Variational Inference in RKHS for Uncertainty Estimation in Deep Learning

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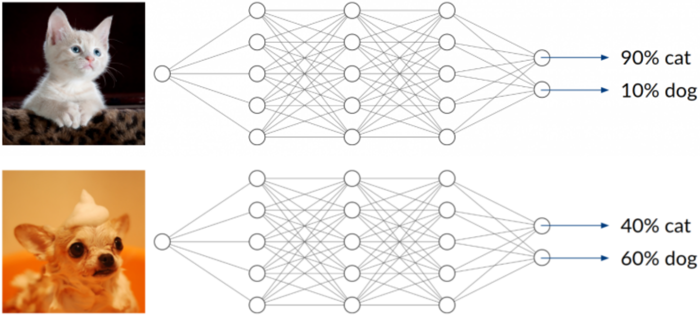
90% cat
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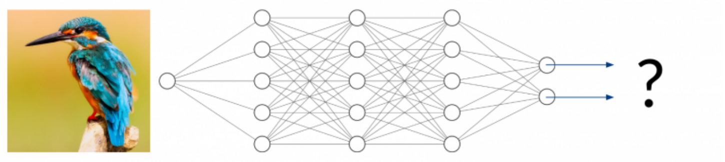
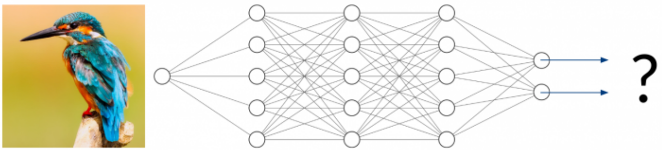
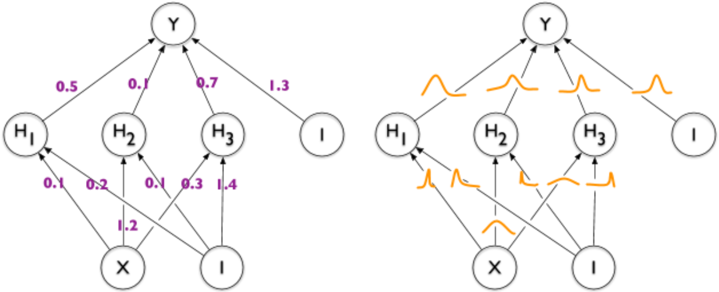




Deep learning methods are unable to quantify the uncertainty of their predictions!

Straight-forward solution: Using a Bayesian model.



Making predictions **requires the posterior** over the parameters of the model $\boldsymbol{\theta}$:

$$p(y^\star|\mathbf{x}^\star, \mathcal{D}) = \int p(y^\star|\mathbf{x}^\star, \boldsymbol{\theta}) p(\boldsymbol{\theta}|\mathcal{D}) \, d\boldsymbol{\theta} \, ,$$

where $p(\boldsymbol{\theta}|\mathcal{D})$ is **intractable for complex models**.

Approximate $p(\boldsymbol{\theta}|\mathcal{D})$ by something simpler $q(\boldsymbol{\theta})$.

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$$\Downarrow$$

Poor performance in many cases.

Approach

1. Learn a DL **deterministic** model h.

High Performance - No Uncertainty

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3. Optimize parameters using function-space VI.

Uncertainty Estimation in function-space

Given a mean $m(\cdot)$ and covariance function $\kappa(\cdot, \cdot)$, defines a **Gaussian prior over function evaluations**:

$$p(f(\mathbf{x})) = \mathcal{N}(m(\mathbf{x}), K(\mathbf{x}, \mathbf{x}))\,.$$

$$f \sim \mathcal{GP}(m, K)\,.$$

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Set of observations $(\mathbf{X}, \mathbf{y})$, the **predictive distribution** is Gaussian

$$p(y^\star|\mathbf{x}^\star, \mathbf{X}, \mathbf{y}) = \mathcal{N}(m^\star(\mathbf{x}^\star), K(\mathbf{x}^\star, \mathbf{x}^\star)) \,.$$

