Function-Space Orthogonality in Probabilistic Learning

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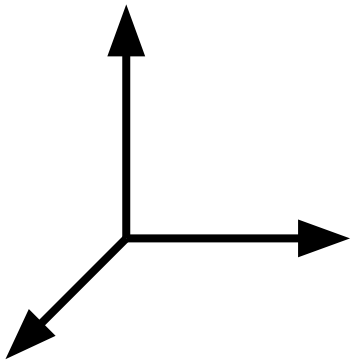
Functions in Probabilistic Learning

- Probability/Cumulative density functions
- Score functions
- Critic/Test functions
- Distributions of functions, e.g., Gaussian Processes

Motivation: Orthogonal Basis in Function Spaces



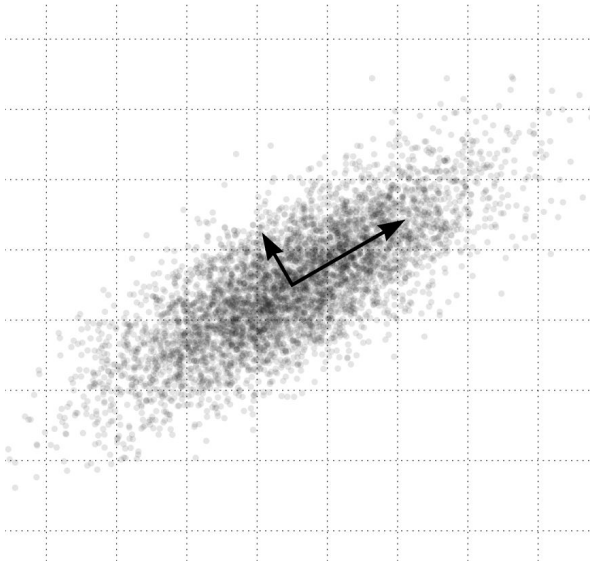
- How to characterize functions in probabilistic computations?
- Goal: Build an orthogonal basis in the function space.

Motivation: Orthogonal Basis in Function Spaces

- Recap: PCA

$$\mathbf{X}^\top \mathbf{X} = \mathbf{U} \mathbf{\Lambda} \mathbf{U}^\top$$

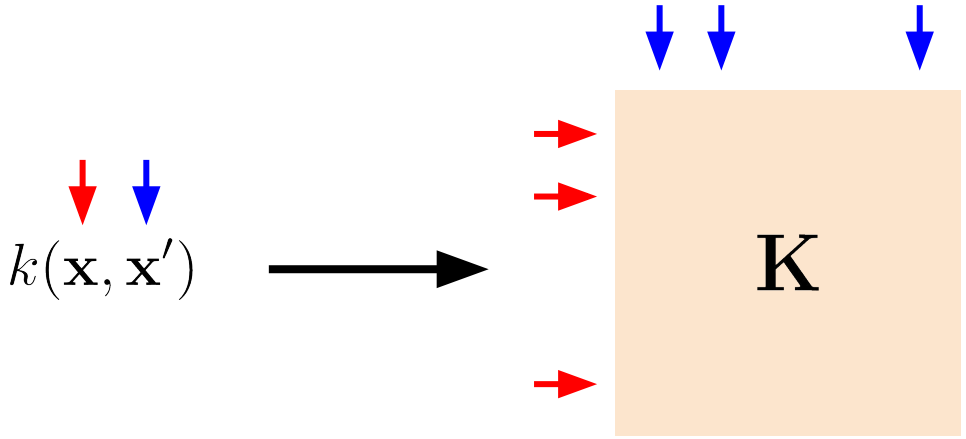
where $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_N]^\top$



- Eigenvectors form a new orthogonal basis
  - u_1: the direction with the largest data variance
  - u_2: the direction orthogonal to u_1 with the second largest data variance
  - ...

Motivation: Orthogonal Basis in Function Spaces

- Kernel: p.s.d. matrix in infinite-dimensional spaces



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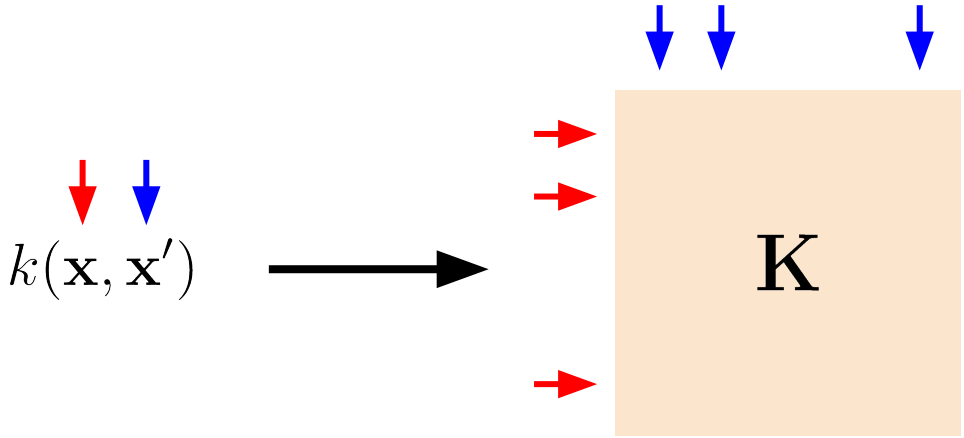
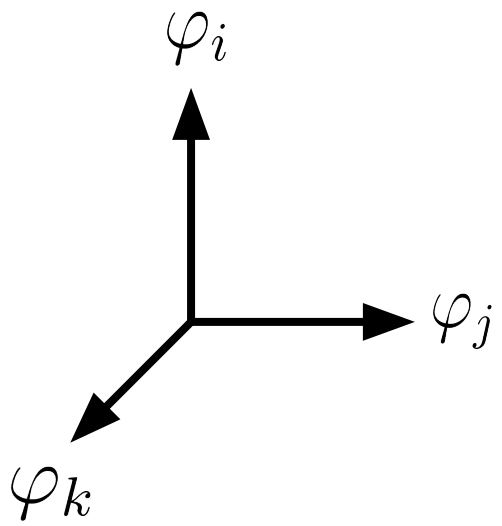


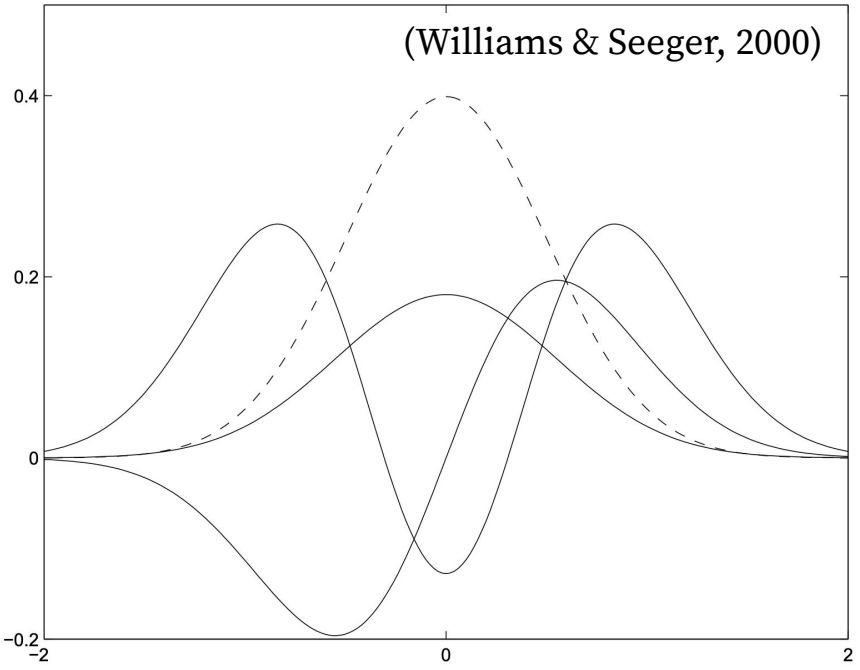
- Mercer's Theorem $k(\mathbf{x}, \mathbf{x}') = \sum_i \mu_i \varphi_i(\mathbf{x}) \varphi_i(\mathbf{x}')$
- Eigenvectors > Eigenfunctions

$$\int k(\mathbf{x}, \mathbf{x}') \varphi_i(\mathbf{x}') p(\mathbf{x}') d\mathbf{x}' = \mu_i \varphi_i(\mathbf{x})$$

Motivation: Orthogonal Basis in Function Spaces

- Eigenfunctions as an orthonormal basis





$$\int \varphi_i \varphi_j dp = 0 \qquad \int \varphi_i^2 dp = 1$$

Outline

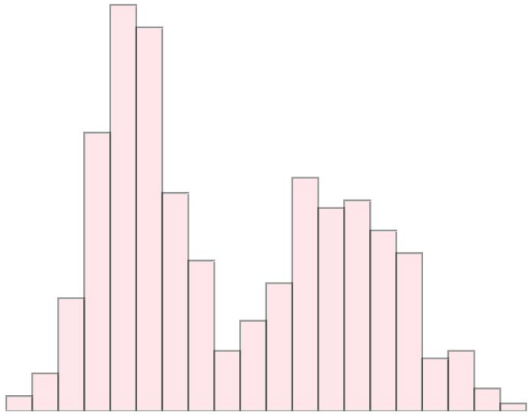
- Orthogonal Series Estimators for Score Functions

  Shi, Shengyang Sun, Jun Zhu, ICML 18

- Sparse Orthogonal Variational Inference for Gaussian Processes

  Shi, Michalis K. Titsias, Andriy Mnih, AISTATS 20

Score Estimation

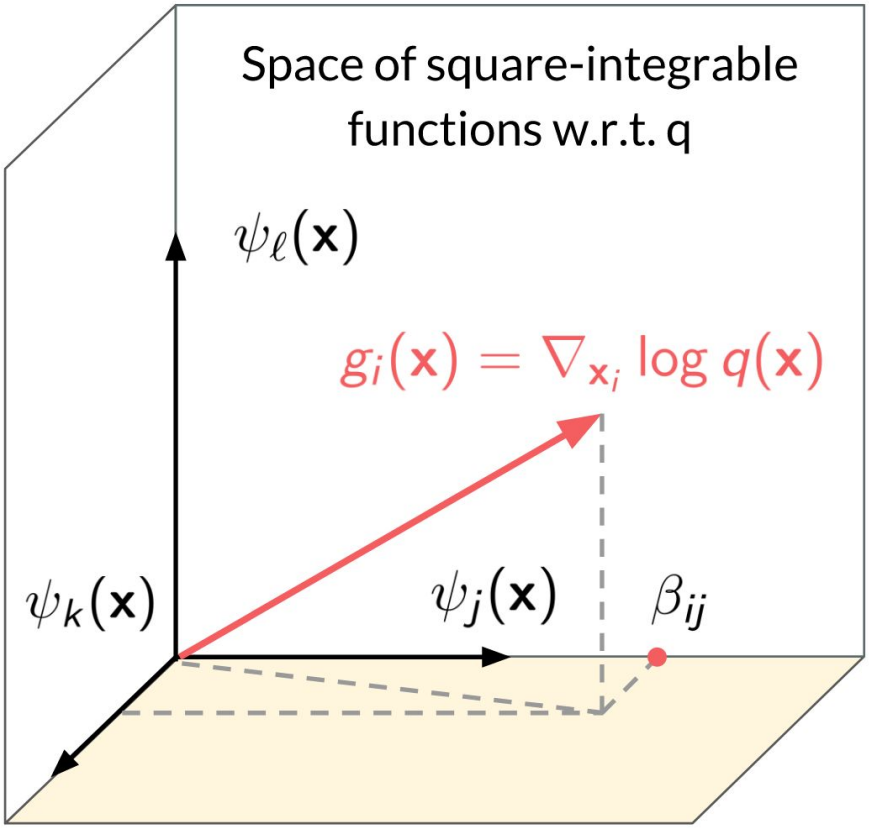


$$\mathbf{x}^{1:M} \sim q$$

$$g_{\mathbf{x}^{1:M}}(\mathbf{x}) \approx \nabla_{\mathbf{x}} \log q(\mathbf{x})$$

(Strathmann et al., 15; Li & Turner, 18; Sutherland et al., 18)

Orthogonal Series Expansion



$$\frac{\partial}{\partial x_i} \log q(\mathbf{x}) = \sum_j \beta_{ij} \varphi_j(\mathbf{x})$$

Main Result

Theorem: Under mild assumptions

$$\frac{\partial}{\partial x_i} \log q(\mathbf{x}) = -\sum_j \mathbb{E}_q \left[\frac{\partial}{\partial x_i} \varphi_j(\mathbf{x}) \right] \varphi_j(\mathbf{x})$$

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Proof:

- Coefficients of the orthogonal series expansion of $\frac{\partial}{\partial x_i} \log q(\mathbf{x})$:

$$\beta_{ij} = \mathbb{E}_q \left[\varphi_j(\mathbf{x}) \frac{\partial}{\partial x_i} \log q(\mathbf{x}) \right]$$

(Shi, Sun, Zhu, 18)

(Generalized) Stein's Lemma

$$\mathbb{E}_q\left[h(\mathbf{x})\nabla_{\mathbf{x}}\log q(\mathbf{x})\right] = \int h(\mathbf{x})\nabla_{\mathbf{x}} q(\mathbf{x}) d\mathbf{x}$$

$$= \int \nabla_{\mathbf{x}}\left[h(\mathbf{x})q(\mathbf{x})\right] d\mathbf{x} - \int \nabla_{\mathbf{x}} h(\mathbf{x}) q(\mathbf{x}) d\mathbf{x}$$

$$= -\mathbb{E}_q\left[\nabla_{\mathbf{x}} h(\mathbf{x})\right]$$

where $\int \nabla_{\mathbf{x}}\left[h(\mathbf{x})q(\mathbf{x})\right] d\mathbf{x} = 0$ holds when $\lim_{\|\mathbf{x}\|\to\infty} h(\mathbf{x})q(\mathbf{x}) = 0$

by divergence theorem

(Stein, 1972; Gorham & Mackey, 2015)

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  where we replace the Stein test function with eigenfunctions.

