtain the optimal expression of $q(\mathbf{U})$:

$$q^*(\mathbf{U}) \propto p_\alpha(\mathbf{Y}|\mathbf{U})^{1/(1-\alpha)} p(\mathbf{U}).$$

Specifically,

$$q^*(\mathbf{U}) = \frac{p_\alpha(\mathbf{Y}|\mathbf{U})^{1/(1-\alpha)} p(\mathbf{U})}{\int p_\alpha(\mathbf{Y}|\mathbf{U})^{1/(1-\alpha)} p(\mathbf{U}) d\mathbf{U}}.$$

Therefore, we can obtain

$$\begin{aligned}\mathcal{L}_\alpha^*(q; \mathbf{Y}) &= \frac{1}{1-\alpha} \log [\mathbb{E}_q \left(\frac{p_\alpha(\mathbf{Y}|\mathbf{U})^{1/(1-\alpha)} p(\mathbf{U})}{q(\mathbf{U})} \right)]^{1-\alpha} \\ &= \log \mathbb{E}_q \left(\frac{p_\alpha(\mathbf{Y}|\mathbf{U})^{1/(1-\alpha)} p(\mathbf{U})}{q(\mathbf{U})} \right) \\ &= \log \int p_\alpha(\mathbf{Y}|\mathbf{U})^{1/(1-\alpha)} p(\mathbf{U}) d\mathbf{U}.\end{aligned}$$

where $\mathcal{L}_\alpha^*(q; \mathbf{Y})$ is $\mathcal{L}_\alpha(q)$ with $q^*(\mathbf{U})$.

A.4 Finding the closed form

So far, we have shown that

$$\mathcal{L}_\alpha^*(q; \mathbf{Y}) = \log \int p_\alpha(\mathbf{Y}|\mathbf{U})^{1/(1-\alpha)} p(\mathbf{U}) d\mathbf{U}.$$

Our final goal is to simplify this integration and obtain our proposed lower bound.

It can be shown that

$$\begin{aligned} p_\alpha(\mathbf{Y}|\mathbf{U})^{\frac{1}{1-\alpha}} &= [(2\pi\sigma_\epsilon^2)^{\frac{\alpha N}{2}} (\frac{1}{1-\alpha})^{\frac{N}{2}}]^{\frac{1}{1-\alpha}} \phi(\mathbf{K}_{f,U} \mathbf{K}_{U,U}^{-1} \mathbf{U}, \frac{\sigma_\epsilon^2}{1-\alpha} I + \mathbf{K}_{f,f} - \mathbf{Q})^{\frac{1}{1-\alpha}} \\ &= [(2\pi\sigma_\epsilon^2)^{\frac{\alpha N}{2(1-\alpha)}} (\frac{1}{1-\alpha})^{\frac{N}{2(1-\alpha)}}] C \phi(\mathbf{K}_{f,U} \mathbf{K}_{U,U}^{-1} \mathbf{U}, \sigma_\epsilon^2 I + (1-\alpha)[\mathbf{K}_{f,f} - \mathbf{Q}]), \end{aligned}$$

where $C = \frac{|2\pi(\frac{\sigma_\epsilon^2}{1-\alpha} I + \mathbf{K}_{f,f} - \mathbf{Q})|^{-0.5/(1-\alpha)}}{|2\pi(\sigma_\epsilon^2 I + (1-\alpha)[\mathbf{K}_{f,f} - \mathbf{Q}])|^{-0.5}} = |2\pi(\frac{\sigma_\epsilon^2}{1-\alpha} I + \mathbf{K}_{f,f} - \mathbf{Q})|^{\frac{-\alpha}{2(1-\alpha)}} (1-\alpha)^{N/2}$. Since $p(\mathbf{U}) = \phi(\mathbf{0}, \mathbf{K}_{U,U})$, we have

$$\begin{aligned} \mathcal{L}_\alpha(q) &= \log \int p_\alpha(\mathbf{Y}|\mathbf{U})^{1/(1-\alpha)} p(\mathbf{U}) d\mathbf{U} \\ &= \log C_x \phi(\mathbf{0}, \sigma_\epsilon^2 I + (1-\alpha)[\mathbf{K}_{f,f} - \mathbf{Q}] + \mathbf{K}_{f,U} \mathbf{K}_{U,U}^{-1} \mathbf{K}_{U,f}) \\ &= \log C_x \phi(\mathbf{0}, \sigma_\epsilon^2 I + (1-\alpha)[\mathbf{K}_{f,f} - \mathbf{Q}] + \mathbf{Q}) \\ &= \log \phi(\mathbf{0}, \sigma_\epsilon^2 I + (1-\alpha)[\mathbf{K}_{f,f}] + \alpha \mathbf{Q}) + \log C_x, \end{aligned}$$

where

$$\begin{aligned} C_x &= [(2\pi\sigma_\epsilon^2)^{\frac{\alpha N}{2(1-\alpha)}} (\frac{1}{1-\alpha})^{\frac{N}{2(1-\alpha)}}] [|2\pi(\frac{\sigma_\epsilon^2}{1-\alpha} I + \mathbf{K}_{f,f} - \mathbf{Q})|^{\frac{-\alpha}{2(1-\alpha)}} (1-\alpha)^{N/2}] \\ &= (2\pi\sigma_\epsilon^2)^{\frac{\alpha N}{2(1-\alpha)}} (1-\alpha)^{\frac{-\alpha N}{2(1-\alpha)}} |2\pi(\frac{\sigma_\epsilon^2}{1-\alpha} I + \mathbf{K}_{f,f} - \mathbf{Q})|^{\frac{-\alpha}{2(1-\alpha)}} \\ &= |I + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q})|^{\frac{-\alpha}{2(1-\alpha)}} \\ &\approx \left\{ 1 + \frac{1-\alpha}{\sigma_\epsilon^2} \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q}) + \mathcal{O}(\frac{(1-\alpha)^2}{\sigma_\epsilon^4}) \right\}^{\frac{-\alpha}{2(1-\alpha)}}. \end{aligned}$$

The last equality comes from the variation of Jacobi's formula. The \approx approximates well only when $\frac{1-\alpha}{\sigma_\epsilon^2}$ is "small". It can be seen that, when α is close to 1, our objective function contains the regularization term $\frac{1-\alpha}{\sigma_\epsilon^2} \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})$, which is similar to the regularization term in \mathcal{L}_{VI} . The tuning parameter α controls how close \mathbf{Q} is to $\mathbf{K}_{f,f}$ and hence it encourages densities q that place their mass on configurations of the latent variables that explain the observed data. This is also true for any $\alpha \in [0, 1)$ yet the regularization effect is conveyed through the

determinant $|\mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2}(\mathbf{K}_{\mathbf{f},\mathbf{f}} - \mathbf{Q})|^{-\frac{\alpha}{2(1-\alpha)}}$.