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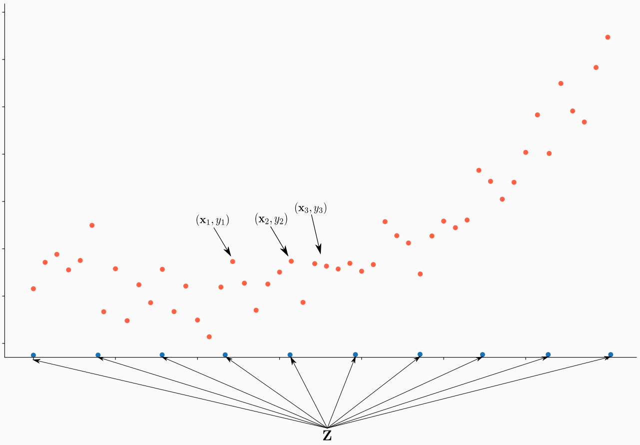
$$m^\star(\mathbf{x}^\star) = \kappa(\mathbf{x}^\star, \mathbf{X})(\kappa(\mathbf{X}, \mathbf{X}) + \sigma^2 \boldsymbol{I})^{-1}(\mathbf{y} - m(\mathbf{x}^\star))\,,$$
$$K(\mathbf{x}^\star, \mathbf{x}^\star) = \kappa(\mathbf{x}^\star, \mathbf{x}^\star) - \kappa(\mathbf{x}^\star, \mathbf{X})(\kappa(\mathbf{X}, \mathbf{X}) + \sigma^2 \boldsymbol{I})^{-1}\kappa(\mathbf{X}, \mathbf{x}^\star)\,.$$

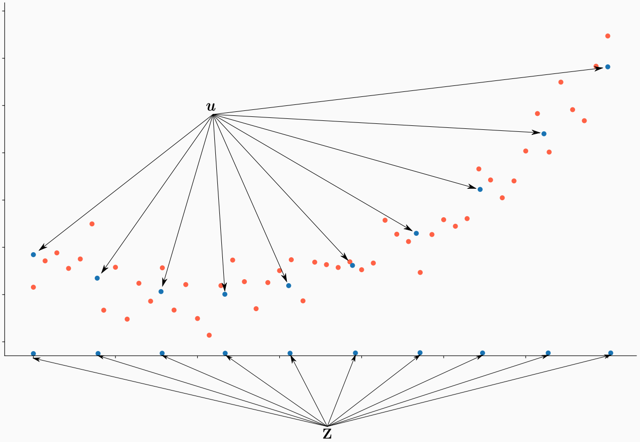
Gaussian noise with variance σ^2 is considered for the targets

Sparse Variational Gaussian Processes

Define a set of *inducing locations* $\mathbf{Z} \subset \mathbb{R}^D$ that "summarize" the training inputs $\mathbf{X}$.

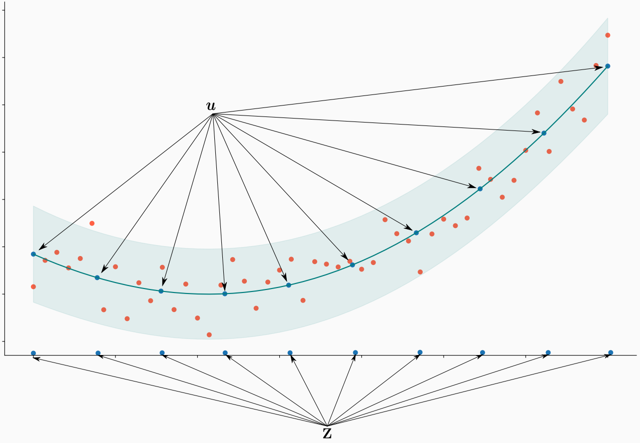


With $\mathbf{u} = f(\mathbf{Z})$, the posterior $p(\mathbf{u}|\mathbf{X}, \mathbf{y})$ is approximated with variational distribution $q(\mathbf{u}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$.