(Shi, Sun, Zhu, 18)

Spectral Stein Gradient Estimator (SSGE)

Theorem: Under mild assumptions

$$\frac{\partial}{\partial x_i} \log q(\mathbf{x}) = -\sum_j \mathbb{E}_q \left[\frac{\partial}{\partial x_i} \varphi_j(\mathbf{x}) \right] \varphi_j(\mathbf{x})$$

Final Step: Estimate φ_i and $\nabla \varphi_i$.

(Shi, Sun, Zhu, 18)

Nyström Methods

$$\int k(\mathbf{x}, \mathbf{x}')\varphi_i(\mathbf{x}')p(\mathbf{x}')d\mathbf{x}' = \mu_i\varphi_i(\mathbf{x})$$

Goal: Estimate φ_i with $\mathbf{x}^{1:M} \sim p$

(Nyström, 1930; Williams & Seeger, 2001)

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$$\mathbf{K} \quad \mathbf{u}_i = \lambda_i \mathbf{u}_i$$

where
$\mathbf{K}_{mn} = k(\mathbf{x}^m, \mathbf{x}^n)$

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$$\varphi_i(\cdot) = \frac{1}{\mu_i}\int k(\mathbf{x}, \cdot)\varphi_i(\mathbf{x})p(\mathbf{x})d\mathbf{x} \approx \frac{\sqrt{M}}{\hat{\lambda}_i}\sum_{m=1}^{M} u_{im}k(\mathbf{x}^m, \cdot)$$

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Estimate φ_i and $\nabla \varphi_i$ with Nyström methods

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$$\nabla \varphi_i(\cdot) = \frac{1}{\mu_i} \int \nabla k(\mathbf{x}, \cdot) \varphi_i(\mathbf{x}) p(\mathbf{x}) d\mathbf{x}$$

(Shi, Sun, Zhu, 18)

Error Analysis

Theorem: Under mild assumptions

$$\int |\hat{g}_i(\mathbf{x}) - g_i(\mathbf{x})|^2 q(\mathbf{x})\, d\mathbf{x}$$

Our estimator True gradient

is bounded by

$$J^2 \left(O_p\left(\frac{1}{M}\right) + O_p\left(\frac{1}{\mu_J \Delta_J^2 M}\right)\right) + J O_p\left(\frac{1}{\mu_J \Delta_J^2 M}\right) + \mu_J \|g_i\|_{\mathcal{H}}^2$$

Sample error Approximation error

where $\Delta_J = \min_{1 \le j \le J} |\mu_j - \mu_{j+1}|$

Related Work

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  - A scalable variant: Sliced Score Matching (Song, Garg, Shi, Ermon, UAI 19).

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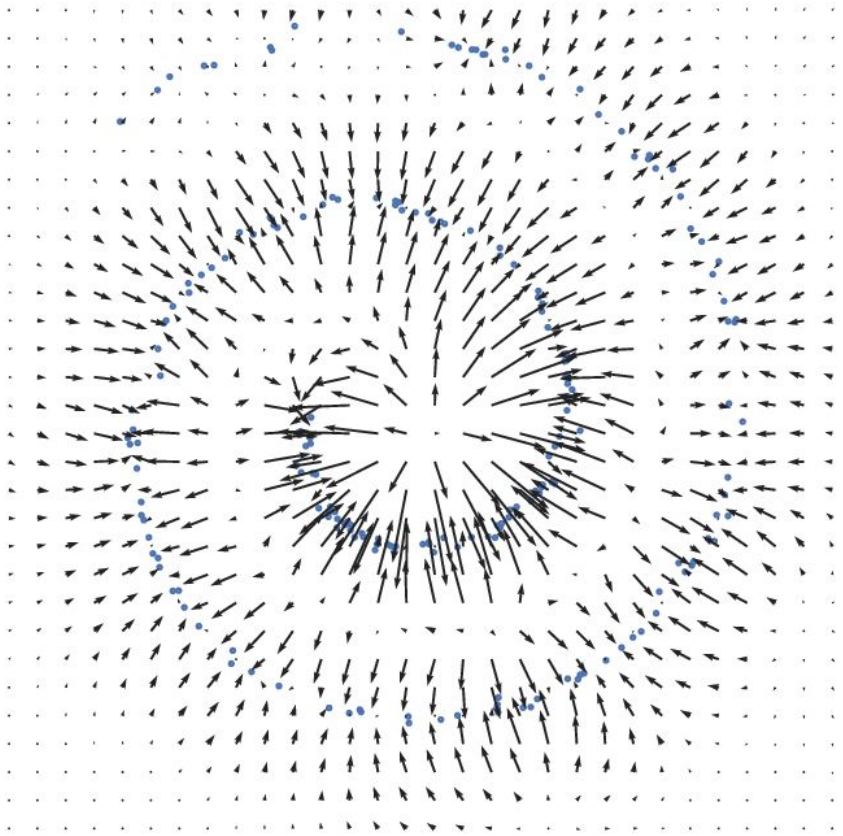
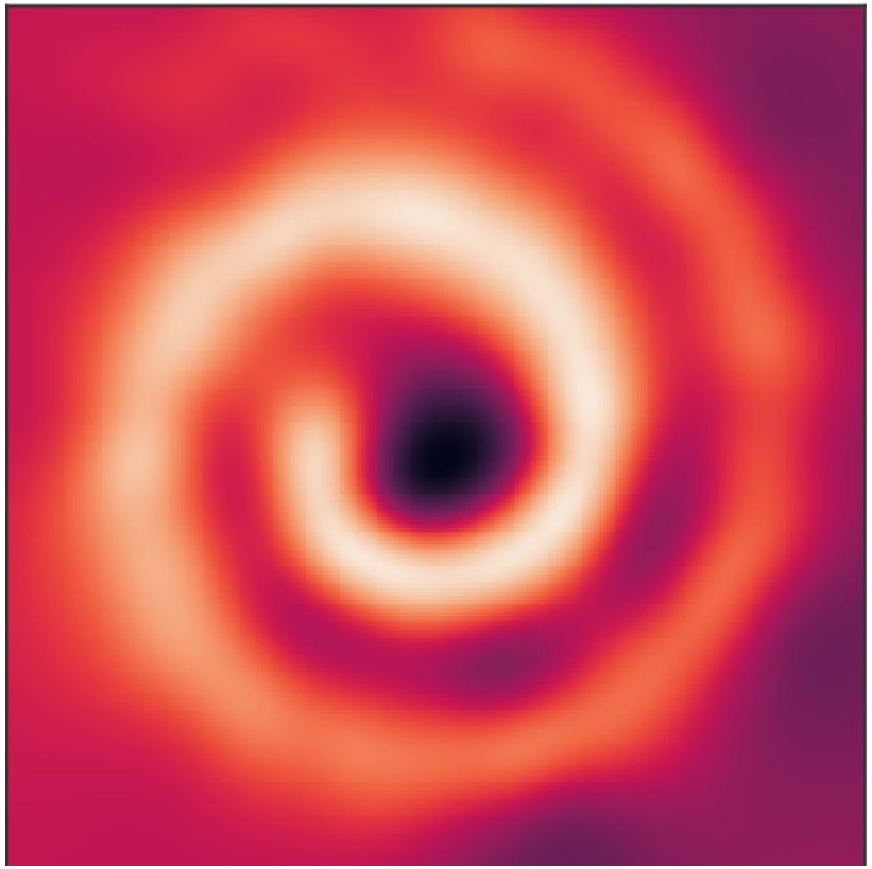
  - A scalable variant: Sliced Score Matching (Song, Garg, Shi, Ermon, UAI 19).
- Nonparametric Score Estimators (coming)
  - A unified view of SSGE, Li & Turner, Score Matching.
  - Vector-valued extensions: Enforce conservative properties of gradient fields

Spiral Data





Entropy/KL-divergence Gradient Estimation

$$\nabla_\phi \mathbb{H}(q) = -\nabla_\phi \mathbb{E}_q \log q_\phi(\mathbf{x}) - \nabla_\phi \mathbb{E}_{q_\phi} \log q(\mathbf{x})$$

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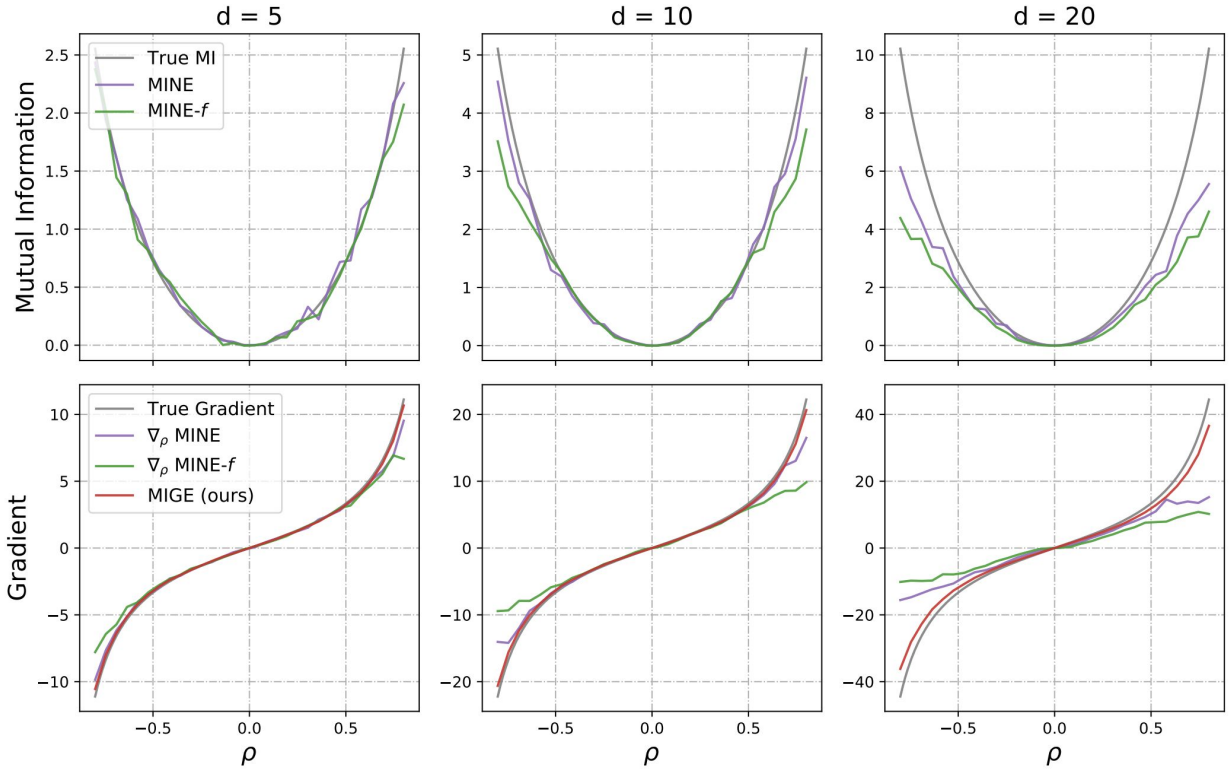
$$= -\mathbb{E}_{\epsilon \sim \nu(\epsilon)} \nabla_{\mathbf{x}} \log q(f(\epsilon; \phi)) \nabla_\phi f(\epsilon; \phi)$$

Entropy/KL-divergence Gradient Estimation

$$\begin{aligned}
\nabla_\phi \mathbb{H}(q) &= -\nabla_\phi \mathbb{E}_q \log q_\phi(\mathbf{x}) - \nabla_\phi \mathbb{E}_{q_\phi} \log q(\mathbf{x}) \\
&= -\nabla_\phi \mathbb{E}_{\epsilon \sim \nu(\epsilon)} \log q(f(\epsilon; \phi)) \\
&= -\mathbb{E}_{\epsilon \sim \nu(\epsilon)} \nabla_{\mathbf{x}} \log q(f(\epsilon; \phi)) \nabla_\phi f(\epsilon; \phi)
\end{aligned}$$

Similarly for cross-entropy (out-of-sample) and KL-divergence.