B Other Bounds

In this section, we provide details on obtaining \mathcal{L}_{jensen} and \mathcal{L}_{VI} .

$$\begin{aligned}
\mathcal{L}_\alpha(q) &:= \frac{1}{1-\alpha} \log \mathbb{E}_q \left[\left(\frac{p(\mathbf{f}, \mathbf{U}, \mathbf{Y} | \mathbf{Z})}{q(\mathbf{f}, \mathbf{U} | \mathbf{Z})} \right)^{1-\alpha} \right] \\
&= \frac{1}{1-\alpha} \log \int \left(\int p(\mathbf{Y} | \mathbf{f})^{1-\alpha} p(\mathbf{f} | \mathbf{U}, \mathbf{Z}) d\mathbf{f} \right) q(\mathbf{U})^{\alpha-1} p(\mathbf{U} | \mathbf{Z})^{1-\alpha} q(\mathbf{U}) d\mathbf{U} \\
&= \frac{1}{1-\alpha} \log \mathbb{E}_{q(\mathbf{U})} \left[\underbrace{\left(\int p(\mathbf{Y} | \mathbf{f})^{1-\alpha} p(\mathbf{f} | \mathbf{U}, \mathbf{Z}) d\mathbf{f} \right) q(\mathbf{U})^{\alpha-1} p(\mathbf{U} | \mathbf{Z})^{1-\alpha}}_{\text{Rényi variational lower bound}} \right] \tag{2} \\
&\geq \frac{1}{1-\alpha} \left\{ \mathbb{E} \log \left[\left(\int p(\mathbf{Y} | \mathbf{f})^{1-\alpha} p(\mathbf{f} | \mathbf{U}, \mathbf{Z}) d\mathbf{f} \right) q(\mathbf{U})^{\alpha-1} p(\mathbf{U} | \mathbf{Z})^{1-\alpha} \right] \right\} \\
&= \frac{1}{1-\alpha} \left\{ \int q(\mathbf{U}) \log \left[\left(\int p(\mathbf{Y} | \mathbf{f})^{1-\alpha} p(\mathbf{f} | \mathbf{U}, \mathbf{Z}) d\mathbf{f} \right) q(\mathbf{U})^{\alpha-1} p(\mathbf{U} | \mathbf{Z})^{1-\alpha} \right] d\mathbf{U} \right\} \\
&= \frac{1}{1-\alpha} \left\{ \int q(\mathbf{U}) \log \left[q(\mathbf{U})^{\alpha-1} p(\mathbf{U} | \mathbf{Z})^{1-\alpha} \right] \right. \\
&\quad \left. + q(\mathbf{U}) \log \left(\int p(\mathbf{Y} | \mathbf{f})^{1-\alpha} p(\mathbf{f} | \mathbf{U}, \mathbf{Z}) d\mathbf{f} \right) d\mathbf{U} \right\} \\
&= -KL[q(\mathbf{U}) || p(\mathbf{U} | \mathbf{Z})] + \frac{1}{1-\alpha} \left\{ \int q(\mathbf{U}) \log \left(\int p(\mathbf{Y} | \mathbf{f})^{1-\alpha} p(\mathbf{f} | \mathbf{U}, \mathbf{Z}) d\mathbf{f} \right) d\mathbf{U} \right\} \tag{3} \\
&\geq -KL[q(\mathbf{U}) || p(\mathbf{U} | \mathbf{Z})] + \frac{1}{1-\alpha} \left\{ \int q(\mathbf{U}) \int p(\mathbf{f} | \mathbf{U}, \mathbf{Z}) \log \left(p(\mathbf{Y} | \mathbf{f})^{1-\alpha} \right) d\mathbf{f} d\mathbf{U} \right\} \\
&= -KL[q(\mathbf{U}) || p(\mathbf{U} | \mathbf{Z})] + \frac{1}{1-\alpha} \left\{ \int q(\mathbf{U}) \int p(\mathbf{f} | \mathbf{U}, \mathbf{Z}) \log \left(p(\mathbf{Y} | \mathbf{f})^{1-\alpha} \right) d\mathbf{f} d\mathbf{U} \right\} \\
&= -KL[q(\mathbf{U}) || p(\mathbf{U} | \mathbf{Z})] + \mathbb{E}_{q(\mathbf{f}, \mathbf{U})} [\log p(\mathbf{Y} | \mathbf{f})] = \mathcal{L}_{VI}. \tag{4}
\end{aligned}$$

Here,

$$\begin{aligned}
\mathcal{L}_\alpha(q) &= \frac{1}{1-\alpha} \log \mathbb{E}_{q(\mathbf{U})} \left[\left(\int p(\mathbf{Y} | \mathbf{f})^{1-\alpha} p(\mathbf{f} | \mathbf{U}, \mathbf{Z}) d\mathbf{f} \right) q(\mathbf{U})^{\alpha-1} p(\mathbf{U} | \mathbf{Z})^{1-\alpha} \right], \\
\mathcal{L}_{Jensen} &= -KL[q(\mathbf{U}) || p(\mathbf{U} | \mathbf{Z})] + \frac{1}{1-\alpha} \left\{ \int q(\mathbf{U}) \log \left(\int p(\mathbf{Y} | \mathbf{f})^{1-\alpha} p(\mathbf{f} | \mathbf{U}, \mathbf{Z}) d\mathbf{f} \right) d\mathbf{U} \right\}, \\
\mathcal{L}_{VI} &= -KL[q(\mathbf{U}) || p(\mathbf{U} | \mathbf{Z})] + \mathbb{E}_{q(\mathbf{f}, \mathbf{U})} [\log p(\mathbf{Y} | \mathbf{f})].
\end{aligned}$$

It can be seen that $\mathcal{L}_\alpha(q) \geq \mathcal{L}_{Jensen} \geq \mathcal{L}_{VI}$. Therefore, \mathcal{L}_{Jensen} is decreasing as $\alpha \rightarrow 1$. This implies $\frac{1}{1-\alpha} \left\{ \int q(\mathbf{U}) \log \left(\int p(\mathbf{Y}|\mathbf{f})^{1-\alpha} p(\mathbf{f}|\mathbf{U}, \mathbf{Z}) d\mathbf{f} \right) d\mathbf{U} \right\}$ is decreasing as $\alpha \rightarrow 1$. Alternatively, one can take a derivative with respect to α and conclude that the aforementioned function is decreasing.