Sparse Variational Gaussian Processes

The inducing points can be marginalized in closed form to make predictions.



A **RKHS** $\mathcal{H}$ is a Hilbert space of functions satisfying the **reproducing property**: $\forall \mathbf{x} \in \mathcal{X}\ \exists \phi_{\mathbf{x}} \in \mathcal{H}$ such that $\forall g \in \mathcal{H}, g(\mathbf{x}) = \langle \phi_{\mathbf{x}}, g \rangle$.

Dual representation of Gaussian Processes

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A **Gaussian process** $f \sim \mathcal{GP}(m, K)$ has a **dual representation** in a RKHS as: there exists $\mu \in \mathcal{H}$ and a linear semi-definite positive operator $\Sigma : \mathcal{H} \to \mathcal{H}$ such that, for any $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$, $\exists \phi_{\mathbf{x}}, \phi_{\mathbf{x}'}$, verifying

$$m(\mathbf{x}) = \langle \phi_{\mathbf{x}}, \mu \rangle \,, \quad K(\mathbf{x}, \mathbf{x}') = \langle \phi_{\mathbf{x}}, \Sigma(\phi_{\mathbf{x}'}) \rangle \ .$$

Dual representation of Gaussian Processes

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$$m(\mathbf{x}) = \langle \phi_{\mathbf{x}}, \mu \rangle \,, \quad K(\mathbf{x}, \mathbf{x}') = \langle \phi_{\mathbf{x}}, \Sigma(\phi_{\mathbf{x}'}) \rangle \ .$$

We write $f \sim \mathcal{N}(\mu, \Sigma)$, which is a **Gaussian measure** in the RKHS.

This characterization in the RKHS allows the **rethink Gaussian Processes as Gaussian Measures** in the Hilbert space:

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The **posterior measure** can be specified as a **Gaussian**:

$$p(f|\mathbf{y}) = \mathcal{N}(\mu^\star, \Sigma^\star)$$

$$\mu^\star = \kappa(\cdot, \mathbf{X})(\kappa(\mathbf{X}, \mathbf{X}) + \sigma^2 \boldsymbol{I})^{-1}(\mathbf{y} - m(\cdot))$$
$$\Sigma^\star = I - \phi_{\mathbf{X}}^T(\kappa(\mathbf{X}, \mathbf{X}) + \sigma^2 \boldsymbol{I})^{-1}\phi_{\mathbf{X}}$$

Theorem. A SVGP is equivalent to restricting the mean and covariance functions in the RKHS to

$$\tilde{\mu} = \Phi_{\mathbf{Z}}(\boldsymbol{a}) \quad \text{and} \quad \tilde{\Sigma} = I + \Phi_{\mathbf{Z}} \boldsymbol{A} \Phi_{\mathbf{Z}}^T \,,$$

where $\Phi_{\mathbf{Z}} : \mathbb{R}^M \to \mathcal{H}$ is defined as

$$\Phi_{\mathbf{Z}}(\boldsymbol{a}) = \sum_{m=1}^{M} a_m \phi_{\mathbf{z}_m} \,, \quad \text{and} \quad \Phi_{\mathbf{Z}} \boldsymbol{A} \Phi_{\mathbf{Z}}^T = \sum_{i=1}^{M} \sum_{j=1}^{M} \phi_{\mathbf{z}_i} A_{i,j} \phi_{\mathbf{z}_j}^T$$

where $\boldsymbol{A} \in \mathbb{R}^{M \times M}$ such that $\tilde{\Sigma} \geq 0$.

Cheng, C.A. and Boots, B., 2016. Incremental variational sparse Gaussian process regression. Advances in Neural Information Processing Systems, 29.