Applications



$$X \sim p_d(X) \quad Z = f_\phi(X) \qquad \max_\phi I(Z; X)$$

Mutual Information Gradient Estimation for Representation Learning
(Wen et al., ICLR 20)

Applications

Model	CIFAR-10			CIFAR-100		
	conv	fc(1024)	Y(64)	conv	fc(1024)	Y(64)
DIM (JSD)	55.81%	45.73%	40.67%	28.41%	22.16%	16.50%
DIM (JSD + PM)	52.2%	52.84%	43.17%	24.40%	18.22%	15.22%
DIM (infoNCE)	51.82%	42.81%	37.79%	24.60%	16.54%	12.96%
DIM (infoNCE + PM)	56.77%	49.42%	42.68%	25.51%	20.15%	15.35%
MIGE	**57.95%**	**57.09%**	**53.75%**	**29.86%**	**27.91%**	**25.84%**

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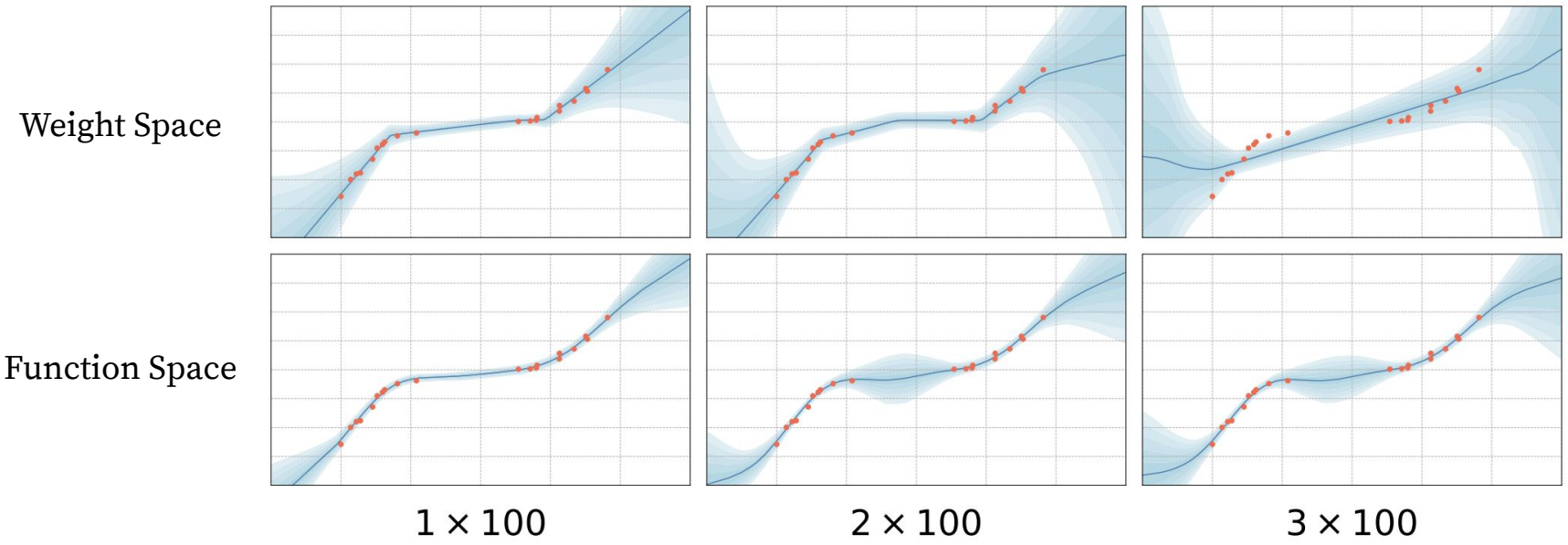

Functional Bayesian Neural Networks
(Sun, Zhang, Shi, Grosse, ICLR 19)

Summary

- Eigenfunction expansions of the score has a simple form.
- Eigenfunctions can be approximated with Nyström Methods.
- Score estimation is useful when samples are easier to obtain than densities.

Main Ref:
A Spectral Approach to Gradient Estimation for Implicit Distributions. Shi, Sun, Zhu, 2018

From Eigenfunctions to Distributions of Functions

$$f = \sum_i \eta_i \varphi_i$$

$$\eta_i \sim p(\eta_i)$$

Eigenfunction Representations of GPs

- GP samples can be represented as series of eigenfunctions

$$f \sim \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x}')) \iff f = \sum_i \eta_i \varphi_i, \quad \eta_i \sim \mathcal{N}(0, \mu_i)$$

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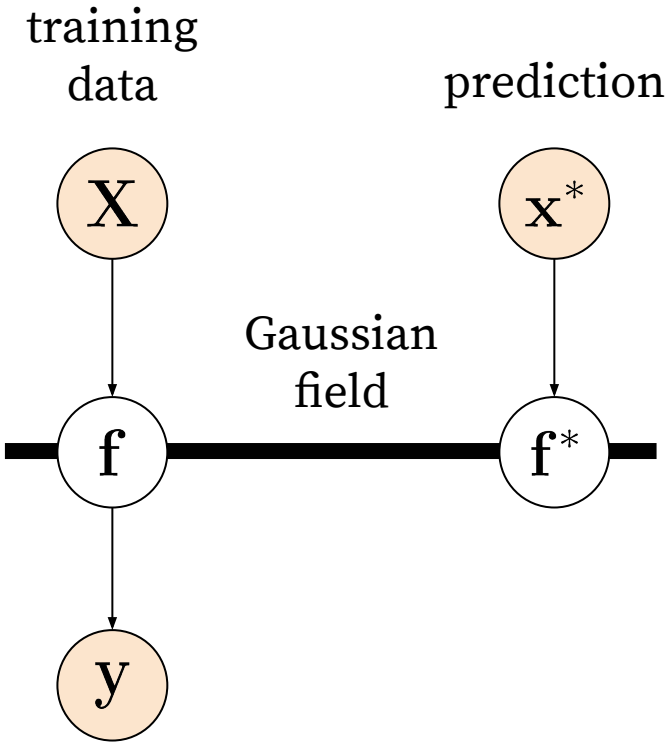
Mercer's theorem

Gaussian Processes (GP)



$$f(\mathbf{x}) \sim \mathcal{GP}\left(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}')\right)$$

mean function

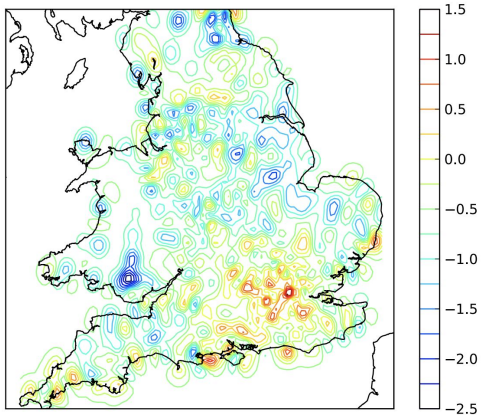
covariance function / kernel

$$p(\mathbf{f}, \mathbf{f}^*) := \mathcal{N}\left(\begin{array}{c|c} \mathbf{f} & \left[\begin{array}{c} m(\mathbf{X}) \\ m(\mathbf{x}^*) \end{array}\right], \left[\begin{array}{cc} \mathbf{K}_{\mathbf{XX}} & \mathbf{K}_{\mathbf{X}*} \\ \mathbf{K}_{*\mathbf{X}} & \mathbf{K}_{**} \end{array}\right] \\ \mathbf{f}^* & \end{array}\right)$$

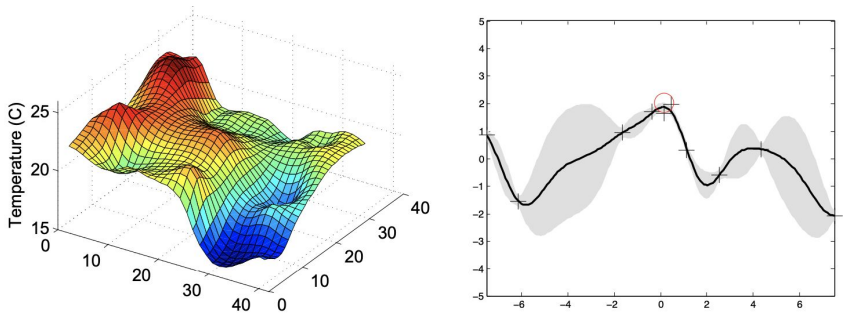
$$\mathbf{f} = f(\mathbf{X}) := [f(\mathbf{x}_1), \ldots, f(\mathbf{x}_N)]^\top$$

$\mathcal{O}(N^3)$ complexity

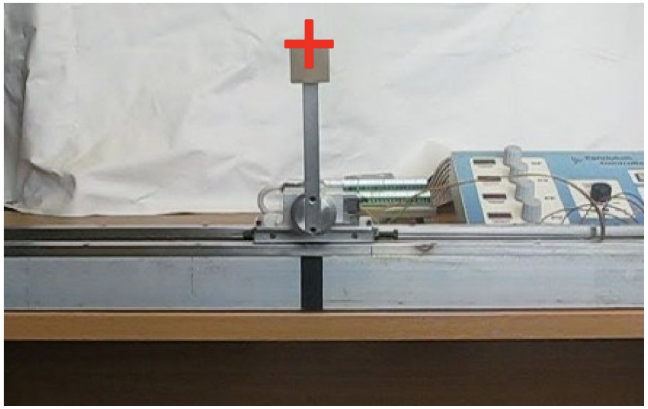
Gaussian Processes (GP)



(Hensman et al., 13)



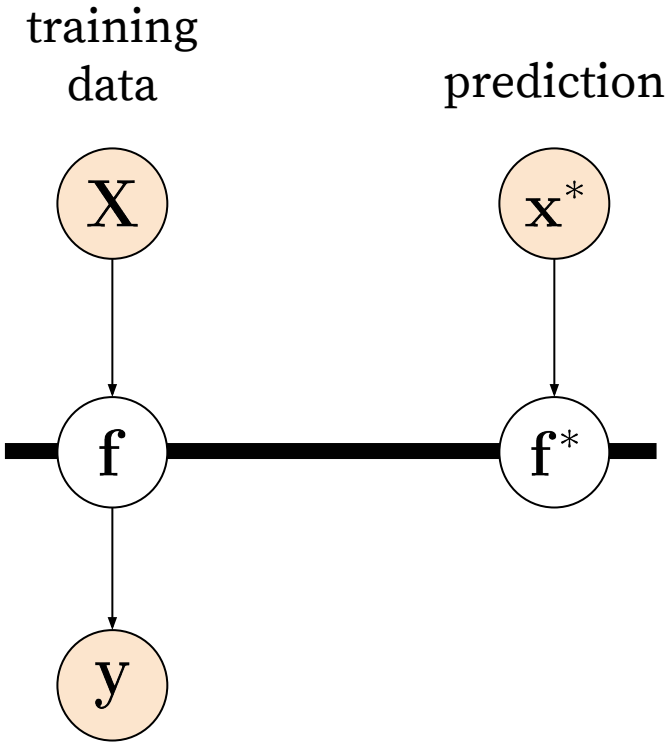
(Srinivas et al., 09)



(Deisenroth & Rasmussen, 11)

(Titsias & Lawrence, 10)

Scalable GPs via Approximate Inference



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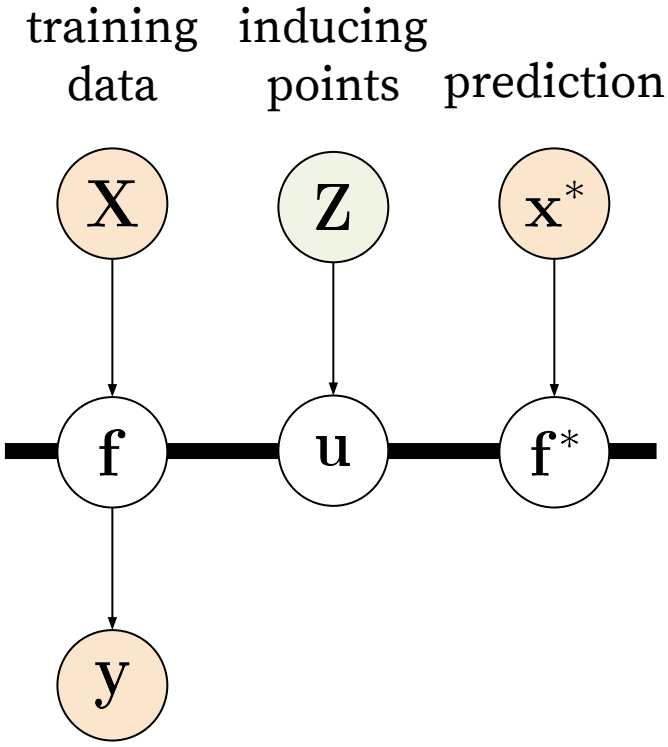


$$\mathbf{u} = f(\mathbf{Z}) := [f(\mathbf{z}_1), \ldots, f(\mathbf{z}_M)]^\top$$

