

Appendix

A Derivative of ELBO

We first derive the (6). Starting from Kullback-Leibler divergence (KL divergence D_{KL}) between the variational approximate posterior $q(\mathbf{f}, \mathbf{f}_m)$ and the true posterior $p(\mathbf{f}, \mathbf{f}_m|\mathbf{y})$, $D_{\text{KL}}[q(\mathbf{f}, \mathbf{f}_m)||p(\mathbf{f}, \mathbf{f}_m|\mathbf{y})]$, we can derive that,

$$\begin{aligned} D_{\text{KL}}[q(\mathbf{f}, \mathbf{f}_m)||p(\mathbf{f}, \mathbf{f}_m|\mathbf{y})] &= \mathbb{E}_q[\log \frac{q(\mathbf{f}, \mathbf{f}_m)}{p(\mathbf{f}, \mathbf{f}_m|\mathbf{y})}] \\ &= \mathbb{E}_q[\log \frac{q(\mathbf{f}, \mathbf{f}_m)p(\mathbf{y})}{p(\mathbf{f}, \mathbf{f}_m, \mathbf{y})}] \\ &= \mathbb{E}_q[\log q(\mathbf{f}, \mathbf{f}_m) + \log p(\mathbf{y}) - \log p(\mathbf{f}, \mathbf{f}_m, \mathbf{y})] \geq 0. \end{aligned} \quad (1)$$

Thus,

$$\begin{aligned} \log p(\mathbf{y}) &\geq \mathbb{E}_q[\log p(\mathbf{f}, \mathbf{f}_m, \mathbf{y}) - \log q(\mathbf{f}, \mathbf{f}_m)] \\ &= \mathbb{E}_q[\log \frac{p(\mathbf{f}, \mathbf{f}_m, \mathbf{y})}{q(\mathbf{f}, \mathbf{f}_m)}] \triangleq \mathcal{L}(\tilde{\mathbf{Z}}, \Phi, q), \end{aligned} \quad (2)$$

which is consistent with (6). $\mathcal{L}(\tilde{\mathbf{Z}}, \Phi, q)$ can be further reduced as,

$$\begin{aligned} \mathcal{L}(\tilde{\mathbf{Z}}, \Phi, q) &= \int_{\mathbf{f}, \mathbf{f}_m} p(\mathbf{f}|\mathbf{f}_m)q(\mathbf{f}_m) \log \frac{p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\mathbf{f}_m)p(\mathbf{f}_m)}{p(\mathbf{f}|\mathbf{f}_m)q(\mathbf{f}_m)} d\mathbf{f}d\mathbf{f}_m \\ &= \int_{\mathbf{f}_m} q(\mathbf{f}_m) \left\{ \int_{\mathbf{f}} p(\mathbf{f}|\mathbf{f}_m) \log p(\mathbf{y}|\mathbf{f}) d\mathbf{f} + \log \frac{p(\mathbf{f}_m)}{q(\mathbf{f}_m)} \right\} d\mathbf{f}_m \\ &= \int_{\mathbf{f}_m} q(\mathbf{f}_m) \left\{ \log \frac{L(\mathbf{f}_m, \mathbf{y})p(\mathbf{f}_m)}{q(\mathbf{f}_m)} \right\} d\mathbf{f}_m, \end{aligned} \quad (3)$$

where $\log L(\mathbf{f}_m, \mathbf{y})$ is the lower bound of the likelihood $\log p(\mathbf{y}|\mathbf{f}_m)$, and $\log L(\mathbf{f}_m, \mathbf{y}) = \log \int_{\mathbf{f}} p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\mathbf{f}_m)d\mathbf{f} = \log \mathcal{N}(\mathbf{y}|\mathbf{K}_{nm}\mathbf{K}_{mm}^{-1}\mathbf{f}_m, \sigma^2 I) - \frac{1}{2\sigma^2} \text{Tr}(\tilde{\mathbf{K}})$, with $\tilde{\mathbf{K}} = \mathbf{K}_{nn} - \hat{\mathbf{K}}_{nn} = \mathbf{K}_{nn} - \mathbf{K}_{nm}\mathbf{K}_{mm}^{-1}\mathbf{K}_{mn}$. By Jensen's inequality,

$$\begin{aligned} \mathcal{L}(\tilde{\mathbf{Z}}, \Phi, q) &\leq \log \int_{\mathbf{f}_m} L(\mathbf{f}_m, \mathbf{y})p(\mathbf{f}_m)d\mathbf{f}_m \\ &= \log \int_{\mathbf{f}_m} \mathcal{N}(\mathbf{y}|\mathbf{K}_{nm}\mathbf{K}_{mm}^{-1}\mathbf{f}_m, \sigma^2 I)d\mathbf{f}_m - \frac{1}{2\sigma^2} \text{Tr}(\tilde{\mathbf{K}}) \\ &= \log \mathcal{N}(\mathbf{y}|\mathbf{0}, \sigma^2 I + \mathbf{K}_{nm}\mathbf{K}_{mm}^{-1}\mathbf{K}_{mn}) - \frac{1}{2\sigma^2} \text{Tr}(\mathbf{K}_{nn} - \hat{\mathbf{K}}_{nn}) \triangleq \mathcal{L}(\tilde{\mathbf{Z}}, \Phi), \end{aligned} \quad (4)$$

which matches (9).