C Computation

We elaborate the modified BBMM approach here. By scrutinizing our objective function, defined below,

$$\begin{aligned} \mathcal{L}_\alpha(q^*) &= \log \int p_\alpha(\mathbf{Y}|\mathbf{U})^{1/(1-\alpha)} p(\mathbf{U}) d\mathbf{U} = \\ &\log \left\{ \mathcal{N}(\mathbf{0}, \sigma_\epsilon^2 I + (1-\alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q}) \right\} + \log \left| I + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right|^{\frac{-\alpha}{2(1-\alpha)}}. \end{aligned} \quad (5)$$

we can see that the computational complexity is dominated by the first term, which has the same complexity as the exact \mathcal{GP} , and the determinant term. The detailed computing procedure is provided as follows. We rewrite the function above as

$$\mathcal{L}_\alpha(q^*) = \log |2\pi\mathbf{\Xi}|^{-\frac{1}{2}} - \frac{1}{2} \mathbf{Y}^T \mathbf{\Xi}^{-1} \mathbf{Y} + \log C_x \quad (6)$$

where matrices $\mathbf{\Xi} := \sigma_\epsilon^2 I + (1-\alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q}$ and $C_x = \left| I + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right|^{\frac{-\alpha}{2(1-\alpha)}}$.

In Eq. (6), two expensive terms $\log |\mathbf{\Xi}|$ and $\mathbf{\Xi}^{-1} \mathbf{Y}$ can be efficiently estimated by the Batched Conjugate Gradients Algorithm (mBCG) [Gardner et al., 2018] with some modifications. The remaining work is to estimate the determinant term. First, we can write it as

$$\log C_x = \log \left| I + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right|^{\frac{-\alpha}{2(1-\alpha)}} = \log \left| \frac{\mathbf{\Xi}}{\sigma_\epsilon^2} + \frac{1-2\alpha}{\sigma_\epsilon^2} \mathbf{Q} \right|^{\frac{-\alpha}{2(1-\alpha)}}.$$

By the matrix determinant lemma, we have

$$\begin{aligned} \log \left| \frac{\Xi}{\sigma_\epsilon^2} + \frac{1-2\alpha}{\sigma_\epsilon^2} \mathbf{Q} \right| &= \log \left| \frac{1}{\sigma_\epsilon^2} \right| \left| \Xi + (1-2\alpha) \mathbf{Q} \right| = \log \left| \frac{1}{\sigma_\epsilon^2} \right| \left| \Xi + (1-2\alpha) \mathbf{K}_{f,U} \mathbf{K}_{U,U}^{-1} \mathbf{K}_{U,f} \right| \\ &= \log \left| \frac{1}{\sigma_\epsilon^2} \right| \left| \frac{1}{(1-2\alpha)} \mathbf{K}_{U,U} + \mathbf{K}_{U,f} \Xi^{-1} \mathbf{K}_{f,U} \right| + \log |(1-2\alpha) \mathbf{K}_{U,U}^{-1}| + \log |\Xi|. \end{aligned}$$

In this equation, $\log |\Xi|$ is already available as aforementioned. Therefore, only $\Xi^{-1} \mathbf{K}_{f,U}$ is expensive to compute. Similarly, we resort to the CG algorithm to overcome this difficulty. Overall, the resulting matrix is of dimension $M \times M$ (note that $M \ll N$) and is cheap to compute.

On Computing Inverse

$\Xi^{-1} \mathbf{Y}$ can be calculated by the conjugate gradient (CG) algorithm. Specifically, we solve the following quadratic optimization problem

$$\Xi^{-1} \mathbf{Y} = \arg \min_{\mathbf{u}} \left(\frac{1}{2} \mathbf{u}^T \Xi \mathbf{u} - \mathbf{u}^T \mathbf{Y} \right).$$

Furthermore, CG can be extended to return a matrix output. Let $\Theta = [\mathbf{Y} \quad \mathbf{K}_{f,U}]$, then we can compute both $\Xi^{-1} \mathbf{Y}$ and $\Xi^{-1} \mathbf{K}_{f,U}$ by solving

$$\Xi^{-1} \Theta = \arg \min_{\mathbf{U}} \left(\frac{1}{2} \mathbf{U}^T \Theta \mathbf{U} - \mathbf{U}^T \Theta \right).$$

On Computing Determinant

$\log |\Xi|$ can be computed in two ways. First, we can use pivoted Cholesky decomposition. Second, we can use Lanczos algorithm. When running Lanczos algorithm, we only need to return the Tridiagonal matrix T and we have $\log |\Xi| = \text{Tr}(\log T)$.

On Computing Gradient

Let $\mathbf{Z} = [\mathbf{z}_1, \dots, \mathbf{z}_t]$ be a set of vectors where \mathbf{z}_i is drawn from $\mathcal{N}(\mathbf{0}, \mathbf{I})$. Then we can use mBCG to compute $\mathbf{\Xi}^{-1}\mathbf{Z}$ and calculate gradient as

$$\text{Tr}\left(\mathbf{\Xi}^{-1}\frac{d\mathbf{\Xi}}{d\mathbf{w}}\right) \approx \frac{1}{t} \sum_{i=1}^t (\mathbf{z}_i^T \mathbf{\Xi}^{-1}) \left(\frac{d\mathbf{\Xi}}{d\mathbf{w}} \mathbf{z}_i\right).$$

where $\mathbf{w} = (\sigma_\epsilon, \boldsymbol{\theta})$ is our model parameters. Please refer to [Gardner et al. \[2018\]](#) for the detailed implementation.