Sparse variational GP methods (SVGP)

- Augmented joint distribution:

$$p(\mathbf{y}, \mathbf{f}, \mathbf{u}) = p(\mathbf{y}|\mathbf{f})p(\mathbf{f}, \mathbf{u})$$

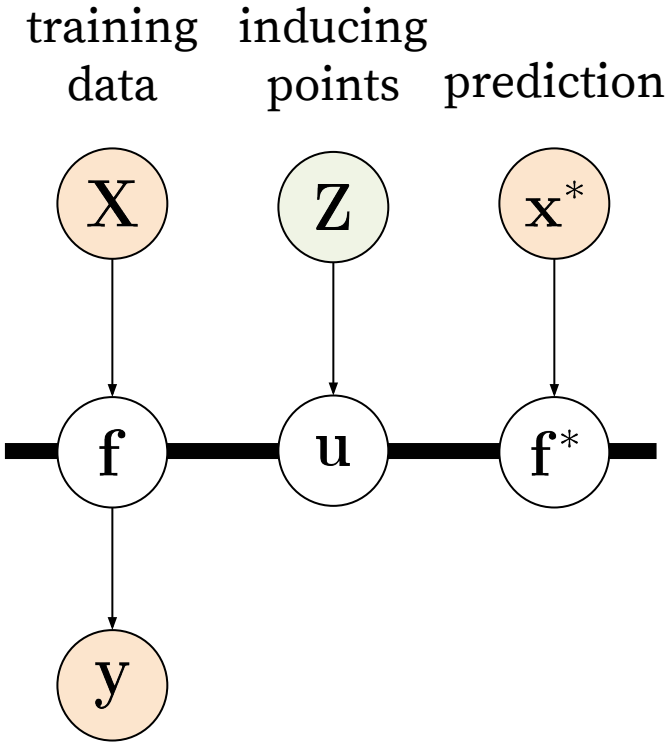
- Variational distribution:

$$q(\mathbf{f}, \mathbf{u}) = p(\mathbf{f}|\mathbf{u})q(\mathbf{u})$$

$$\mathrm{KL}\left[q(\mathbf{f}, \mathbf{u}) \| p(\mathbf{f}, \mathbf{u}|\mathbf{y})\right] = \mathbb{E}_q \log \frac{p(\mathbf{f}|\mathbf{u})q(\mathbf{u}) \cdot p(\mathbf{y})}{p(\mathbf{y}|\mathbf{f}) \cdot p(\mathbf{f}|\mathbf{u})p(\mathbf{u})}$$

(Titsias, 09; Hensman et al., 13 & 15)

Scalable GPs via Approximate Inference



$$\mathbf{u} = f(\mathbf{Z}) := [f(\mathbf{z}_1), \ldots, f(\mathbf{z}_M)]^\top$$

Sparse variational GP methods (SVGP)

- Augmented joint distribution:

$$p(\mathbf{y}, \mathbf{f}, \mathbf{u}) = p(\mathbf{y}|\mathbf{f})p(\mathbf{f}, \mathbf{u})$$

- Variational distribution:

$$q(\mathbf{f}, \mathbf{u}) = p(\mathbf{f}|\mathbf{u})q(\mathbf{u})$$

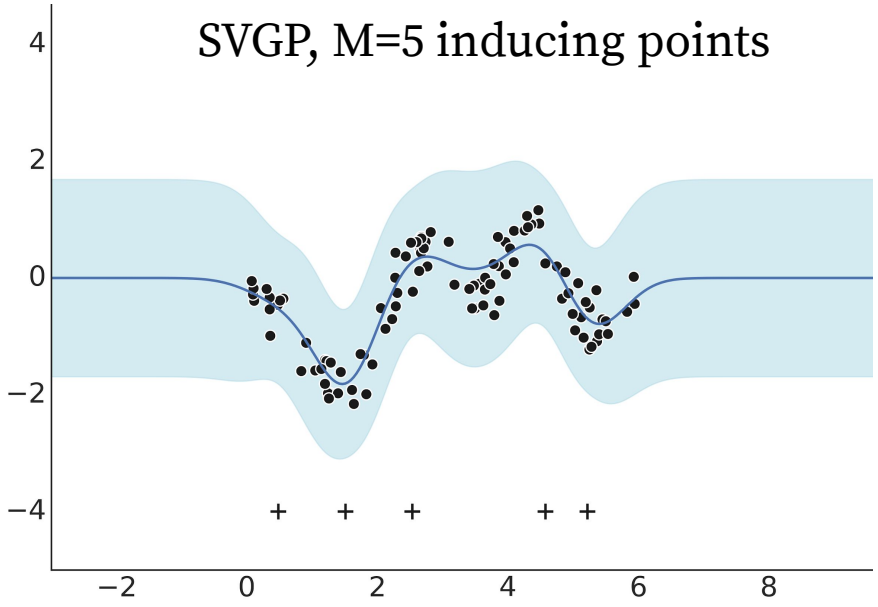
$$\mathrm{KL}\left[q(\mathbf{f}, \mathbf{u}) \| p(\mathbf{f}, \mathbf{u}|\mathbf{y})\right] = \mathbb{E}_q \log \frac{p(\mathbf{f}|\mathbf{u})q(\mathbf{u}) \cdot p(\mathbf{y})}{p(\mathbf{y}|\mathbf{f}) \cdot p(\mathbf{f}|\mathbf{u})p(\mathbf{u})}$$

$$\mathbb{E}_{q(\mathbf{u})p(\mathbf{f}|\mathbf{u})}\left[\log p(\mathbf{y}|\mathbf{f})\right] - \mathrm{KL}[q(\mathbf{u})\|p(\mathbf{u})]$$

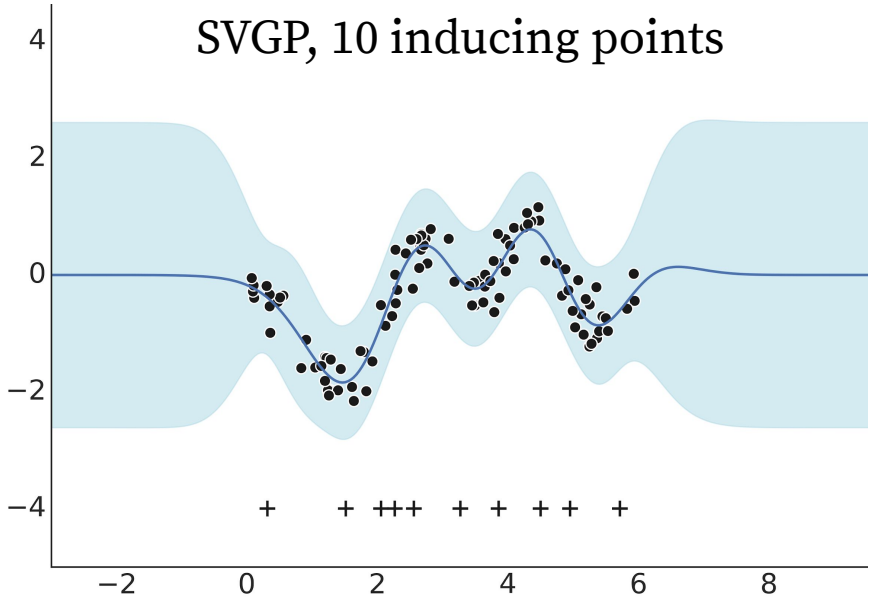
$\mathcal{O}(M^3)$ complexity per update

(Titsias, 09; Hensman et al., 13 & 15)

Inducing Points Are Expensive

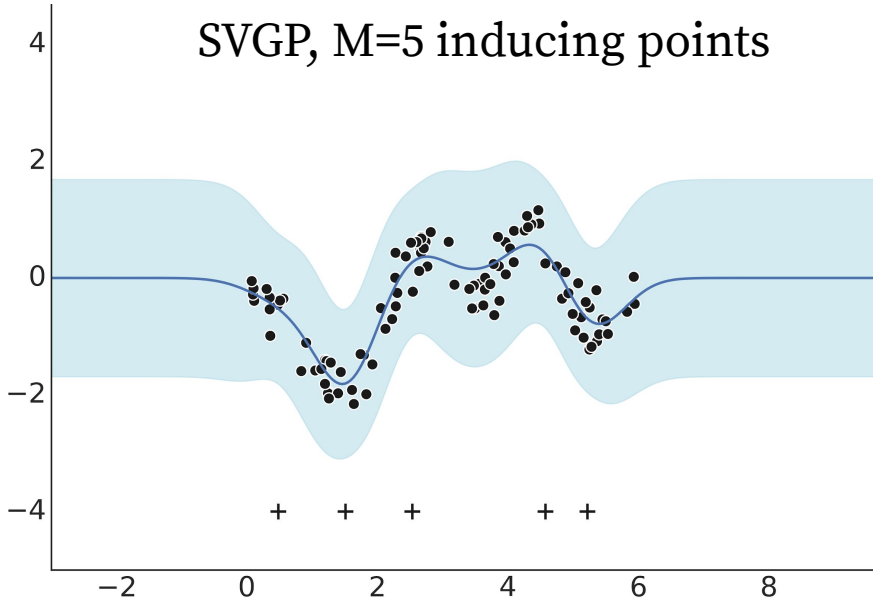


Cholesky: cM^3



Cholesky: $8cM^3$

Inducing Points Are Expensive



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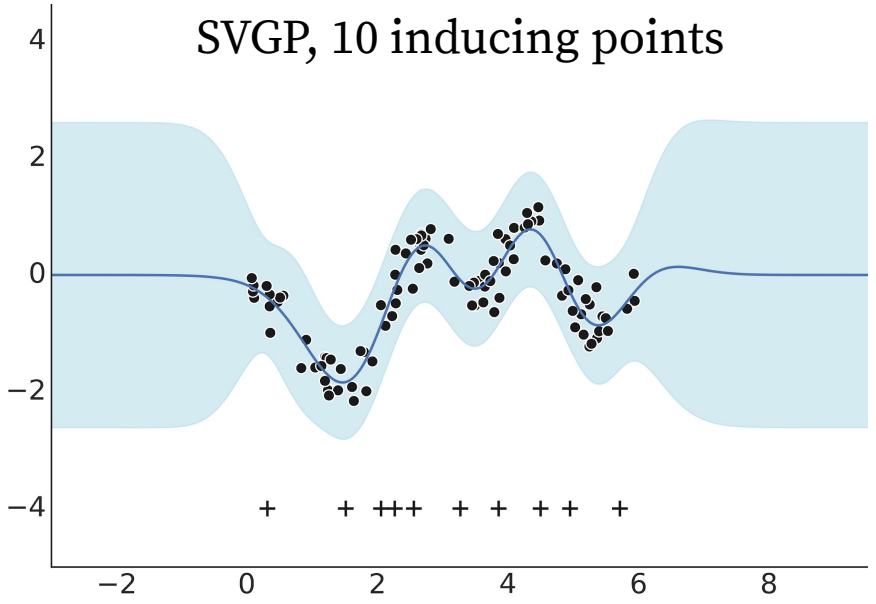

Cholesky: $8cM^3$

Can we do better?

Reinterpreting SVGP

$$\mathbf{f} \sim p(\mathbf{f}) \quad \begin{cases} \mathbf{u} \sim p(\mathbf{u}) \equiv \mathcal{N}(\mathbf{0}, \mathbf{K_{ZZ}}) \\ \mathbf{f} \sim p(\mathbf{f}|\mathbf{u}) \end{cases}$$

(Shi, Titsias, Mnih, 20)

Reinterpreting SVGP

$$\mathbf{f} \sim p(\mathbf{f}) \quad \begin{cases} \mathbf{u} \sim p(\mathbf{u}) \equiv \mathcal{N}(\mathbf{0}, \mathbf{K_{ZZ}}) \\ \mathbf{f} \sim p(\mathbf{f}|\mathbf{u}) \end{cases} \qquad p(\mathbf{f}|\mathbf{u}) \equiv \mathcal{N}(\mathbf{K_{XZ}}\mathbf{K_{ZZ}^{-1}}\mathbf{u}, \mathbf{K_{XX}} - \mathbf{K_{XZ}}\mathbf{K_{ZZ}^{-1}}\mathbf{K_{ZX}})$$

(Shi, Titsias, Mnih, 20)

Reinterpreting SVGP

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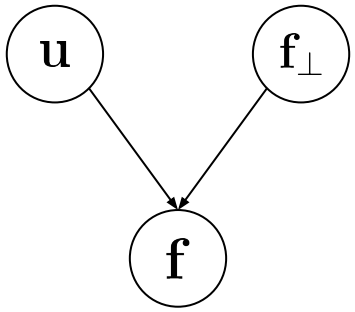
$$\mathbf{u} \sim p(\mathbf{u}) \equiv \mathcal{N}(\mathbf{0}, \mathbf{K_{zz}})$$

$$\begin{cases} \mathbf{f}_\perp \sim p_\perp(\mathbf{f}_\perp) \equiv \mathcal{N}(\mathbf{0}, \mathbf{K_{xx}} - \mathbf{K_{xz}}\mathbf{K_{zz}^{-1}}\mathbf{K_{zx}}) \\ \mathbf{f} = \mathbf{K_{xz}}\mathbf{K_{zz}^{-1}}\mathbf{u} + \mathbf{f}_\perp \end{cases}$$



(Shi, Titsias, Mnih, 20)

Reinterpreting SVGP

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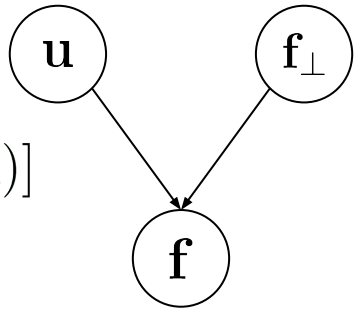
$$\mathbb{E}_{q(\mathbf{u})p(\mathbf{f}|\mathbf{u})}\left[\log p(\mathbf{y}|\mathbf{f})\right] - \mathrm{KL}[q(\mathbf{u})\|p(\mathbf{u})]$$

$$\rightarrow \quad \mathbb{E}_{q(\mathbf{u})p_\perp(\mathbf{f}_\perp)}\left[\log p(\mathbf{y}|\mathbf{f}_\perp + \mathbf{K_{XZ}}\mathbf{K_{ZZ}^{-1}}\mathbf{u})\right] - \mathrm{KL}\left[q(\mathbf{u})\|p(\mathbf{u})\right]$$



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Reinterpreting SVGP

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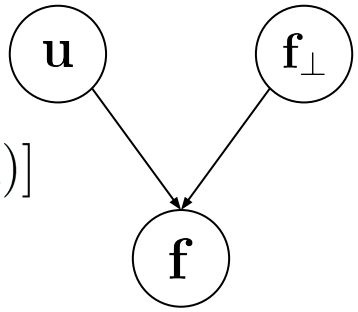


The variational posterior distribution over $\mathbf{f}_\perp$ is simply chosen to be the prior distribution.

