Stochastic Gradient Descent for Gaussian Processes

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Computational and Biological Learning
DEPARTMENT OF ENGINEERING

UNIVERSITY OF CAMBRIDGE

Why do we need Uncertainty Estimates?

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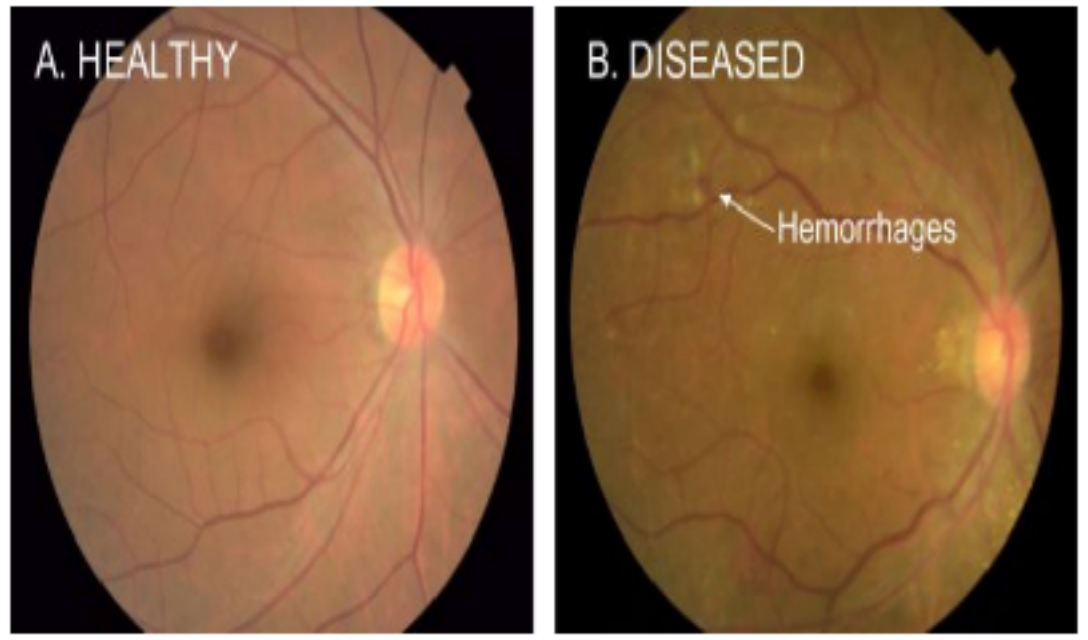
- Deep Learning is massively scalable and extremely powerful at modelling data



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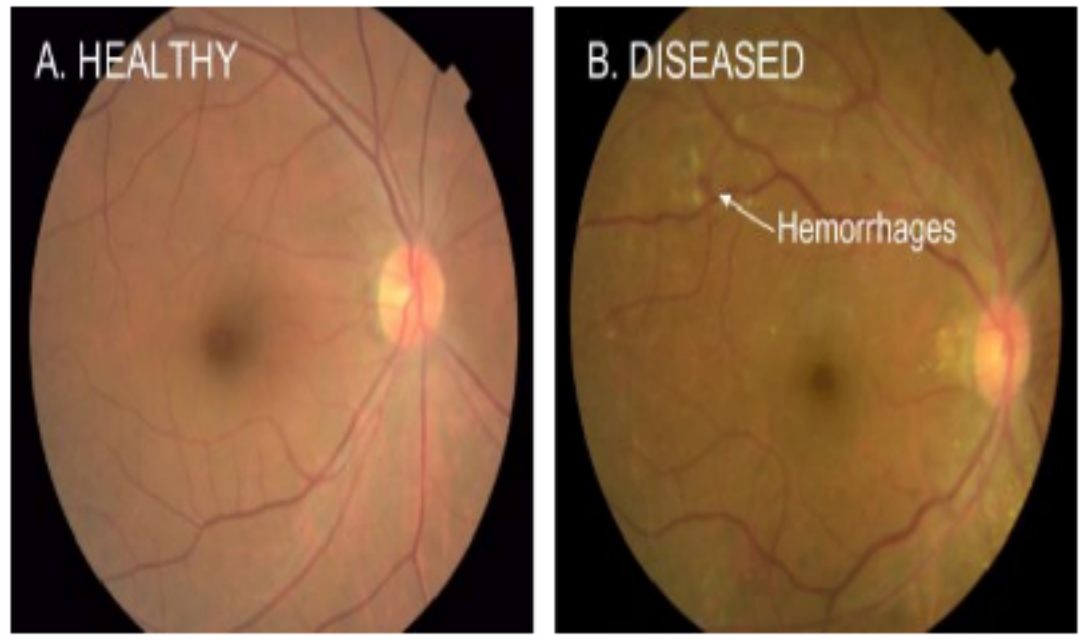

Low Degree of Belief on Prediction

Defer predictions

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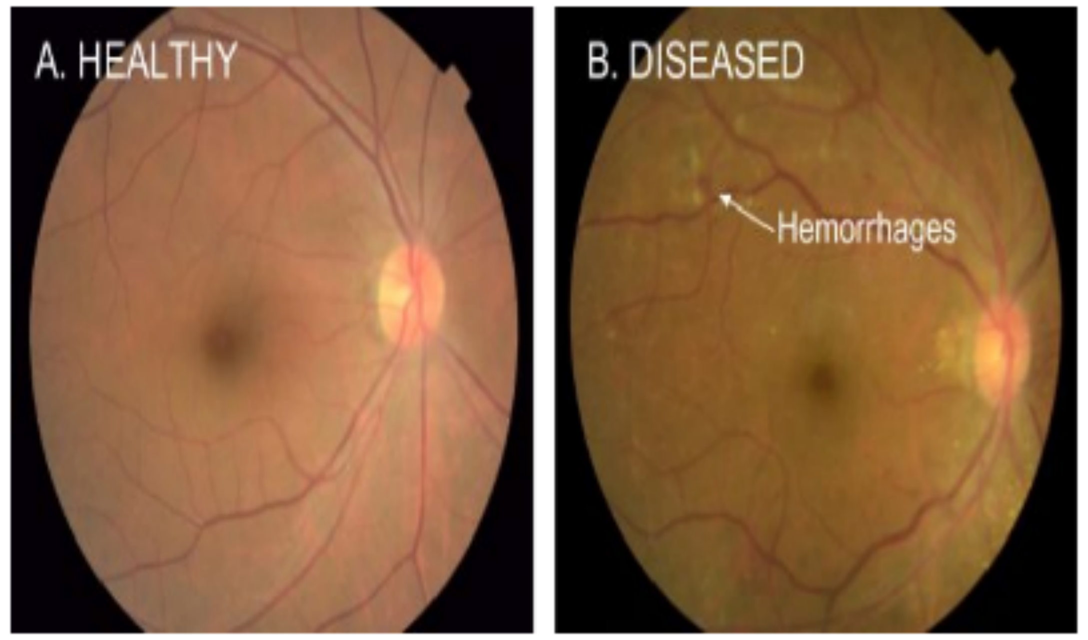

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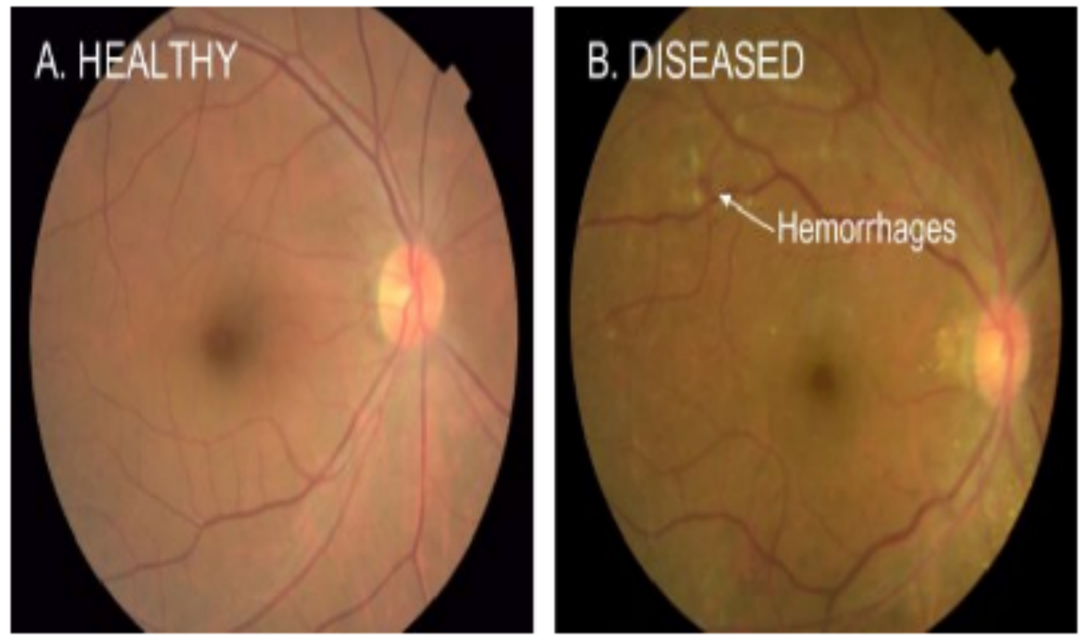

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If we use numerical values to model "uncertainty", simple axioms on these uncertainties follow the laws of probability => Bayes' Rule

[Cox, 1946], [Jaynes, 2003]

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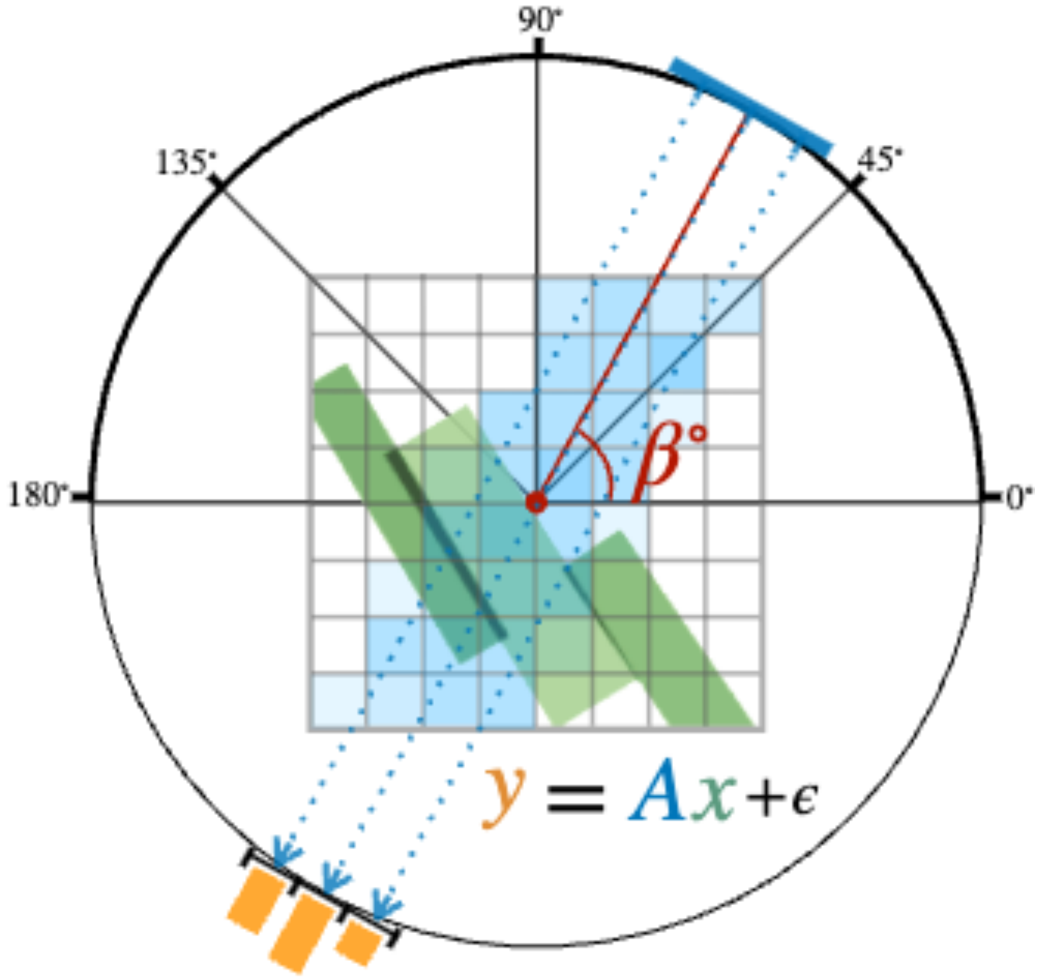

Image

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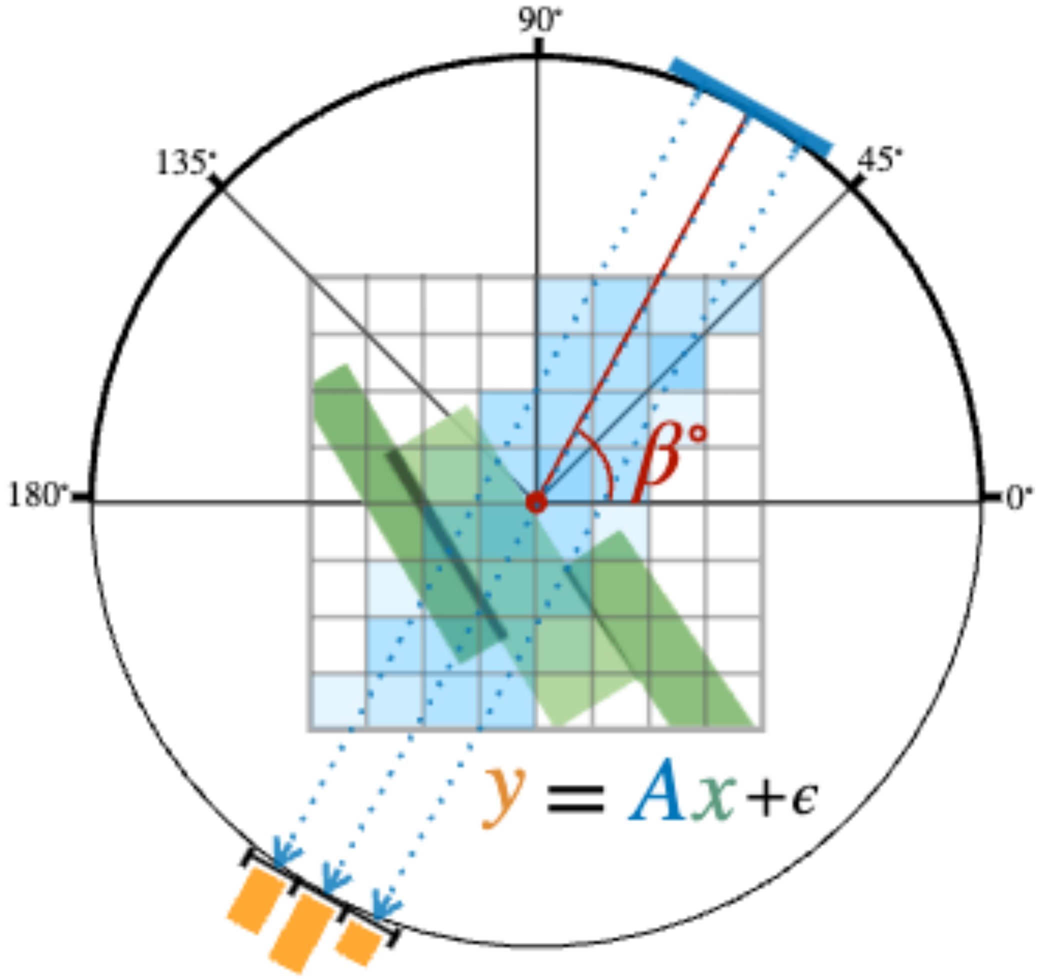

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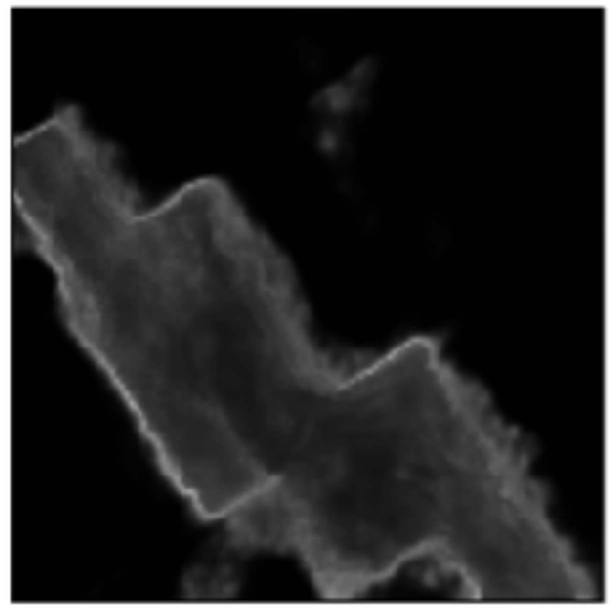

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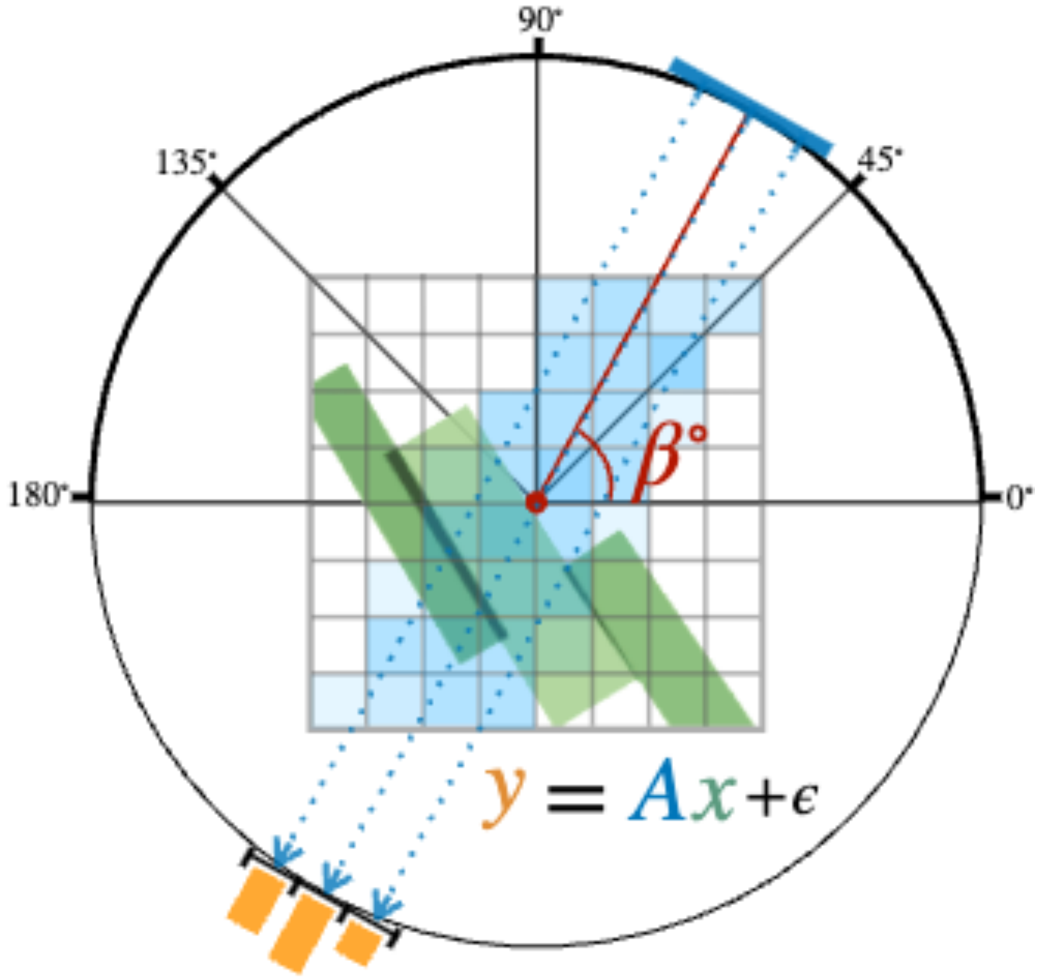

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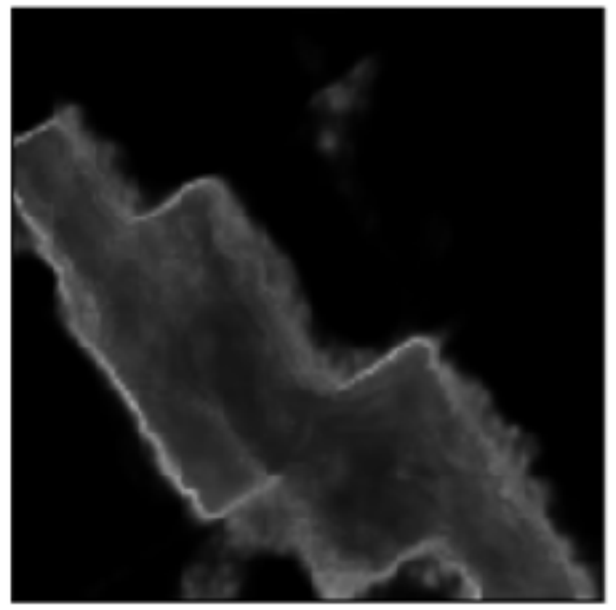

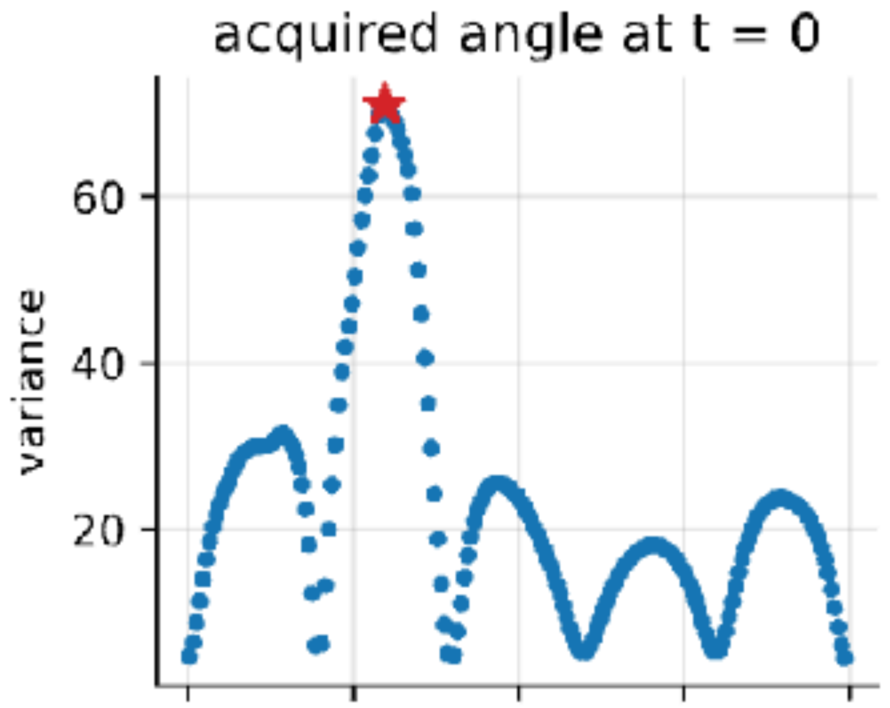

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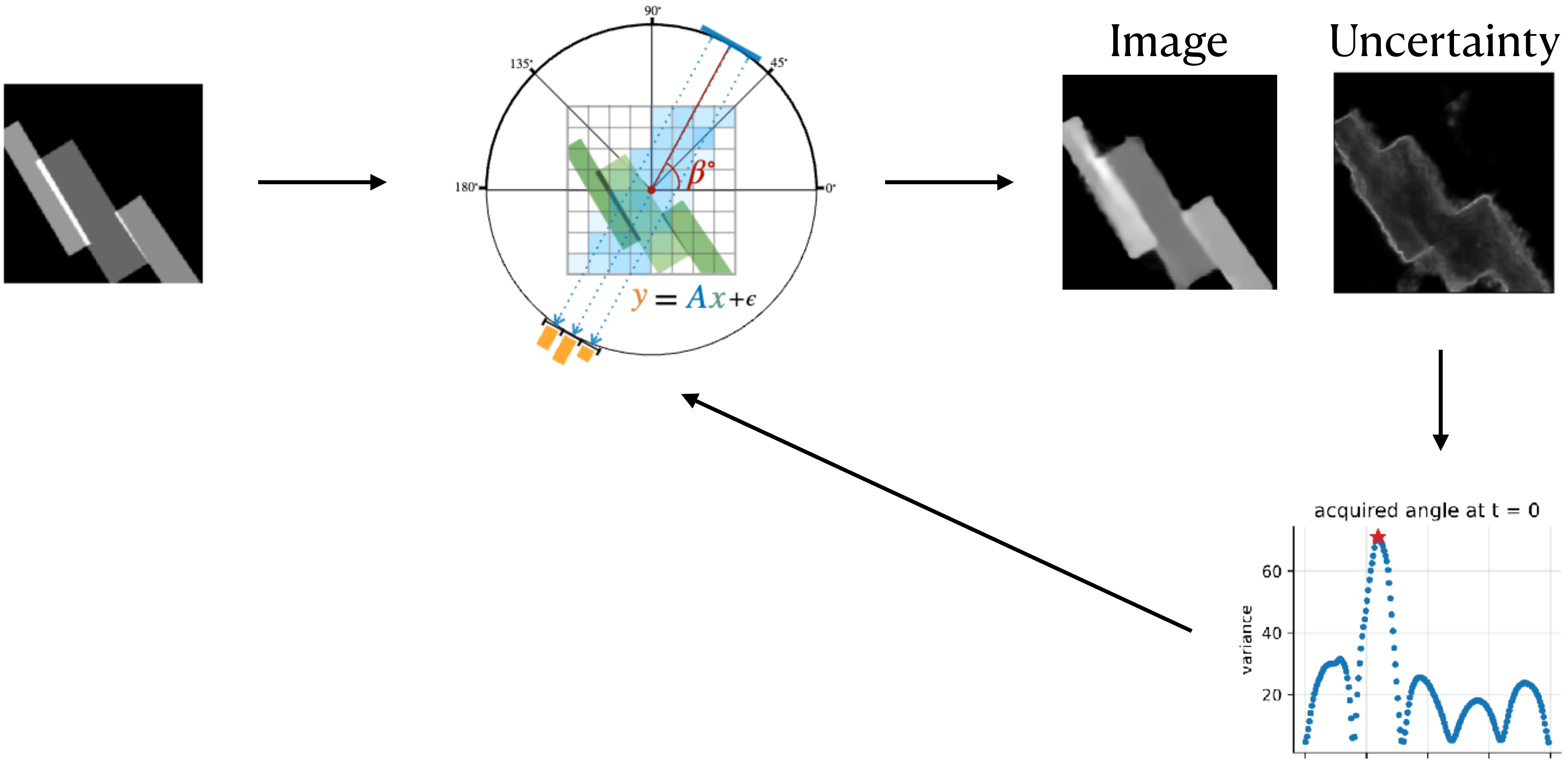

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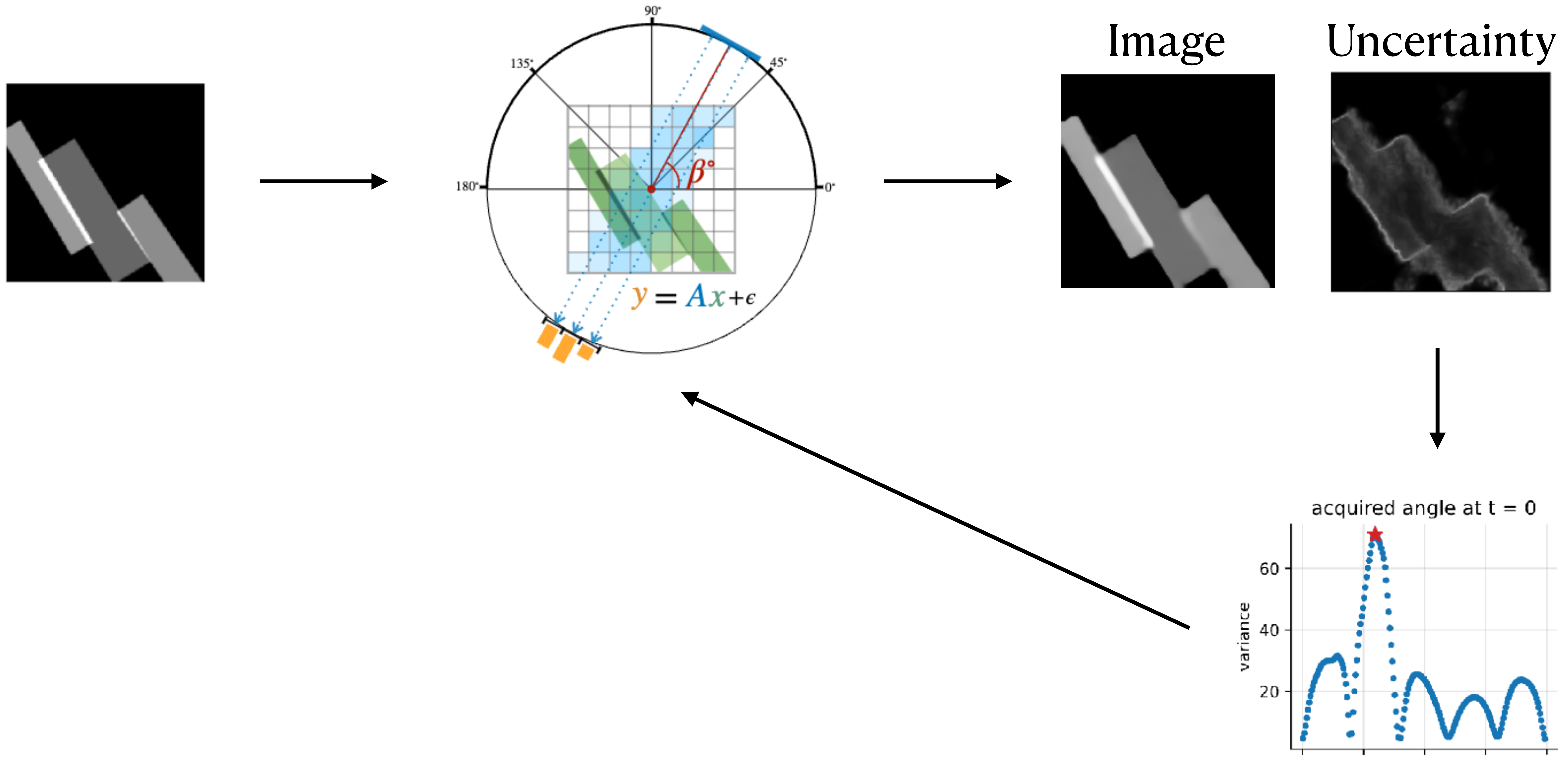

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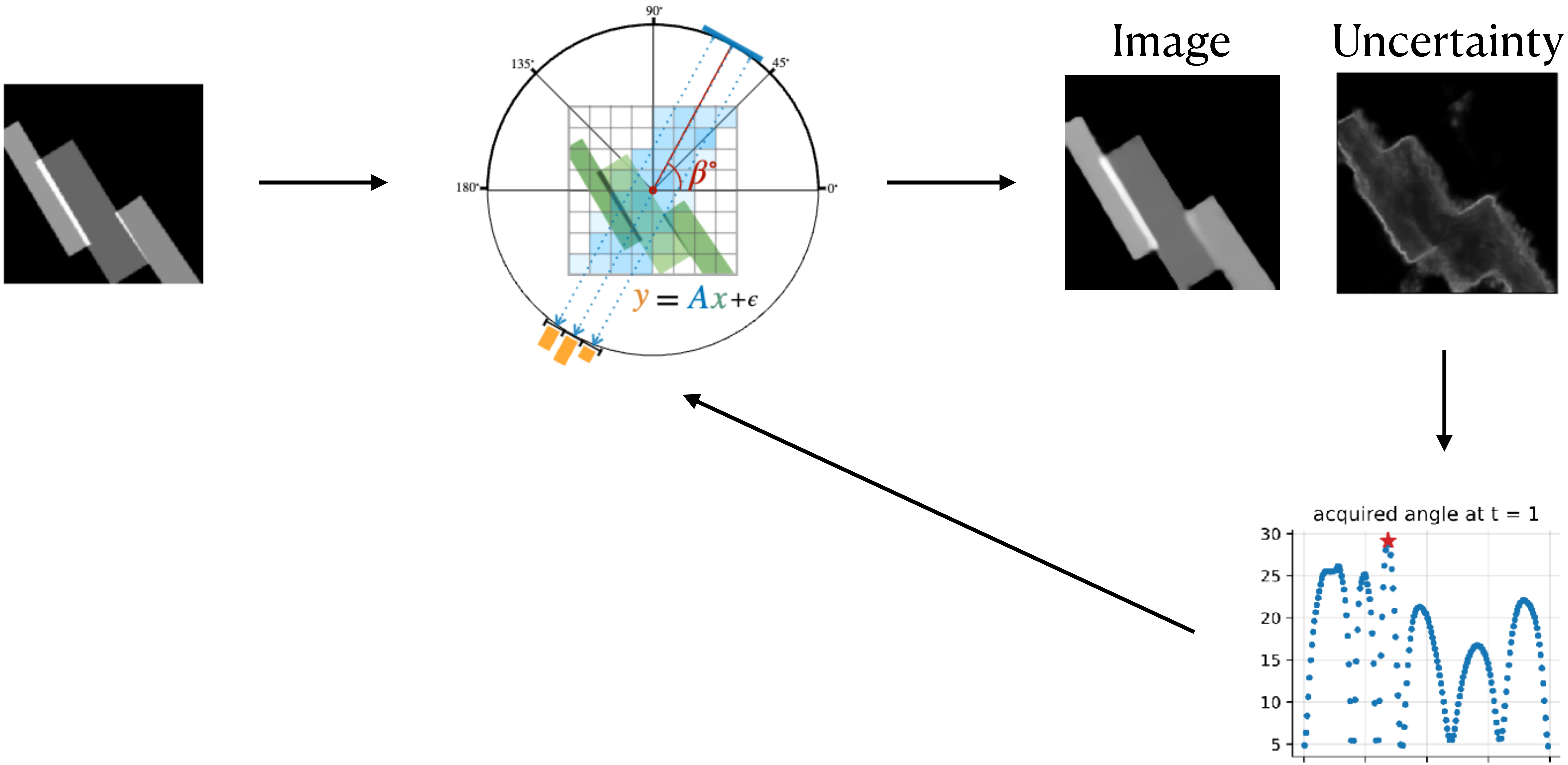