D Convergence Results

D.1 An Upper Bound

Lemma 1. *Suppose we have two positive semi-definite (PSD) matrices A and B such that $A - B$ is also a PSD matrix, then $|A| \geq |B|$. Furthermore, if A and B are positive definite (PD), then $B^{-1} \geq A^{-1}$.*

The proof of this Lemma can be found in any matrix theory textbook. Based on this lemma, we can compute a data-dependent upper bound on the log-marginal likelihood [[Titsias, 2014](#)].

Claim 1. $\log p(\mathbf{Y}) \leq \log \frac{1}{|2\pi((1-\alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \sigma_\epsilon^2\mathbf{I})|^{\frac{1}{2}}} e^{-\frac{1}{2}\mathbf{Y}^T((1-\alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \sigma_\epsilon^2\mathbf{I})^{-1}\mathbf{Y}} := \mathcal{L}_{upper}.$

Proof. Since

$$\mathbf{K}_{f,f} + \sigma_\epsilon^2\mathbf{I} = (1-\alpha)\mathbf{K}_{f,f} + \alpha\mathbf{K}_{f,f} + \sigma_\epsilon^2\mathbf{I} \succeq (1-\alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \sigma_\epsilon^2\mathbf{I} \succeq 0,$$

where $\mathbf{A} \succeq \mathbf{B}$ means $\mathbf{x}^T \mathbf{A} \mathbf{x} \geq \mathbf{x}^T \mathbf{B} \mathbf{x} \geq 0, \forall \mathbf{x}$. Then, we can obtain $|\mathbf{K}_{f,f} + \sigma_\epsilon^2\mathbf{I}| \geq$

$|(1 - \alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \sigma_\epsilon^2\mathbf{I}|$ since they are both PSD matrix. Therefore,

$$\frac{1}{|2\pi(\mathbf{K}_{f,f} + \sigma_\epsilon^2\mathbf{I})|^{\frac{1}{2}}} \leq \frac{1}{|2\pi((1 - \alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \sigma_\epsilon^2\mathbf{I})|^{\frac{1}{2}}}.$$

Let $\mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$ be the eigen-decomposition of $\mathbf{K}_{f,f} - \mathbf{Q}$. This decomposition exists since the matrix is PD. Then

$$\begin{aligned} \mathbf{Y}^T\mathbf{U}\mathbf{\Lambda}\mathbf{U}^T\mathbf{Y} &= \mathbf{z}^T\mathbf{\Lambda}\mathbf{z} = \sum_{i=1}^N \lambda_i z_i^2 \leq \lambda_{max} \sum_{i=1}^N z_i^2 = \lambda_{max} \|\mathbf{z}\|^2 \\ &= \lambda_{max} \|\mathbf{Y}\|^2 \leq \sum_{i=1}^N \lambda_i \|\mathbf{Y}\|^2 \leq \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q}) \|\mathbf{Y}\|^2, \end{aligned}$$

where $\mathbf{z} = \mathbf{U}^T\mathbf{Y}$, $\{\lambda_i\}_{i=1}^N$ are eigenvalues of $\mathbf{K}_{f,f} - \mathbf{Q}$ and $\lambda_{max} = \max(\lambda_1, \dots, \lambda_N)$. Therefore, we have $\mathbf{Y}^T(\mathbf{K}_{f,f} - \mathbf{Q})\mathbf{Y} \leq \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q}) \|\mathbf{Y}\|^2 = \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})\mathbf{Y}^T\mathbf{Y}$. Apparently, $\alpha\mathbf{Y}^T(\mathbf{K}_{f,f} - \mathbf{Q})\mathbf{Y} \leq \alpha\text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})\mathbf{Y}^T\mathbf{Y}$. Therefore, we can obtain

$$\begin{aligned} \mathbf{Y}^T(\mathbf{K}_{f,f} + \sigma_\epsilon^2\mathbf{I})\mathbf{Y} &\leq \mathbf{Y}^T((1 - \alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \sigma_\epsilon^2\mathbf{I})\mathbf{Y} + \alpha\text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})\mathbf{Y}^T\mathbf{Y} \\ &= \mathbf{Y}^T((1 - \alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \alpha\text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})\mathbf{I} + \sigma_\epsilon^2\mathbf{I})\mathbf{Y}. \end{aligned}$$

Based on this inequality, it is easy to show that

$$e^{-\frac{1}{2}\mathbf{Y}^T(\mathbf{K}_{f,f} + \sigma_\epsilon^2\mathbf{I})^{-1}\mathbf{Y}} \leq e^{-\frac{1}{2}\mathbf{Y}^T((1 - \alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \alpha\text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})\mathbf{I} + \sigma_\epsilon^2\mathbf{I})^{-1}\mathbf{Y}}.$$

Finally, we obtain

$$\begin{aligned} &\frac{1}{|2\pi(\mathbf{K}_{f,f} + \sigma_\epsilon^2\mathbf{I})|^{\frac{1}{2}}} e^{-\frac{1}{2}\mathbf{Y}^T(\mathbf{K}_{f,f} + \sigma_\epsilon^2\mathbf{I})^{-1}\mathbf{Y}} \\ &\leq \frac{1}{|2\pi((1 - \alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \sigma_\epsilon^2\mathbf{I})|^{\frac{1}{2}}} e^{-\frac{1}{2}\mathbf{Y}^T((1 - \alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \alpha\text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})\mathbf{I} + \sigma_\epsilon^2\mathbf{I})^{-1}\mathbf{Y}}. \end{aligned}$$

□

We will use this upper bound to prove our main theorem.

D.2 Rate of Convergence and Related Lemmas

Claim 2. $-\log |\mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2}(\mathbf{K}_{f,f} - \mathbf{Q})|^{\frac{-\alpha}{2(1-\alpha)}} \leq \frac{\alpha}{2(1-\alpha)} \log \left(\frac{\text{Tr}(\mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2}(\mathbf{K}_{f,f} - \mathbf{Q}))}{N} \right)^N$.

Proof. Based on the inequality of arithmetic and geometric means, we have

$$\frac{\text{Tr}(M)}{N} \geq |M|^{1/N},$$

given an positive semi-definite matrix M with dimension N . Therefore, we can obtain

$$|\mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2}(\mathbf{K}_{f,f} - \mathbf{Q})|^{1/N} \leq \frac{\text{Tr}(\mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2}(\mathbf{K}_{f,f} - \mathbf{Q}))}{N}.$$

By some simple algebra manipulation, we will obtain

$$\frac{\alpha}{2(1-\alpha)} \log |\mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2}(\mathbf{K}_{f,f} - \mathbf{Q})| \leq \frac{\alpha}{2(1-\alpha)} \log \left(\frac{\text{Tr}(\mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2}(\mathbf{K}_{f,f} - \mathbf{Q}))}{N} \right)^N.$$

□

We first provide a lower bound and an upper bound on the Rényi divergence.