(Shi, Titsias, Mnih, 20)

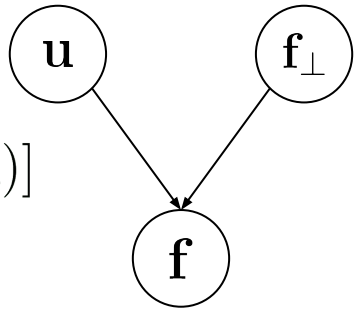
Reinterpreting SVGP

$$\mathbf{f} \sim p(\mathbf{f}) \quad \begin{cases} \mathbf{u} \sim p(\mathbf{u}) \equiv \mathcal{N}(\mathbf{0}, \mathbf{K_{ZZ}}) \\ \mathbf{f} \sim p(\mathbf{f}|\mathbf{u}) \end{cases} \qquad \mathbf{u} \sim p(\mathbf{u}) \equiv \mathcal{N}(\mathbf{0}, \mathbf{K_{ZZ}})$$

$$\begin{cases} \mathbf{f}_\perp \sim p_\perp(\mathbf{f}_\perp) \equiv \mathcal{N}(\mathbf{0}, \mathbf{K_{XX}} - \mathbf{K_{XZ}}\mathbf{K_{ZZ}^{-1}}\mathbf{K_{ZX}}) \\ \mathbf{f} = \mathbf{K_{XZ}}\mathbf{K_{ZZ}^{-1}}\mathbf{u} + \mathbf{f}_\perp \end{cases}$$

$$\mathbb{E}_{q(\mathbf{u})p(\mathbf{f}|\mathbf{u})}\left[\log p(\mathbf{y}|\mathbf{f})\right] - \mathrm{KL}[q(\mathbf{u})\|p(\mathbf{u})]$$

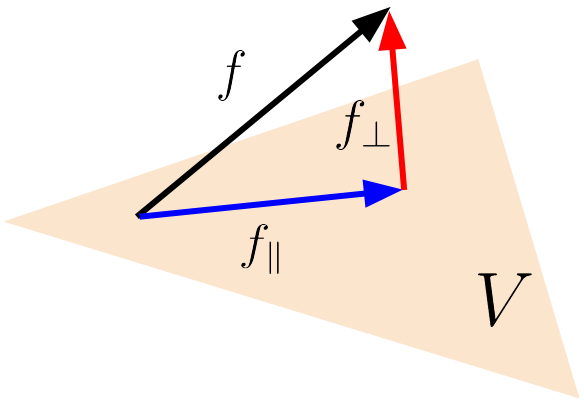
$$\rightarrow \quad \mathbb{E}_{q(\mathbf{u})p_\perp(\mathbf{f}_\perp)}\left[\log p(\mathbf{y}|\mathbf{f}_\perp + \mathbf{K_{XZ}}\mathbf{K_{ZZ}^{-1}}\mathbf{u})\right] - \mathrm{KL}\left[q(\mathbf{u})\|p(\mathbf{u})\right]$$

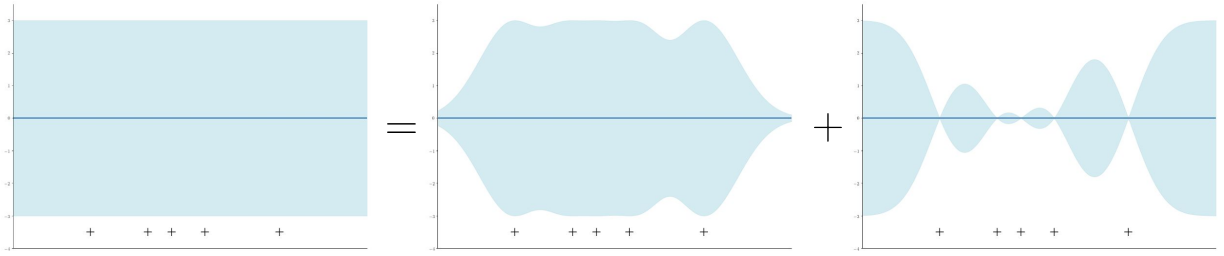


- Can we improve the variational approximation for $\mathbf{f}_\perp$?
- Full Gaussian parameterization of $q(\mathbf{f}_\perp)$ has $\mathcal{O}(N^3)$ cost.

(Shi, Titsias, Mnih, 20)

Orthogonal Decomposition





$$V = \left\{ \sum_{i=1}^{M} a_i k(\mathbf{z}_i, \cdot) \;\middle|\; \mathbf{a} \in \mathbb{R}^M \right\}$$

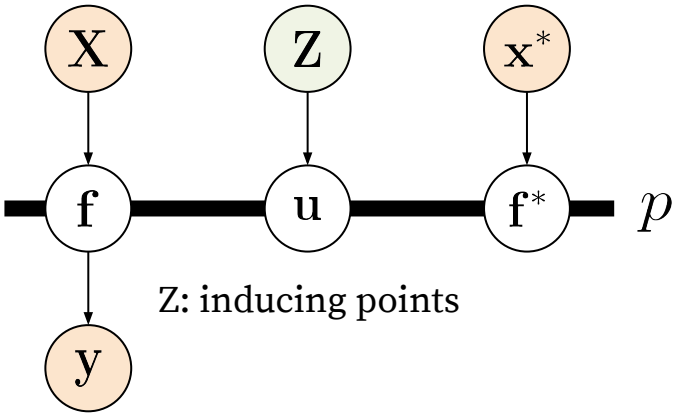
$$p_\parallel : f_\parallel = k(\mathbf{x}, \mathbf{Z})^\top \mathbf{K}_{\mathbf{ZZ}}^{-1} \mathbf{u} \sim \mathcal{GP}(0, k(\mathbf{x}, \mathbf{Z}) \mathbf{K}_{\mathbf{ZZ}}^{-1} k(\mathbf{Z}, \mathbf{x}'))$$

$$p_\perp : f_\perp \sim \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x}') - k(\mathbf{x}, \mathbf{Z}) \mathbf{K}_{\mathbf{ZZ}}^{-1} k(\mathbf{Z}, \mathbf{x}'))$$

$$p : f = f_\perp + f_\parallel \sim \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x}'))$$

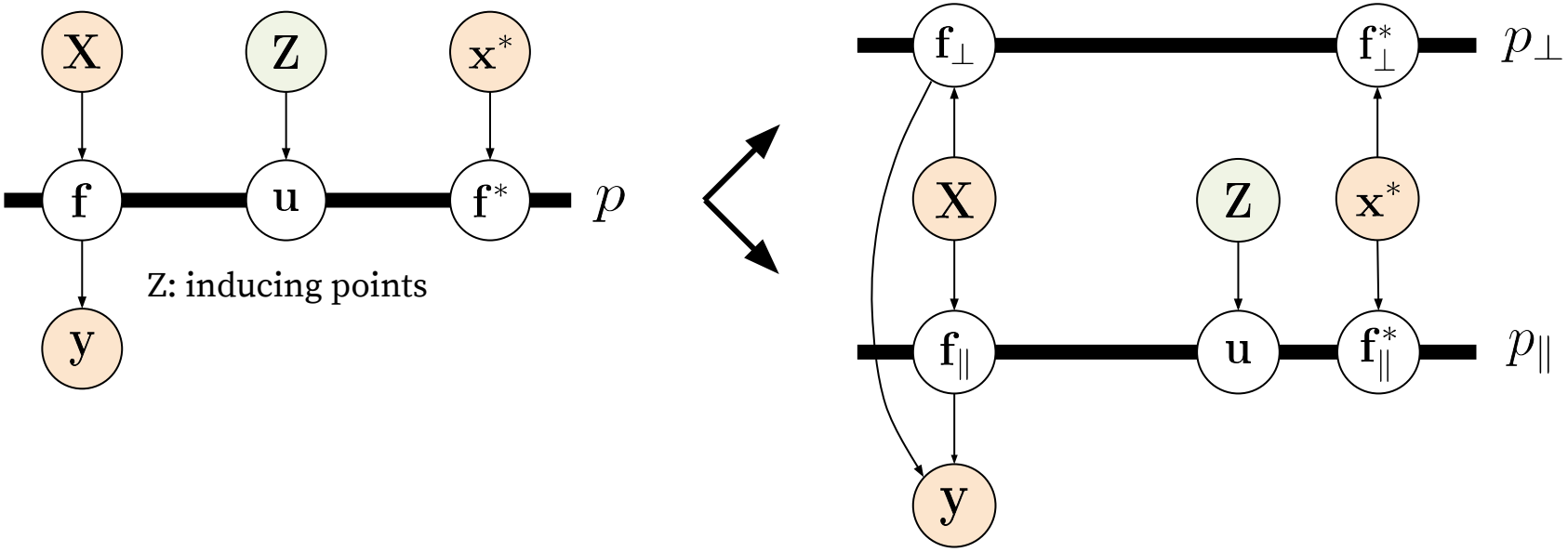
(Shi, Titsias, Mnih, 20)

Orthogonal Inducing Points



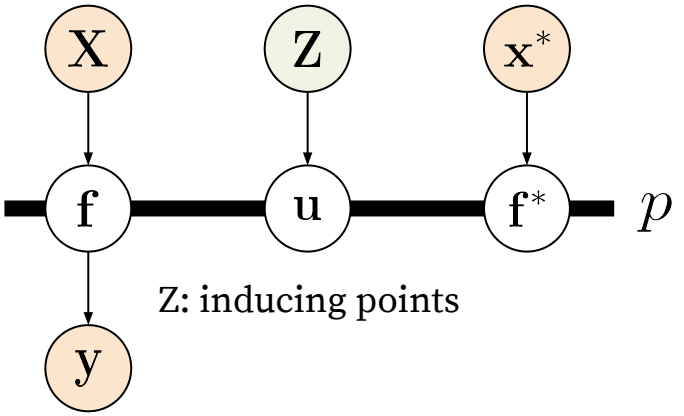
(Shi, Titsias, Mnih, 20)

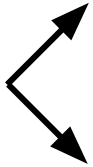
Orthogonal Inducing Points

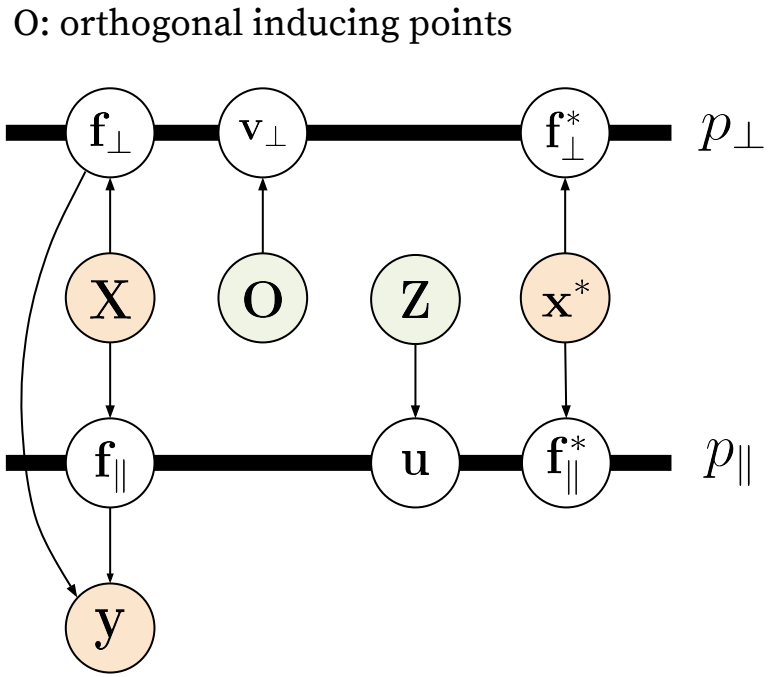


(Shi, Titsias, Mnih, 20)