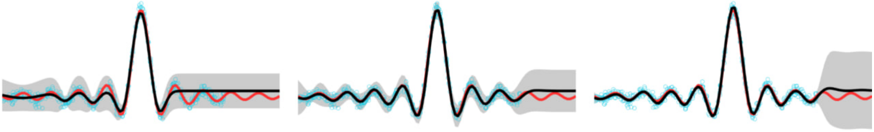
A SVGP can be generalized with mean and covariance functions of the dual representation in the RKHS to

$$\tilde{\mu} = \Phi_{\mathbf{Z}_\alpha}(\boldsymbol{a}) \quad \text{and} \quad \tilde{\Sigma} = I + \Phi_{\mathbf{Z}_\beta} \boldsymbol{A} \Phi_{\mathbf{Z}_\beta}{}^T \,,$$

where $\mathbf{Z}_\alpha$ and $\mathbf{Z}_\beta$ are two sets of inducing locations.

Cheng, C.A. and Boots, B., 2017. Variational inference for Gaussian process models with linear complexity. Advances in Neural Information Processing Systems, 30.

Comparison between models with shared and decoupled basis



(a) $M = 10$ (b) $M_\alpha = 100, M_\beta = 10$ (c) $M = 100$

- (a) and (c) denote the models with shared basis of size M.
- (b) denotes the model of decoupled basis with size (M_α, M_β).

Figure from Cheng, C.A. and Boots, B., 2017. Variational inference for Gaussian process models with linear complexity. Advances in Neural Information Processing Systems, 30.

Variational Optimization

SVGPs are optimized using the Evidence Lower Bound:

$$\mathsf{KL}\big(p(\mathbf{f},\mathbf{u}|\mathbf{y})|q(\mathbf{f},\mathbf{u})\big) = \log p(\mathbf{y}) \underbrace{- \mathbb{E}_{q(\mathbf{f})}[\log p(\mathbf{y}|\mathbf{f})] + \mathsf{KL}\big(q(\mathbf{u})|p(\mathbf{u})\big)}_{-ELBO}$$

with $\mathbf{f} = f(\mathbf{X})$ and $\mathbf{u} = f(\mathbf{Z})$.

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Which is **equivalent** to optimize the ELBO in function-space

$$\mathsf{KL}\big(p(f|\mathbf{y})|q(f)\big) = \log p(\mathbf{y}) \underbrace{- \mathbb{E}_{q(f)}[\log p(\mathbf{y}|f)] + \mathsf{KL}\big(q(f)|p(f)\big)}_{-ELBO}$$

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Variational Optimization

Optimizing the ELBO in the Hilbert space:

$$\max_{q(f)} \mathcal{L}(q(f)) = \max_{q(f)} \mathbb{E}_{q(f)}\left[\log p(\mathbf{y}|f)\right] - \mathsf{KL}\left(q|p\right) \,.$$

Where

$$\mathsf{KL}\left(q|p\right) = \underbrace{\frac{1}{2}\boldsymbol{a}^T\boldsymbol{K}_\alpha\boldsymbol{a}}_{\boldsymbol{a},\mathbf{Z}_\alpha} + \underbrace{\frac{1}{2}\log|\boldsymbol{I} - \boldsymbol{K}_\beta(\boldsymbol{A}+\boldsymbol{K}_\beta)^{-1}| + \frac{1}{2}\mathsf{tr}\left(\boldsymbol{K}_\beta\boldsymbol{A}^{-1}\right)}_{\boldsymbol{A},\mathbf{Z}_\beta}$$

and $\mathbb{E}_{q(f)}\left[\log p(\mathbf{y}|f)\right]$ can be computed in regression and estimated in classification.