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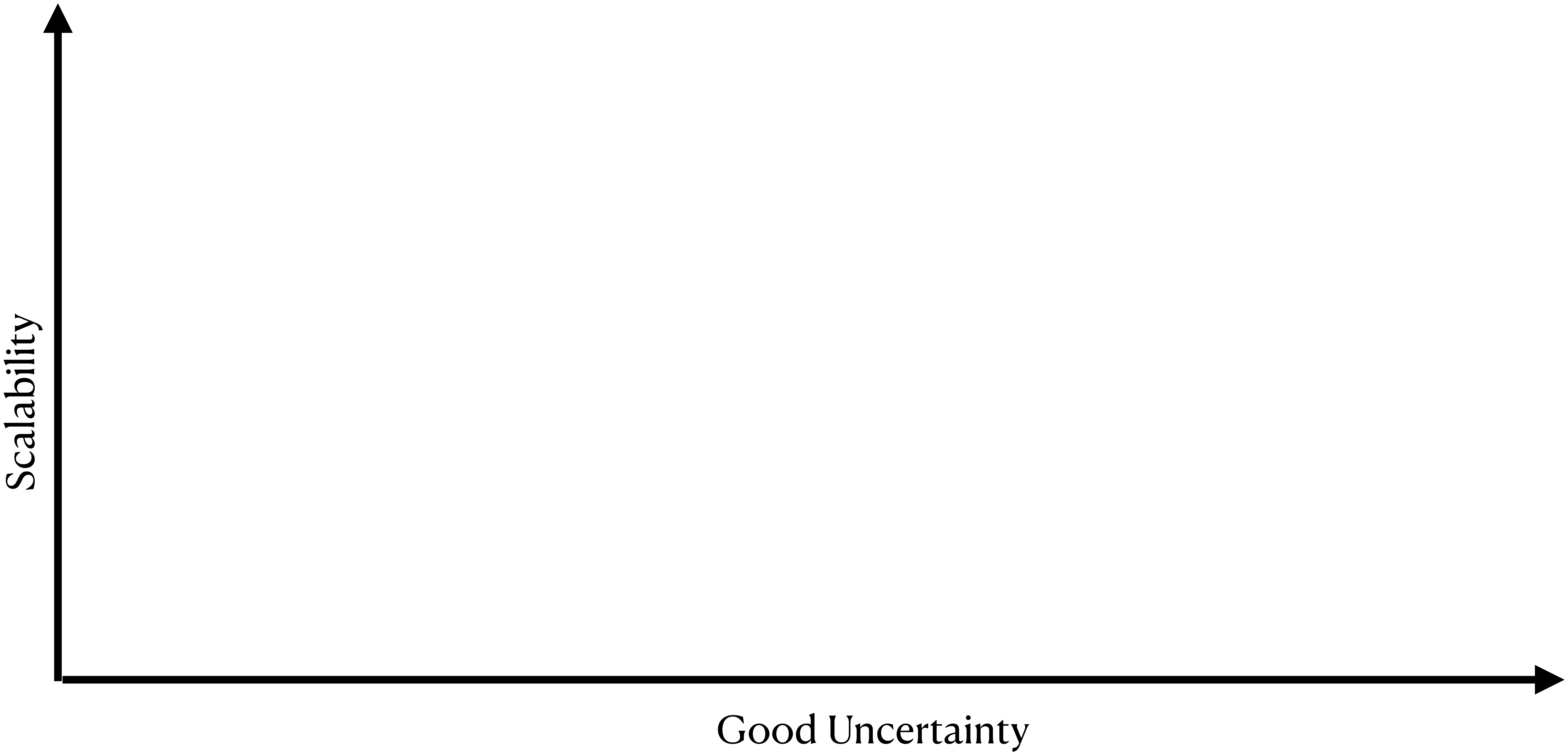

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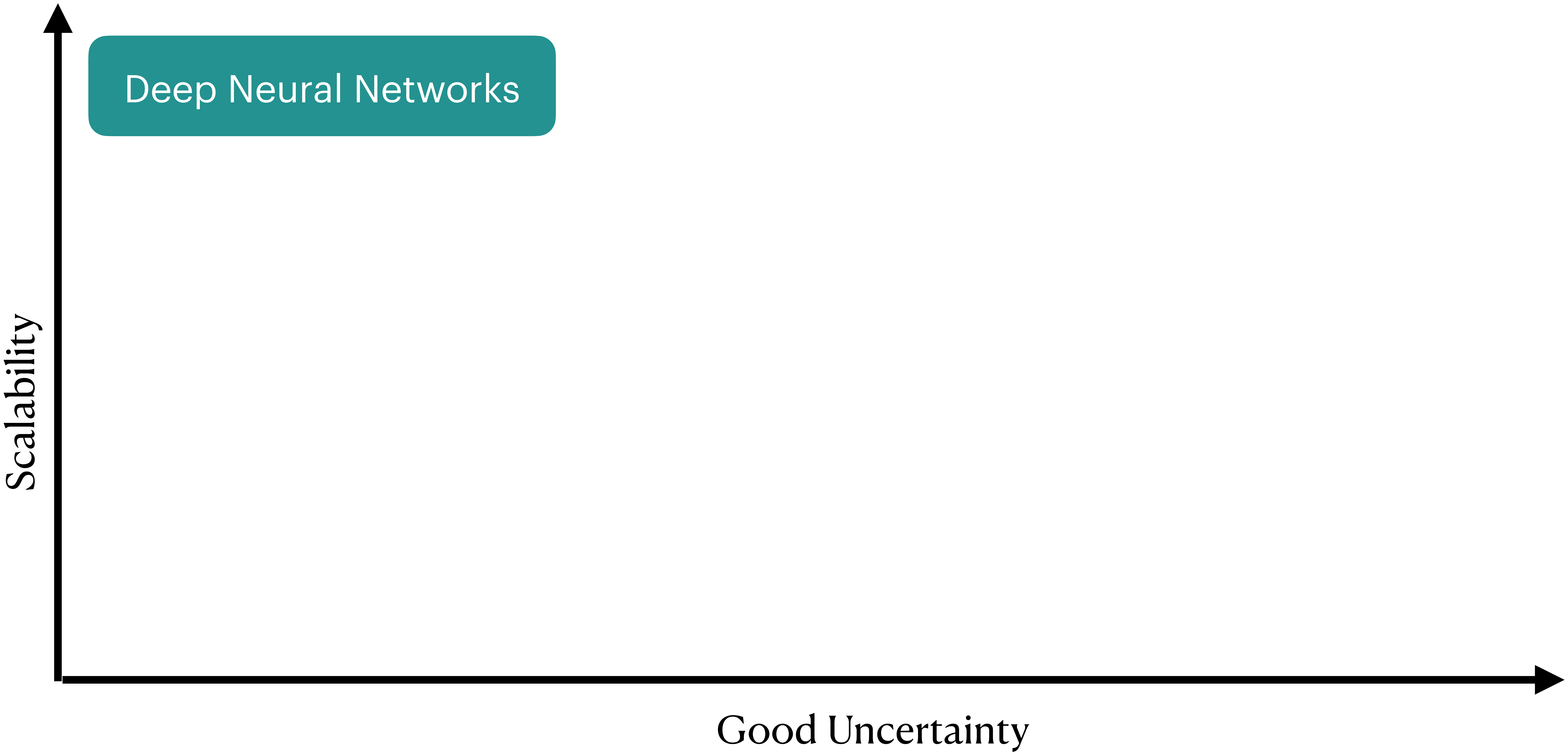

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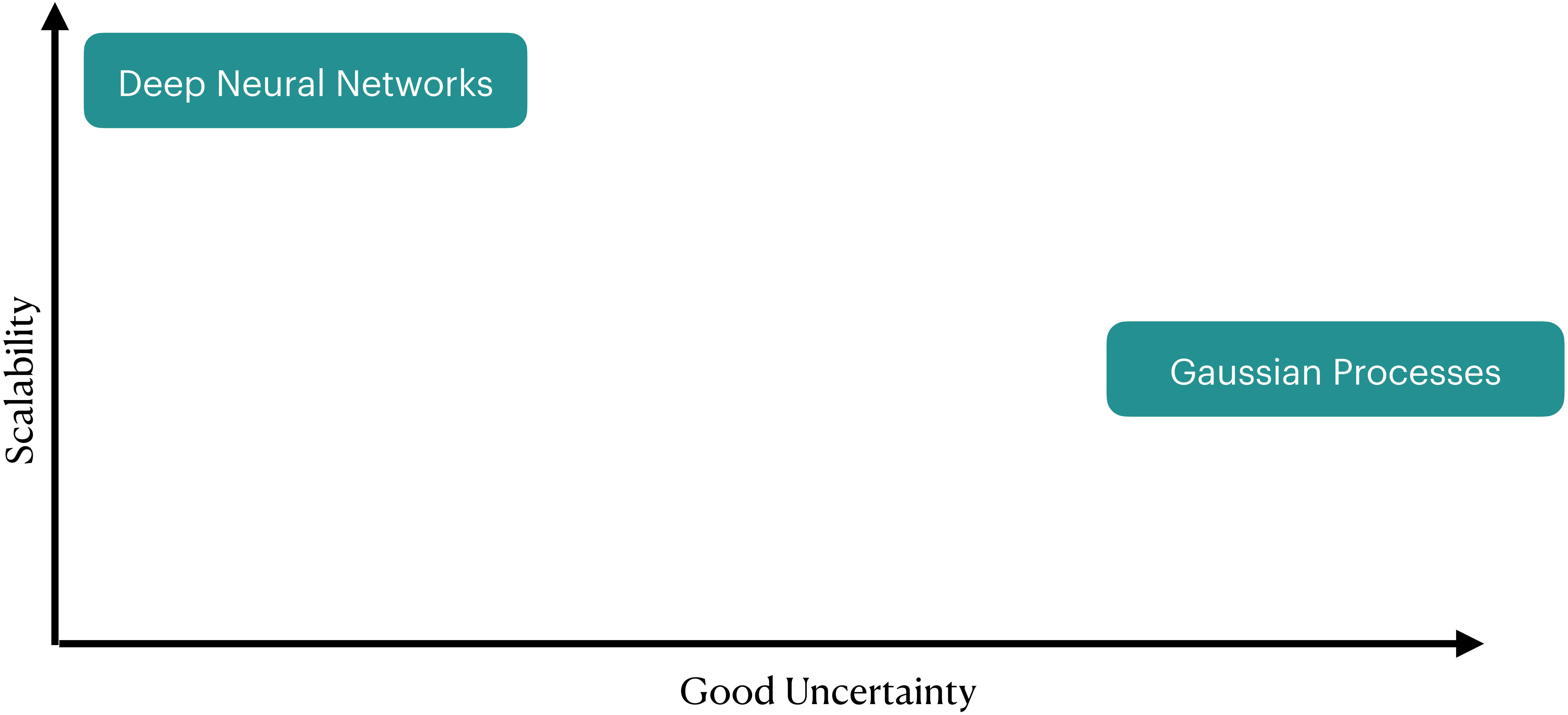

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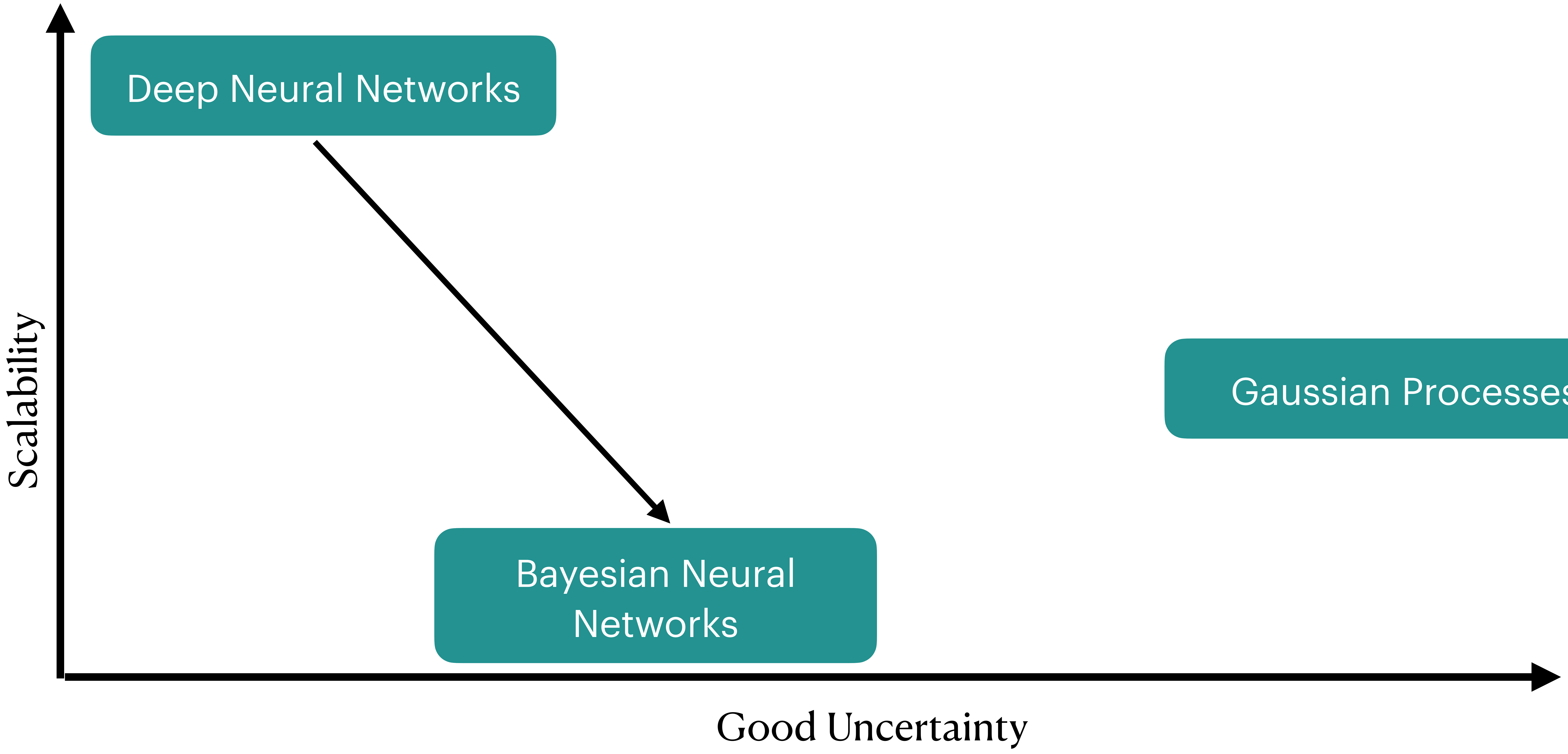

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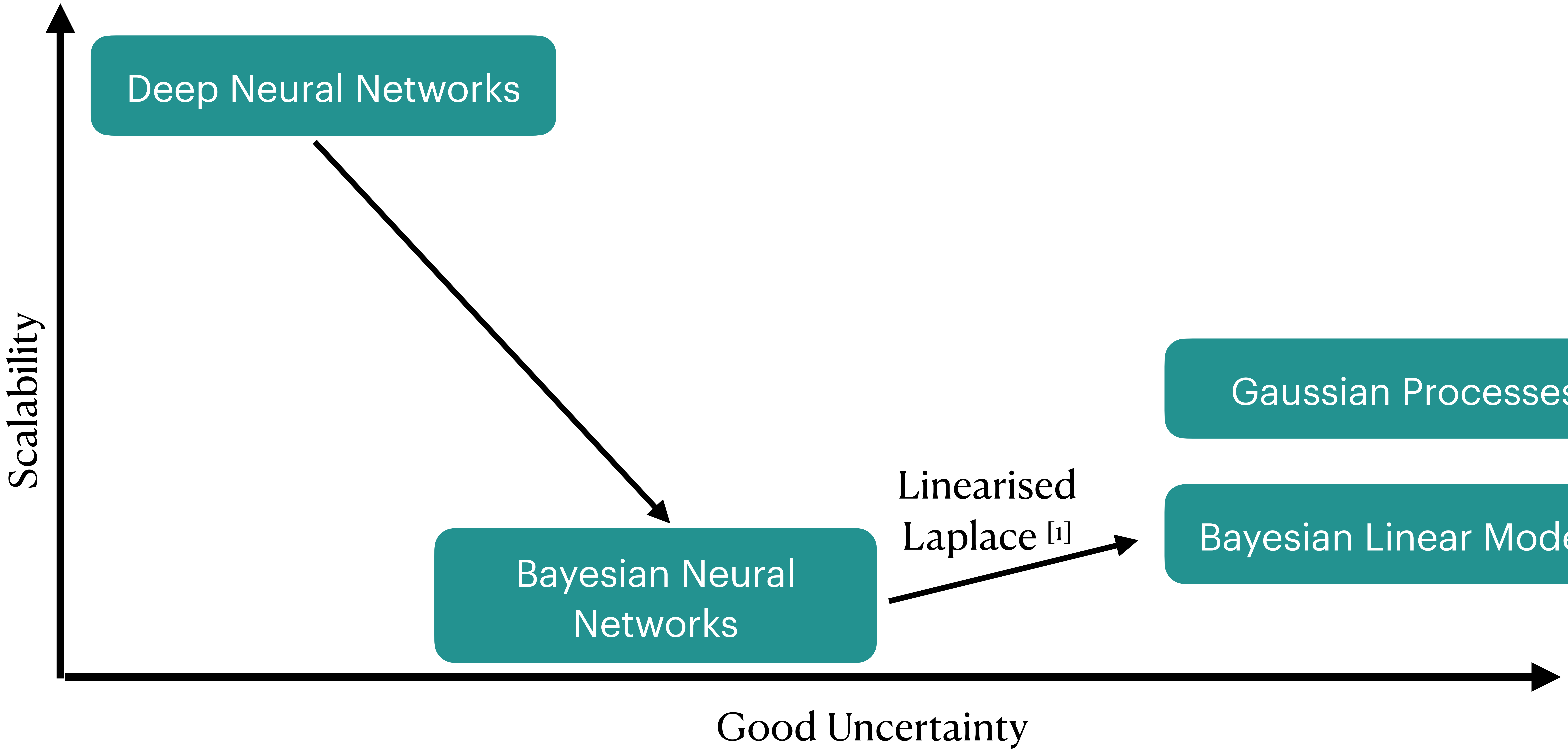

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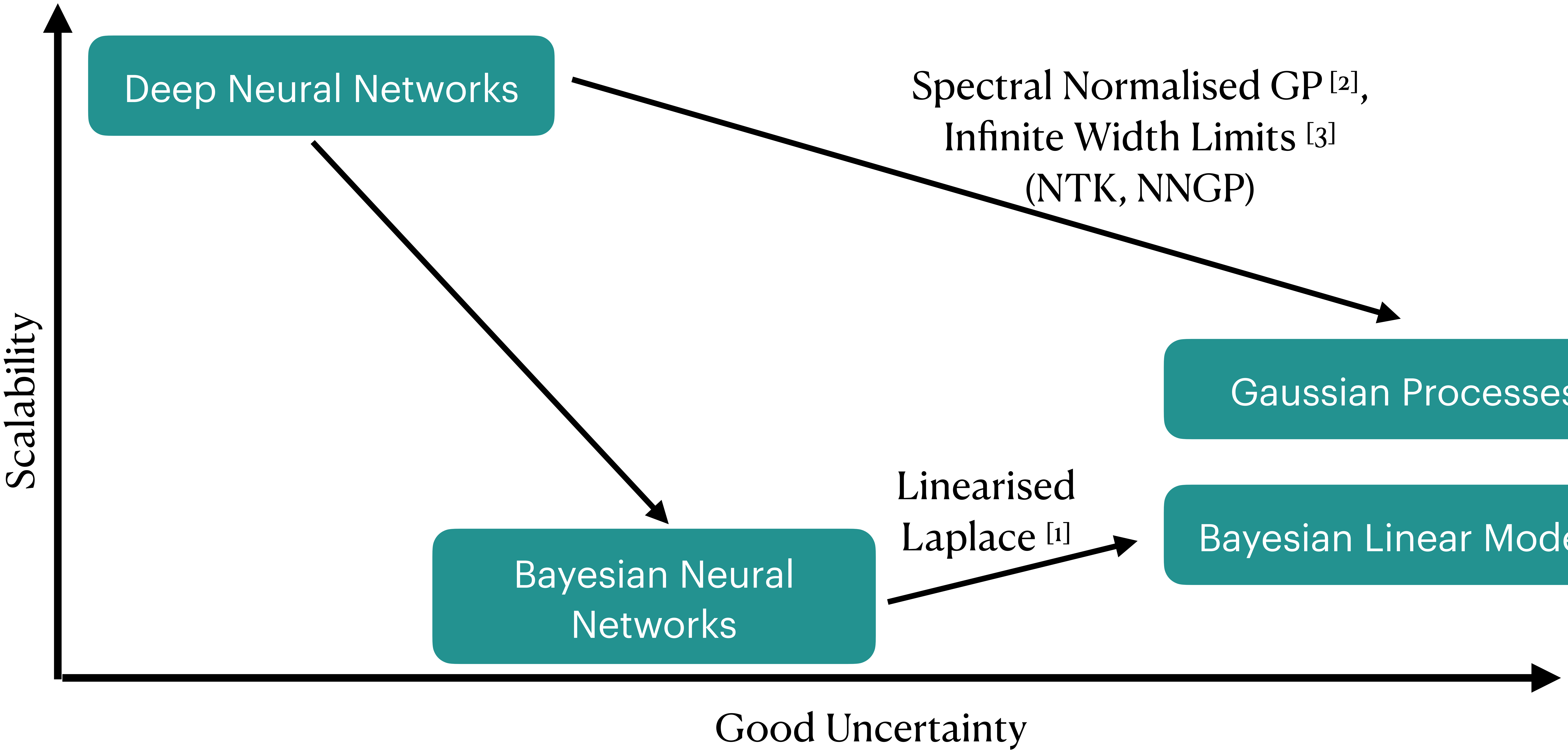

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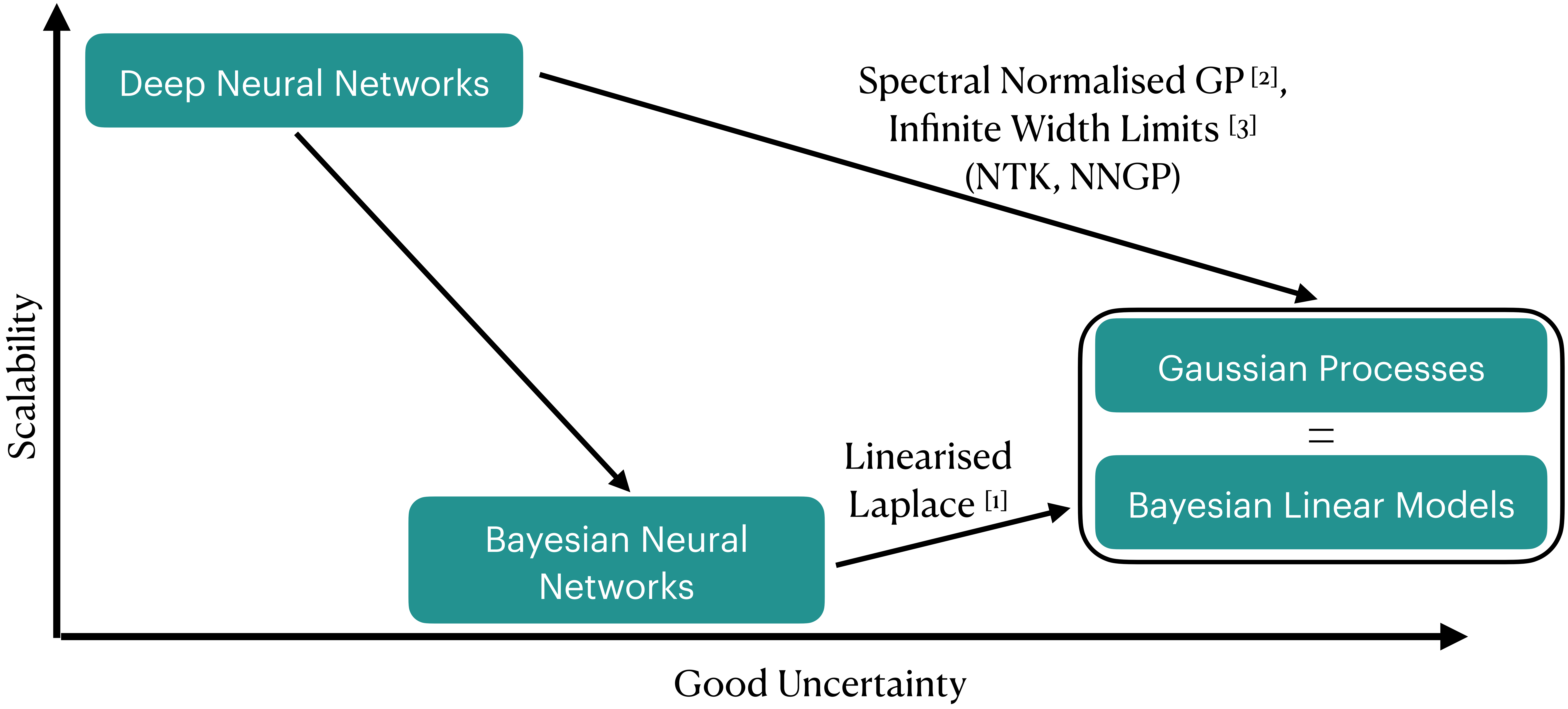

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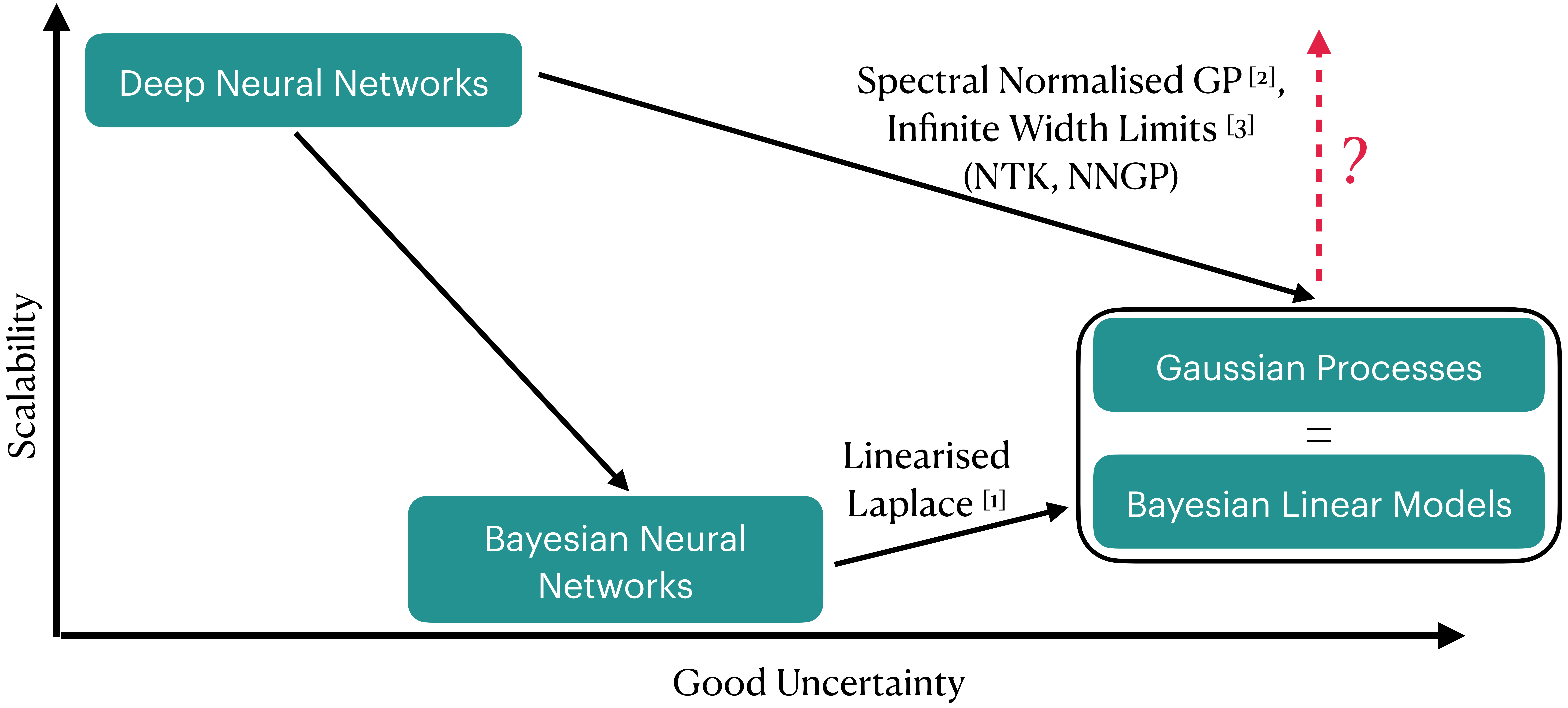

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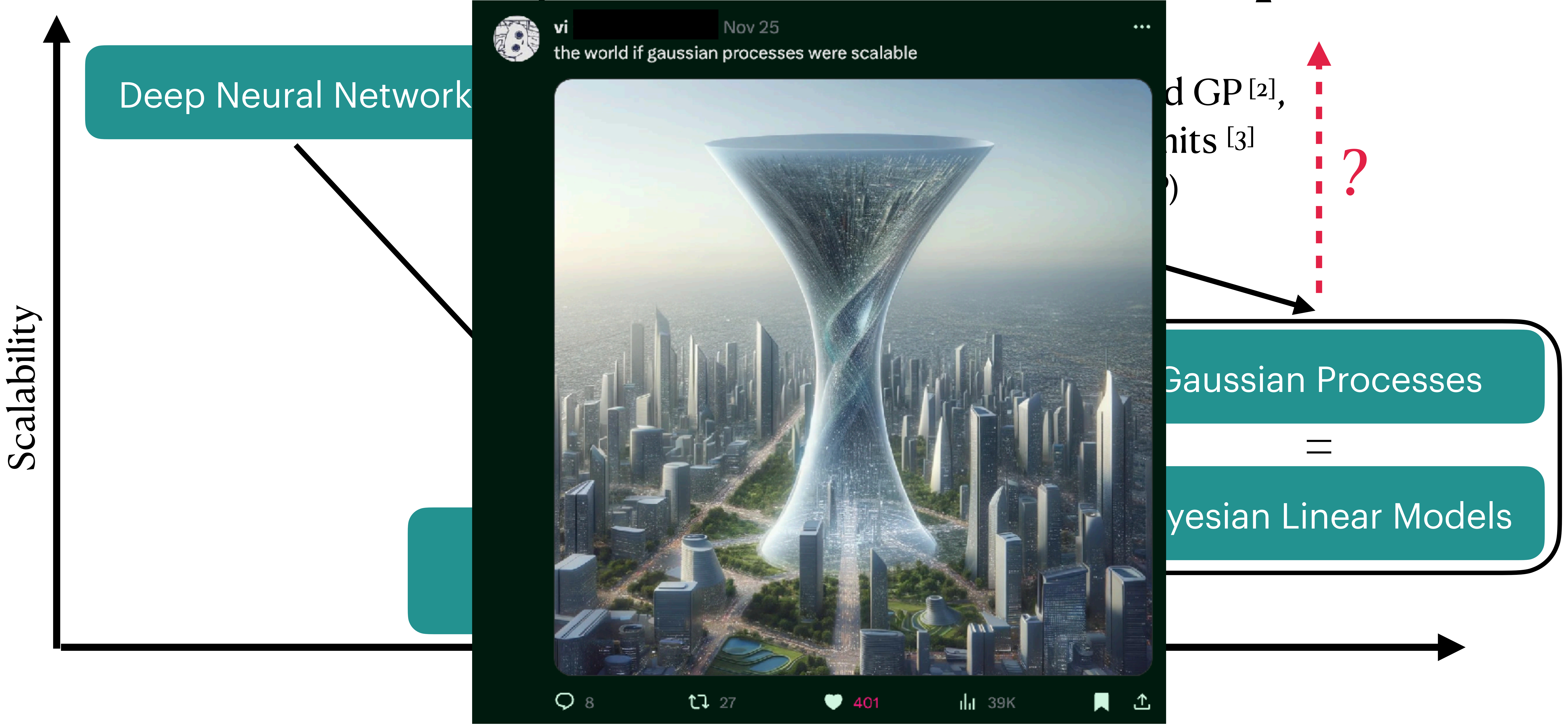