Orthogonal Inducing Points





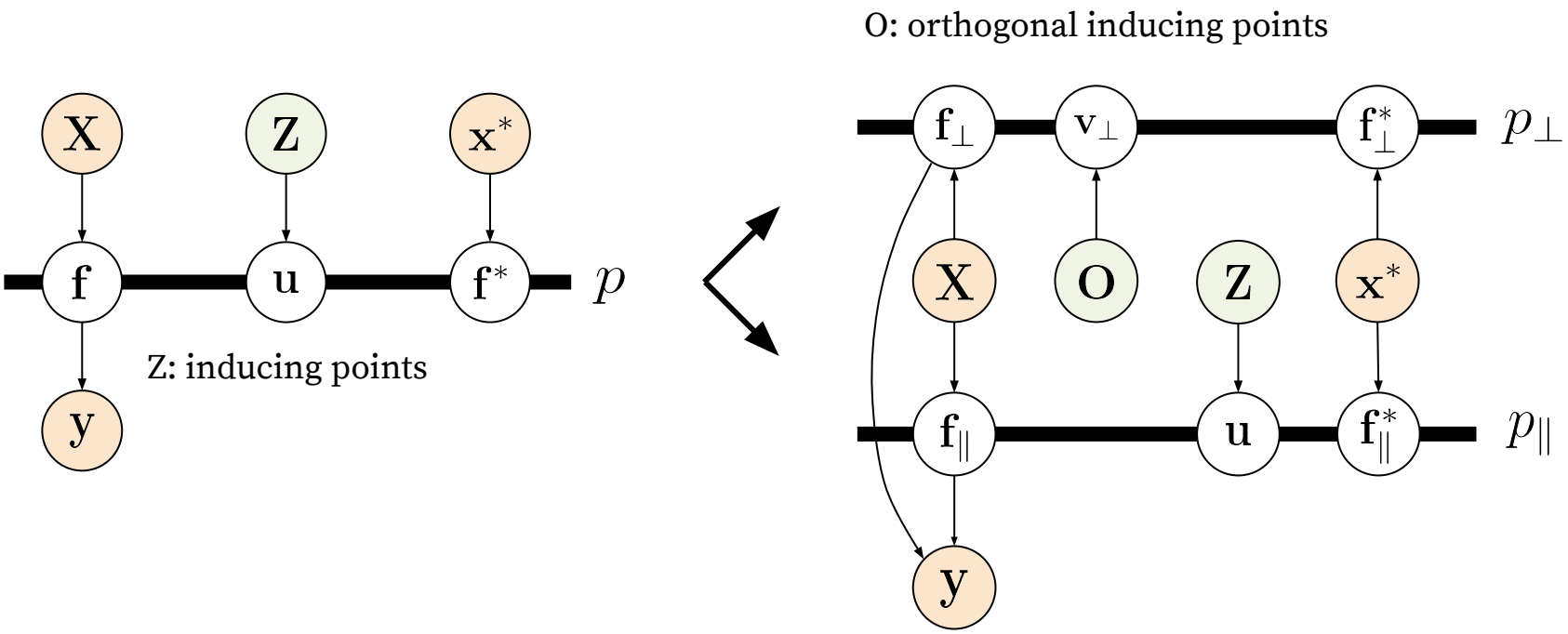


Idea

- After reparameterization, posterior inference for f is equivalent to posterior inference for $f_\perp$, u
- introducing inducing variables $v_\perp$ in the orthogonal process to summarize $f_\perp$.

(Shi, Titsias, Mnih, 20)

Sparse Orthogonal Variational Inference for Gaussian Processes

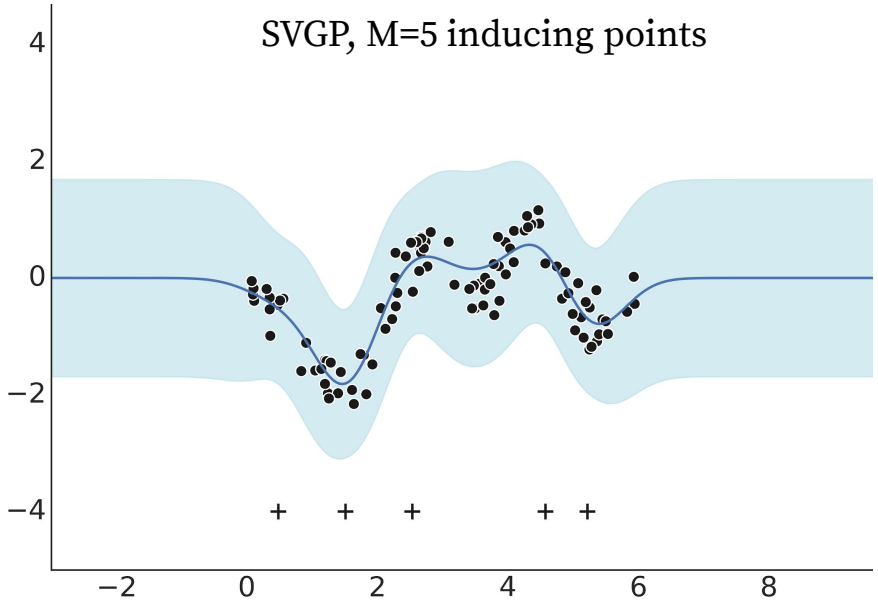


SOLVE-GP lower bound

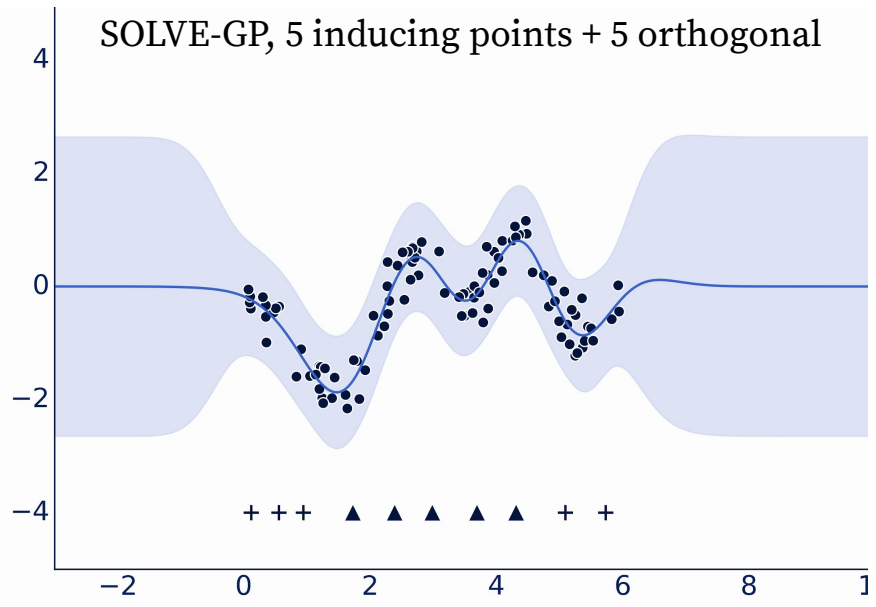
$$\mathbb{E}_{q(\mathbf{u})q(\mathbf{v}_\perp)p_\perp(\mathbf{f}_\perp|\mathbf{v}_\perp)}\left[\log p(\mathbf{y}|\mathbf{f}_\perp + \mathbf{K_{xz}}\mathbf{K_{zz}^{-1}}\mathbf{u})\right] - \mathrm{KL}\left[q(\mathbf{v}_\perp)\|p_\perp(\mathbf{v}_\perp)\right] - \mathrm{KL}\left[q(\mathbf{u})\|p(\mathbf{u})\right]$$

(Shi, Titsias, Mnih, 20)

Orthogonal Inducing Points Are Cheaper



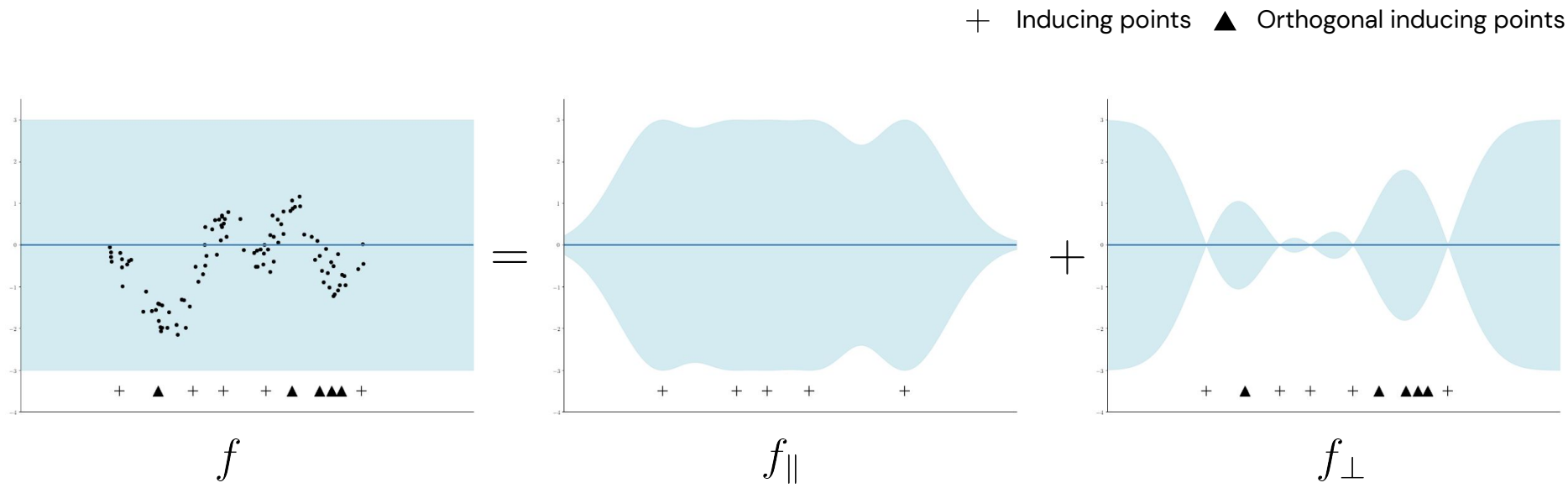
Cholesky: cM^3



Cholesky: $2cM^3$

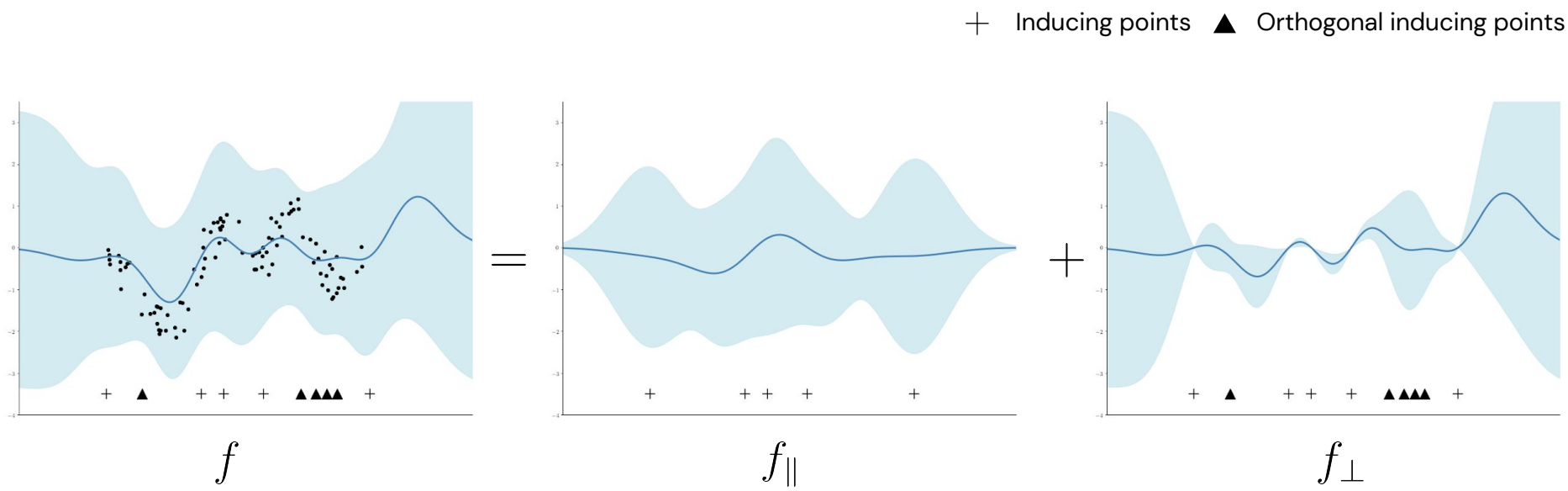
+ Inducing points ▲ Orthogonal inducing points