Lemma 2. *For any set of $\{\mathbf{x}_i\}_{i=1}^N$, if the output $\{y_i\}_{i=1}^N$ are generated according to some generative model, then*

$$\begin{aligned} -\log |\mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2}(\mathbf{K}_{f,f} - \mathbf{Q})|^{\frac{-\alpha}{2(1-\alpha)}} &\leq \mathbb{E}_y \left[D_\alpha[p||q] \right] \\ &\leq -\log |\mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2}(\mathbf{K}_{f,f} - \mathbf{Q})|^{\frac{-\alpha}{2(1-\alpha)}} + \frac{\alpha \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})}{2\sigma_\epsilon^2}. \end{aligned} \tag{7}$$

Proof. We have

$$\begin{aligned} &\mathbb{E}_y \left[D_\alpha[p||q] \right] \\ &= \mathbb{E}_y \left[\log p(\mathbf{Y}) - \log \phi(\mathbf{0}, \sigma_\epsilon^2 \mathbf{I} + (1-\alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q}) - \log |\mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2}(\mathbf{K}_{f,f} - \mathbf{Q})|^{\frac{-\alpha}{2(1-\alpha)}} \right] \\ &= -\log |\mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2}(\mathbf{K}_{f,f} - \mathbf{Q})|^{\frac{-\alpha}{2(1-\alpha)}} + \mathbb{E}_y \left[\log \frac{\phi(\mathbf{0}, \mathbf{K}_{f,f} + \sigma_\epsilon^2 \mathbf{I})}{\phi(\mathbf{0}, \sigma_\epsilon^2 \mathbf{I} + (1-\alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q})} \right]. \end{aligned}$$

It is apparent that the lower bound to (7) is

$$-\log \left| \mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right|^{\frac{-\alpha}{2(1-\alpha)}},$$

since the KL divergence is non-negative. We then provide an upper bound to (7). We have

$$\begin{aligned} & -\log \left| \mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right|^{\frac{-\alpha}{2(1-\alpha)}} + \mathbb{E}_y \left[\log \frac{\phi(\mathbf{0}, \mathbf{K}_{f,f} + \sigma_\epsilon^2 \mathbf{I})}{\phi(\mathbf{0}, \sigma_\epsilon^2 \mathbf{I} + (1-\alpha) \mathbf{K}_{f,f} + \alpha \mathbf{Q})} \right] \\ &= -\log \left| \mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right|^{\frac{-\alpha}{2(1-\alpha)}} \\ &\quad - \frac{N}{2} + \frac{1}{2} \log \left(\frac{|\sigma_\epsilon^2 \mathbf{I} + (1-\alpha) \mathbf{K}_{f,f} + \alpha \mathbf{Q}|}{|\mathbf{K}_{f,f} + \sigma_\epsilon^2 \mathbf{I}|} \right) + \frac{1}{2} \text{Tr} \left((\sigma_\epsilon^2 \mathbf{I} + (1-\alpha) \mathbf{K}_{f,f} + \alpha \mathbf{Q})^{-1} (\mathbf{K}_{f,f} + \sigma_\epsilon^2 \mathbf{I}) \right) \\ &\leq -\log \left| \mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right|^{\frac{-\alpha}{2(1-\alpha)}} - \frac{N}{2} + \frac{1}{2} \text{Tr} \left((\sigma_\epsilon^2 \mathbf{I} + (1-\alpha) \mathbf{K}_{f,f} + \alpha \mathbf{Q})^{-1} (\mathbf{K}_{f,f} + \sigma_\epsilon^2 \mathbf{I}) \right). \end{aligned}$$

This inequality follows from the fact that $\mathbf{K}_{f,f} + \sigma_\epsilon^2 \mathbf{I} \succeq \sigma_\epsilon^2 \mathbf{I} + (1-\alpha) \mathbf{K}_{f,f} + \alpha \mathbf{Q}$. Since

$$\begin{aligned} & \frac{1}{2} \text{Tr} \left((\sigma_\epsilon^2 \mathbf{I} + (1-\alpha) \mathbf{K}_{f,f} + \alpha \mathbf{Q})^{-1} (\mathbf{K}_{f,f} + \sigma_\epsilon^2 \mathbf{I}) \right) \\ &= \frac{1}{2} \text{Tr}(\mathbf{I}) + \frac{1}{2} \text{Tr} \left((\sigma_\epsilon^2 \mathbf{I} + (1-\alpha) \mathbf{K}_{f,f} + \alpha \mathbf{Q})^{-1} (\tilde{\mathbf{K}}) \right) \\ &\leq \frac{N}{2} + \alpha \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q}) \lambda_1((\sigma_\epsilon^2 \mathbf{I} + (1-\alpha) \mathbf{K}_{f,f} + \alpha \mathbf{Q})^{-1})/2 \\ &\leq \frac{N}{2} + \frac{\alpha \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})}{2\sigma_\epsilon^2}, \end{aligned}$$

where $\tilde{\mathbf{K}} = \mathbf{K}_{f,f} + \sigma_\epsilon^2 \mathbf{I} - (\sigma_\epsilon^2 \mathbf{I} + (1-\alpha) \mathbf{K}_{f,f} + \alpha \mathbf{Q})$ and $\lambda_1(\mathbf{M})$ is the largest eigenvalue of an arbitrary matrix \mathbf{M} . We apply the Hölder's inequality for Schatten norms to the second last inequality. Therefore, we obtain the upper bound as follow.

$$-\log \left| \mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right|^{\frac{-\alpha}{2(1-\alpha)}} + \frac{\alpha \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})}{2\sigma_\epsilon^2}.$$

□

As $\alpha \rightarrow 1$, we recover the bounds for the KL divergence. Specifically, we get the lower bound $\frac{\text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})}{2\sigma_\epsilon^2}$ and upper bound $\frac{\text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})}{\sigma_\epsilon^2}$ [?].