Fixing the Mean Function

If the kernel $\kappa(\cdot, \cdot)$ is universal, then, $\forall \epsilon > 0$, there exists a set of M_α points $\mathbf{Z}_\alpha \subset \mathbb{R}^D$ and coefficients $\boldsymbol{a} \in \mathbb{R}^{M_\alpha}$, such that

$$d_{\mathcal{H}}(h, \Phi_{\mathbf{Z}_\alpha}(\boldsymbol{a})) \leq \epsilon, \quad \text{with} \quad \Phi_{\mathbf{Z}_\alpha}(\boldsymbol{a}) := \sum_{m=1}^{M_\alpha} a_m \phi_{\mathbf{z}_m} .$$

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$$
\begin{aligned}
m^\star(\mathbf{x}) &= \kappa(\mathbf{x}, \mathbf{Z}_\alpha)\boldsymbol{a}\,, \\
K^\star(\mathbf{x}, \mathbf{x}') &= \kappa(\mathbf{x}, \mathbf{x}') + \kappa(\mathbf{x}, \mathbf{Z}_\beta)\boldsymbol{A}^{-1}\kappa(\mathbf{Z}_\beta, \mathbf{x}')\,,
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$$

where $\mathbf{Z}_\beta \subset \mathbb{R}^D$ is a set of M_β inducing points, $\boldsymbol{A} \in \mathbb{R}^{M_\beta \times M_\beta}$ such that $\tilde{\Sigma} \geq 0$ and it verifies

$$
d_{\mathcal{H}}(h, m^\star) \leq \epsilon
$$

Distributions over function-space with fixed mean to h.

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Parameters: $\mathbf{Z}_\beta \subset \mathbb{R}^D$ and $\boldsymbol{A} \in \mathbb{R}^{M_\beta \times M_\beta}$ (such that $\tilde{\Sigma} \geq 0$).

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Parameters: $\mathbf{Z}_\beta \subset \mathbb{R}^D$ and $\boldsymbol{A} \in \mathbb{R}^{M_\beta \times M_\beta}$ (such that $\tilde{\Sigma} \geq 0$).

Gaussian process posterior approximation $\mathcal{GP}(m^\star, K^\star)$:

$$
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m^\star(\mathbf{x}) &\approx h(\mathbf{x})\,, \\
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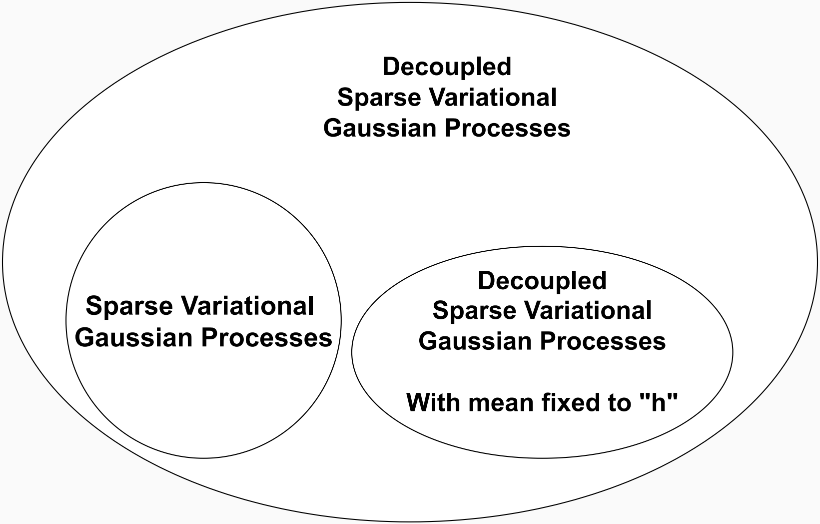
Diagram - Distribution over function-space