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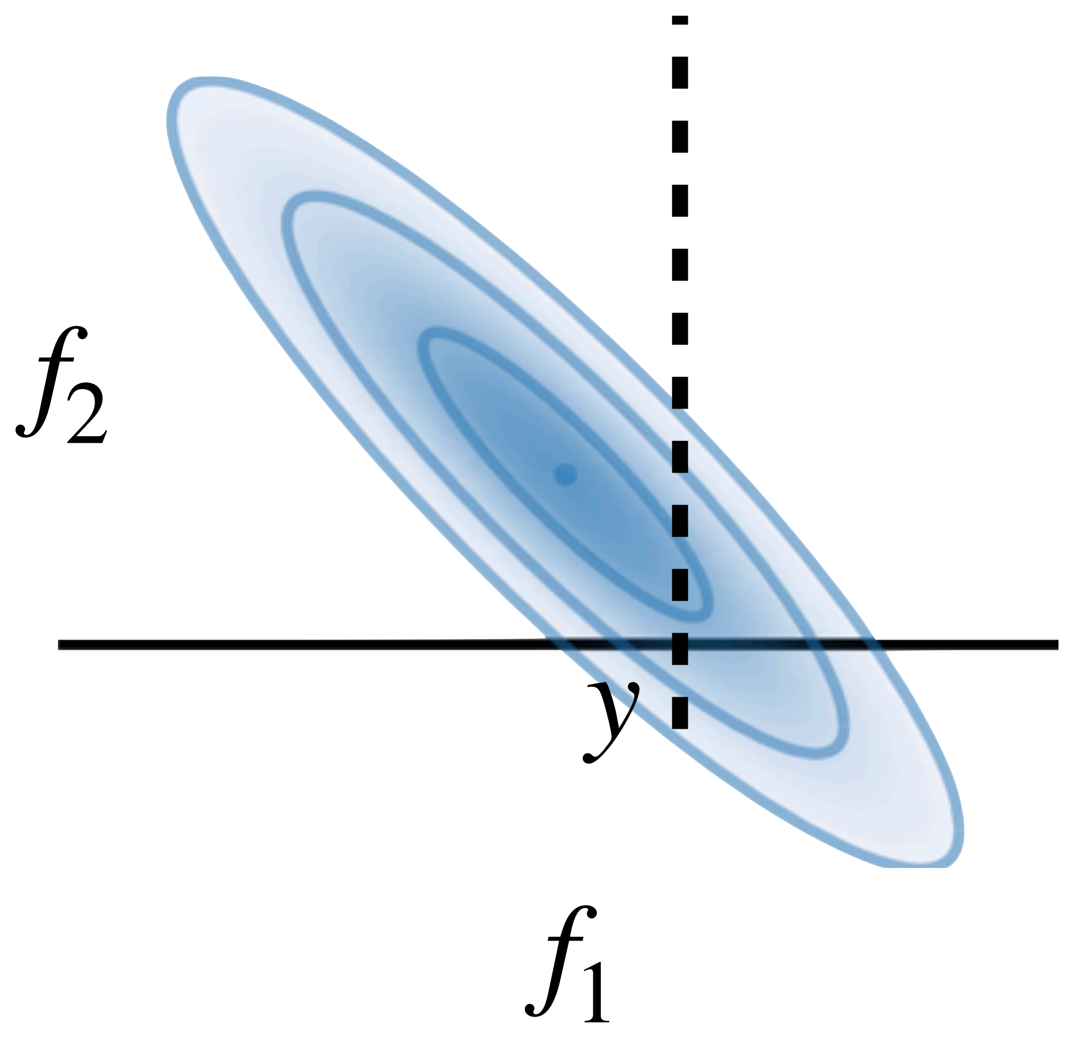

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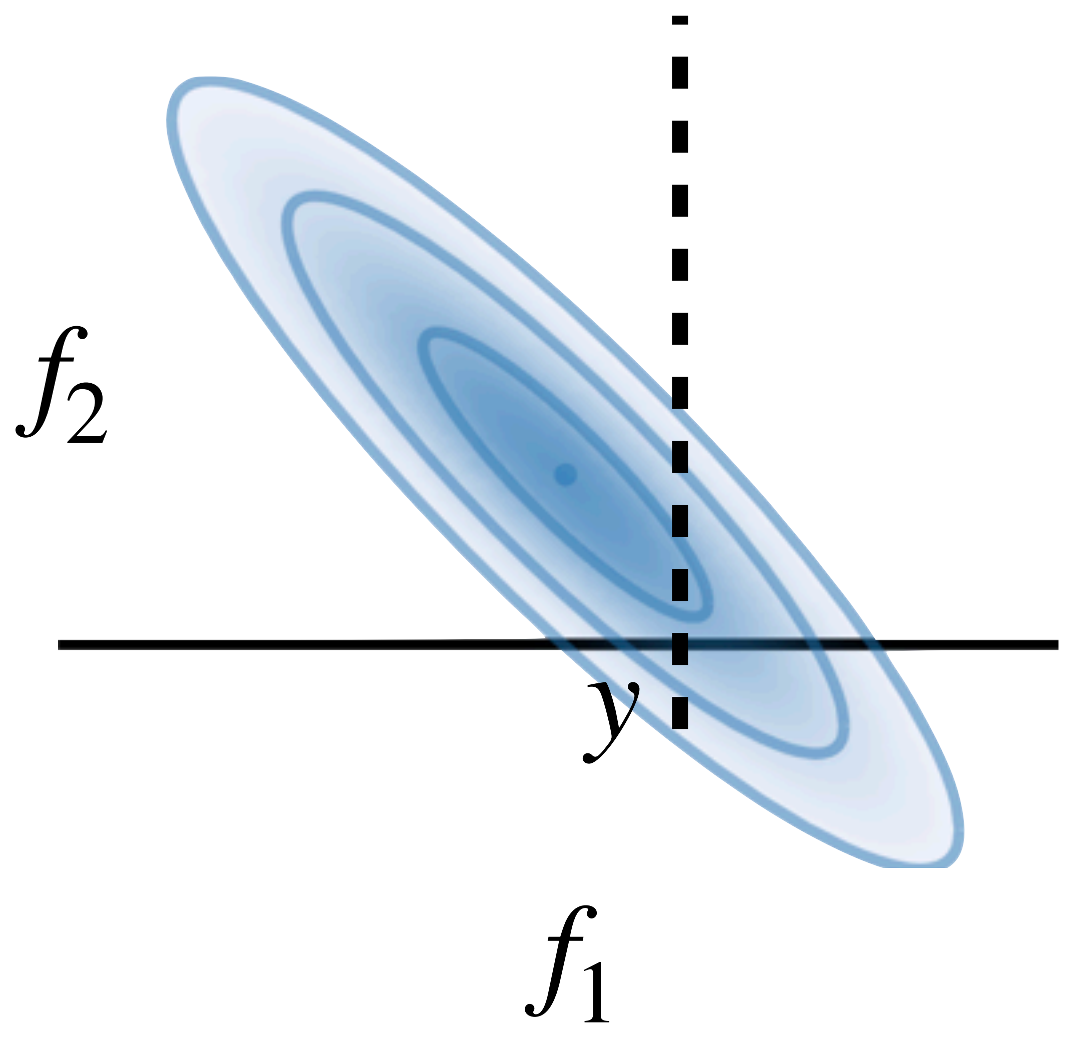

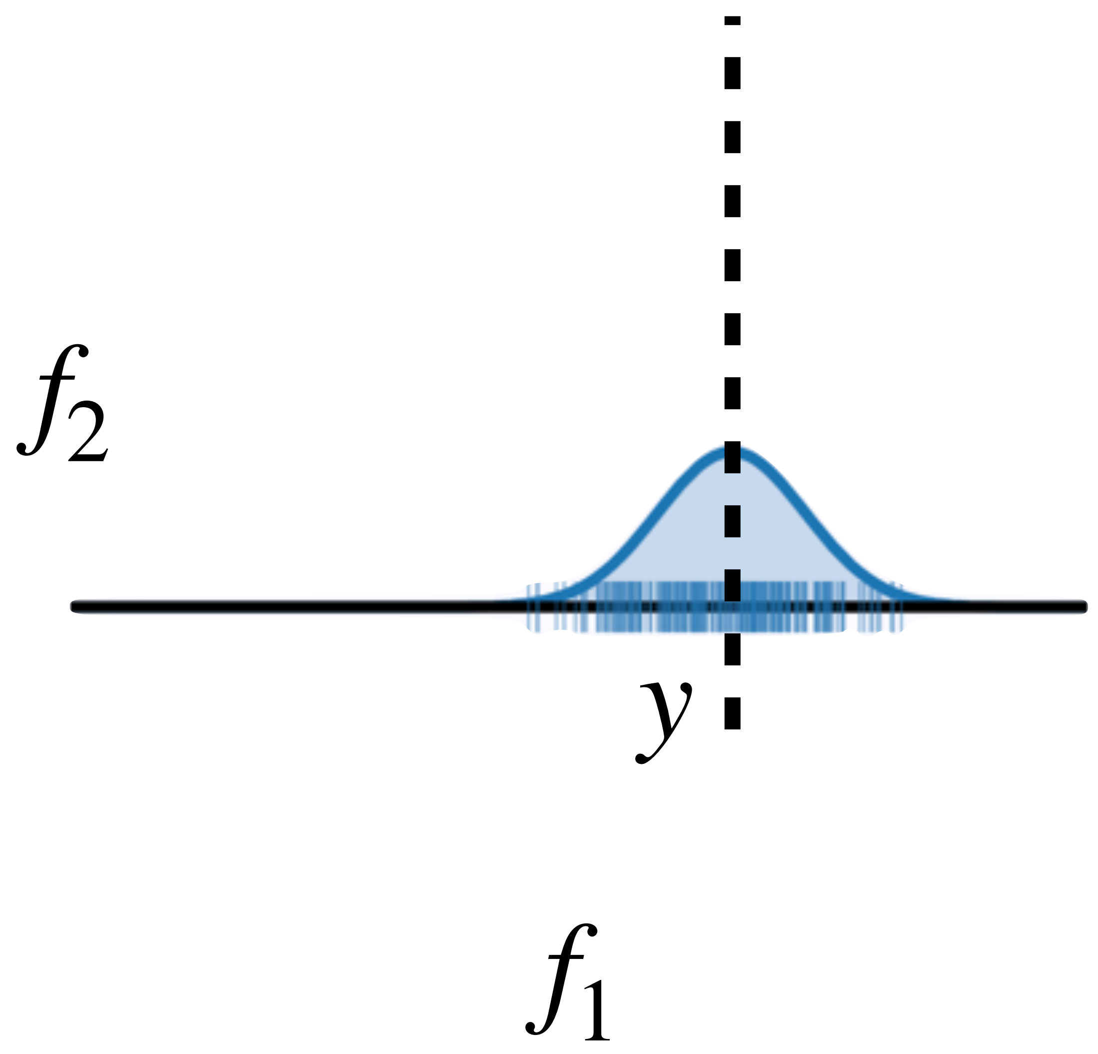

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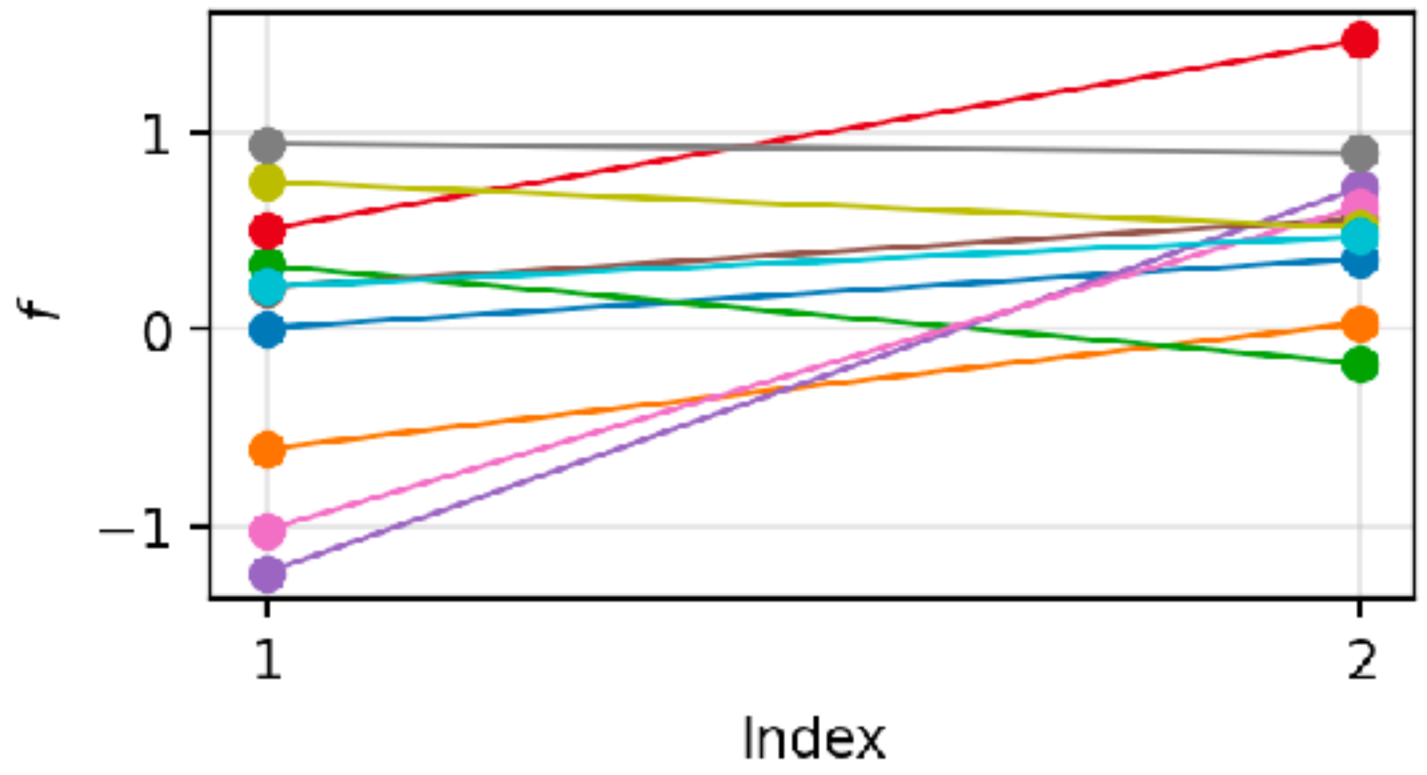

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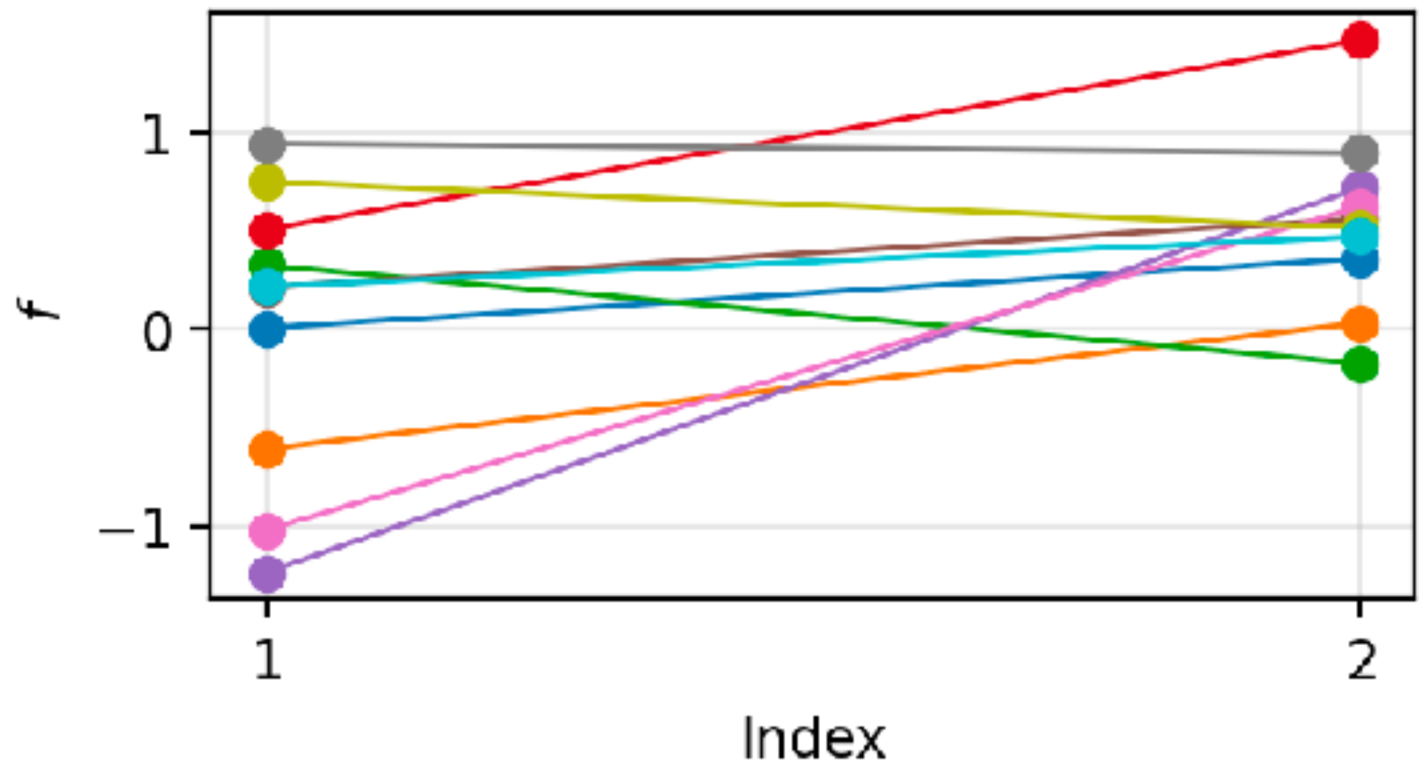

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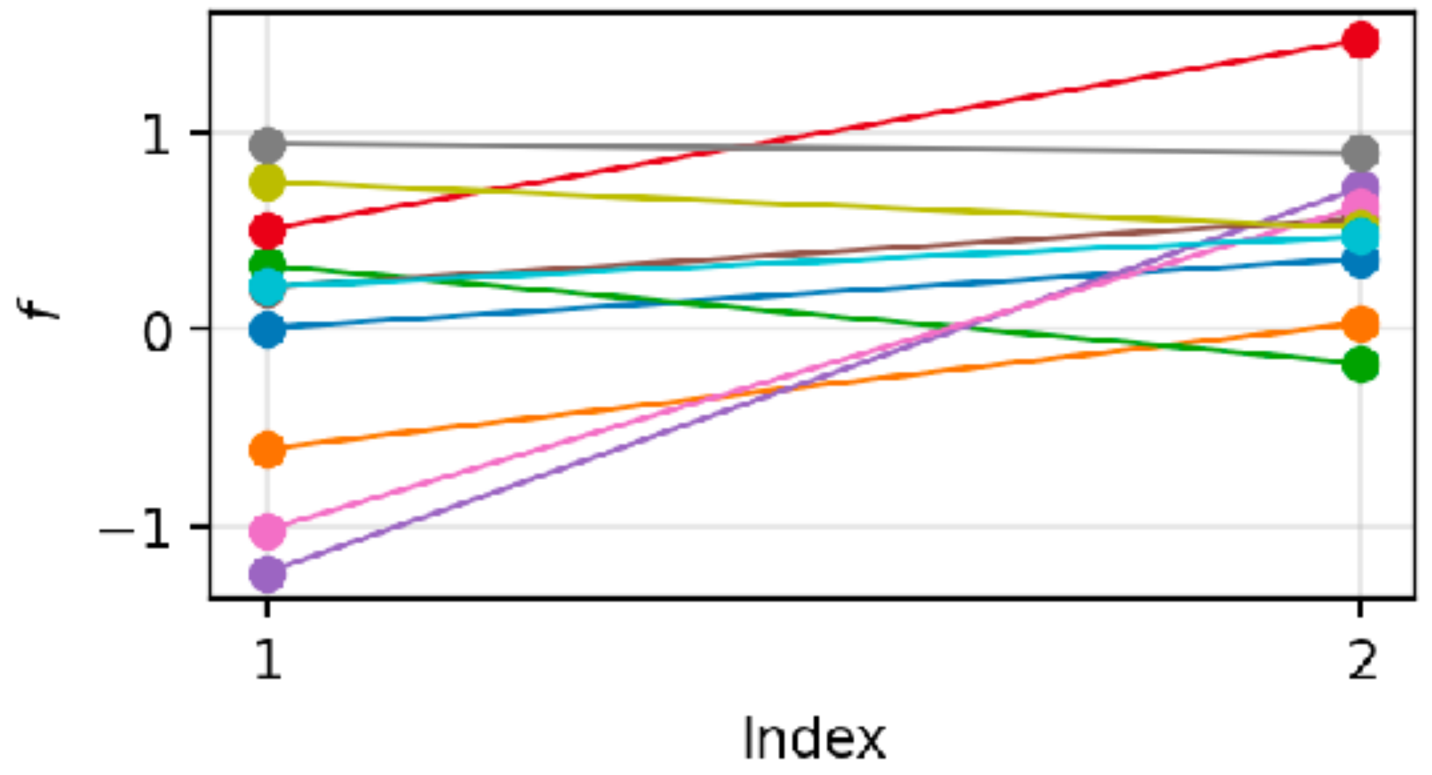

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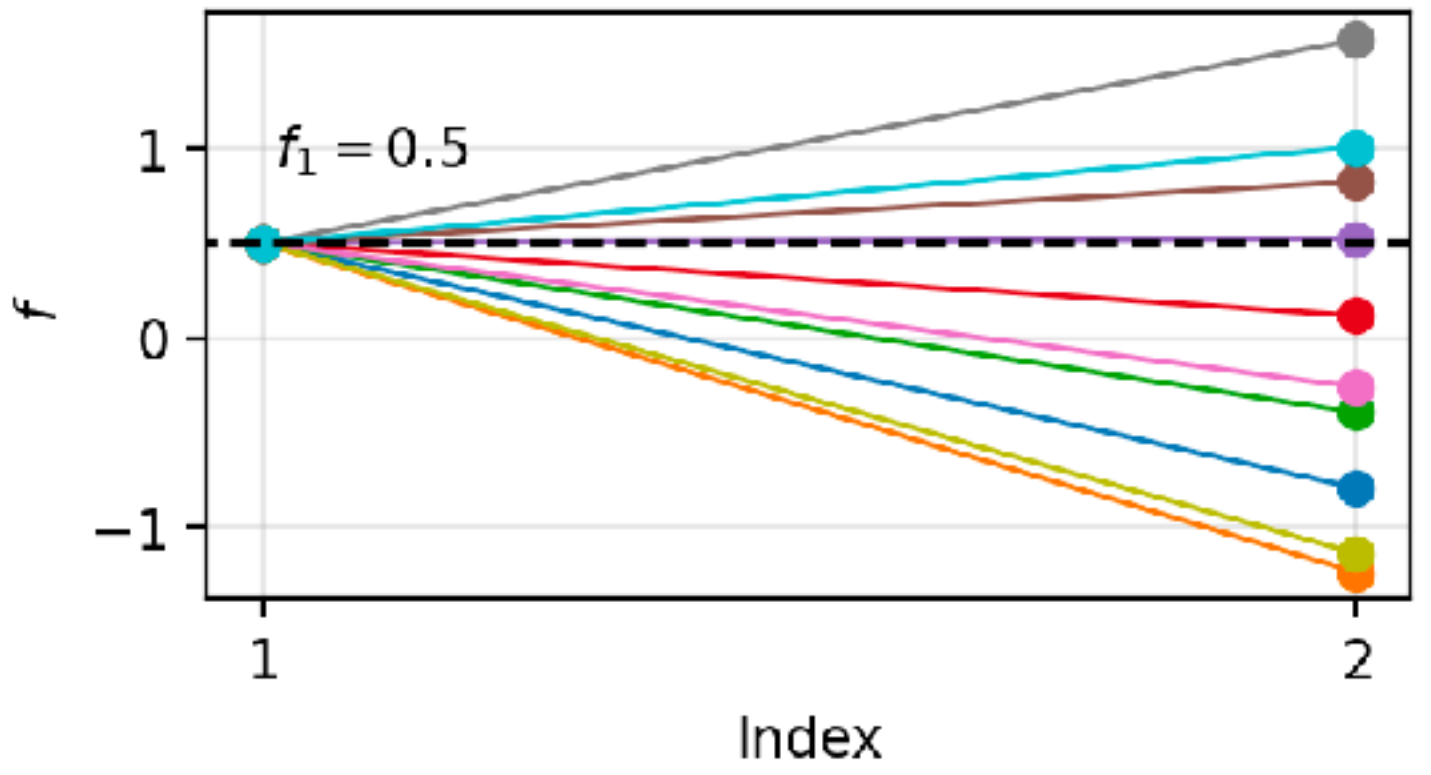

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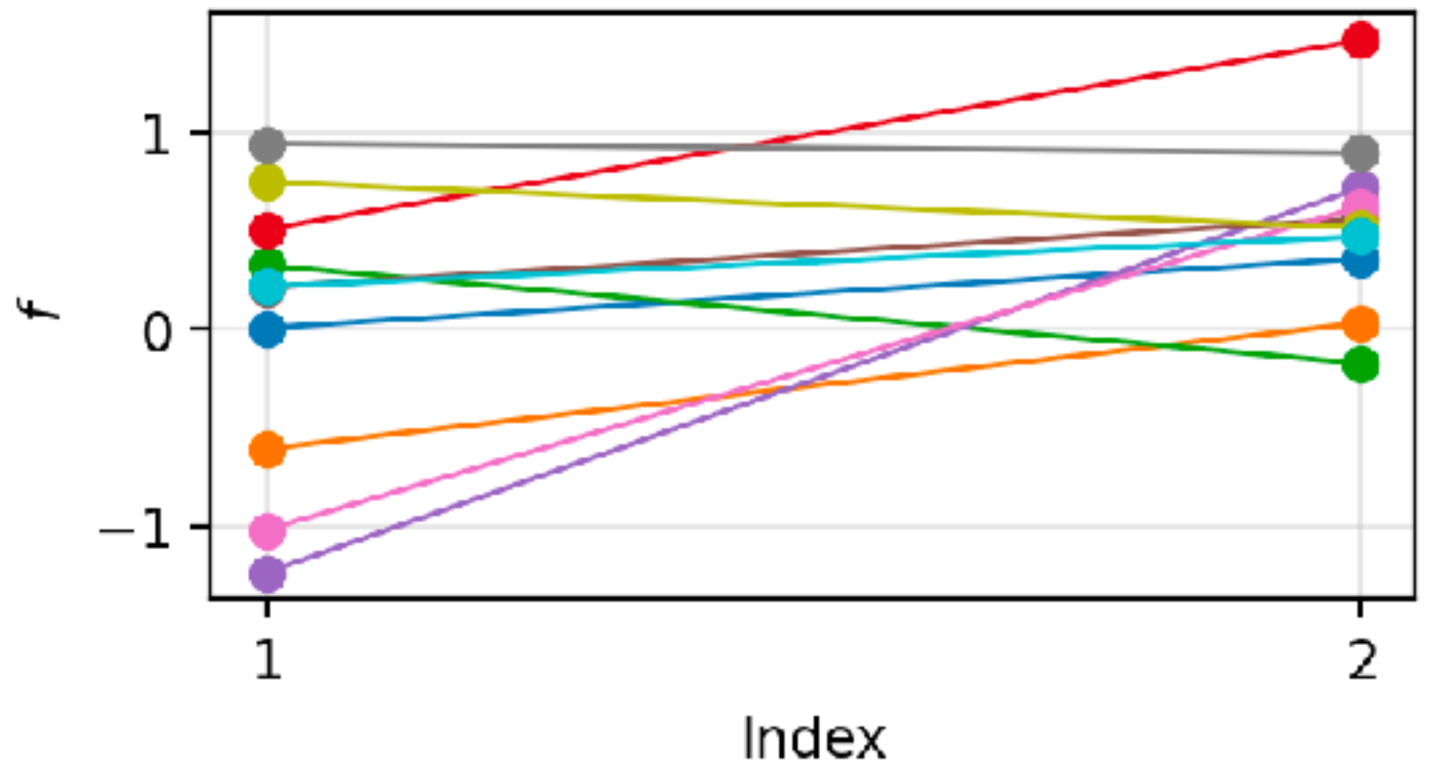

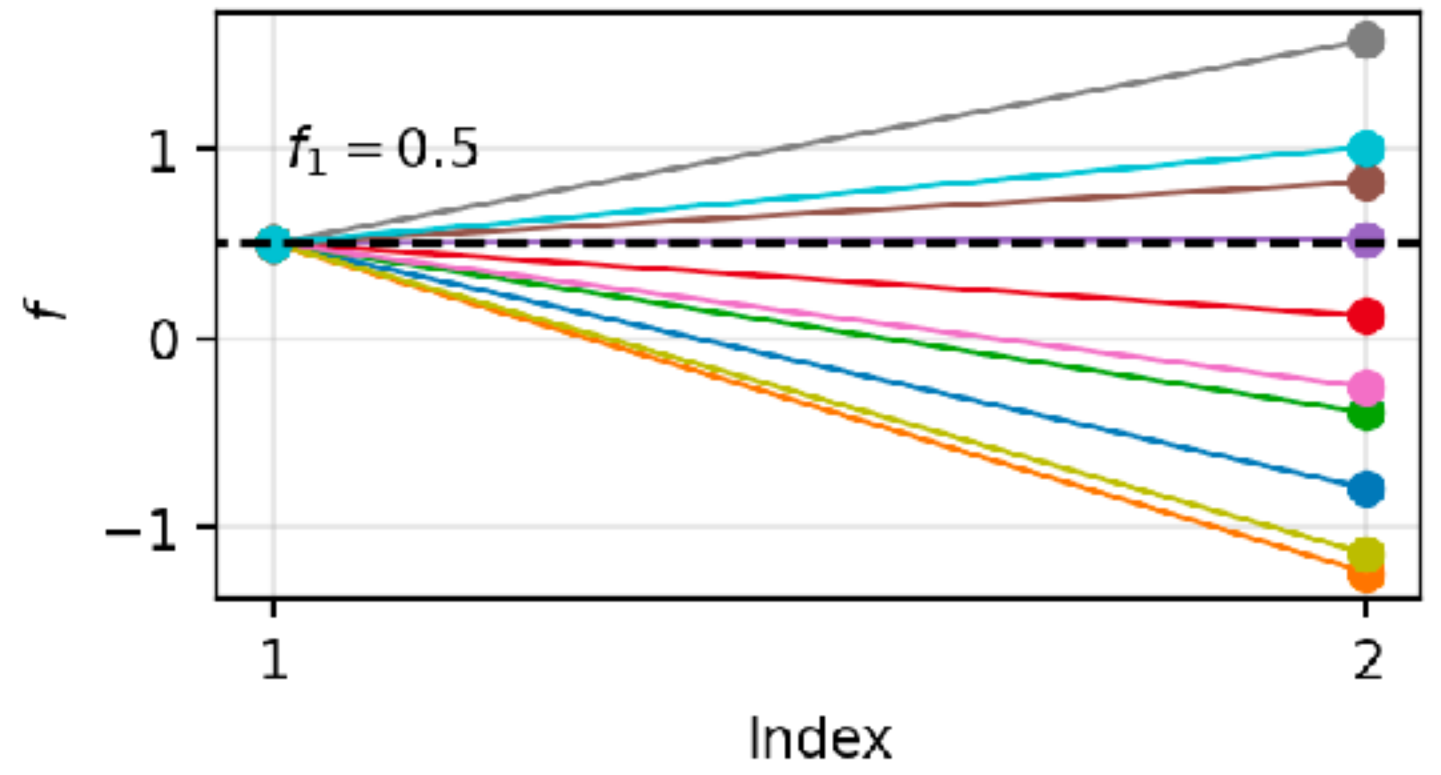

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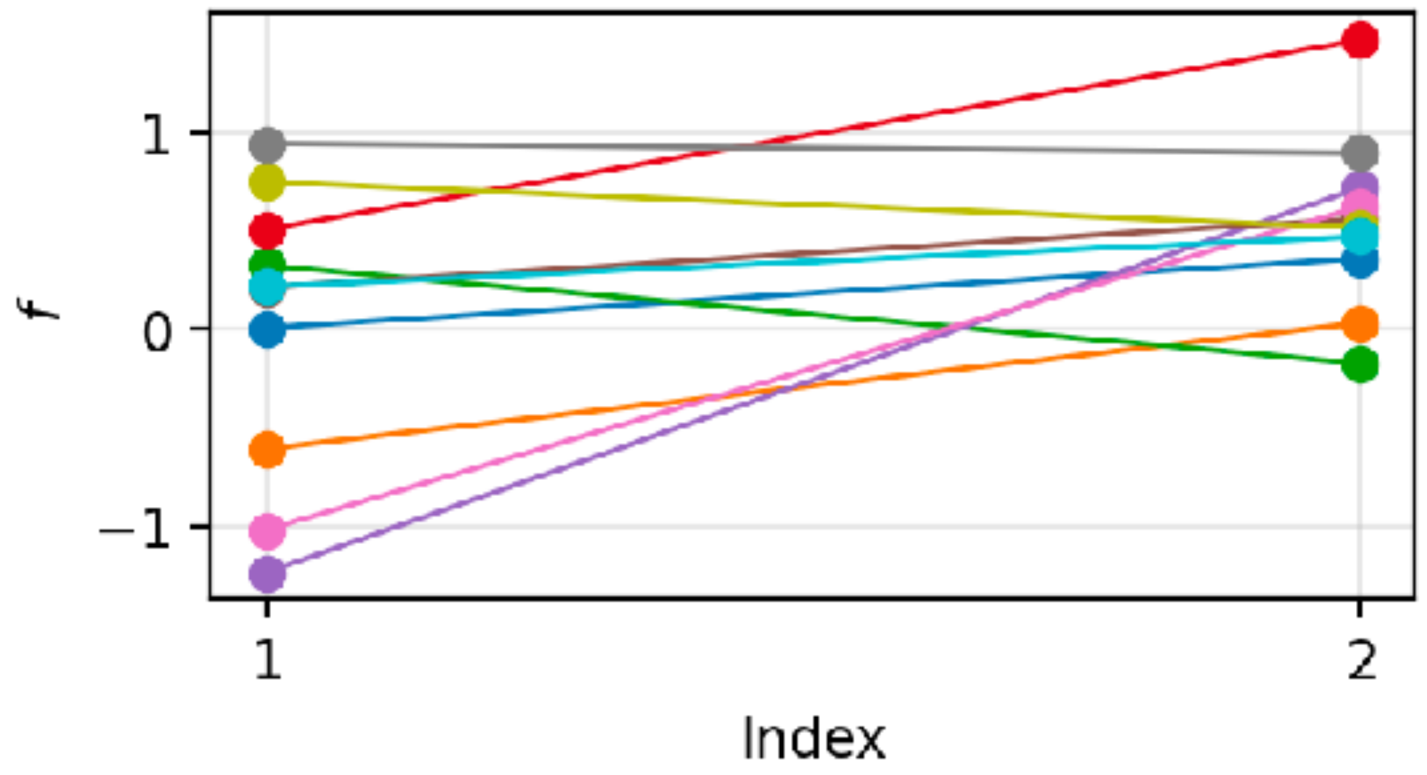