Lemma 3. *Given a symmetric positive semidefinite matrix $\mathbf{K}_{f,f}$, if M columns are selected to form a Nystrom approximation such that the probability of selecting a subset of columns Z is proportional to the determinant of the principal submatrix formed by these columns and the matching rows, then*

$$\mathbb{E}_Z \left[\text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q}) \right] \leq (M+1) \sum_{m=M+1}^N \lambda_m(\mathbf{K}_{f,f}).$$

This lemma is proved in [?]. Following this lemma and by Lemma 2, we can show that

$$\begin{aligned} & \mathbb{E}_Z \left[-\log \left| \mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right|^{\frac{-\alpha}{2(1-\alpha)}} \right] \\ &= \mathbb{E}_Z \left[\frac{\alpha}{2(1-\alpha)} \log \left| \mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right| \right] \\ &\leq \mathbb{E}_Z \left[\frac{\alpha}{2(1-\alpha)} \log \left(\frac{\text{Tr}(\mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}))}{N} \right)^N \right] \\ &\leq \frac{\alpha N}{2(1-\alpha)} \log \mathbb{E}_Z \left[\left(\frac{\text{Tr}(\mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}))}{N} \right) \right] \\ &\leq \frac{\alpha N}{2(1-\alpha)} \log \left\{ 1 + \frac{1-\alpha}{\sigma_\epsilon^2} \frac{(M+1) \sum_{m=M+1}^N \lambda_m(\mathbf{K}_{f,f})}{N} \right\}. \end{aligned}$$

As $\alpha \rightarrow 1$, this bound becomes $\frac{1}{2\sigma_\epsilon^2} (M+1) \sum_{m=M+1}^N \lambda_m(\mathbf{K}_{f,f})$. Following the inequality and lemma above, we can obtain the following corollary.

Corollary 1.

$$\mathbb{E}_{Z \sim v} [\text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})] \leq (M+1) \sum_{m=M+1}^N \lambda_m(\mathbf{K}_{f,f}) + 2Nv\epsilon.$$

This inequality is from [?]. Using this fact, we can show that

$$\begin{aligned}
& \mathbb{E}_{Z \sim v} \left[-\log \left| \mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right|^{\frac{-\alpha}{2(1-\alpha)}} \right] \\
& \leq \frac{\alpha}{2(1-\alpha)} \mathbb{E}_{Z \sim v} \left[\log \left(\frac{\text{Tr}(\mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}))}{N} \right)^N \right] \\
& \leq \frac{\alpha N}{2(1-\alpha)} \log \left[1 + \frac{1-\alpha}{\sigma_\epsilon^2} \frac{[(M+1) \sum_{m=M+1}^N \lambda_m(\mathbf{K}_{f,f}) + 2Nv\epsilon]}{N} \right].
\end{aligned}$$

The next theorem is based on a lemma. We will prove this lemma first.

Lemma 4.

$$D_\alpha[p||q] \leq -\log \left| \mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right|^{\frac{-\alpha}{2(1-\alpha)}} + \|\mathbf{Y}\|^2 \frac{\alpha \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})}{\sigma_\epsilon^4 + \alpha \sigma_\epsilon^2 \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})}$$

where $\tilde{\lambda}_{max}$ is the largest eigenvalue of $\mathbf{K}_{f,f} - \mathbf{Q}$.

Proof. Based on Claim 1, we have

$$\begin{aligned}
\mathcal{L}_{upper} &= \log \frac{1}{|2\pi((1-\alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \sigma_\epsilon^2\mathbf{I})|^{\frac{1}{2}}} e^{-\frac{1}{2}\mathbf{Y}^T((1-\alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \sigma_\epsilon^2\mathbf{I})^{-1}\mathbf{Y}} \\
&\leq -\frac{1}{2} \log |(1-\alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \sigma_\epsilon^2\mathbf{I}| - \frac{N}{2} \log(2\pi) - \frac{1}{2} \mathbf{Y}^T((1-\alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \alpha\tilde{\lambda}_{max}\mathbf{I} + \sigma_\epsilon^2\mathbf{I})^{-1}\mathbf{Y} \\
&:= \mathcal{L}'_{upper},
\end{aligned}$$

using the fact that $\text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q}) \geq \tilde{\lambda}_{max}$. Then, we have

$$\begin{aligned}
& \mathcal{L}'_{upper} - \mathcal{L}_\alpha(q) \\
&= -\log \left| \mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right|^{\frac{-\alpha}{2(1-\alpha)}} \\
&+ \frac{1}{2} \mathbf{Y}^T \left(((1-\alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \sigma_\epsilon^2\mathbf{I})^{-1} - ((1-\alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \alpha\tilde{\lambda}_{max}\mathbf{I} + \sigma_\epsilon^2\mathbf{I})^{-1} \right) \mathbf{Y}.
\end{aligned}$$

Let $(1-\alpha)\mathbf{K}_{f,f} + \alpha\mathbf{Q} + \sigma_\epsilon^2\mathbf{I} = \mathbf{V}\mathbf{\Lambda}_\alpha\mathbf{V}^T$ be the eigenvalue decomposition and denote by

$\gamma_1 \geq \dots \geq \gamma_N$ all eigenvalues. Then we can obtain

$$\begin{aligned}
& \frac{1}{2}(\mathbf{V}^T \mathbf{Y})^T \left(\Lambda_{\alpha}^{-1} - (\Lambda_{\alpha} + \alpha \tilde{\lambda}_{max} \mathbf{I})^{-1} \right) (\mathbf{V}^T \mathbf{Y}) \\
&= \frac{1}{2} \mathbf{z}'^T \left(\Lambda_{\alpha}^{-1} - (\Lambda_{\alpha} + \alpha \tilde{\lambda}_{max} \mathbf{I})^{-1} \right) \mathbf{z}' \\
&= \frac{1}{2} \sum_i z_i'^2 \frac{\alpha \tilde{\lambda}_{max}}{\gamma_i^2 + \alpha \gamma_i \tilde{\lambda}_{max}} \\
&\leq \frac{1}{2} \|\mathbf{Y}\|^2 \frac{\alpha \tilde{\lambda}_{max}}{\gamma_N^2 + \alpha \gamma_N \tilde{\lambda}_{max}} \\
&\leq \frac{1}{2} \|\mathbf{Y}\|^2 \frac{\alpha \tilde{\lambda}_{max}}{\sigma_{\epsilon}^4 + \alpha \sigma_{\epsilon}^2 \tilde{\lambda}_{max}},
\end{aligned}$$