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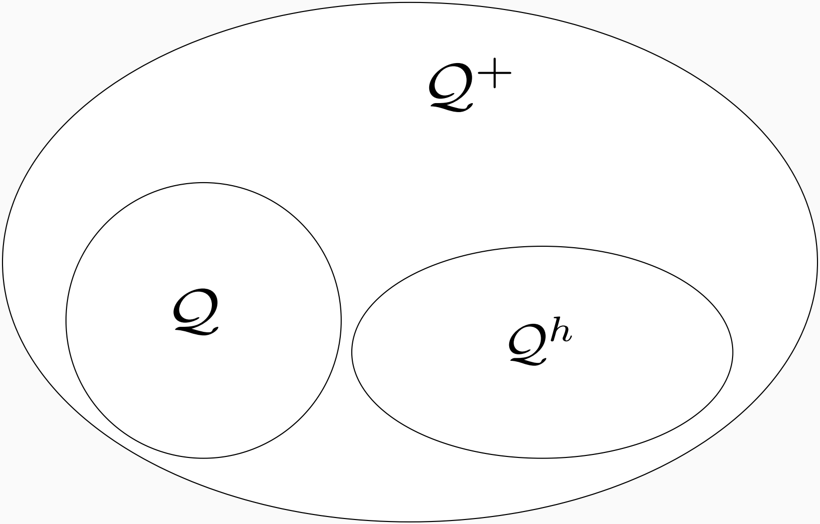

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Decoupled Sparse Variational Gaussian Processes

$$q^\star = \underset{q \in \mathcal{Q}^+}{\arg\max}\ \mathbb{E}_{q(f)}[\log p(\mathbf{y}|f)] - \mathsf{KL}\big(q|p\big)$$

Variational Inference in Different Families

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Fixed Mean Sparse Variational Gaussian Processes

$$q^\star = \underset{q \in \mathcal{Q}^h}{\arg\max}\ \mathbb{E}_{q(f)}[\log p(\mathbf{y}|f)] - \mathsf{KL}\big(q|p\big)$$

Optimizing the ELBO in the Hilbert space:

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where

$$\mathsf{KL}\left(q|p\right) = \frac{1}{2}\boldsymbol{a}^T\boldsymbol{K}_\alpha\boldsymbol{a} + \frac{1}{2}\log|\boldsymbol{I} - \boldsymbol{K}_\beta(\boldsymbol{A} + \boldsymbol{K}_\beta)^{-1}| + \frac{1}{2}\mathrm{tr}\left(\boldsymbol{K}_\beta\boldsymbol{A}^{-1}\right)$$

and $\mathbb{E}_{q(f)}\left[\log p(\mathbf{y}|f)\right]$ can be computed in regression and estimated in classification.

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In regression: $\kappa_\theta(\cdot, \cdot) \to 0$ is a **local optima** in $\mathcal{Q}^h$.

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Solution: α-divergences.

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$$\boxed{q^\star = \arg\max_{q \in \mathcal{Q}^h} \; \frac{1}{\alpha} \log \; \mathbb{E}_{q(f)} \left[p(\mathbf{y}|f)^\alpha\right] - \mathsf{KL}\left(q|p\right)}$$

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$$q^\star = \arg\max_{q \in \mathcal{Q}^h} \; \text{Train LL} - \mathsf{KL}\left(q|p\right)$$

Intuitive Recap

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5. Train the (non-fixed) parameters using **function-space VI** and mini-batch optimization.
6. The resulting method **provides uncertainty estimation** for the deterministic model.

Results in Regression Problems

	Airline		Year		Taxi	
Model	NLL	CRPS	NLL	CRPS	NLL	CRPS
Deterministic	5.087	18.436	3.674	5.056	3.763	3.753
LLA Diag	5.096	**18.317**	3.650	4.957	3.714	3.979
LLA KFAC	5.097	**18.317**	3.650	4.955	3.705	3.977
LLA*	5.097	18.319	3.650	**4.954**	3.718	**3.975**
LLA* KFAC	5.097	**18.317**	3.650	**4.954**	3.718	3.976
ELLA	5.086	18.437	3.674	5.056	3.753	3.754
VaLLA	**4.923**	18.610	**3.527**	5.071	**3.287**	3.968
This Method	**4.903**	**17.552**	**3.485**	**4.721**	**3.208**	**3.493**

Limitations

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Multi-class Classification

Zero Uncertainty $\implies$ Train LL $= h$ Train LL.

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2. Sparse GPs can be generalized to **decouple the inducing points**.
3. There exists a **subspace** with posterior mean h.
4. Preliminary results on **regression** are promising.
5. Limited on **multi-class classification**.

Thank you for your attention!