Posterior Approximation during Training



N=100, M=5+5, Minibatch Size 20

Posterior Approximation during Training



N=100, M=5+5, Minibatch Size 20

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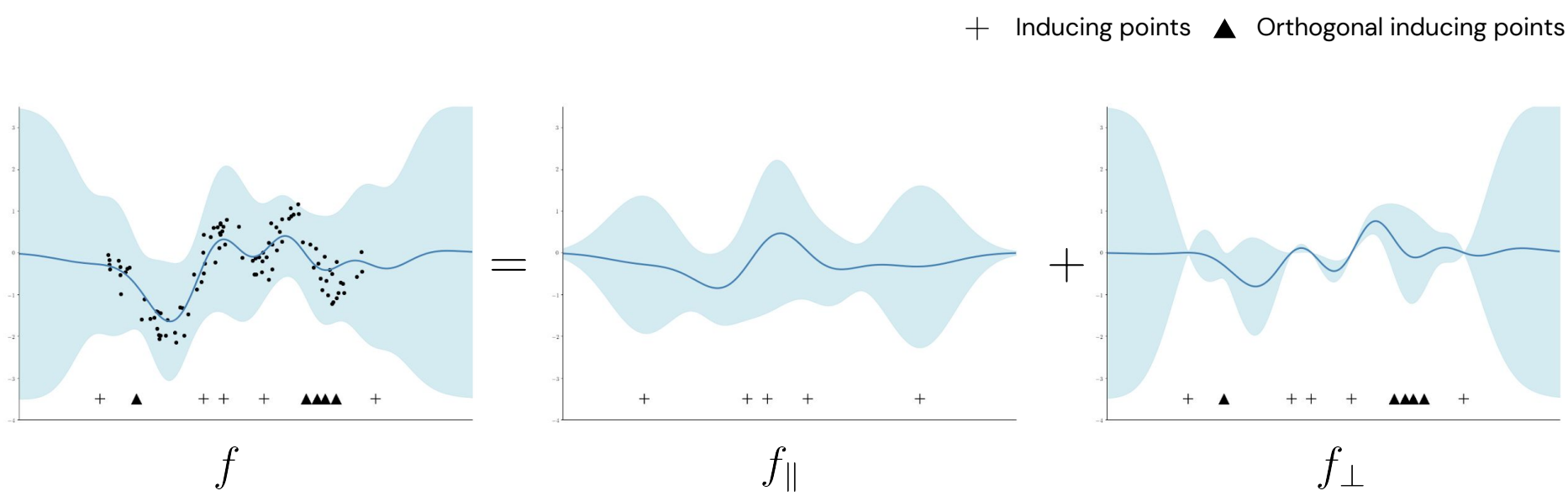

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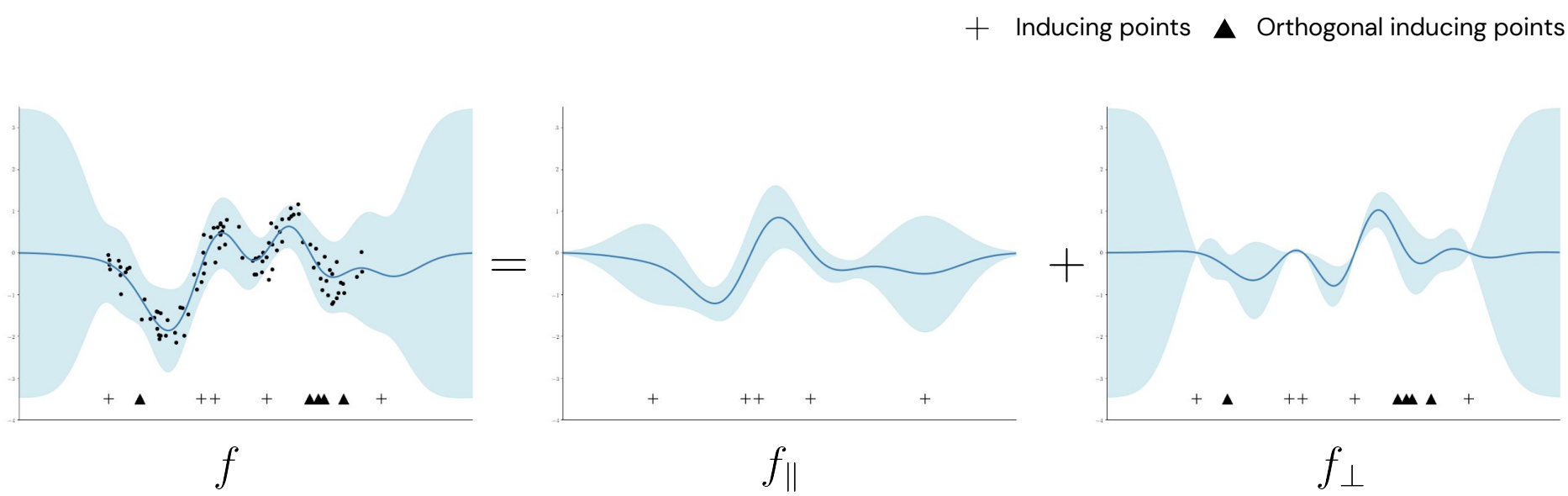

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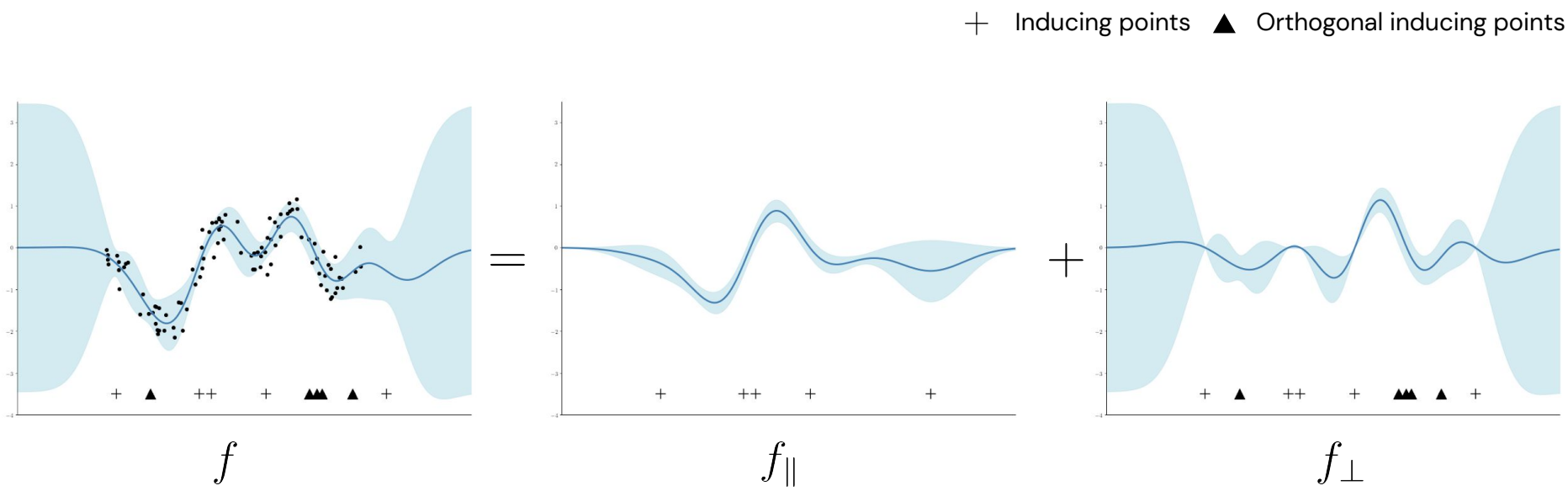
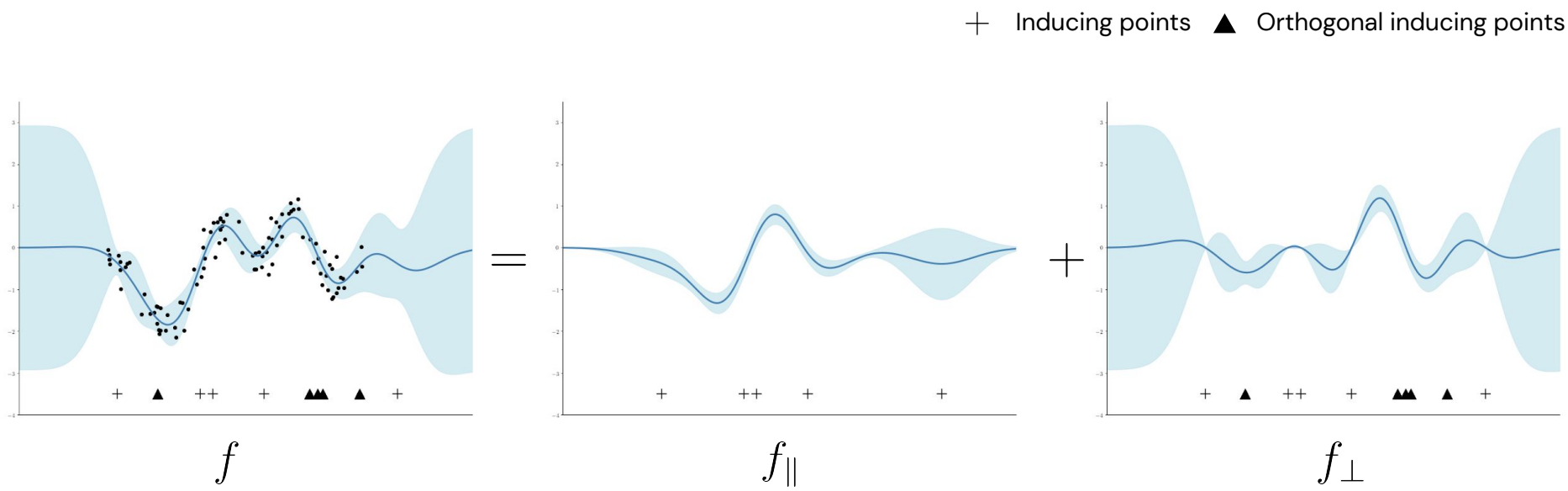