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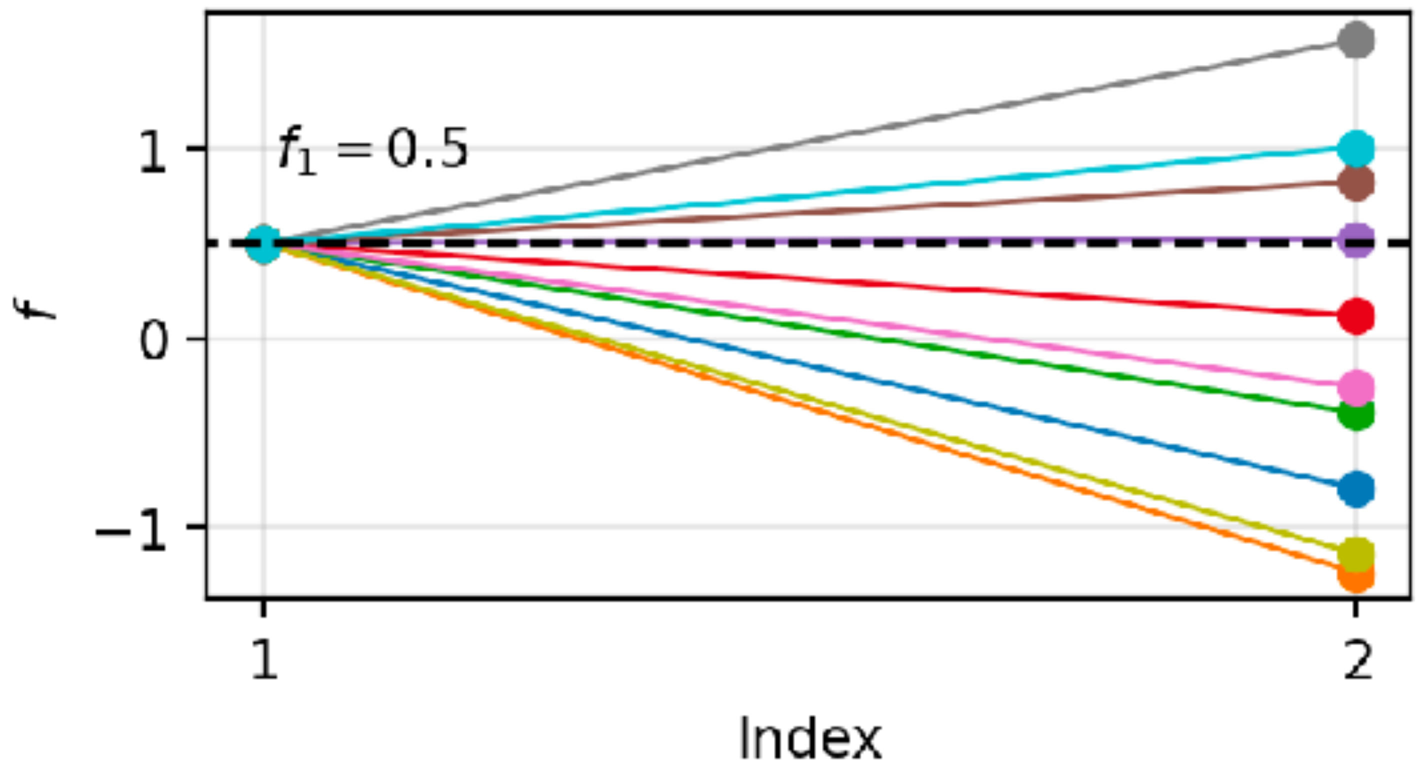

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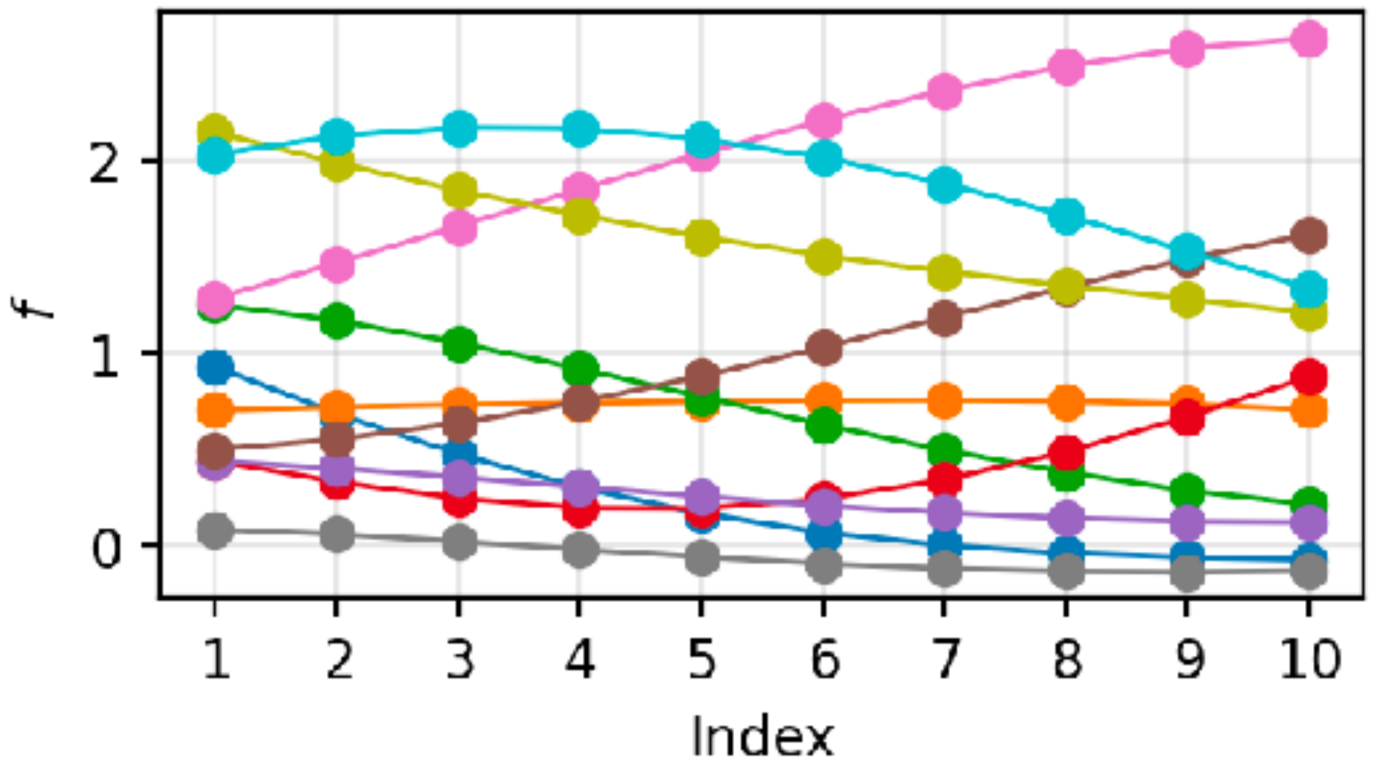

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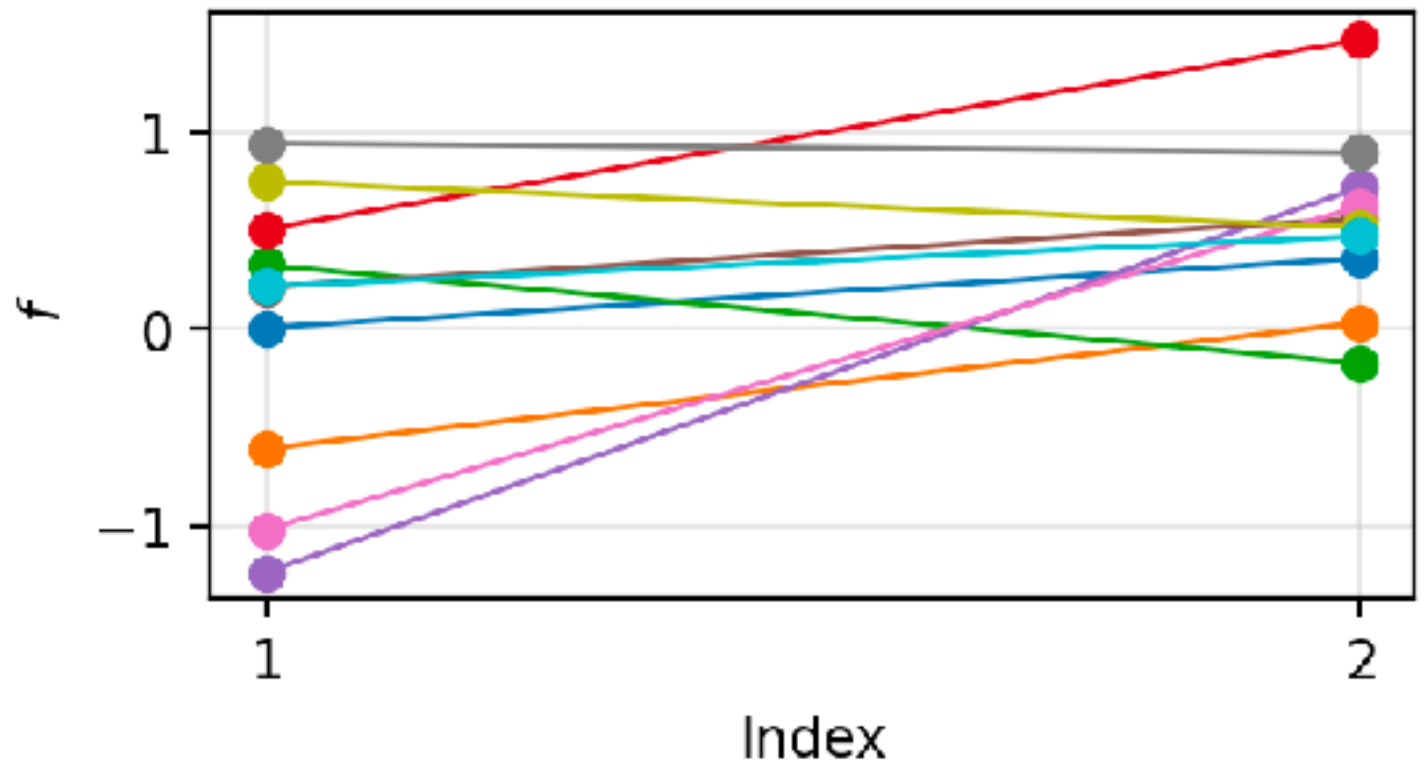

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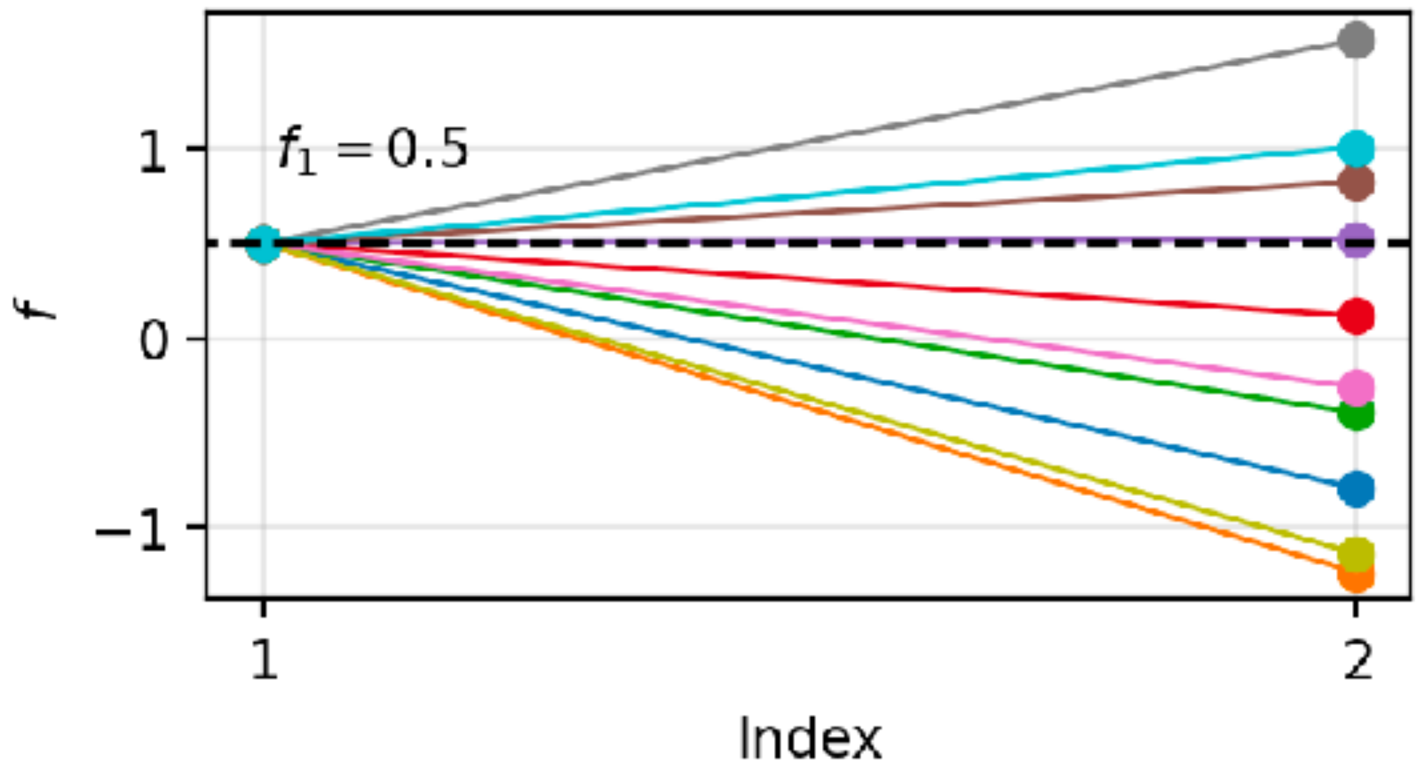

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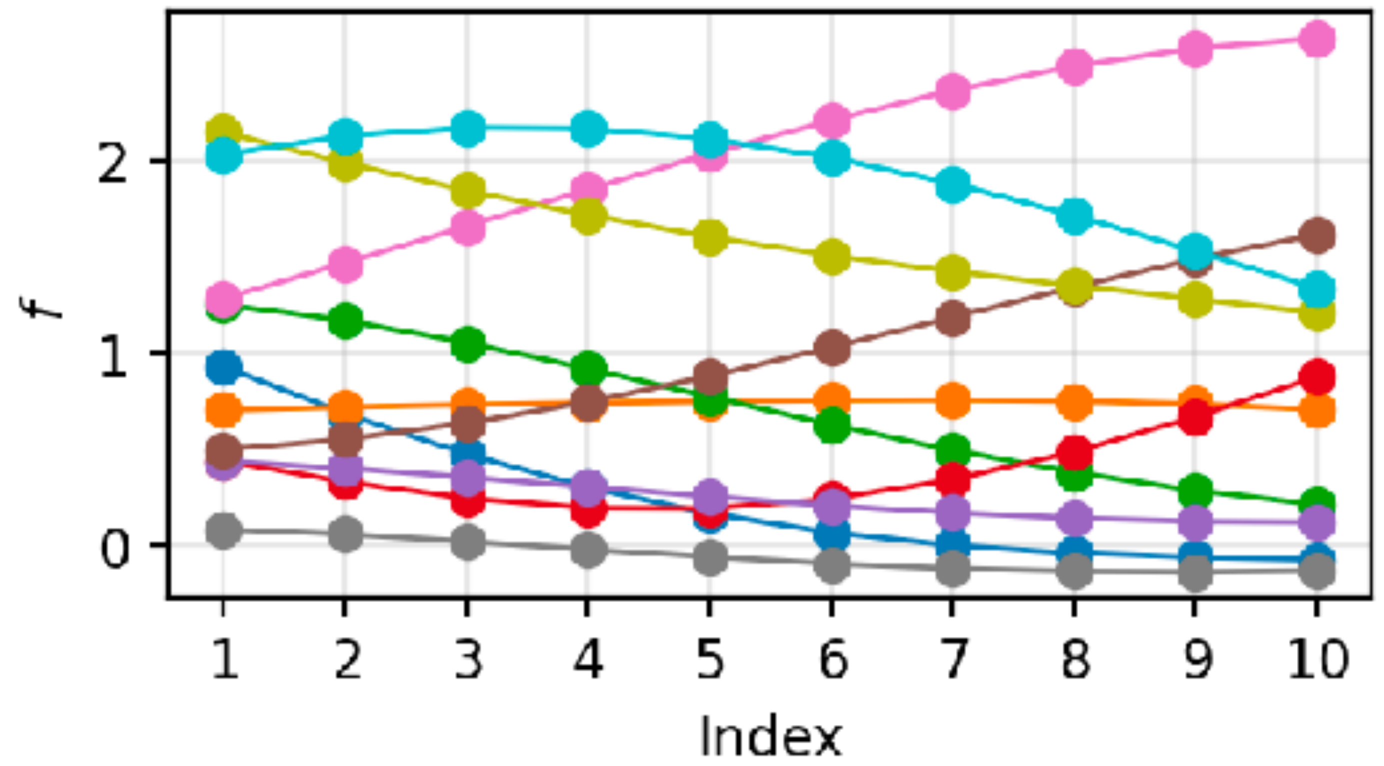

$$f \mid f_6 = 0.5 \sim \mathcal{N}\left(K_{*6}K_{66}^{-1}y, K_{**} - K_{*6}K_{66}^{-1}K_{*6}^T\right)$$

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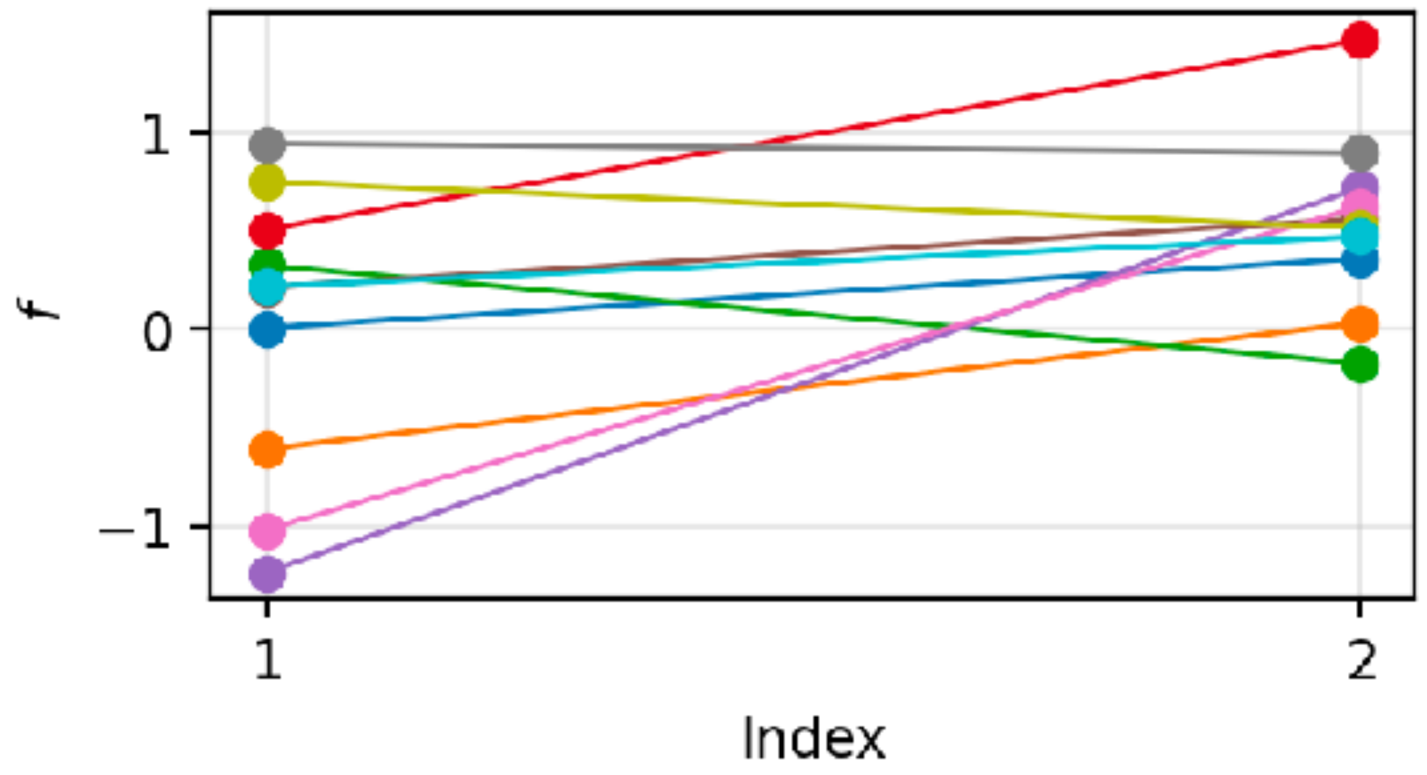

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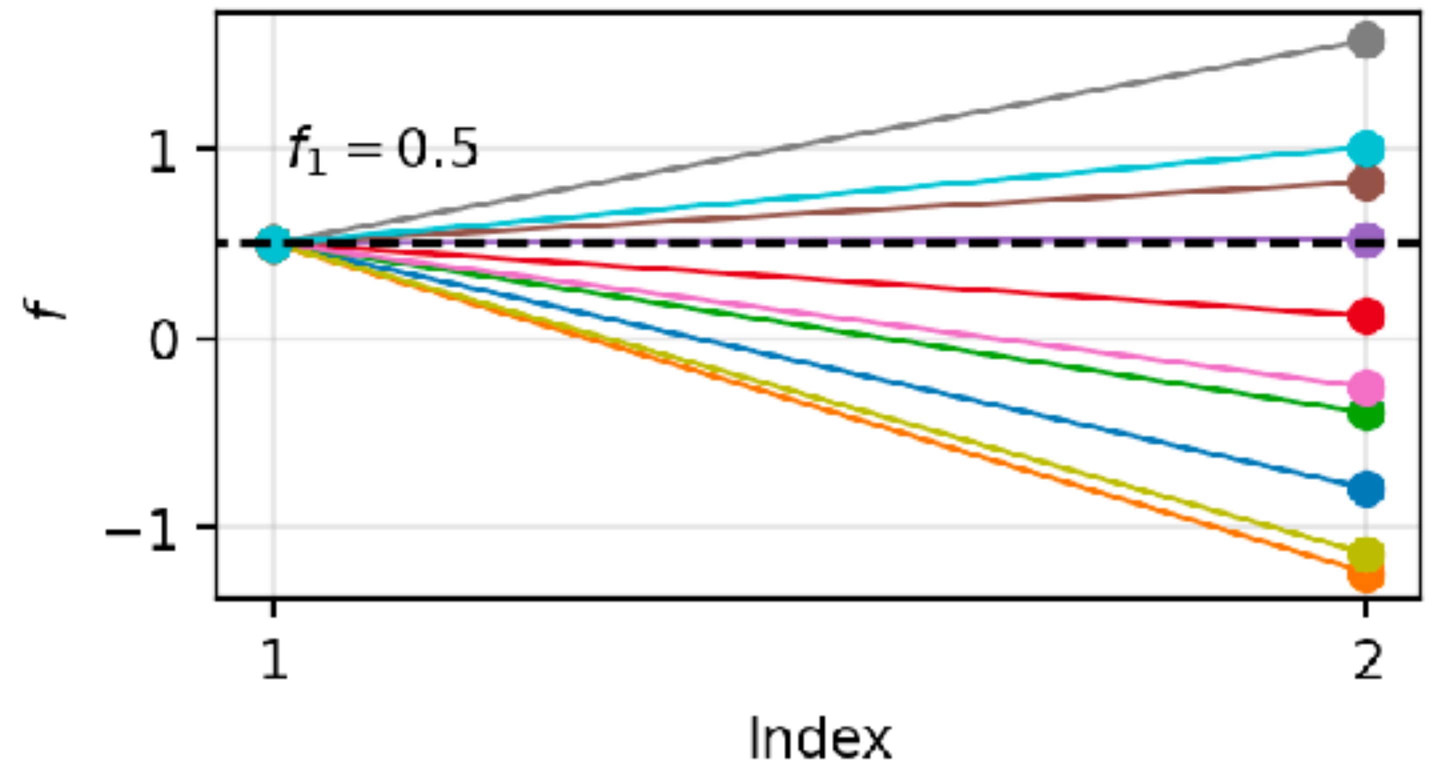
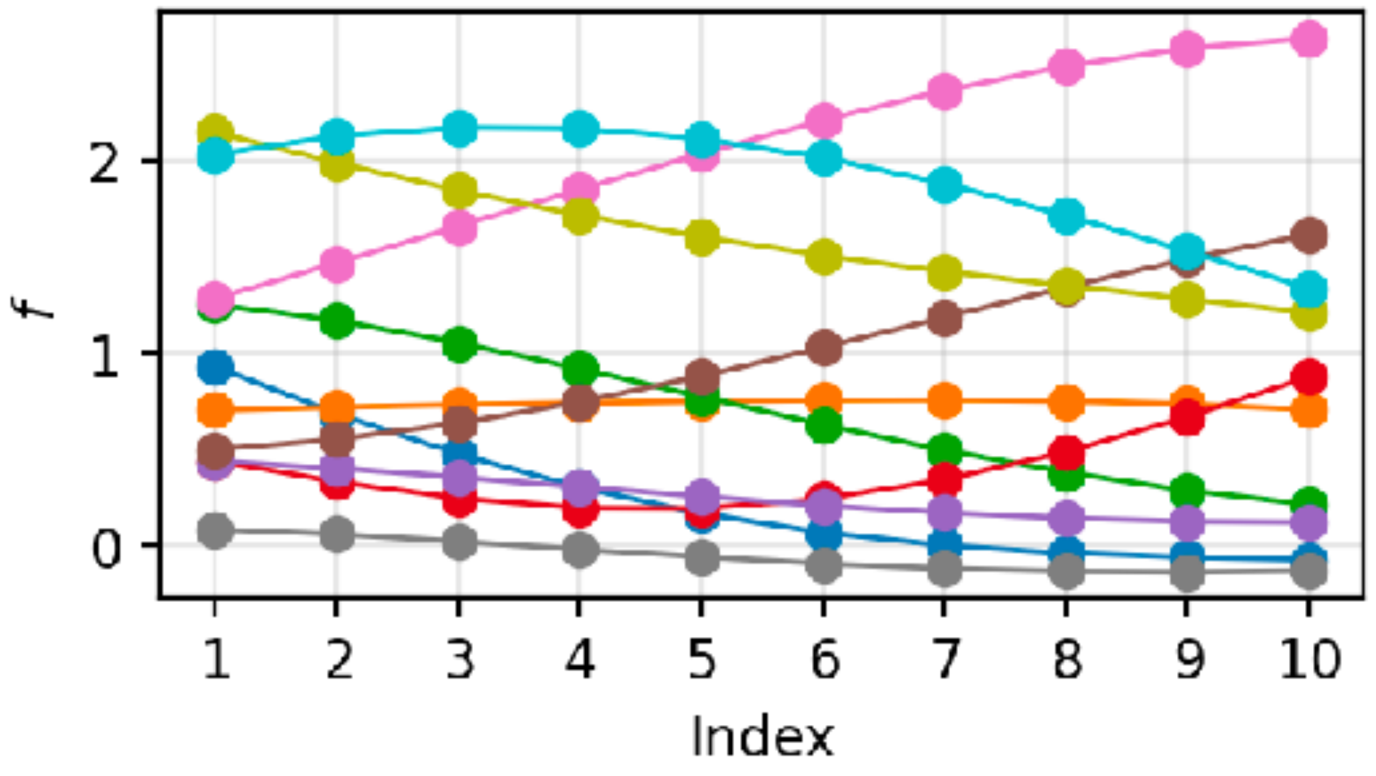
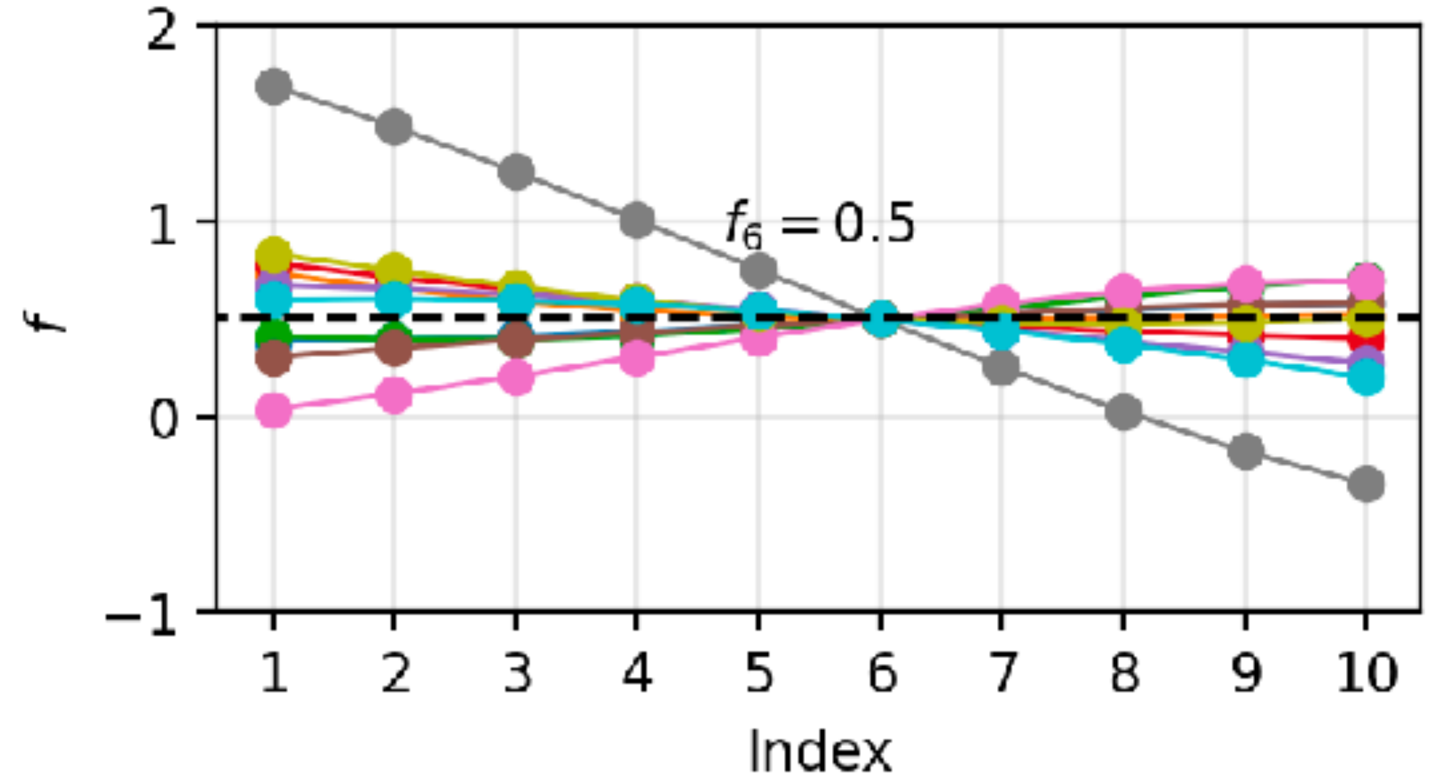


$$\begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_{10} \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} m_1 \\ m_2 \\ \vdots \\ m_{10} \end{pmatrix}, \mathbf{K}\right), \qquad K_{ij} = \exp(-(i-j)^2)$$