where $\mathbf{z}' = \mathbf{V}^T \mathbf{Y}$. Therefore, we have

$$\begin{aligned}
D_{\alpha}[p||q] &\leq -\log |\mathbf{I} + \frac{1-\alpha}{\sigma_{\epsilon}^2} (\mathbf{K}_{f,f} - \mathbf{Q})|^{\frac{-\alpha}{2(1-\alpha)}} + \frac{1}{2} \|\mathbf{Y}\|^2 \frac{\alpha \tilde{\lambda}_{max}}{\sigma_{\epsilon}^4 + \alpha \sigma_{\epsilon}^2 \tilde{\lambda}_{max}} \\
&\leq -\log |\mathbf{I} + \frac{1-\alpha}{\sigma_{\epsilon}^2} (\mathbf{K}_{f,f} - \mathbf{Q})|^{\frac{-\alpha}{2(1-\alpha)}} + \frac{1}{2} \|\mathbf{Y}\|^2 \frac{\alpha \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})}{\sigma_{\epsilon}^4 + \alpha \sigma_{\epsilon}^2 \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})}.
\end{aligned}$$

□

For simplicity, we split our main theorem into two theorems and prove them separately.

Theorem 1. Suppose N data points are drawn i.i.d from input distribution $p(\mathbf{x})$ and $k(\mathbf{x}, \mathbf{x}) \leq v, \forall \mathbf{x} \in \mathcal{X}$. Sample M inducing points from the training data with the probability assigned to any set of size M equal to the probability assigned to the corresponding subset by an ϵ k -Determinantal Point Process (k -DPP) [?] with $k = M$. If \mathbf{Y} is distributed according to a sample from the prior generative model, with probability at least $1 - \delta$,

$$\begin{aligned}
D_{\alpha}[p||q] &\leq \alpha \frac{(M+1)N \sum_{m=M+1}^{\infty} \lambda_m + 2Nv\epsilon}{2\delta\sigma_{\epsilon}^2} + \\
&\frac{1}{\delta} \frac{\alpha}{2(1-\alpha)} \log \left[1 + \frac{1-\alpha}{\sigma_{\epsilon}^2} \frac{[(M+1)N \sum_{m=M+1}^{\infty} \lambda_m + 2Nv\epsilon]}{N} \right]^N.
\end{aligned}$$

where λ_m are the eigenvalues of the integral operator \mathcal{K} associated to kernel, k and $p(\mathbf{x})$.

Proof. We have

$$\begin{aligned}
& \mathbb{E}_{\mathbf{X}} \left[\mathbb{E}_{Z|\mathbf{X}} \left[\mathbb{E}_{\mathbf{Y}} \left[D_{\alpha}[p||q] \right] \right] \right] \\
& \leq \mathbb{E}_{\mathbf{X}} \left[\mathbb{E}_{Z|\mathbf{X}} \left[-\log \left| \mathbf{I} + \frac{1-\alpha}{\sigma_{\epsilon}^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right|^{\frac{-\alpha}{2(1-\alpha)}} + \frac{\alpha \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})}{2\sigma_{\epsilon}^2} \right] \right] \\
& \leq \mathbb{E}_{\mathbf{X}} \left[\frac{\alpha N}{2(1-\alpha)} \log \left[1 + \frac{1-\alpha}{\sigma_{\epsilon}^2} \frac{[(M+1) \sum_{m=M+1}^N \lambda_m(\mathbf{K}_{f,f}) + 2Nv\epsilon]}{N} \right] + \right. \\
& \quad \left. \alpha \frac{(M+1) \sum_{m=M+1}^N \lambda_m(\mathbf{K}_{f,f}) + 2Nv\epsilon}{2\sigma_{\epsilon}^2} \right] \\
& \leq \frac{\alpha N}{2(1-\alpha)} \log \left[1 + \frac{1-\alpha}{\sigma_{\epsilon}^2} \frac{[(M+1)N \sum_{m=M+1}^{\infty} \lambda_m + 2Nv\epsilon]}{N} \right] + \\
& \quad \alpha \frac{(M+1)N \sum_{m=M+1}^{\infty} \lambda_m + 2Nv\epsilon}{2\sigma_{\epsilon}^2}.
\end{aligned}$$

By the Markov's inequality, we have the following bound with probability at least $1 - \delta$ for any $\delta \in (0, 1)$.

$$\begin{aligned}
D_{\alpha}[p||q] & \leq \alpha \frac{(M+1)N \sum_{m=M+1}^{\infty} \lambda_m + 2Nv\epsilon}{2\delta\sigma_{\epsilon}^2} + \\
& \quad \frac{1}{\delta} \frac{\alpha}{2(1-\alpha)} \log \left[1 + \frac{1-\alpha}{\sigma_{\epsilon}^2} \frac{[(M+1)N \sum_{m=M+1}^{\infty} \lambda_m + 2Nv\epsilon]}{N} \right]^N.
\end{aligned}$$

□

As $\alpha \rightarrow 1$, we obtain the bound for the KL divergence.

Theorem 2. Suppose N data points are drawn i.i.d from input distribution $p(\mathbf{x})$ and $k(\mathbf{x}, \mathbf{x}) \leq v, \forall \mathbf{x} \in \mathcal{X}$. Sample M inducing points from the training data with the probability assigned to any set of size M equal to the probability assigned to the corresponding subset by an ϵ k -Determinantal Point Process (k -DPP) [?] with $k = M$. With probability at least $1 - \delta$,

$$\begin{aligned}
D_{\alpha}[q||p] & \leq \frac{1}{\delta} \frac{\alpha}{2(1-\alpha)} \log \left[1 + \frac{1-\alpha}{\sigma_{\epsilon}^2} \frac{[(M+1)N \sum_{m=M+1}^{\infty} \lambda_m + 2Nv\epsilon]}{N} \right]^N + \\
& \quad \alpha \frac{(M+1)N \sum_{m=M+1}^{\infty} \lambda_m + 2Nv\epsilon}{2\delta\sigma_{\epsilon}^2} \frac{\|\mathbf{Y}\|^2}{\sigma_{\epsilon}^2}
\end{aligned}$$

where $C = N \sum_{m=M+1}^{\infty} \lambda_m$ and λ_m are the eigenvalues of the integral operator \mathcal{K} associated to kernel, k and $p(\mathbf{x})$.