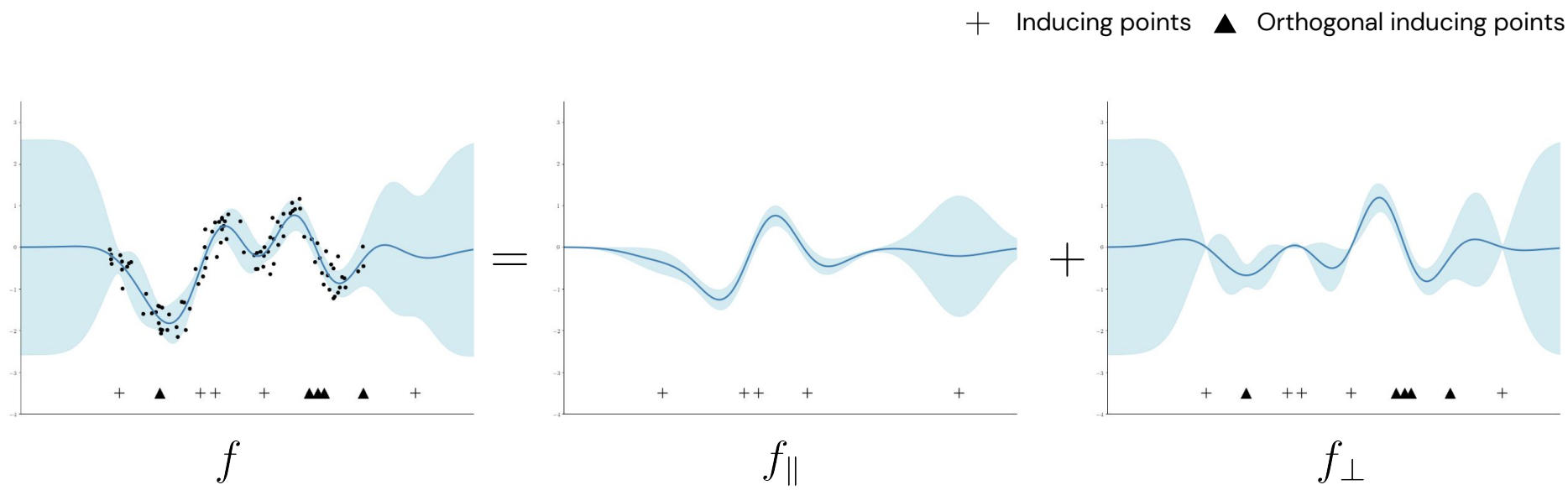
N=100, M=5+5, Minibatch Size 20

Posterior Approximation during Training



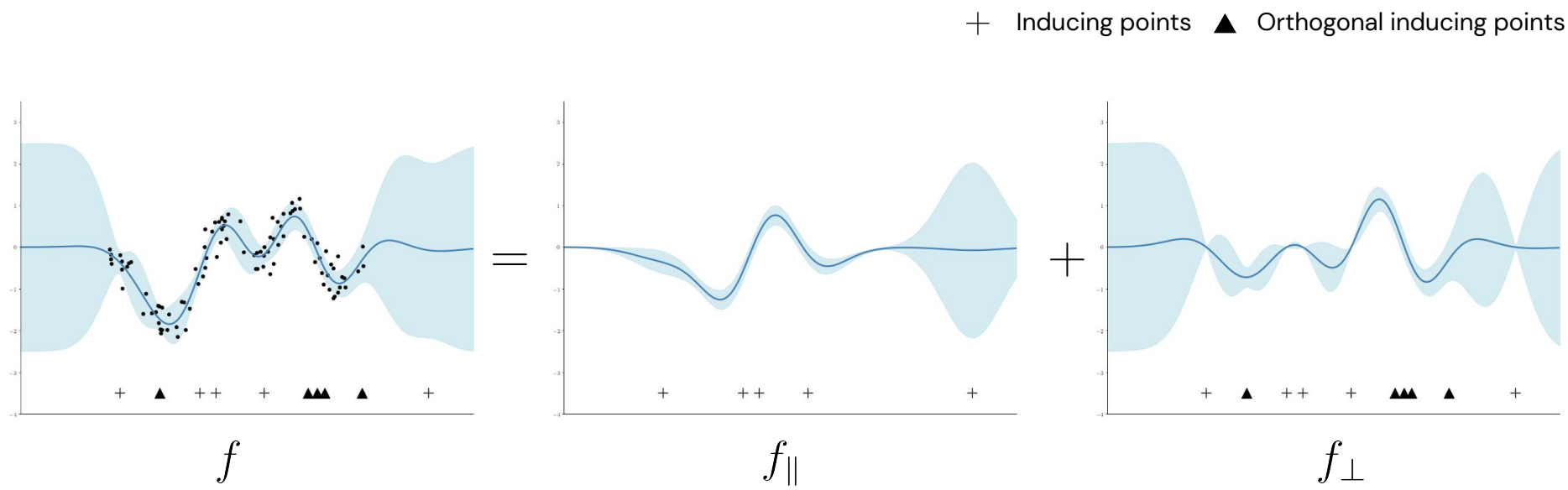
N=100, M=5+5, Minibatch Size 20

Posterior Approximation during Training



N=100, M=5+5, Minibatch Size 20

Posterior Approximation during Training



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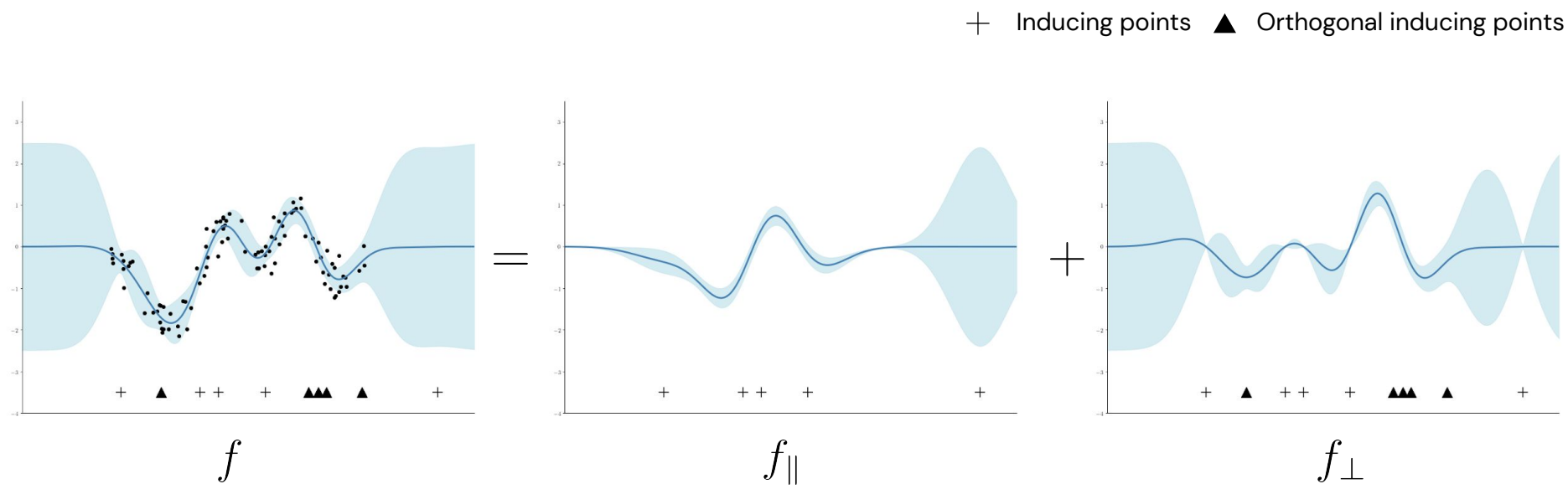

N=100, M=5+5, Minibatch Size 20

Orthogonal Decomposition: Details

$$f = \sum_i \eta_i \varphi_i \qquad g = \sum_j \xi_j \varphi_j$$

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- Define $\langle f, g \rangle = \sum_i \frac{\eta_i \xi_i}{\mu_i}$

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$$\langle f, k(\mathbf{x}, \cdot) \rangle = \left\langle \sum_i \eta_i \varphi_i, \sum_j \mu_j \varphi_j(\mathbf{x}) \varphi_j \right\rangle = \sum_i \frac{\eta_i \cdot \mu_i \varphi_i(\mathbf{x})}{\mu_i} = f(\mathbf{x})$$

Orthogonal Decomposition: Details

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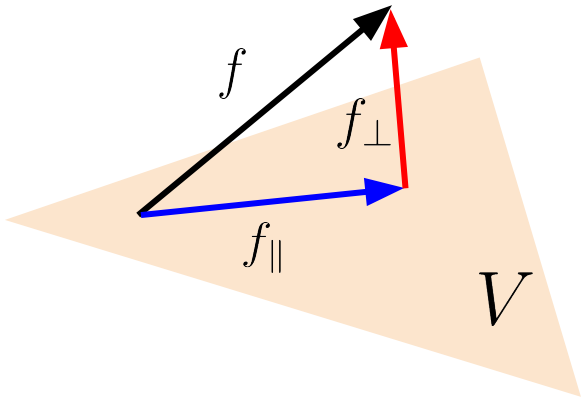


- Define $\langle f, g \rangle = \sum_i \frac{\eta_i \xi_i}{\mu_i}$

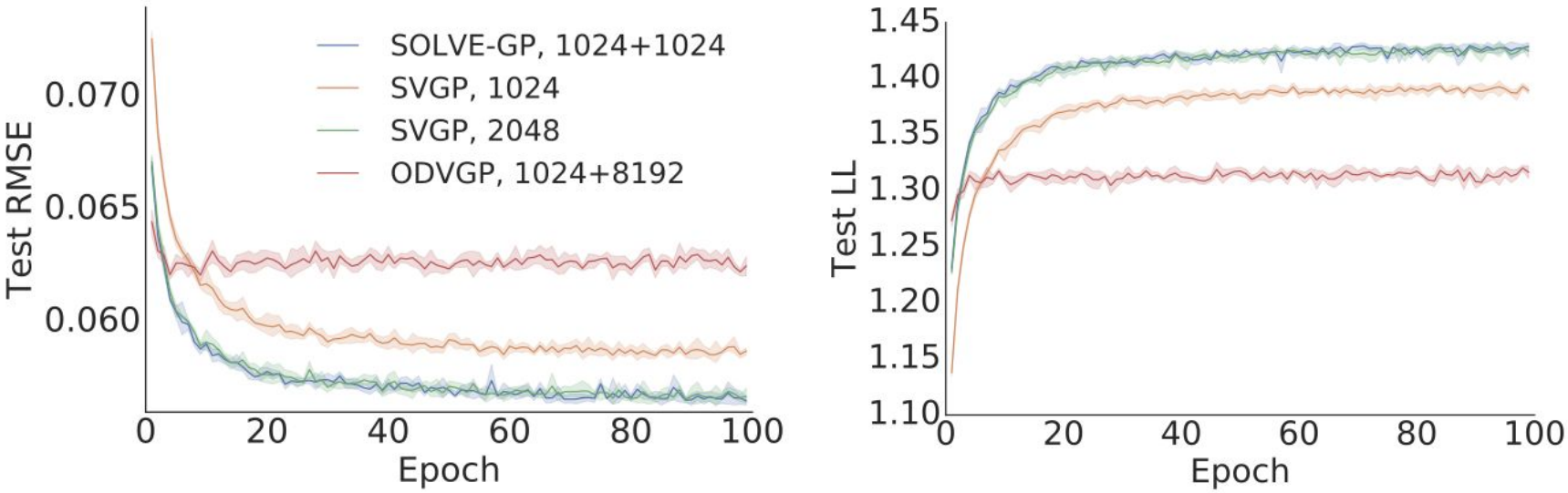
$$\langle f, k(\mathbf{x}, \cdot) \rangle = \left\langle \sum_i \eta_i \varphi_i, \sum_j \mu_j \varphi_j(\mathbf{x}) \varphi_j \right\rangle = \sum_i \frac{\eta_i \cdot \mu_i \varphi_i(\mathbf{x})}{\mu_i} = f(\mathbf{x})$$

- Solve the projections to the subspace:

$$\langle f, f_\parallel \rangle = \langle f, g \rangle \quad \forall g \in V \quad \Longrightarrow \quad f_\parallel = k(\cdot, \mathbf{Z}) \mathbf{K}_{\mathbf{ZZ}}^{-1} \mathbf{u}$$

$$V = \left\{ \sum_{i=1}^{M} a_i k(\mathbf{z}_i, \cdot) \;\middle|\; \mathbf{a} \in \mathbb{R}^M \right\}$$

Regression



HouseElectric (N=1,311,539, D=9)

Classification - CIFAR 10

Convolutional GPs[1]

new SOTA: 64.6% -> 68.2%

Methods	SVGP		SOLVE-GP	SVGP
M	1K	1.6K	1K+1K	2K*
Test LL	-1.59	-1.54	**-1.51**	**-1.48**
Test Acc	66.07%	67.18%	**68.19%**	68.06%
Time /iter	0.241	0.380	0.370	0.474

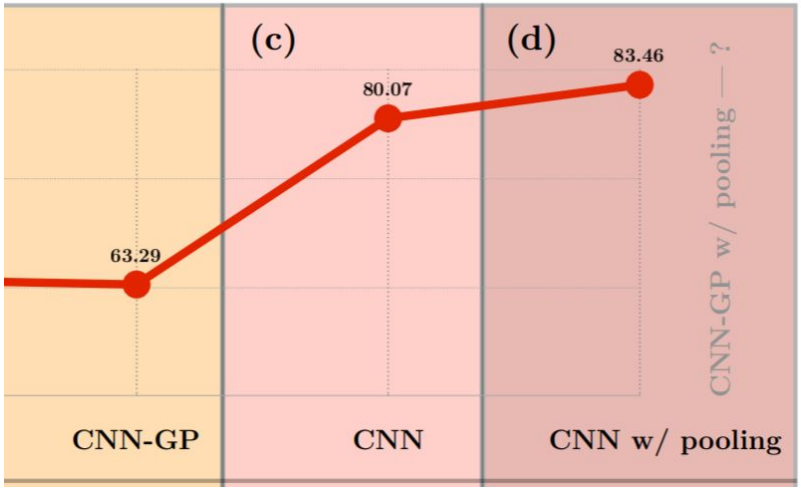
Deep Convolutional GPs[2]

new SOTA: 76.2% -> 80.3%

Methods	SVGP	SOLVE-GP	SVGP
M	384, 384, 1K	384+384, 384 +384, 1K+1K	768,768, 2K*
Test LL	-0.88	**-0.79**	-0.82
Test Acc	78.76%	**80.3%**	**80.33%**
Time /iter	0.418	0.752	1.246

[1,2] Neither neural network components nor data augmentation is used.

Why is 80% interesting?



Radford Neal's NN-as-GP kernel
CNN-GP vs. CNN
(Novak et al., 2019)

Neural Tangent Kernel
CNTK vs. CNN
(Arora et al., 2019)

Depth	CNN-GAP	CNTK-GAP
3	57.96%	70.47%
4	80.58%	75.93%
6	80.97%	76.73%
11	75.45%	77.43%
21	81.23%	77.08%

Conclusion

- Eigenfunctions are powerful tools. They can be used for
  - nonparametric estimation of score functions.
  - analyzing orthogonal decomposition of GPs.
- Functionally “orthogonal” learning
  - Inducing points are feature detectors.
  - Feature detectors need to be functionally “orthogonal” to be efficient.
  - Implications for ML methods in general?

Main Refs:
A Spectral Approach to Gradient Estimation for Implicit Distributions. Shi, Sun, Zhu, ICML 18
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