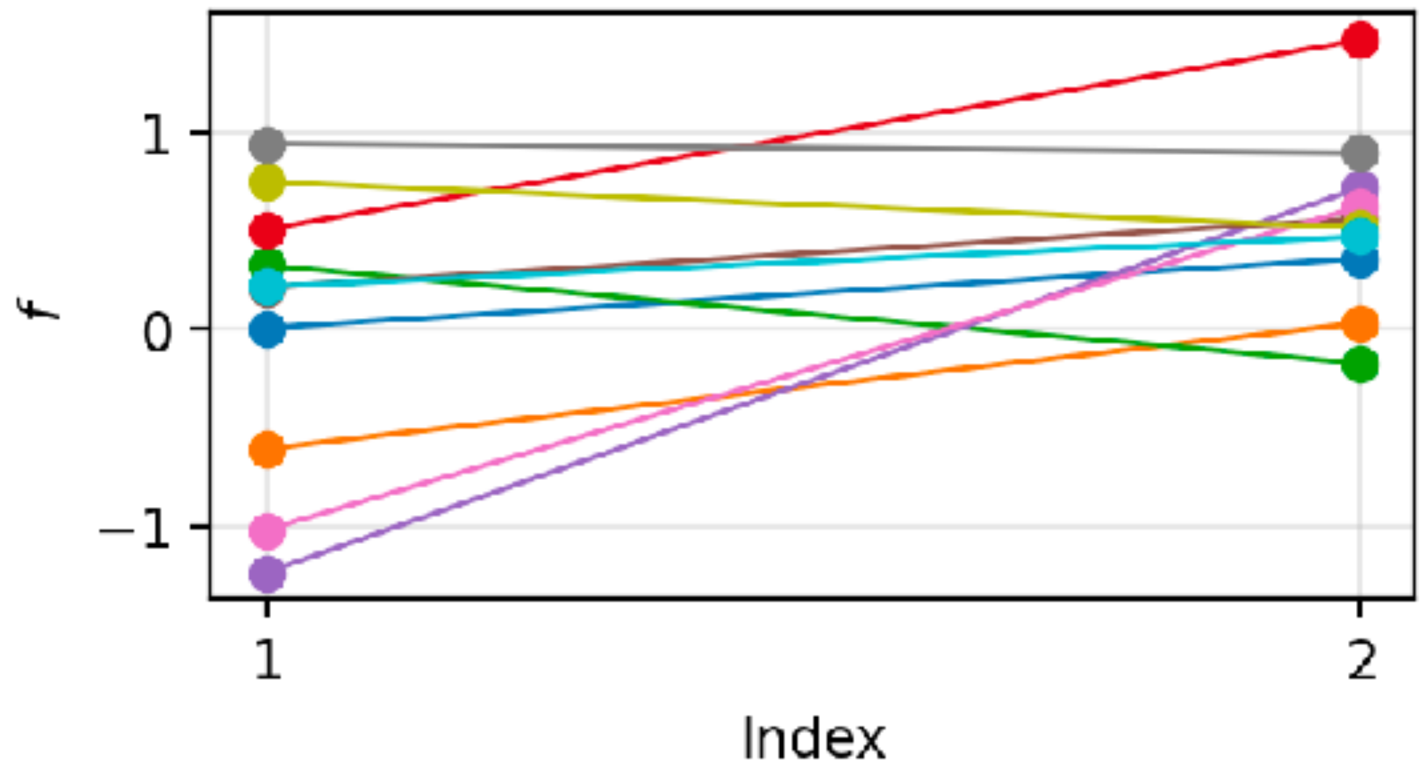


$$f \mid f_6 = 0.5 \sim \mathcal{N}\left(K_{*6}K_{66}^{-1}y, K_{**} - K_{*6}K_{66}^{-1}K_{*6}^{T}\right)$$



Gaussian Processes: A Primer

$$\begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} m_1 \\ m_2 \end{pmatrix}, \begin{pmatrix} k_{11} & k_{12} \\ k_{21} & k_{21} \end{pmatrix}\right)$$



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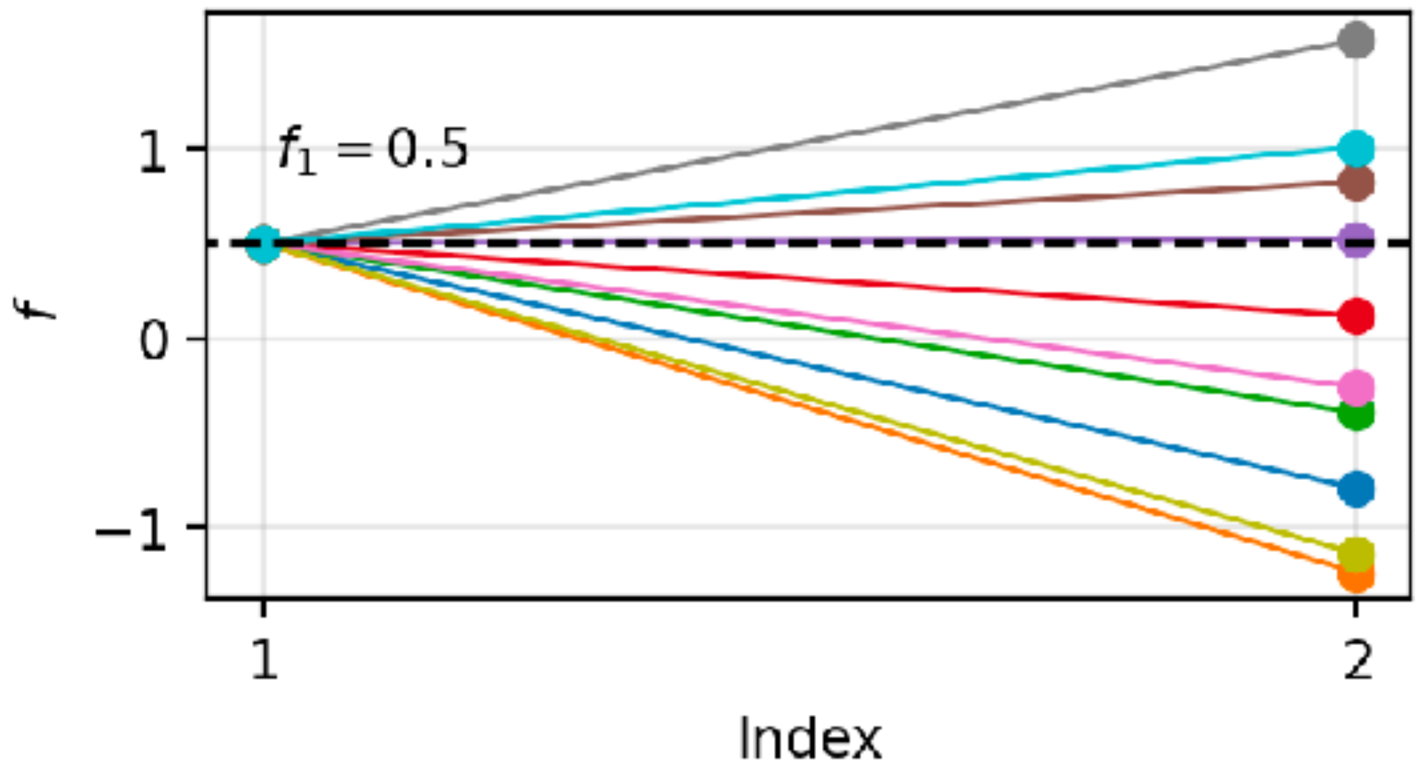

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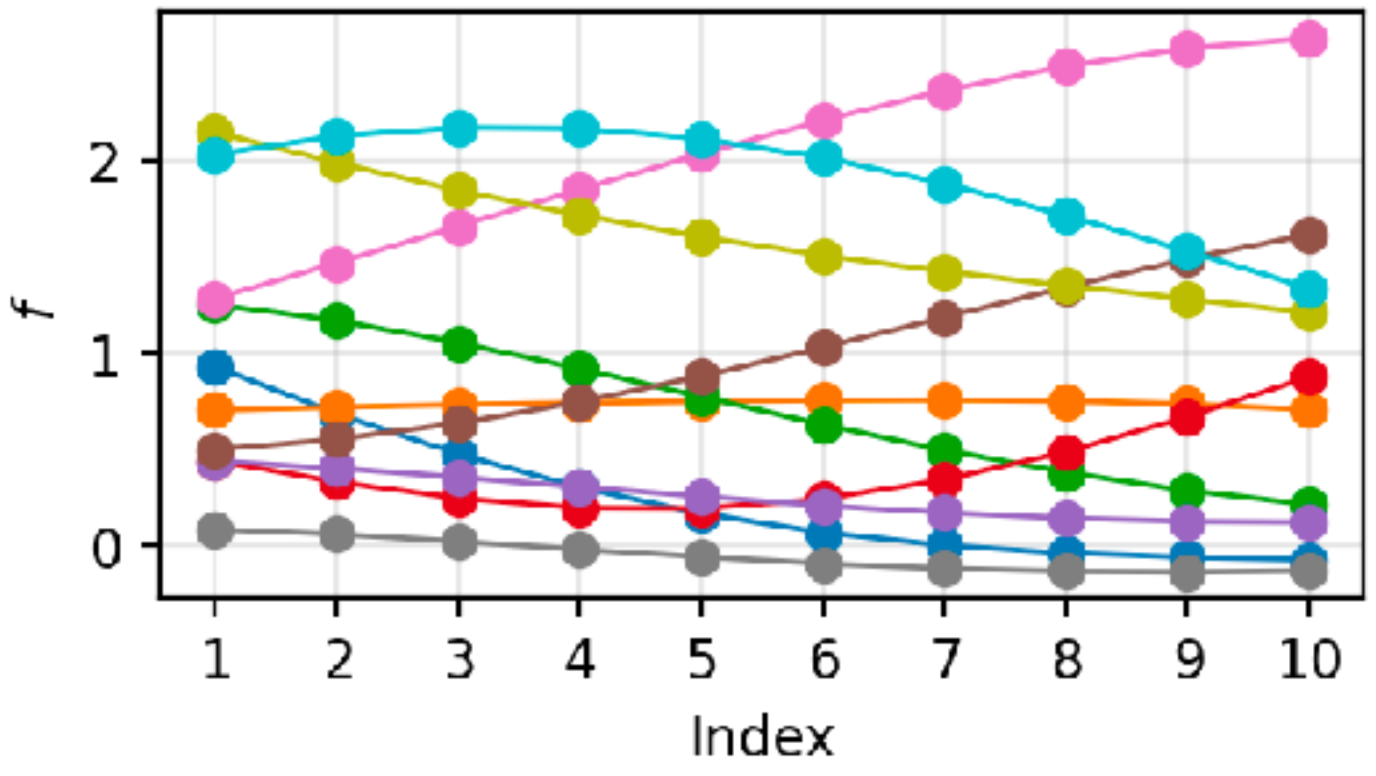
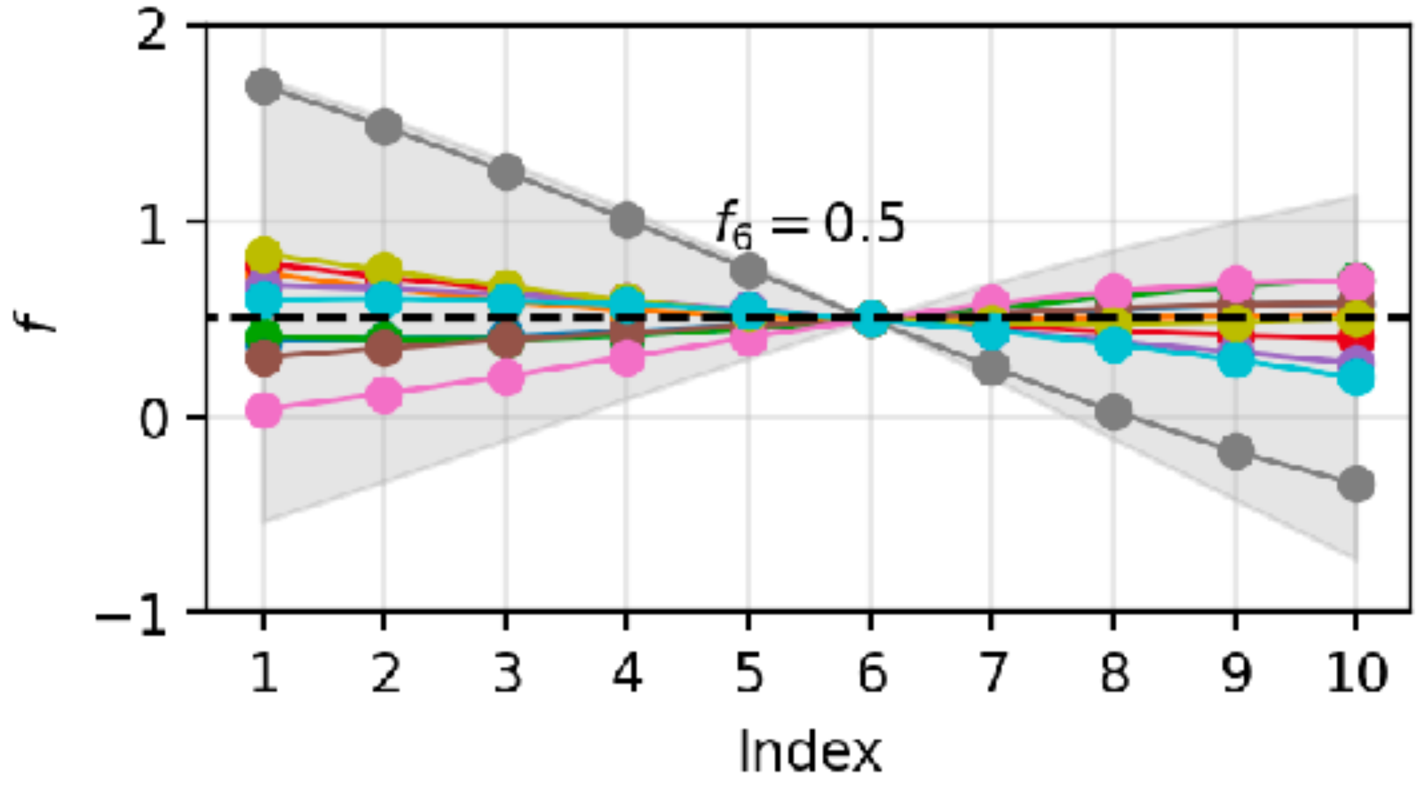
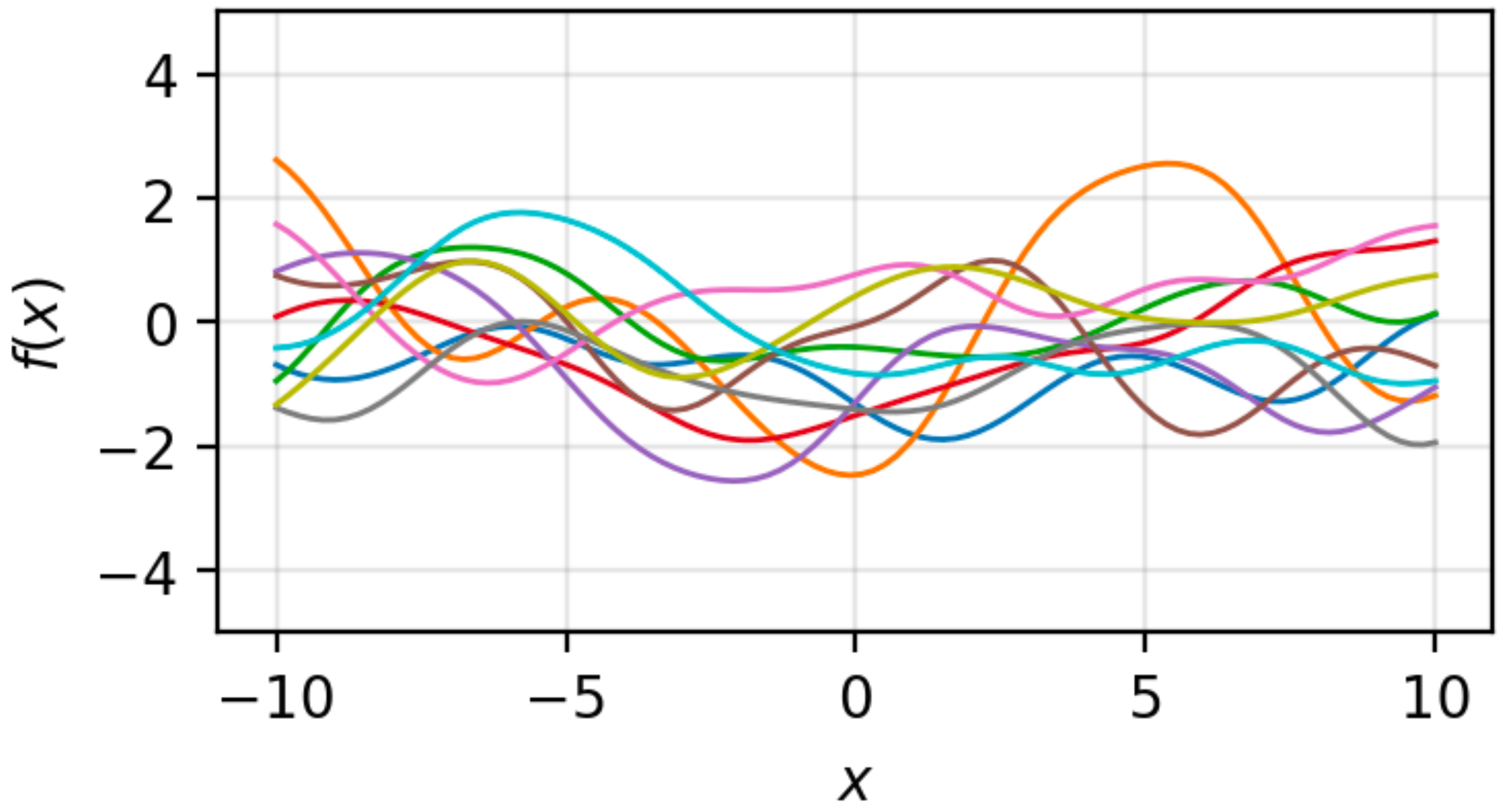


$$f \mid f_6 = 0.5 \sim \mathcal{N}\left(K_{*6}K_{66}^{-1}y, K_{**} - K_{*6}K_{66}^{-1}K_{*6}^T\right)$$



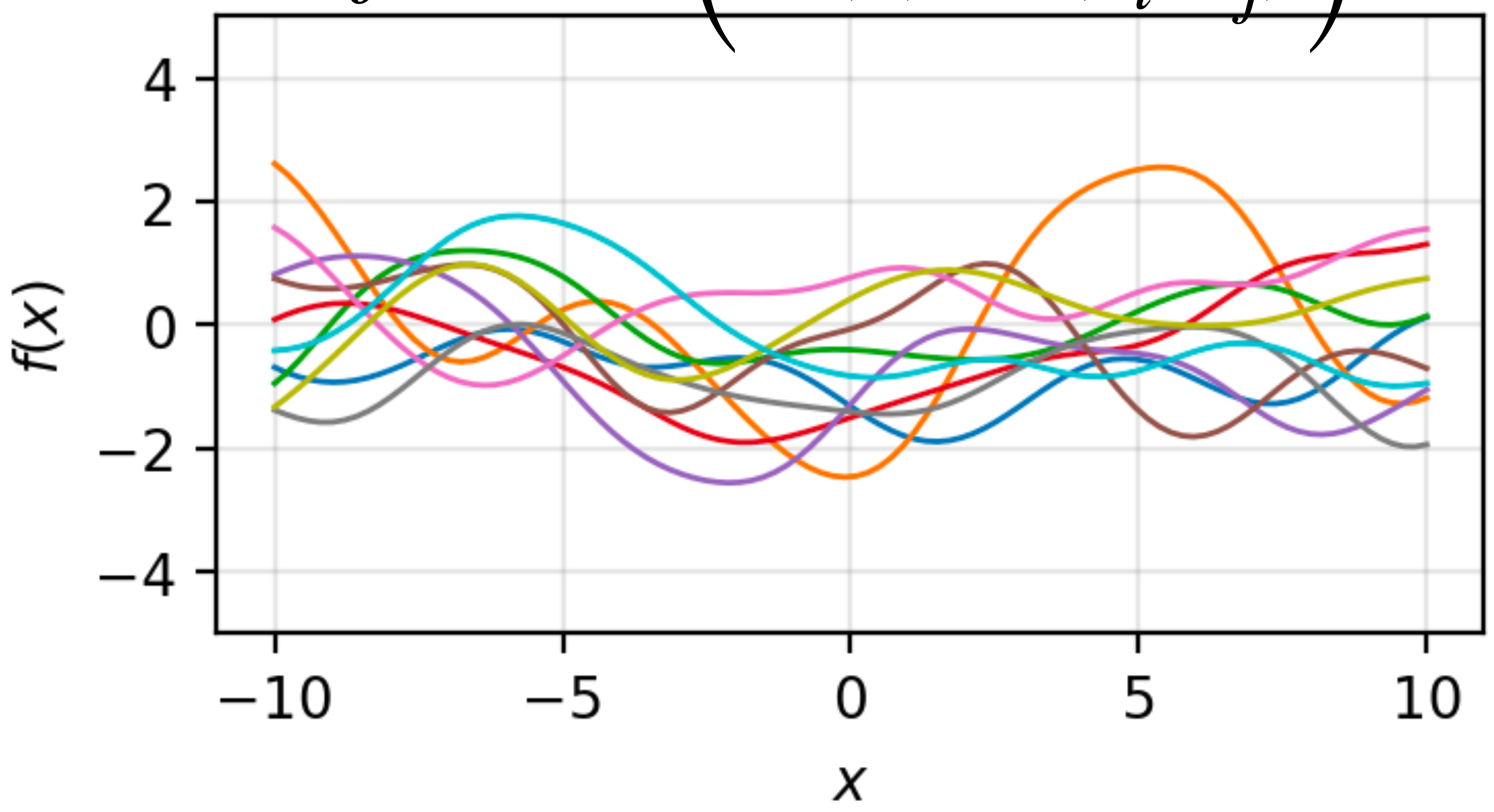
Gaussian Processes: A Primer

Gaussian Processes: A Primer



Gaussian Processes: A Primer

$$f \sim \mathrm{GP}\left(m(x), K(x_i, x_j)\right)$$



Gaussian Processes: A Primer

Dataset

$$(X, y) = \left\{(X_1, y_1), \ldots, (X_n, y_n)\right\}$$

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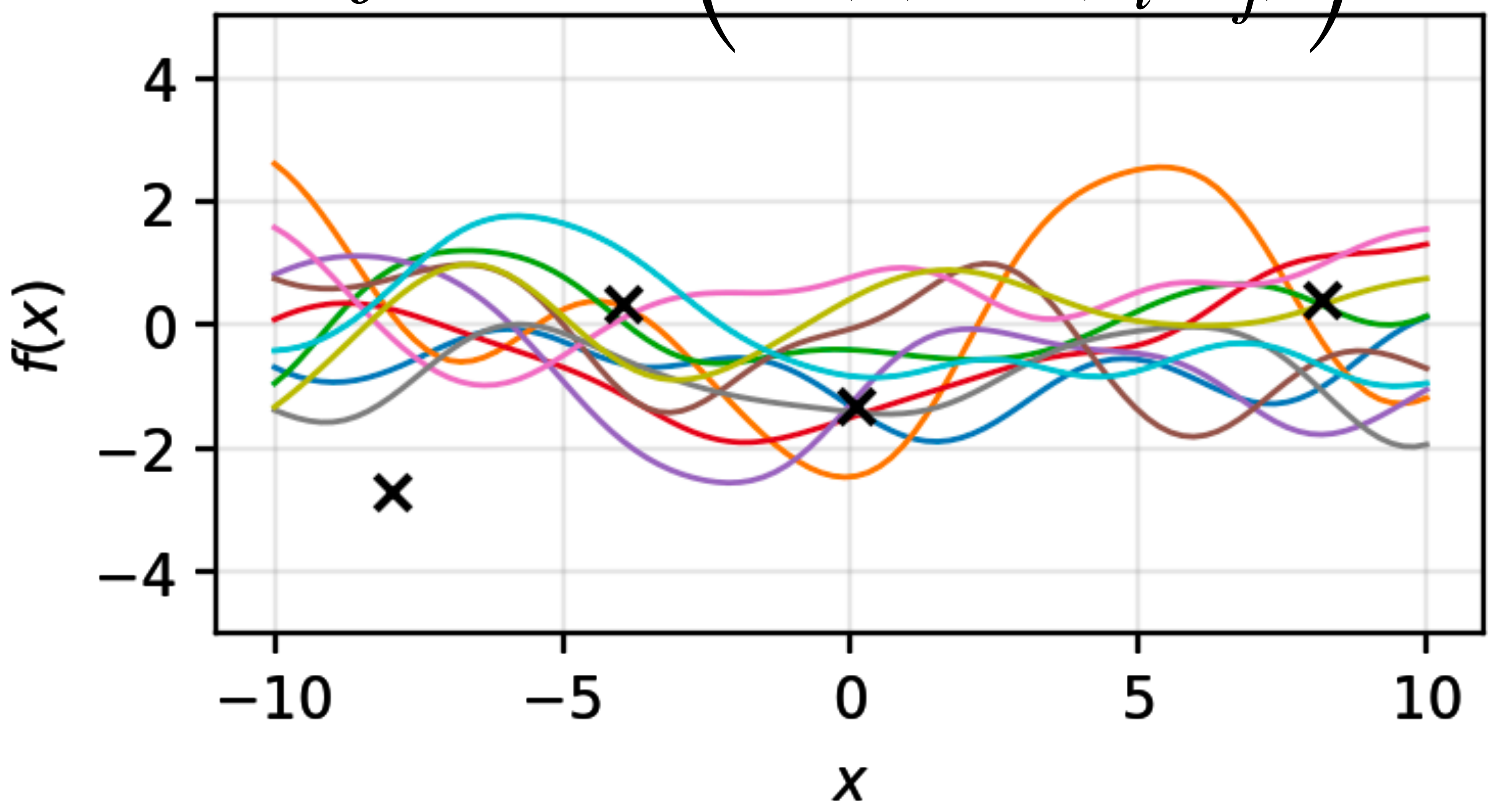

Gaussian Processes: A Primer

$$\left[\begin{pmatrix} f(X_*) \\ f(X) \end{pmatrix}\right] \sim \mathcal{N}\left(0, \left[\begin{pmatrix} K_{**} & K_{*n} \\ K_{*n}^\top & K_{nn} \end{pmatrix}\right]\right)$$

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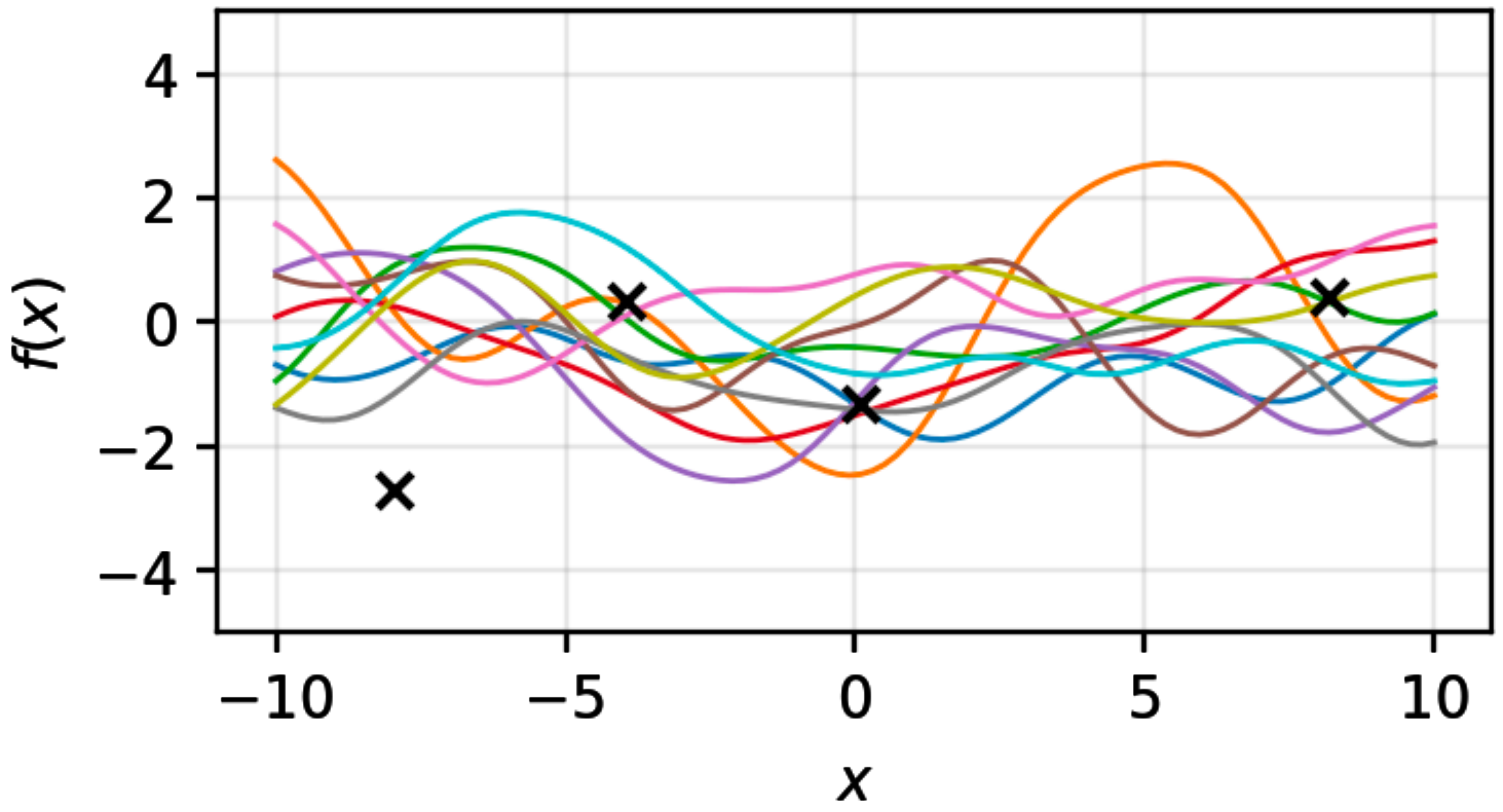