B Implementation Details

In this section, we provide implementation details regarding the proposed method.

All experiments are conducted on a server with 8 Nvidia RTX 3090 graphic cards, and each has 24GB memory. Every experiment we report can be trained and tested on a single card. The machine is also equipped with 512GB memory and two AMD EPYC 7502 CPUs. We use PyTorch for the implementations of all experiments.

Every experiment is trained with the ADAM optimizer, with a learning rate of 0.001. We train all networks for a total of 80,000 iterations, with the learning rate decays at the 60,000-th and the 70,000-th iteration. In practice, to improve the stability of training, we clip the predicted $(\sigma^2)_*$ to values between 0.01 to 100.0.

Network architectures.

Table A: The architectures of CNNs.

Conv-4 architecture	
Output size	Layers
84×84×3	Input images
42×42×64	Conv (3×3), BatchNorm, ReLU, MaxPool (2×2, stride=2)
21×21×64	Conv (3×3), BatchNorm, ReLU, MaxPool (2×2, stride=2)
10×10×64	Conv (3×3), BatchNorm, ReLU, MaxPool (2×2, stride=2)
5×5×64	Conv (3×3), BatchNorm, ReLU, MaxPool (2×2, stride=2)
1600	flatten
ResNet-12	
Output size	Layers
84×84×3	Input images
42×42×64	[Conv (3×3), BatchNorm, ReLU] × 3, MaxPool (2×2, stride=2)
21×21×128	[Conv (3×3), BatchNorm, ReLU] × 3, MaxPool (2×2, stride=2)
10×10×256	[Conv (3×3), BatchNorm, ReLU] × 3, MaxPool (2×2, stride=2)
5×5×512	[Conv (3×3), BatchNorm, ReLU] × 3, MaxPool (2×2, stride=2)
1×1×512	Global Average Pool
512	flatten
ResNet-10	
Output size	Layers
224×224×3	Input images
56×56×3	Conv(7×7, stride=2), BatchNorm, ReLU, MaxPool(3×3, stride=2)
56×56×64	[Conv (3×3), BatchNorm, ReLU] × 2, Conv (3×3, stride=2), BatchNorm, ReLU,
28×28×128	Conv (3×3), BatchNorm, Conv (1×1, stride=2), ReLU
14×14×256	Conv (3×3, stride=2), BatchNorm, ReLU, Conv (3×3), BatchNorm, Conv (1×1, stride=2), ReLU
7×7×512	Conv (3×3, stride=2), BatchNorm, ReLU, Conv (3×3), BatchNorm, Conv (1×1, stride=2), ReLU
1×1×512	Global Average Pool
512	flatten

Table B: Performance with different kernels. Numbers are obtained on 5-way 5-shot experiments on CUB with Conv-4 backbone.

Kernel	Linear	Cosine	RBF
Accuracy	80.38	81.48	77.62

Kernel. The pair-wise integration $k(\cdot)$ is decided by the kernel function. Here we present the results obtained with different kernels in Table B. We adopt cosine kernels in all the experiments in Section 4.

C Few-shot Regression

We present in Figure A the results of few-shot regression with uncertainty visualized. The setting of the few-shot regression experiments follows exactly the one introduced in [9] with sine waves.

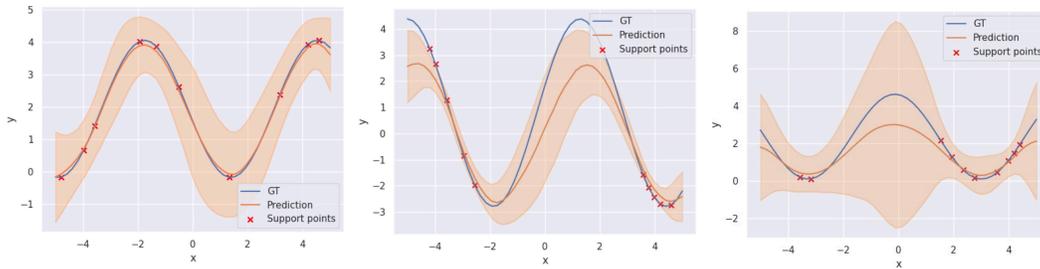


Figure A: Visualizations of the uncertainty quantification in few-shot regression experiments.