Proof. Using lemma in appendix, we have

$$\begin{aligned} D_\alpha[p||q] &\leq -\log \left| \mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right|^{\frac{-\alpha}{2(1-\alpha)}} + \frac{1}{2} \|\mathbf{Y}\|^2 \frac{\alpha \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})}{\sigma_\epsilon^4 + \alpha \sigma_\epsilon^2 \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})} \\ &\leq -\log \left| \mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right|^{\frac{-\alpha}{2(1-\alpha)}} + \frac{1}{2} \frac{\|\mathbf{Y}\|^2}{\sigma_\epsilon^2} \frac{\alpha \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})}{\sigma_\epsilon^2 + \alpha \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})} \\ &\leq -\log \left| \mathbf{I} + \frac{1-\alpha}{\sigma_\epsilon^2} (\mathbf{K}_{f,f} - \mathbf{Q}) \right|^{\frac{-\alpha}{2(1-\alpha)}} + \frac{1}{2} \frac{\|\mathbf{Y}\|^2}{\sigma_\epsilon^2} \frac{\alpha \text{Tr}(\mathbf{K}_{f,f} - \mathbf{Q})}{\sigma_\epsilon^2}. \end{aligned}$$

Following the same argument in the proof of Theorem 1, we have

$$\begin{aligned} &\frac{\alpha}{2(1-\alpha)} \log \left[1 + \frac{1-\alpha}{\sigma_\epsilon^2} \frac{[(M+1)N \sum_{m=M+1}^{\infty} \lambda_m + 2Nv\epsilon]}{N} \right]^N + \\ &\alpha \frac{(M+1)N \sum_{m=M+1}^{\infty} \lambda_m + 2Nv\epsilon}{2\sigma_\epsilon^2} \frac{\|\mathbf{Y}\|^2}{\sigma_\epsilon^2}. \end{aligned}$$

□

As $\alpha \rightarrow 1$, we reach the bound for the KL divergence.

D.3 Smooth Kernel

Proof. We know $\frac{C(M+1)}{2\delta\sigma_\epsilon^2} < \frac{1}{N^{\gamma+1}}$. By Theorem 2, we can obtain the following bound

$$D_\alpha[p||q] \leq 2\alpha \frac{R}{\sigma_\epsilon^2} \frac{1}{N^\gamma} + \frac{1}{\delta} \frac{\alpha}{2(1-\alpha)} \log \left[1 + (1-\alpha) \left(\frac{4\delta}{N^{\gamma+2}} \right) \right]^N.$$

□

D.4 Non-smooth Kernel

For the Matérn $r + \frac{1}{2}$, $\lambda_m \asymp \frac{1}{m^{2r+2}}$ kernel, where \asymp means “asymptotically equivalent to”, we can obtain $\sum_{m=M+1}^{\infty} \lambda_m = \mathcal{O}(\frac{1}{M^{2r+1}})$. Let $\sum_{m=M+1}^{\infty} \lambda_m \leq A \frac{1}{M^{2r+1}}$. Then by Theorem 1, we

have

$$\begin{aligned} \alpha \frac{(M+1)N \sum_{m=M+1}^{\infty} \lambda_m + 2Nv_0\epsilon}{2\delta\sigma_\epsilon^2} \frac{\|\mathbf{Y}\|^2}{\sigma_\epsilon^2} &\leq \alpha \frac{(M+1)NA \frac{1}{M^{2k+1}} + 2Nv_0\epsilon}{2\delta\sigma_\epsilon^2} \frac{RN}{\sigma_\epsilon^2} \\ &= \frac{\alpha R}{2\delta\sigma_\epsilon^4} \left(\frac{(M+1)N^2A}{M^{2r+1}} + 2N^2v_0\epsilon \right). \end{aligned}$$

In order to let $\lim_{N \rightarrow \infty} \frac{(M+1)N^2}{M^{2r+1}} \rightarrow 0$, we require $M = N^t$ (t will be clarified shortly).

Therefore,

$$\frac{(M+1)N^2A}{M^{2r+1}} = \frac{(N^t+1)N^2A}{N^{(2r+1)t}} \leq \frac{A}{N^{2rt-2}}.$$

Let $2rt - 2 \geq \gamma$, then $t \geq \frac{\gamma+2}{2r}$. Therefore, we have

$$\frac{\alpha R}{2\sigma_\epsilon^4} \left(\frac{(M+1)N^2A}{M^{2r+1}} + 2N^2v_0\epsilon \right) \leq \frac{\alpha R}{N^\gamma \sigma_\epsilon^2} + \frac{\alpha RA}{2\delta\sigma_\epsilon^4 N^\gamma}.$$

Another term in the bound can also be simplified as

$$\frac{\alpha}{2(1-\alpha)} \log \left[1 + \frac{1-\alpha}{\sigma_\epsilon^2} \frac{[(M+1)C + 2Nv_0\epsilon]}{N} \right]^N \leq \frac{\alpha N}{2(1-\alpha)} \log \left[1 + (1-\alpha) \left(\frac{A + 2\delta}{\sigma_\epsilon^2 N^{\gamma+2}} \right) \right].$$

It can be seen that we require more inducing points ($\mathcal{O}(N^t)$) when we are using non-smooth kernels and t decreases as we increase the smoothness (i.e., r) of the Matérn kernel.

E More Results

We provide more detailed results in this section. In table 1, we report the negative loss (NL) of each method.

Table 1: NL of all models on many datasets. The NL is calculated over 30 experiments with different initial points.

Dataset	EGP	SGP	PEP	Rényi
Bike	0.41 ± 0.02	0.15 ± 0.03	0.10 ± 0.01	0.45 ± 0.01
C-MAPSS	-1.00 ± 0.01	-1.45 ± 0.01	-1.55 ± 0.02	-0.01 ± 0.01
Protein	2.15 ± 0.01	1.42 ± 0.01	1.97 ± 0.05	2.99 ± 0.04
Traffic	-0.42 ± 0.01	-0.47 ± 0.02	-1.07 ± 0.01	-0.20 ± 0.04
Battery	2.23 ± 0.06	2.10 ± 0.02	2.17 ± 0.02	2.55 ± 0.01

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