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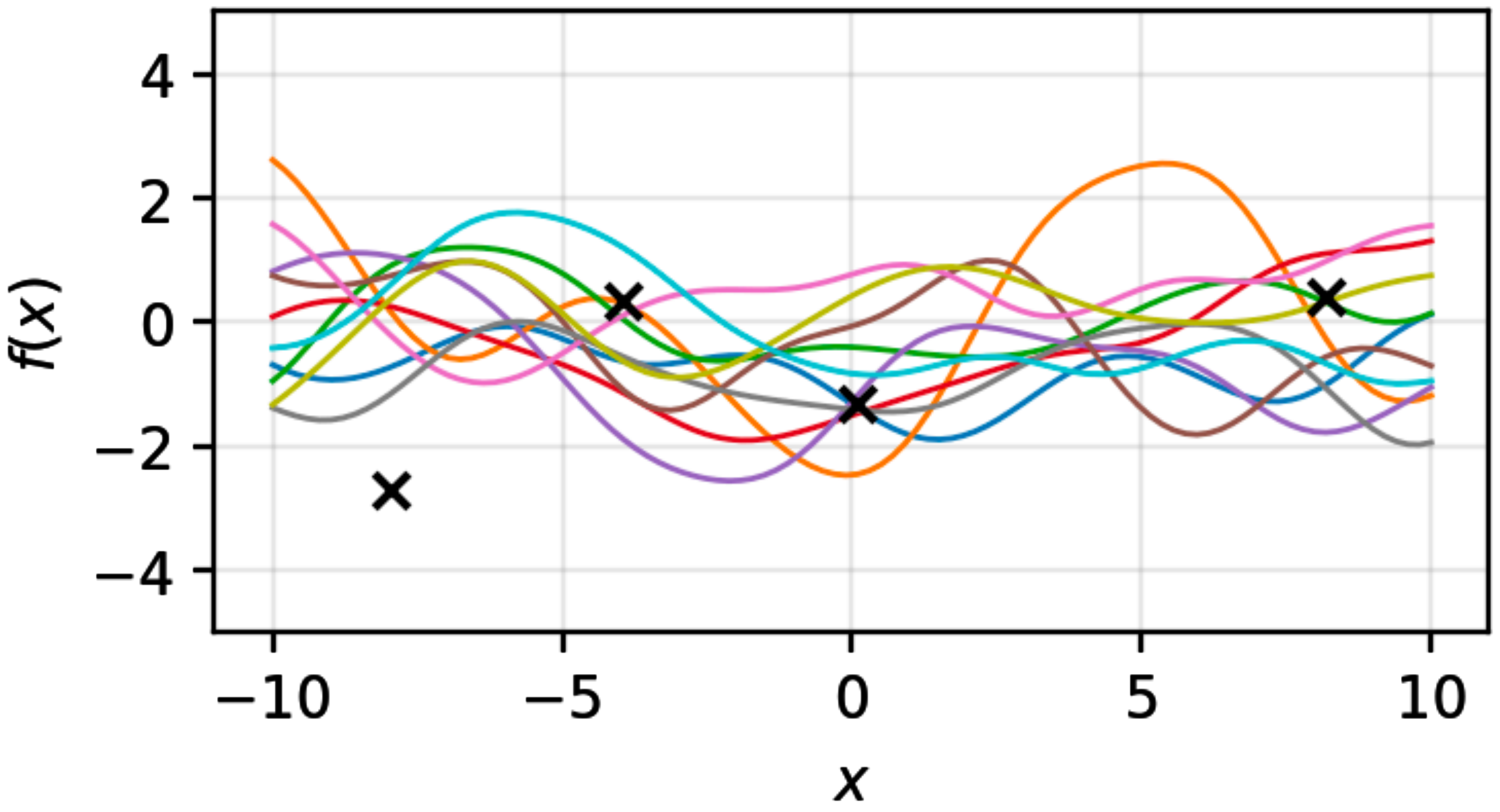
Dataset

$$(X, y) = \{(X_1, y_1), \ldots, (X_n, y_n)\}$$

Observation noise assumption

$$y_i \sim \mathcal{N}(f(X_i), \sigma^2)$$



Gaussian Processes: A Primer

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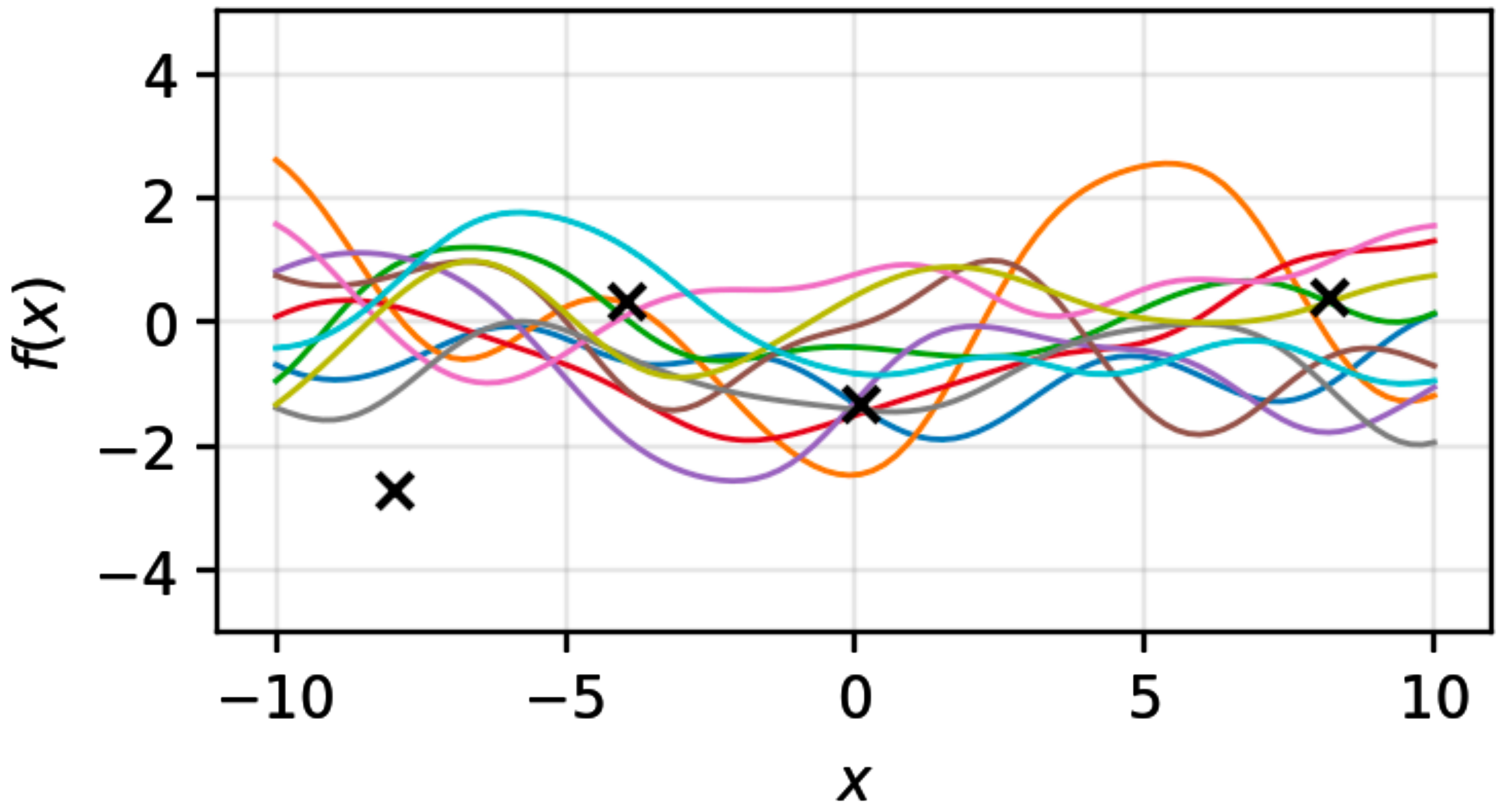

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Posterior Distribution

$$p(f_* \mid f, X, y) = \mathcal{N}(\mu_{f|y}, \Sigma_{f|y})$$

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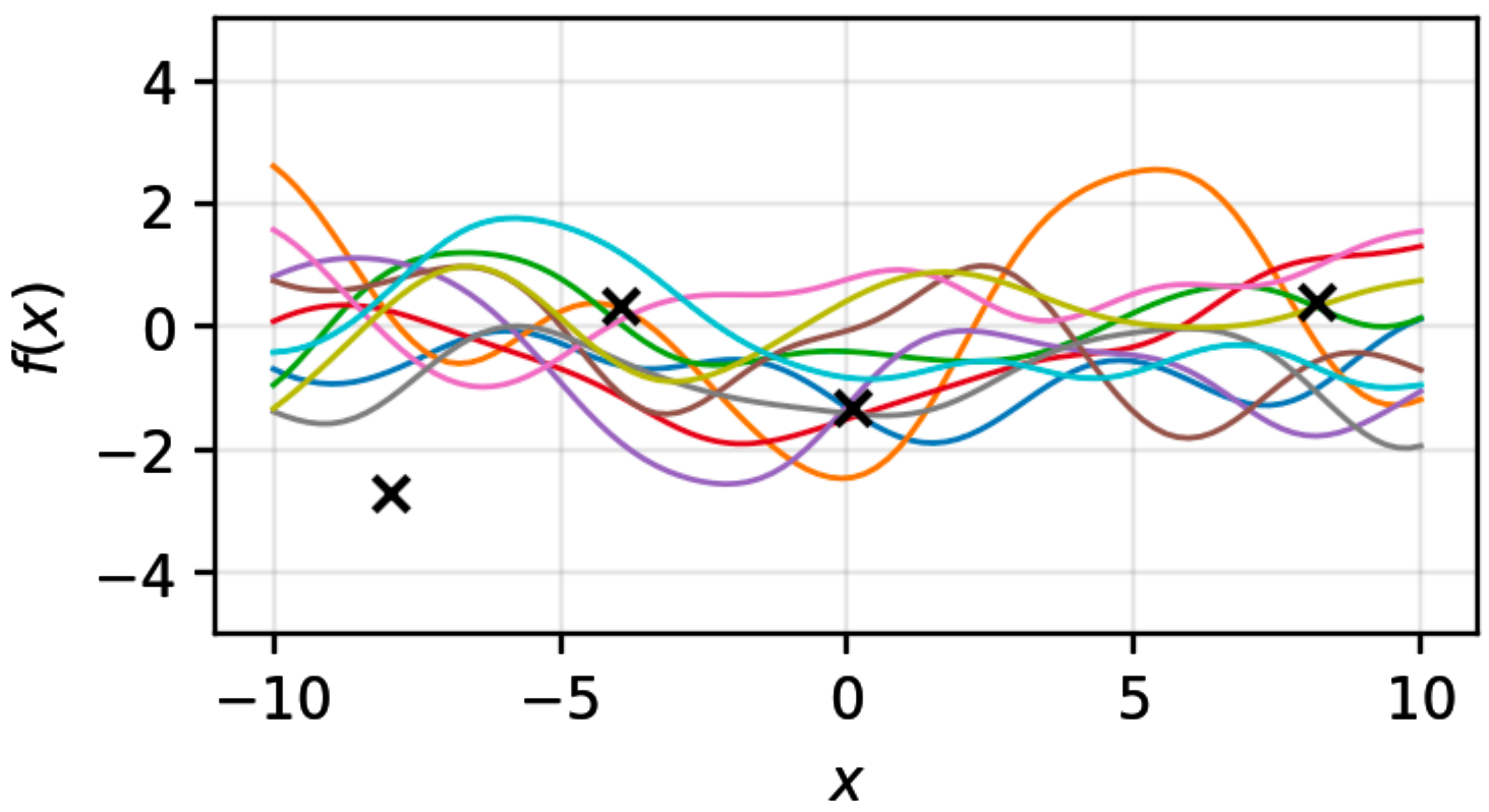

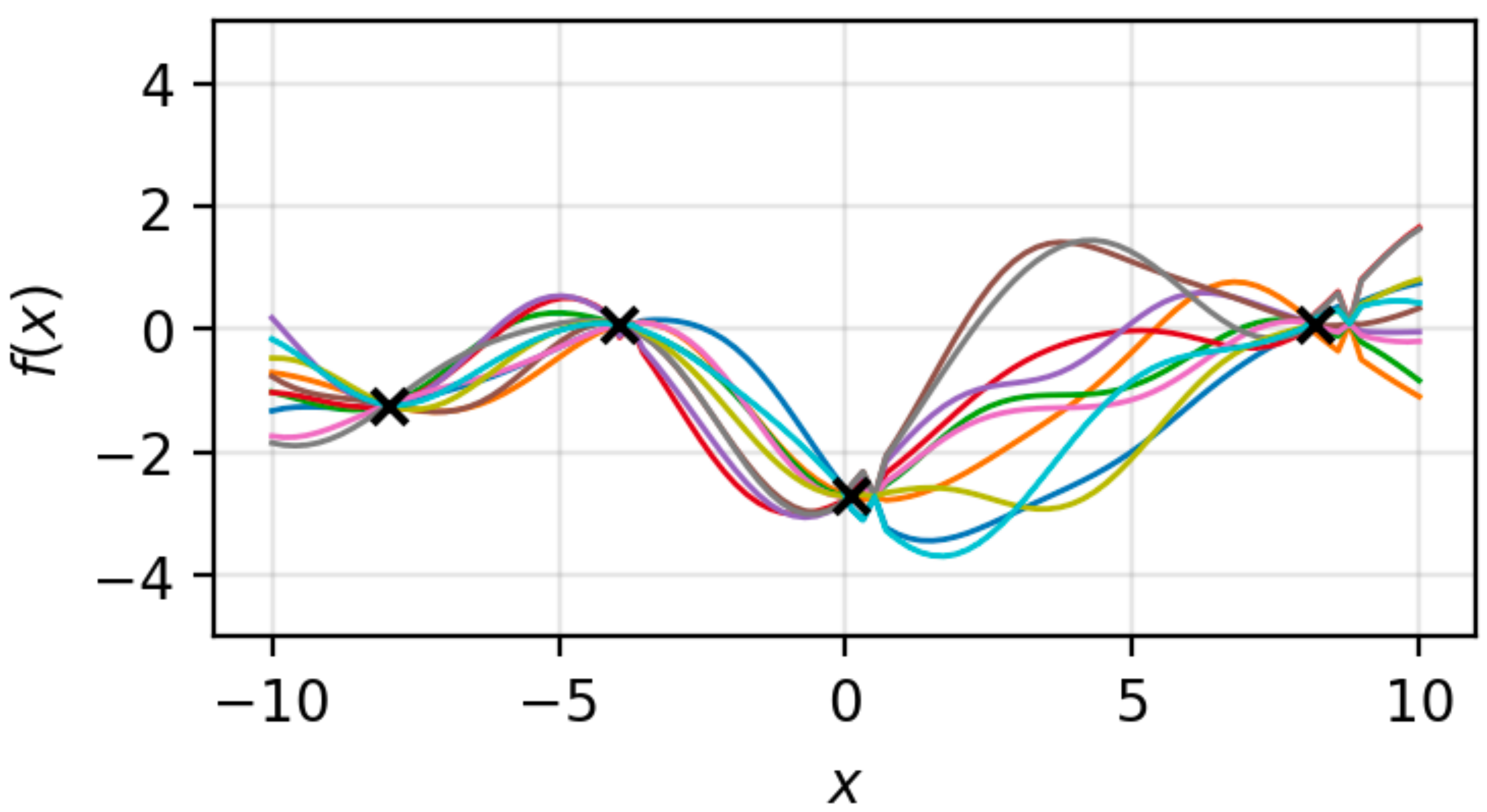

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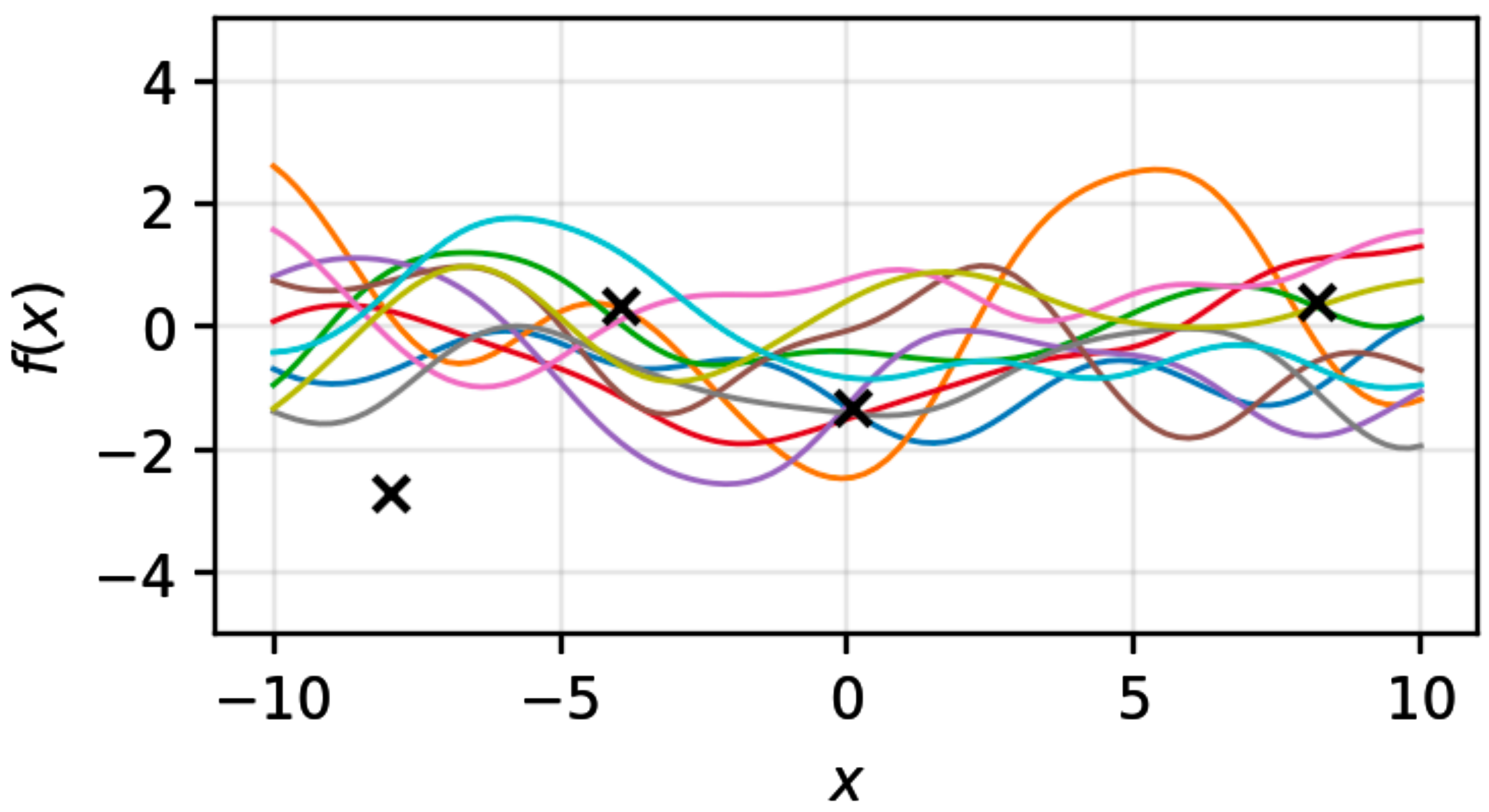
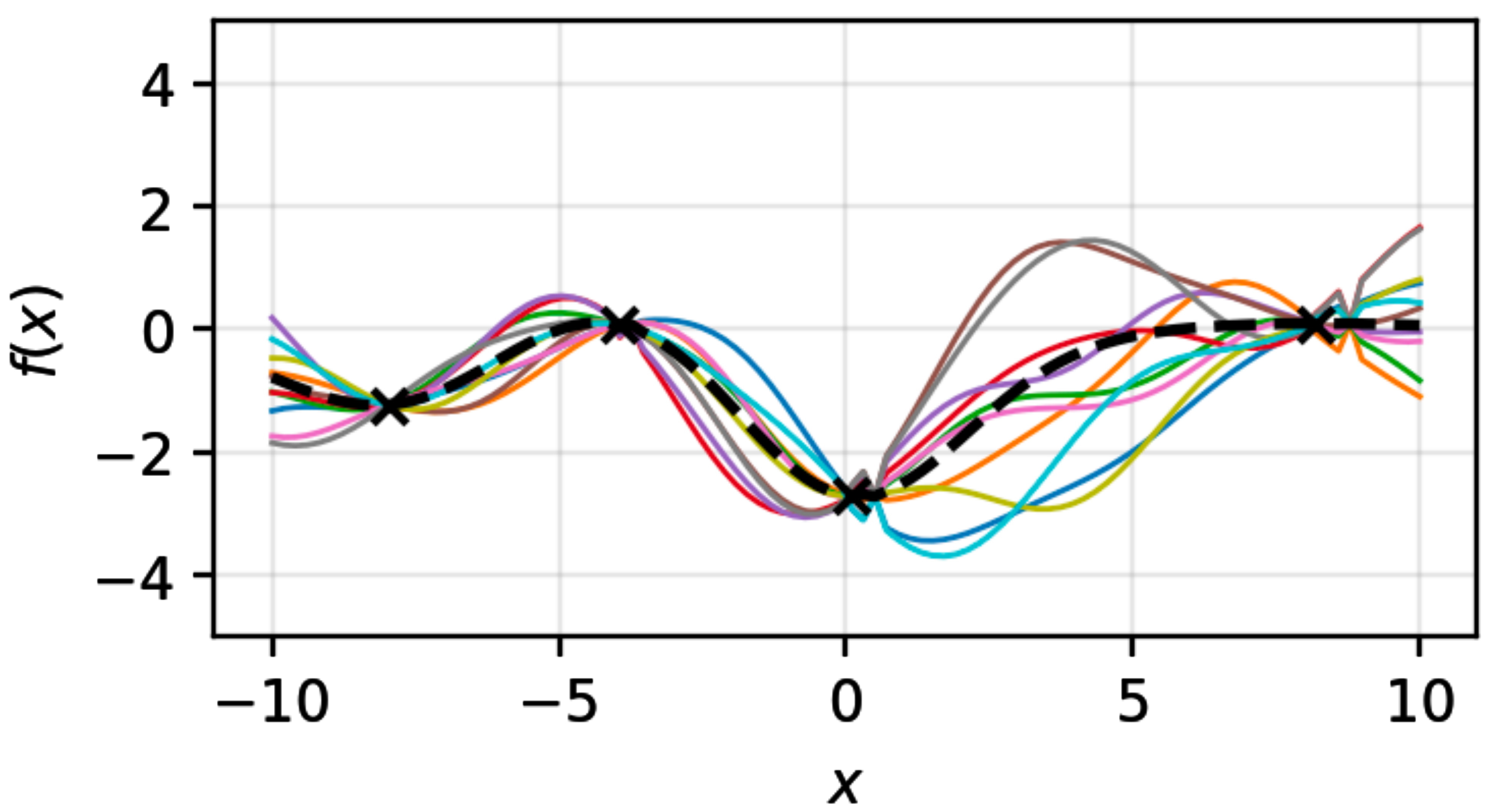
Predictive Mean

$$\mu_{f|y} = K_{*n}(K_{nn} + \sigma^2 I)^{-1} y$$





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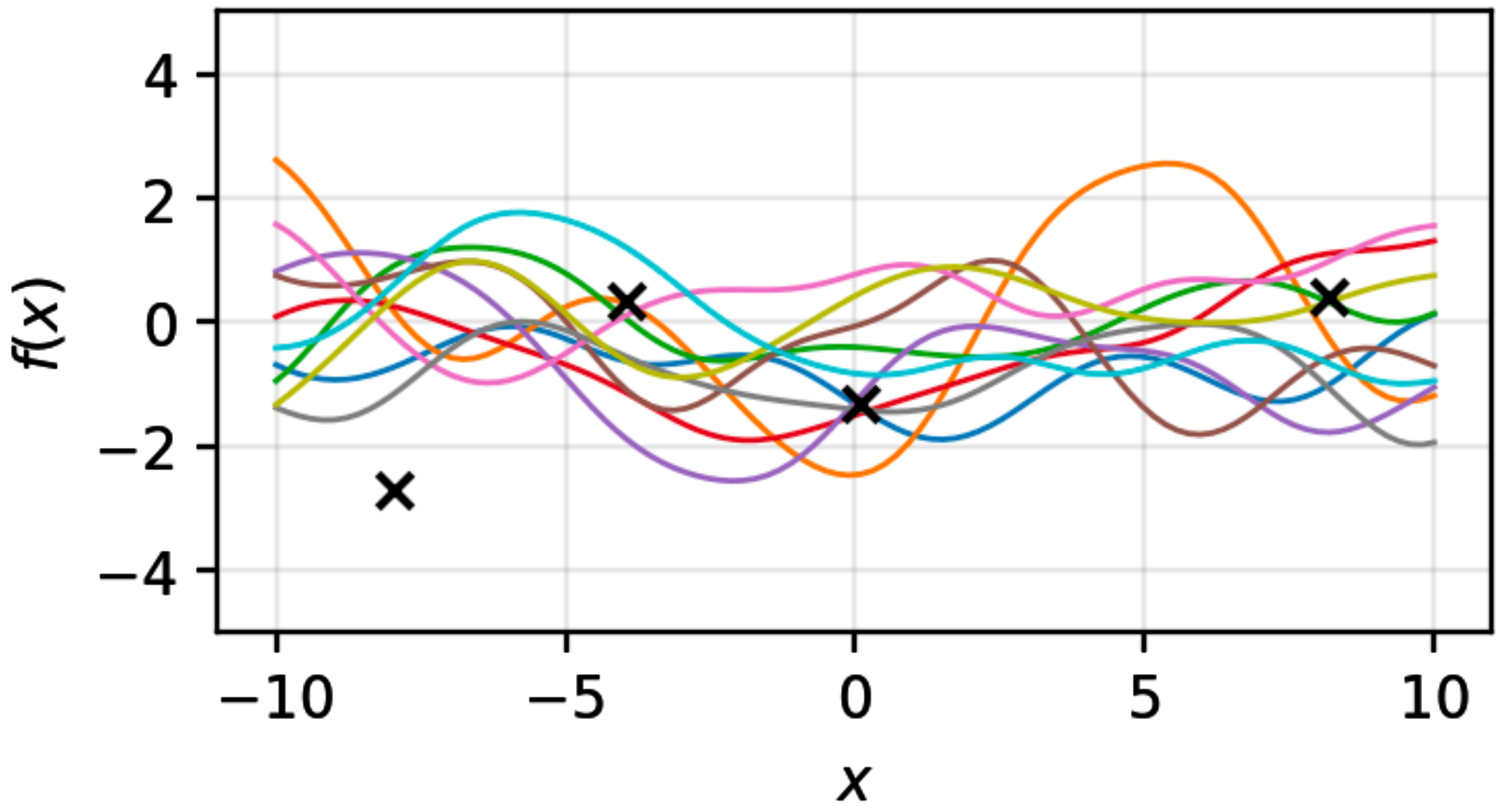
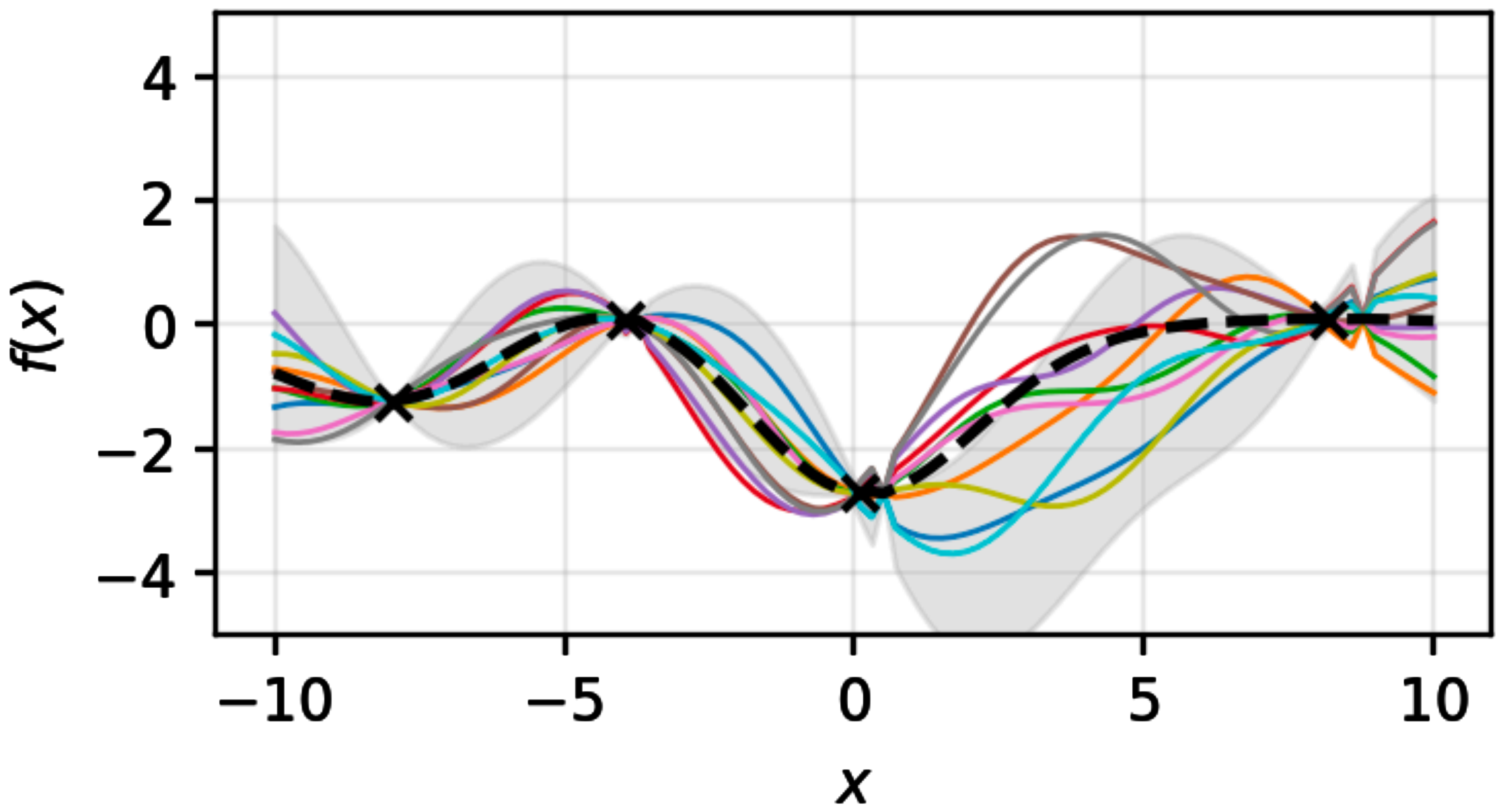
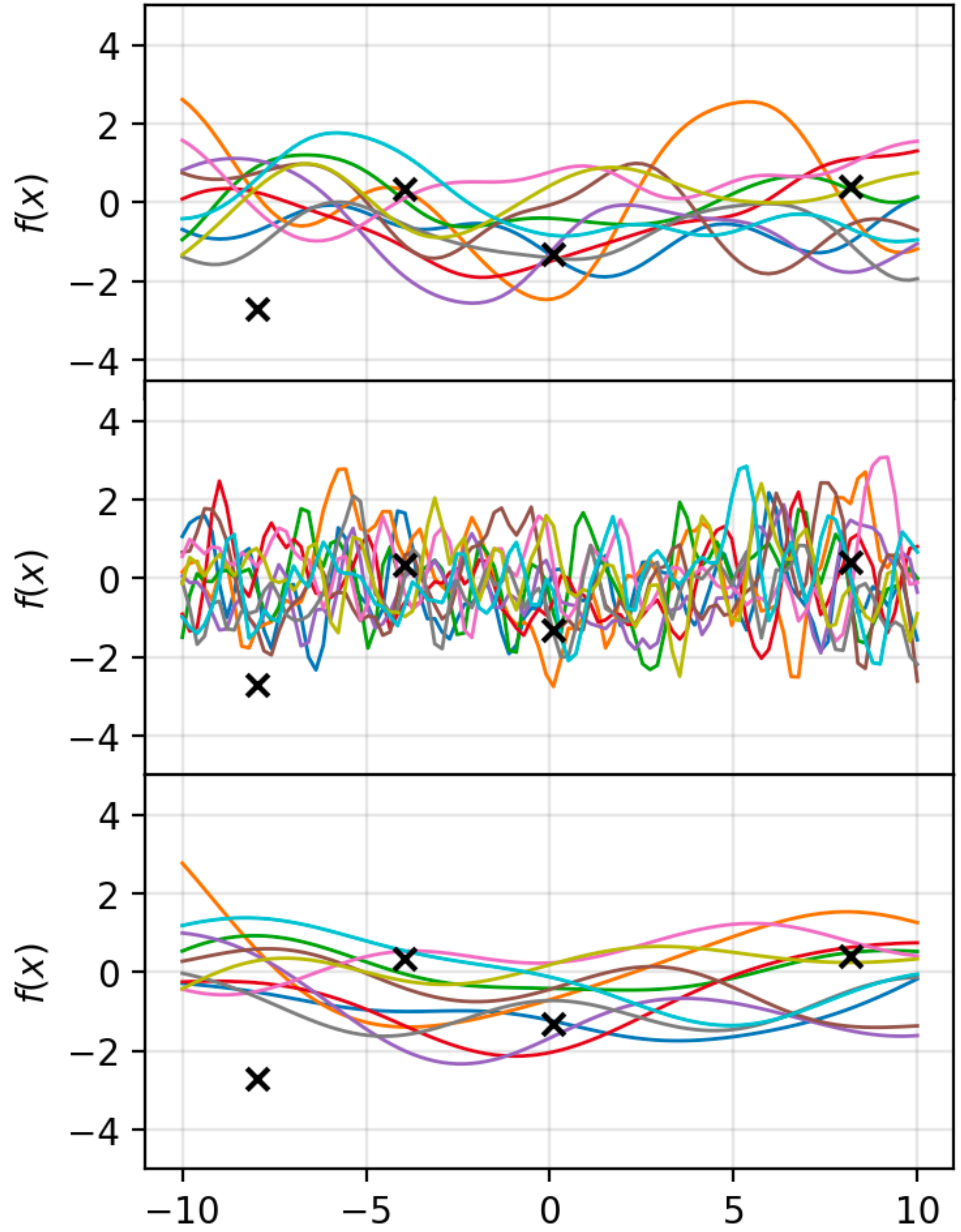
Uncertainty Estimate

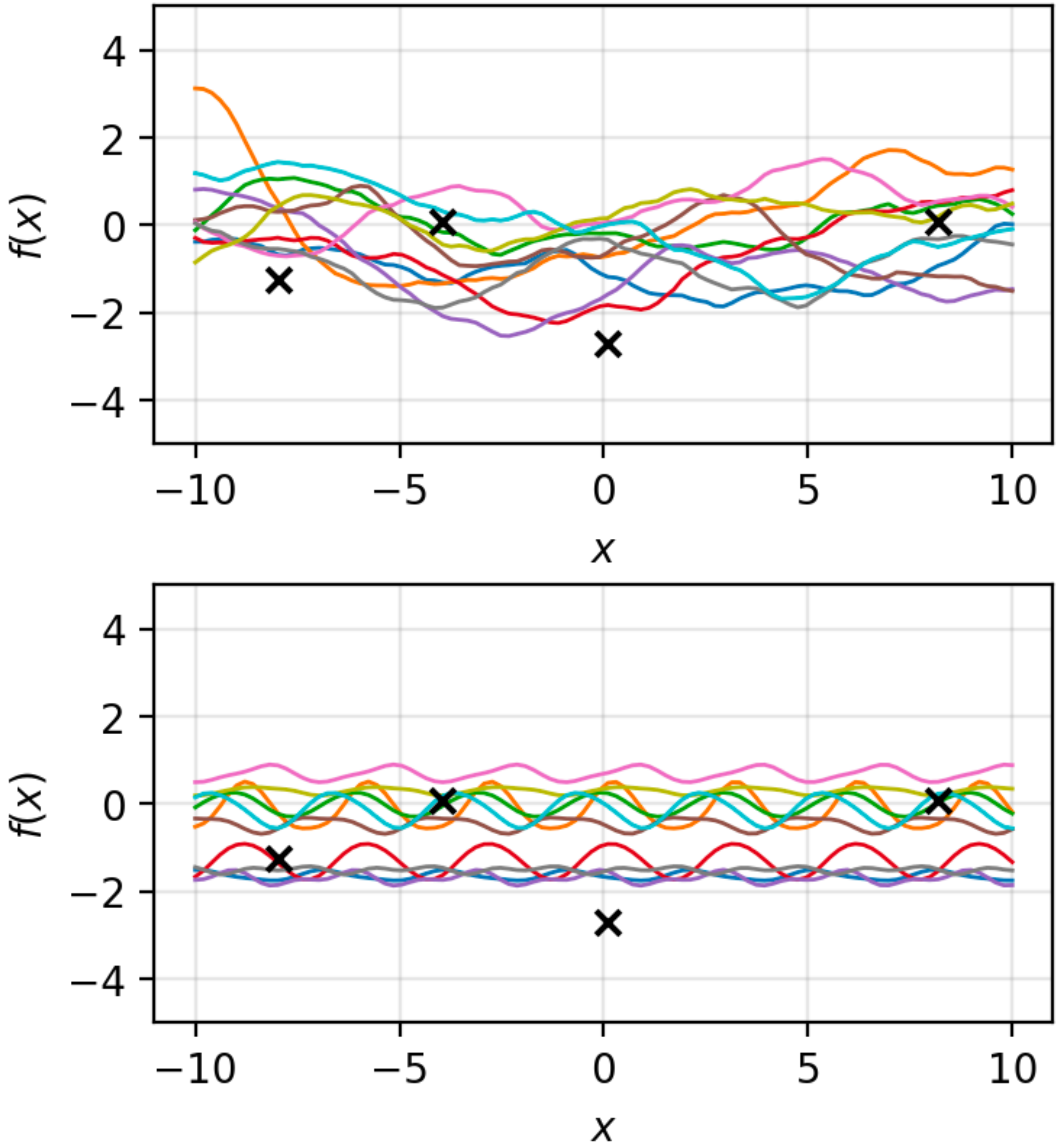
$$\Sigma_{f|y} = K_{**} - K_{*n}^\top (K_{nn} + \sigma^2 I)^{-1} K_{n*}$$





Different Kernels and Hparams





Different Modalities

Different Modalities

$k($  ,  $)$ $>$ $k($  ,  $)$

NNGP/NTK kernels [1]

Linearised Laplace [2]

Deep convolutional kernels

SNGP [3]

[1] Adlam, B., Lee, J., **Padhy, S.,** Nado, Z. and Snoek, J., 2023. Kernel Regression with Infinite-Width Neural Networks on Millions of Examples. *arXiv preprint*

[2] **Padhy, S.***, Antorán, J.,*, **Barbano, R.,** Nalisnick, E., ... and Hernández-Lobato, J.M.. Sampling-based inference for large linear models, with application to linearised Laplace. ***ICLR 2023***

[3] **Padhy, S.***, Liu, J. Z.*, Ren, J.*, Lin, Z., Wen, Y., Jerfel, G., ... & Lakshminarayanan, B. A simple approach to improve single-model deep uncertainty via distance-awareness. ***JMLR 2023***

[4] **Padhy, S.***, Lin, J. A.*, Antorán, J.*, Tripp, A., Terenin, A., Szepesvári, C., ... & Janz, D. Stochastic Gradient Descent for Gaussian Processes Done Right. ***ICLR 2024***

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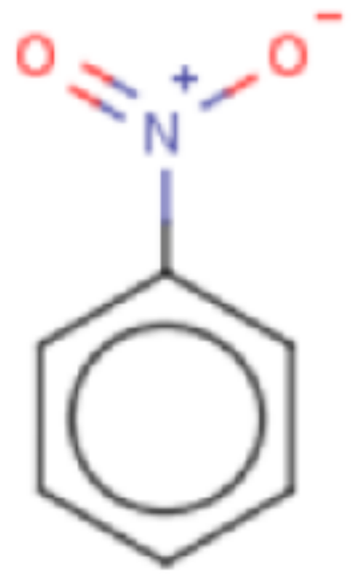
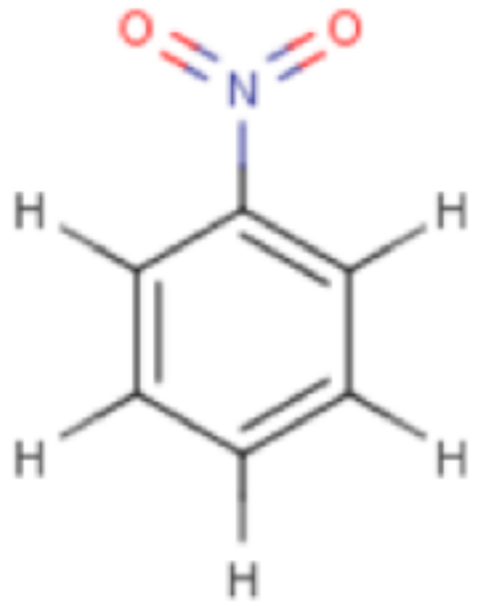
$k($  ,  $)$

Tanimoto kernels [4]

Graph NNGP kernels [1]

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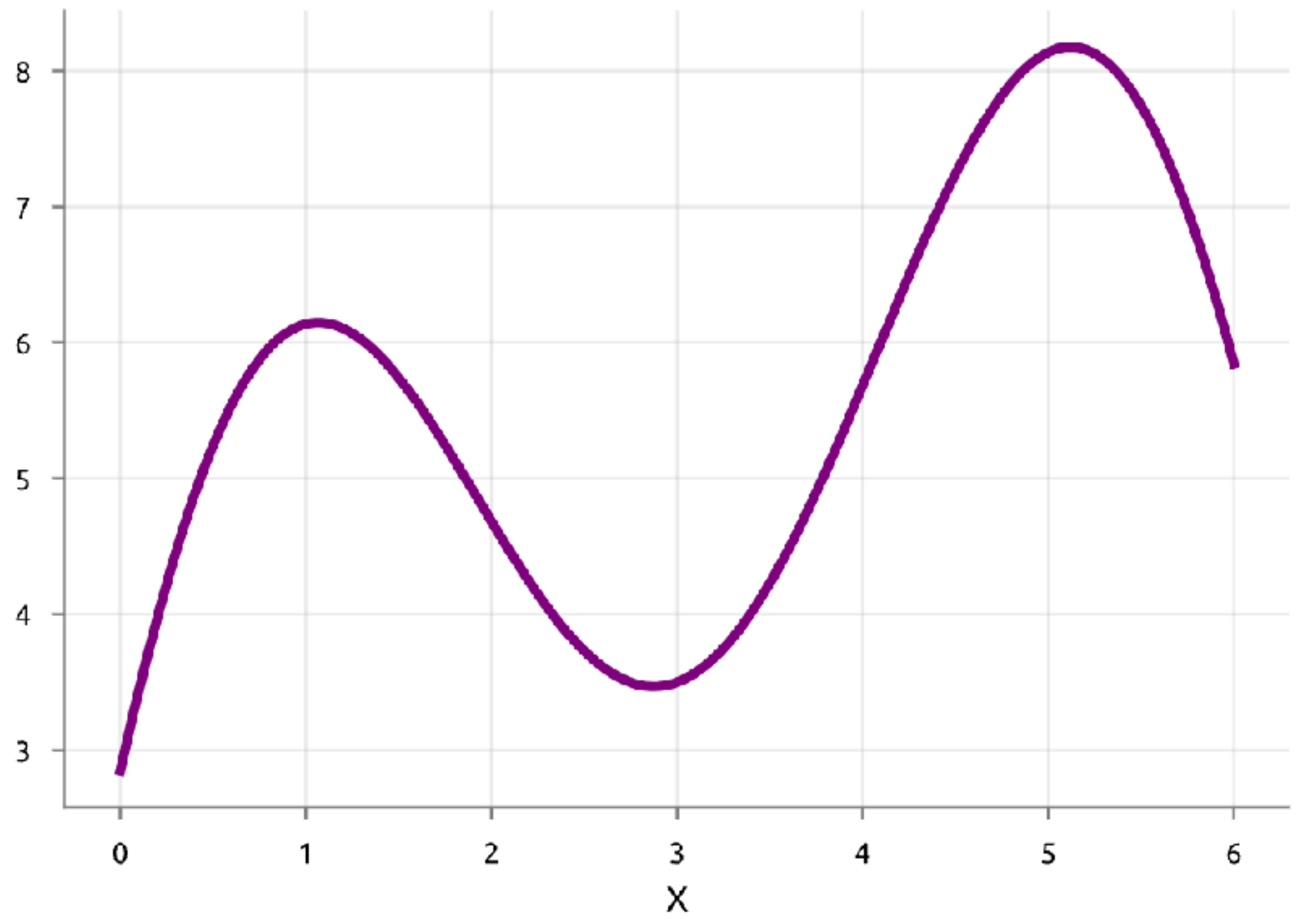
Applications where GPs shine

- We have a function $f(x)$ that is very expensive to evaluate
  - We want to approximate this function cheaply: **Active Learning**
  - We want to find the max value of $f(x)$: **BayesOpt**



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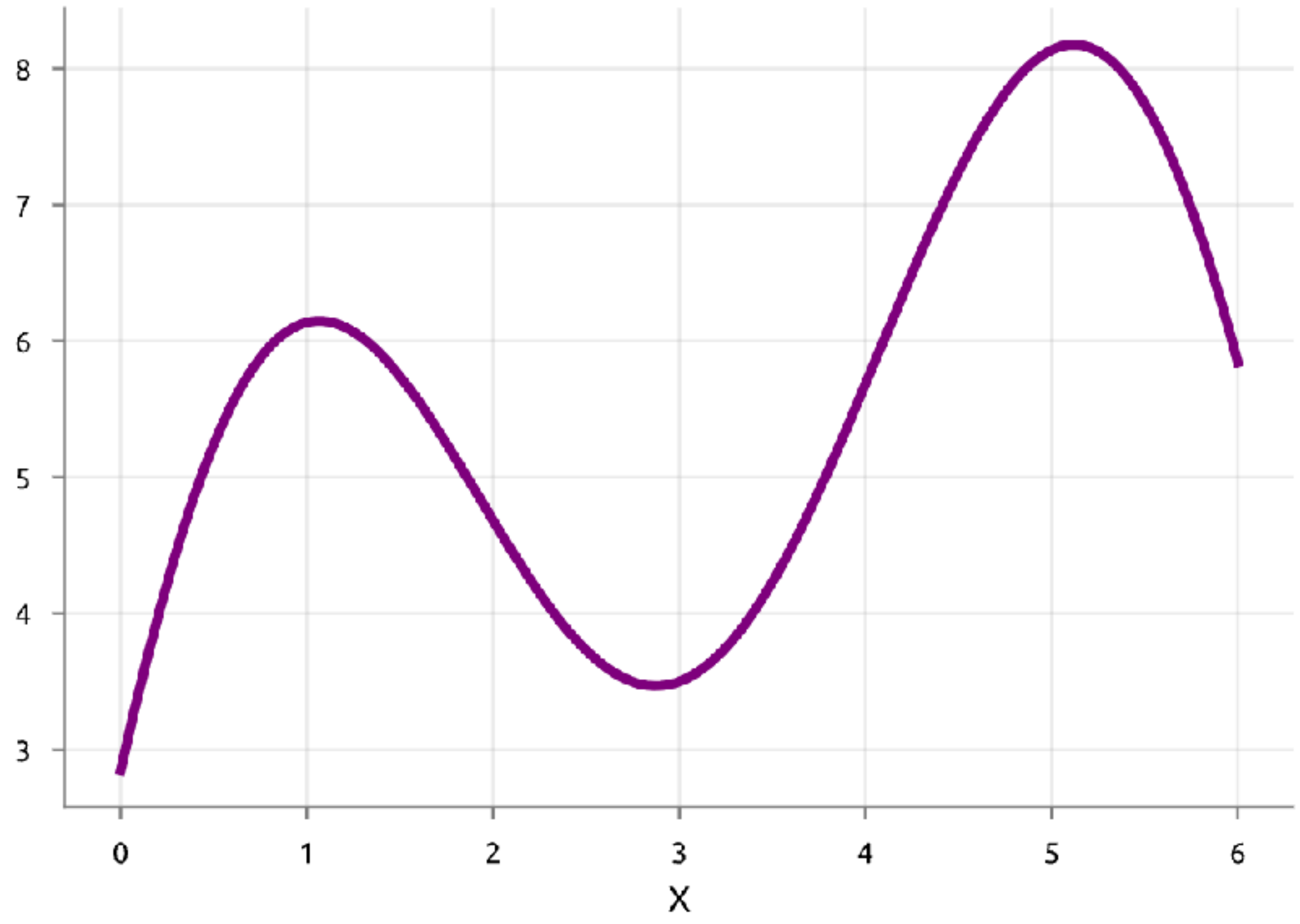
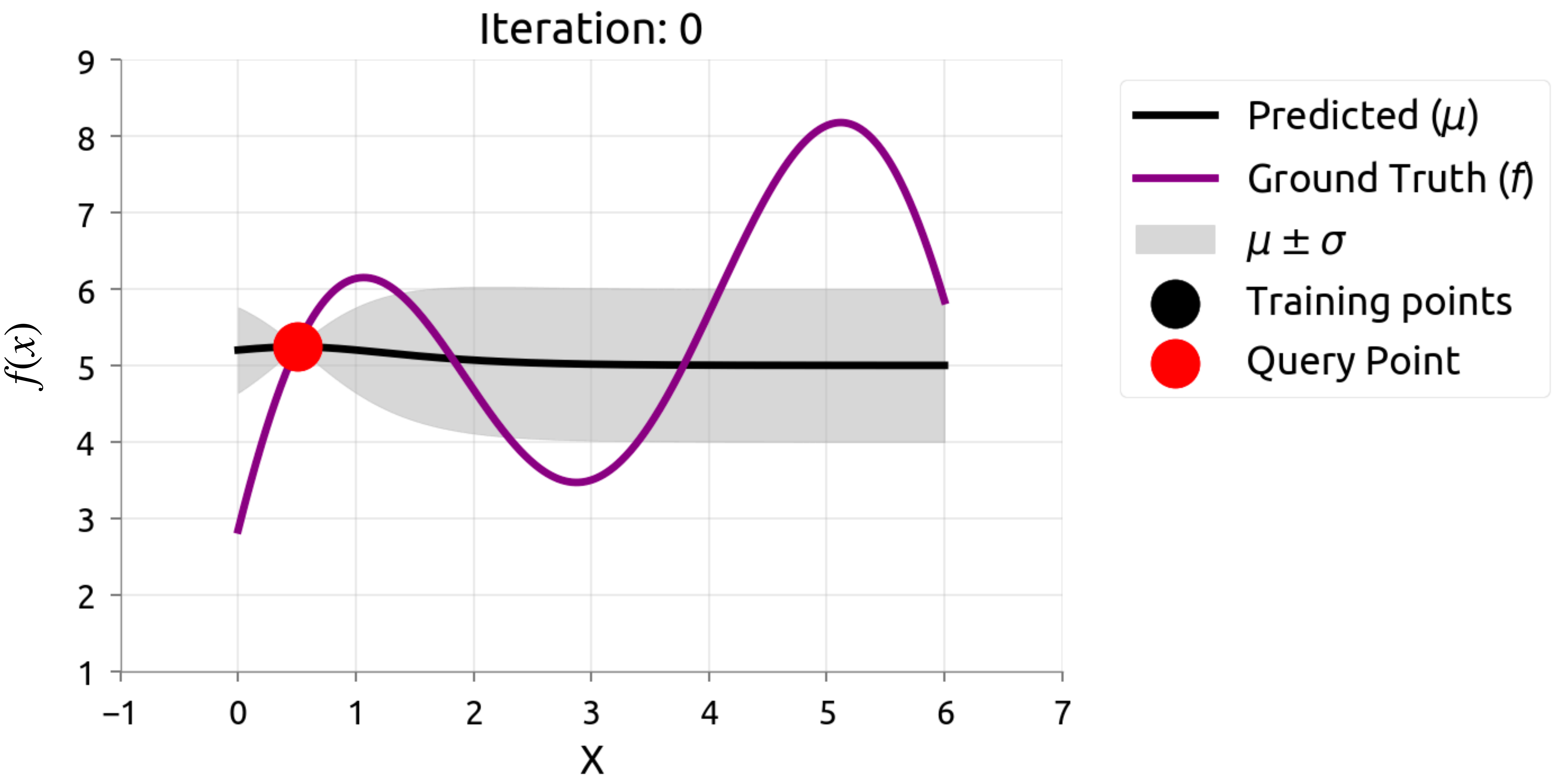


[1] https://distill.pub/2020/bayesian-optimization/

Active Learning



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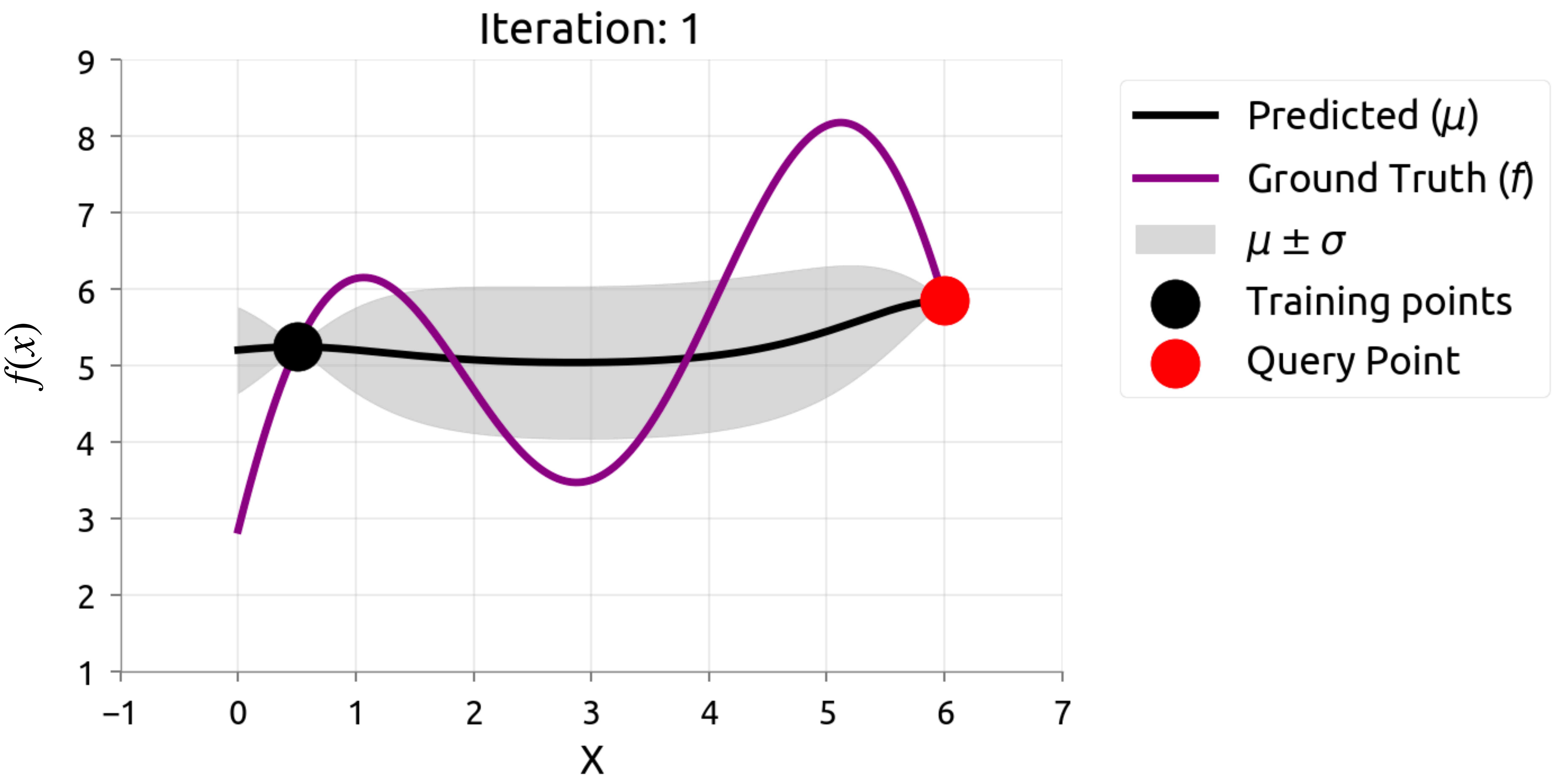

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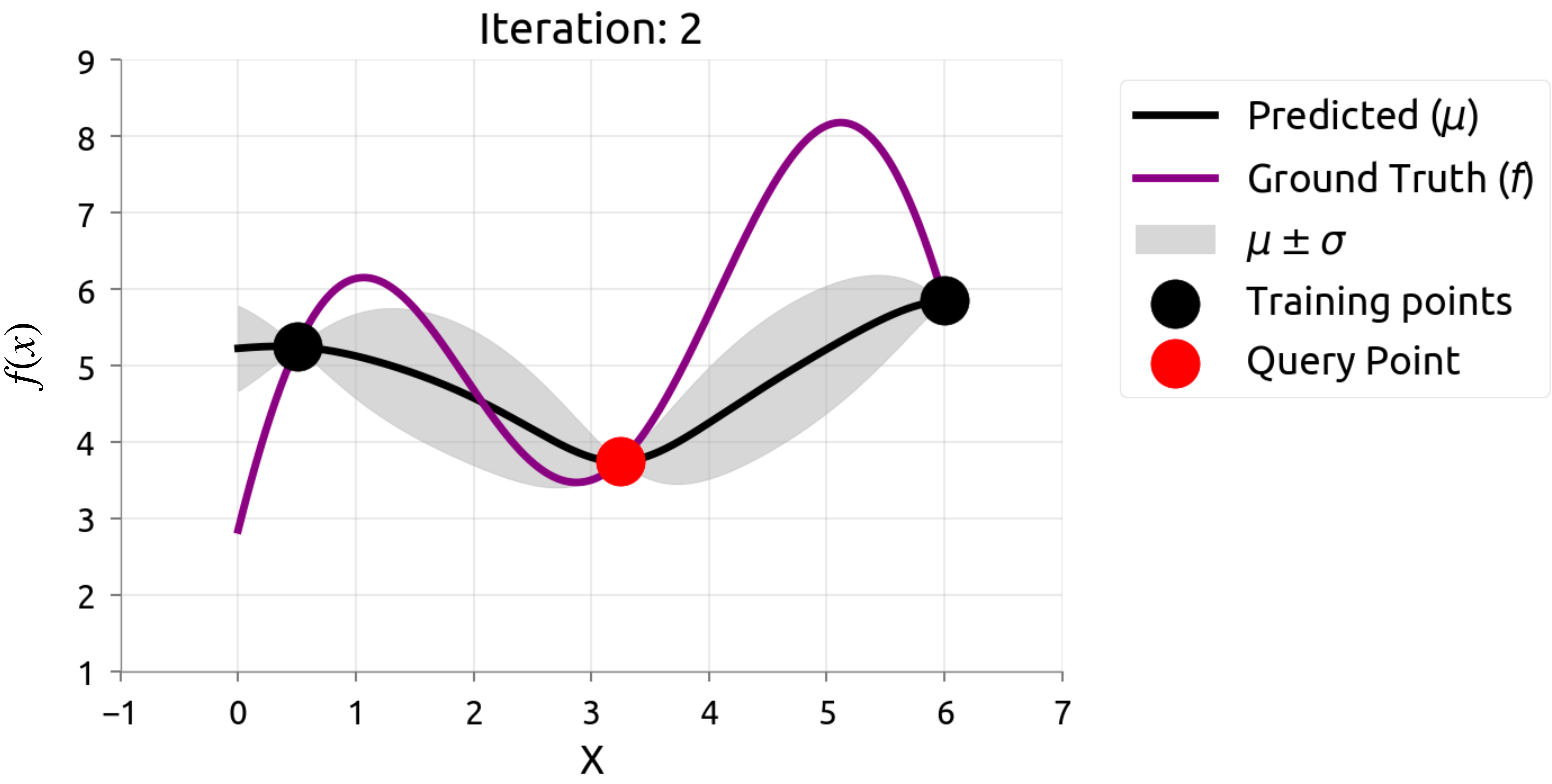

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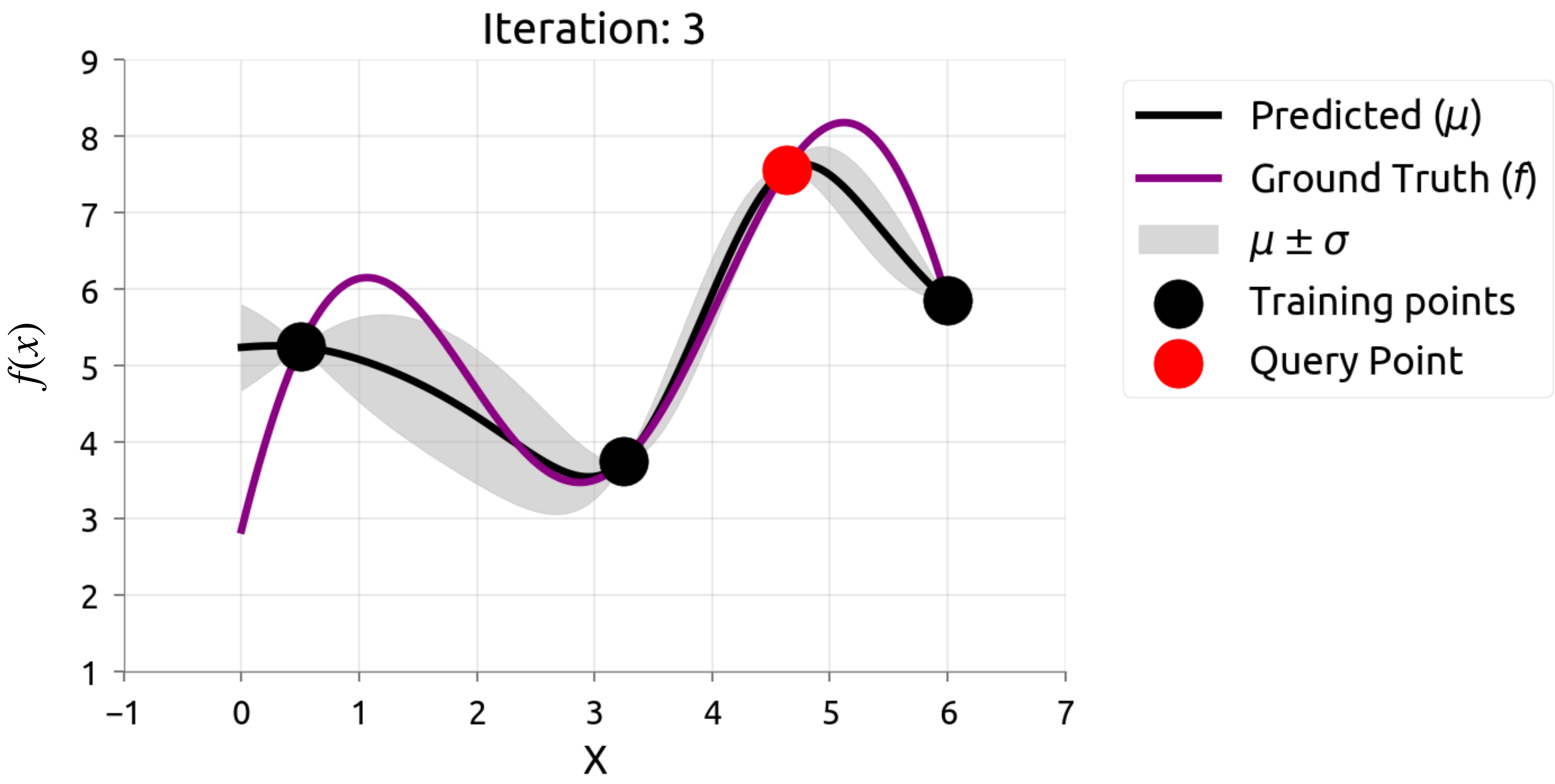

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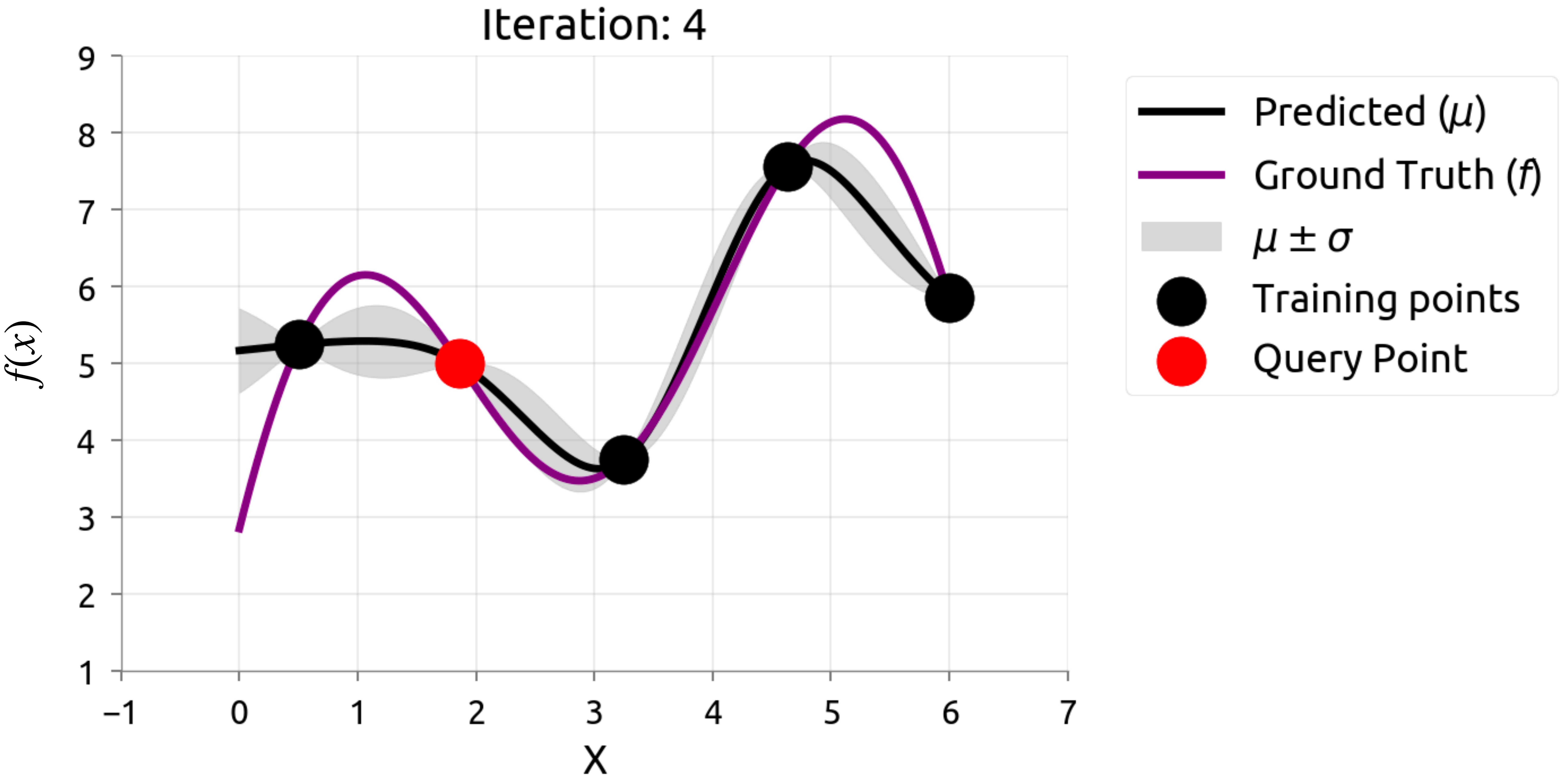

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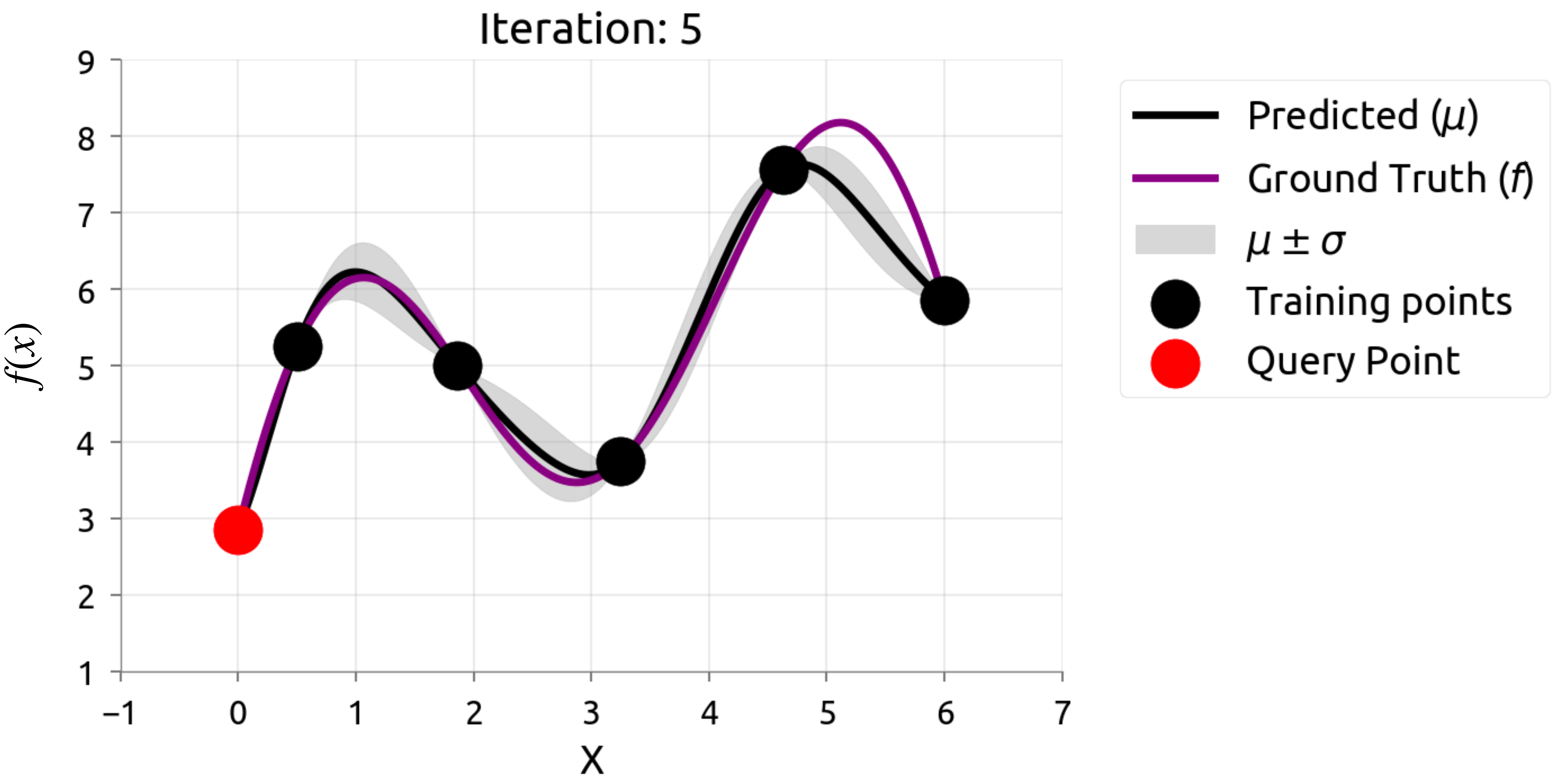

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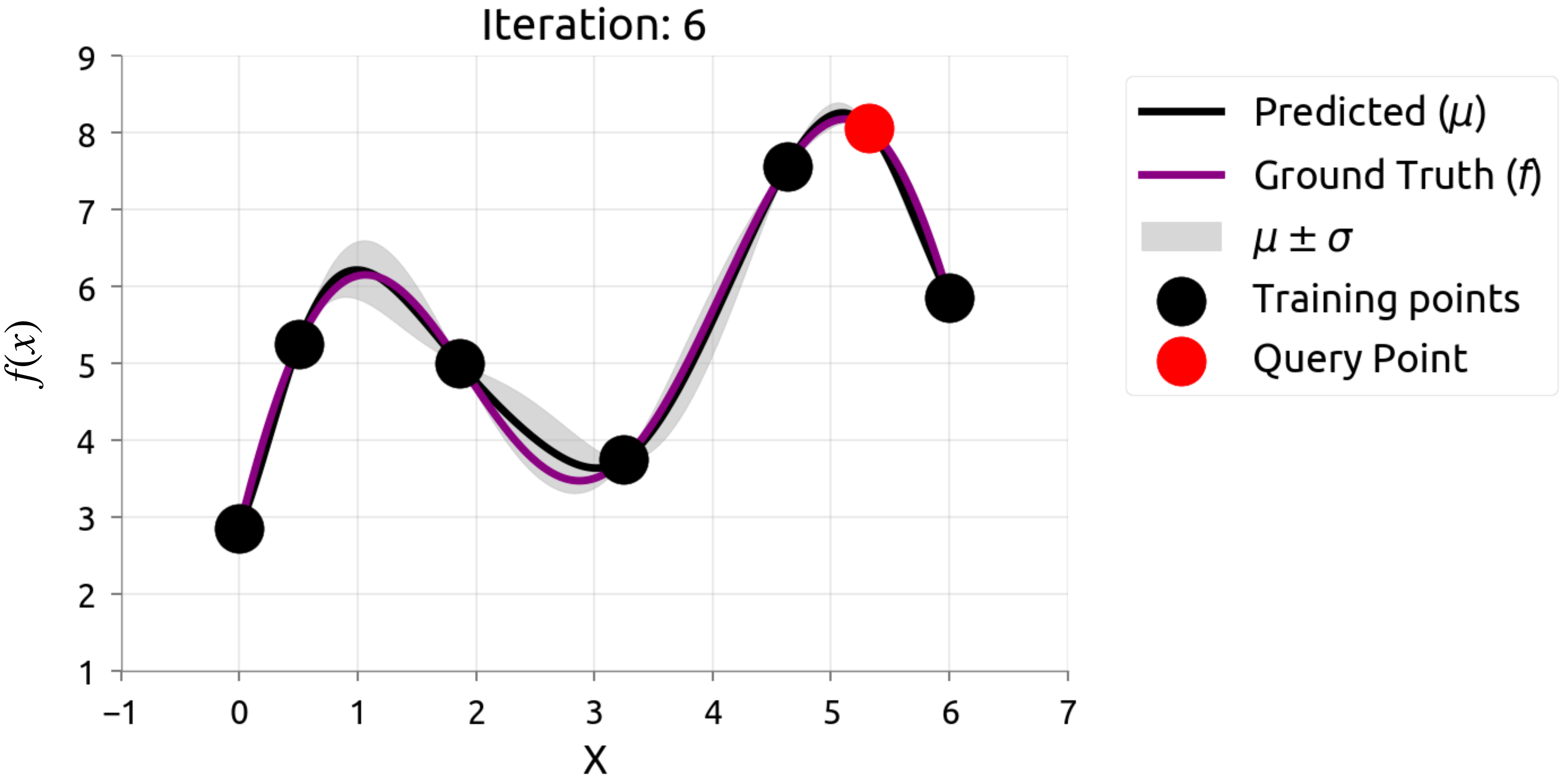

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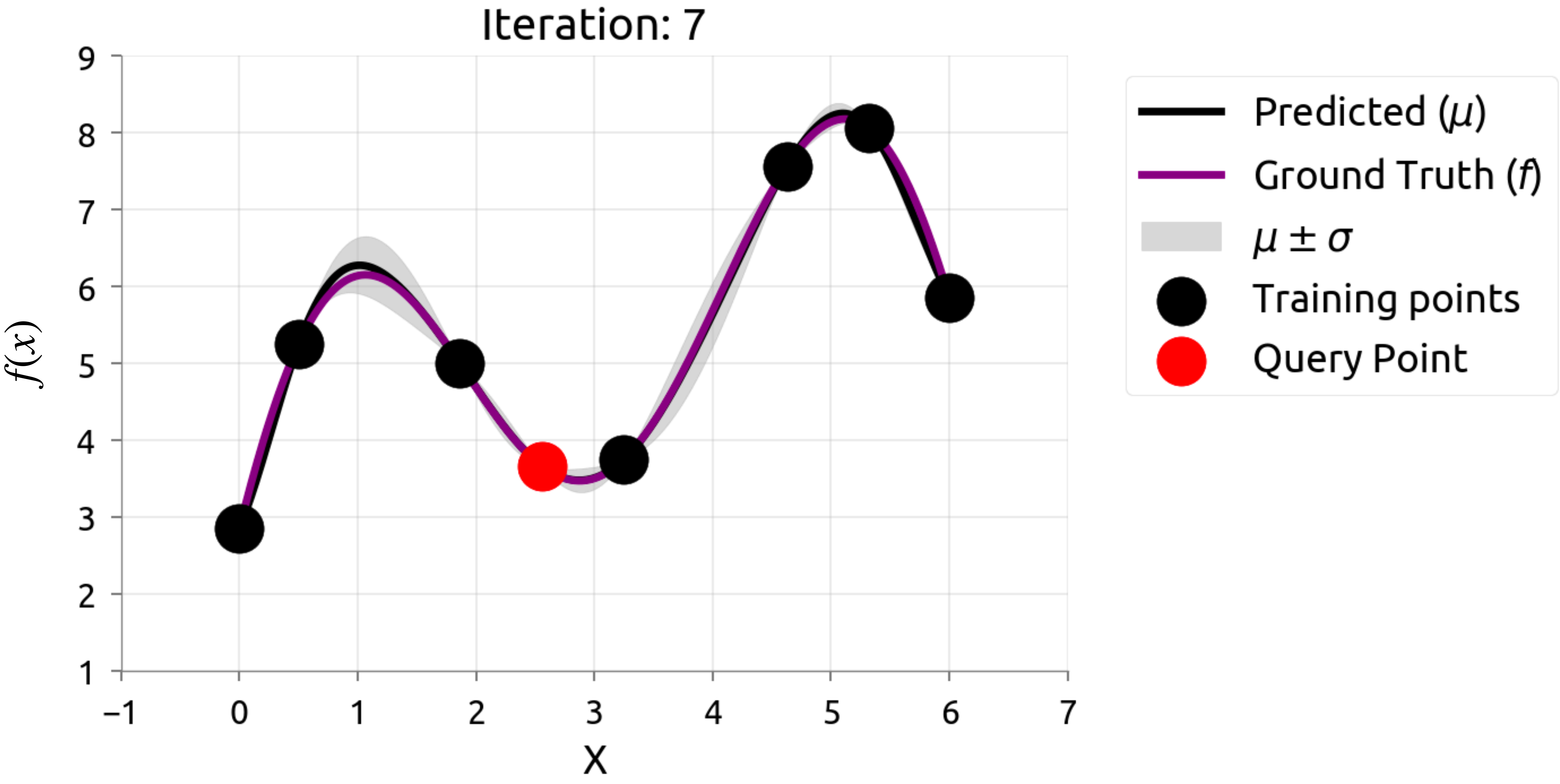

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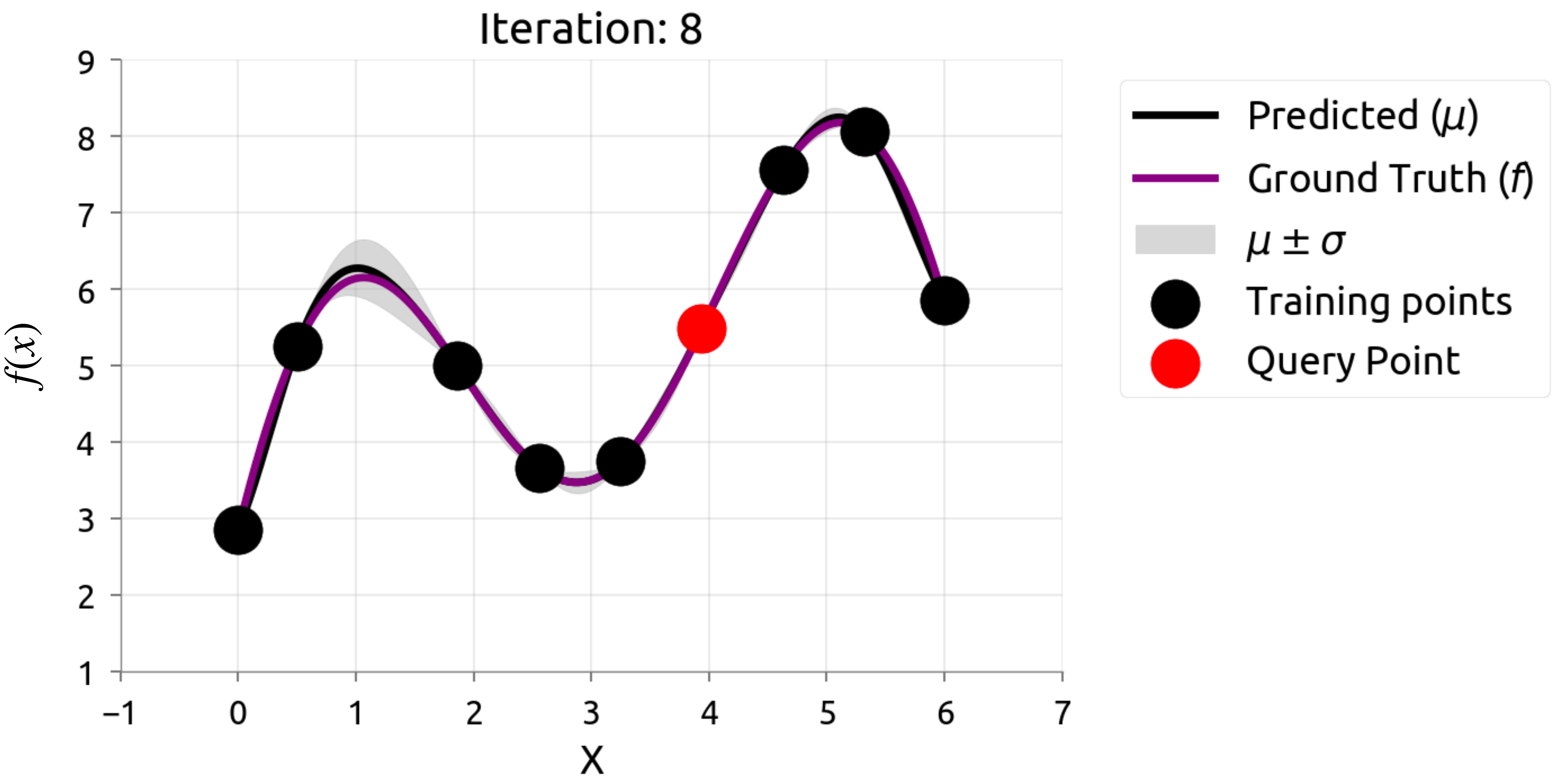

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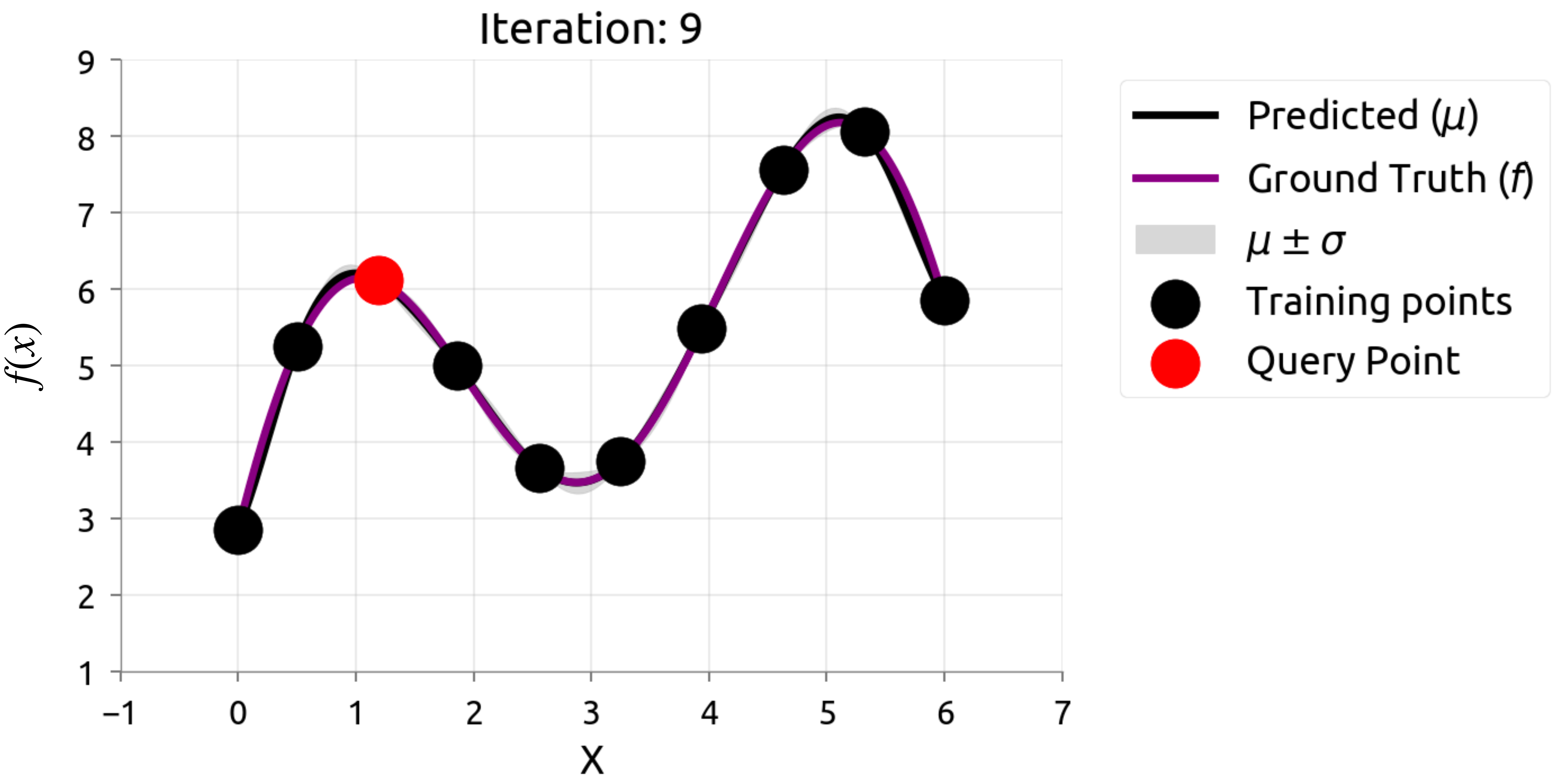
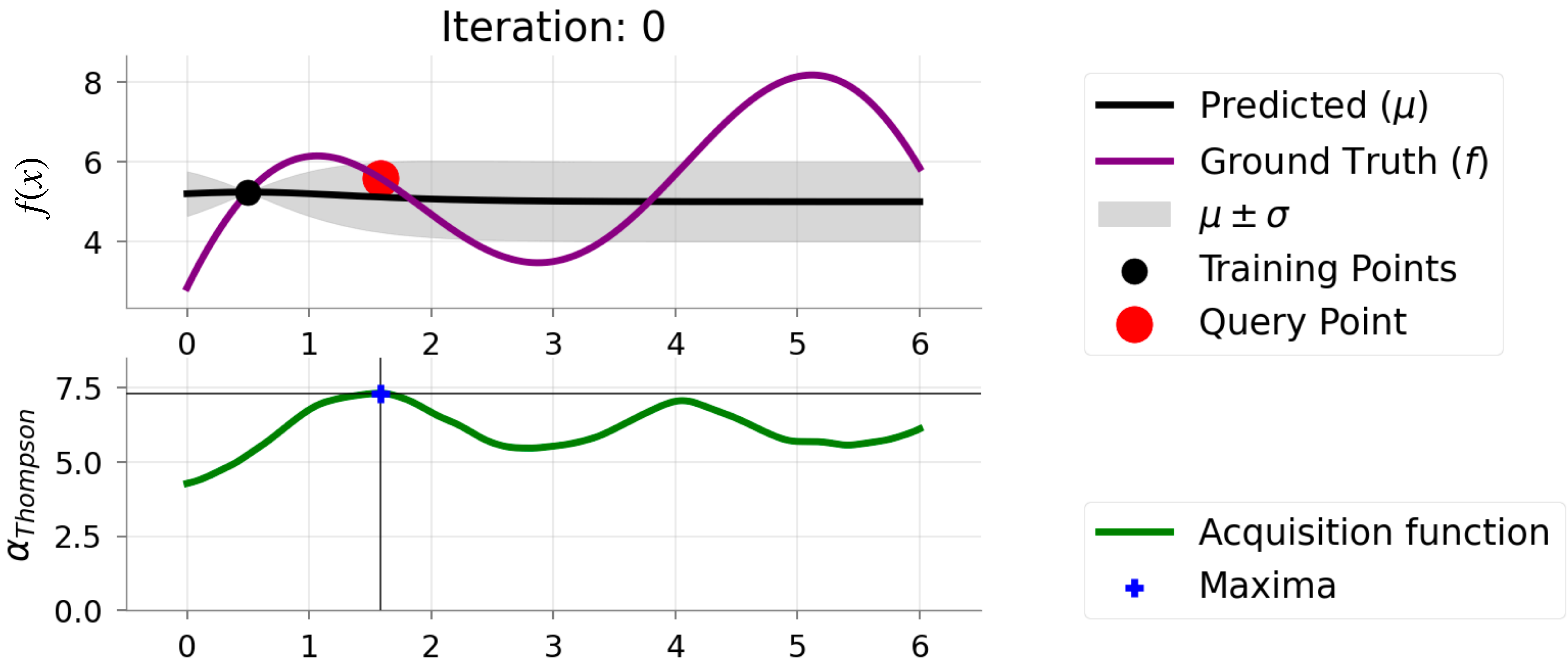


[1] https://distill.pub/2020/bayesian-optimization/

BayesOpt w/ Thompson Sampling



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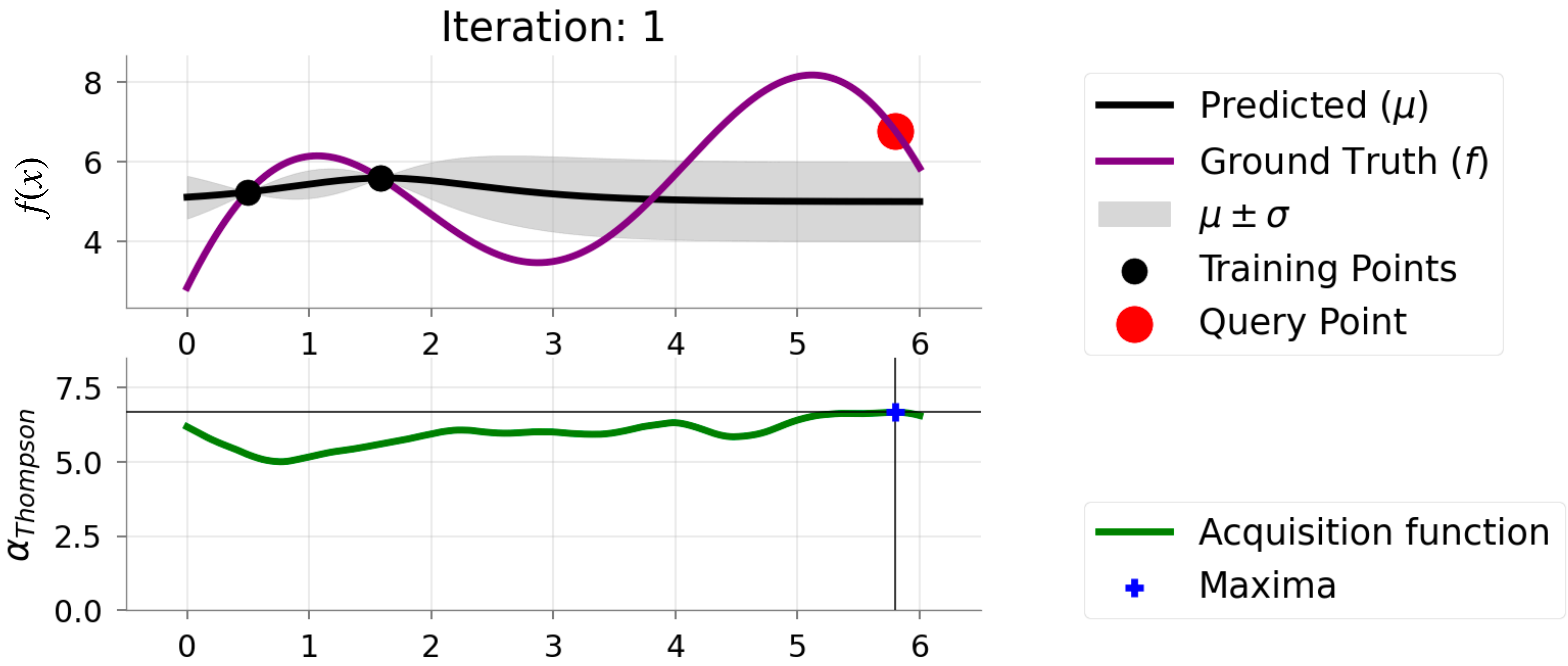

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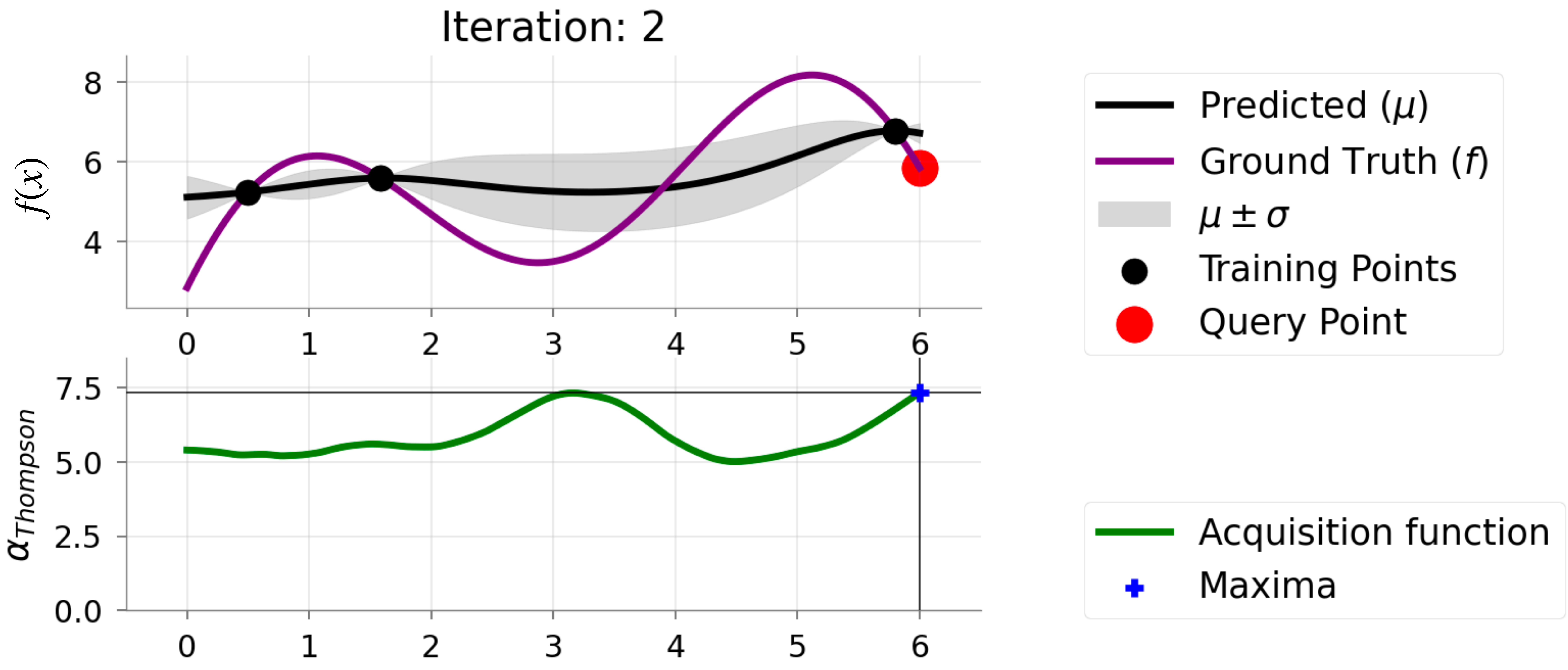

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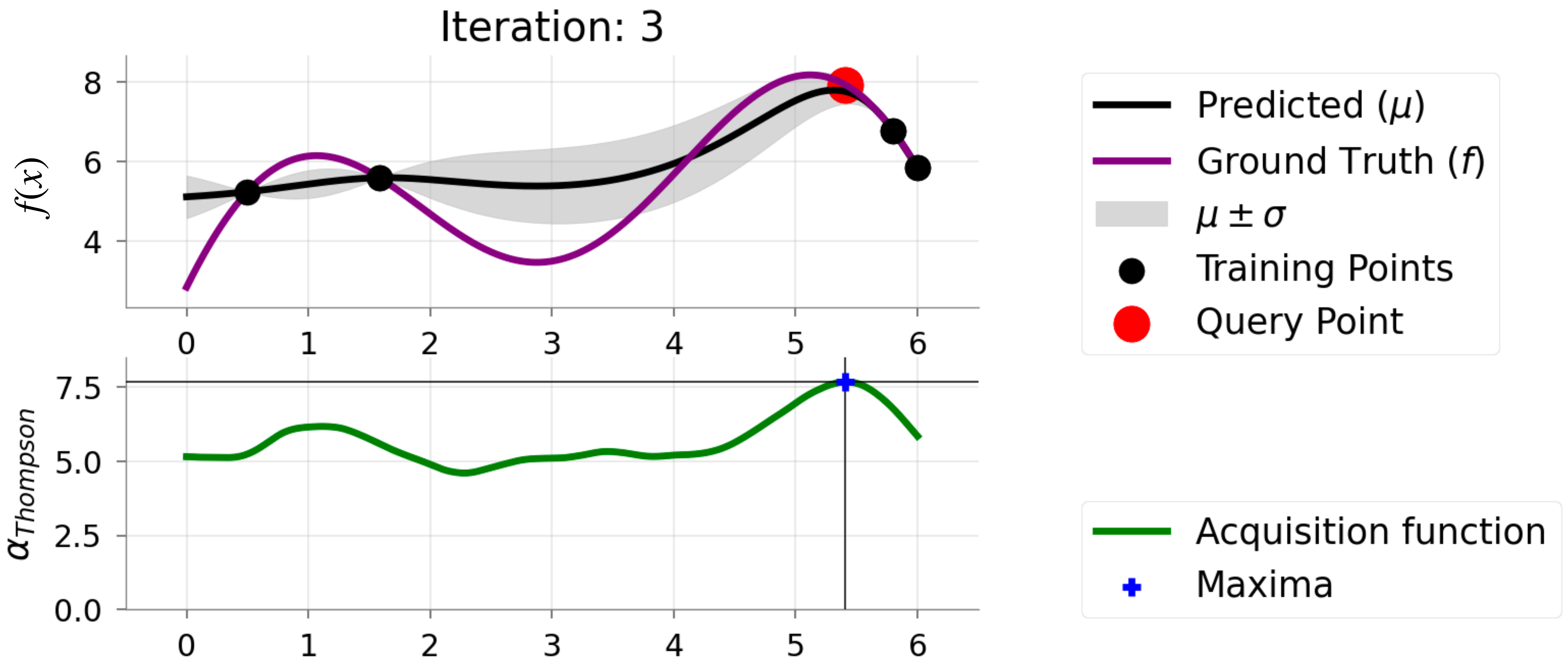

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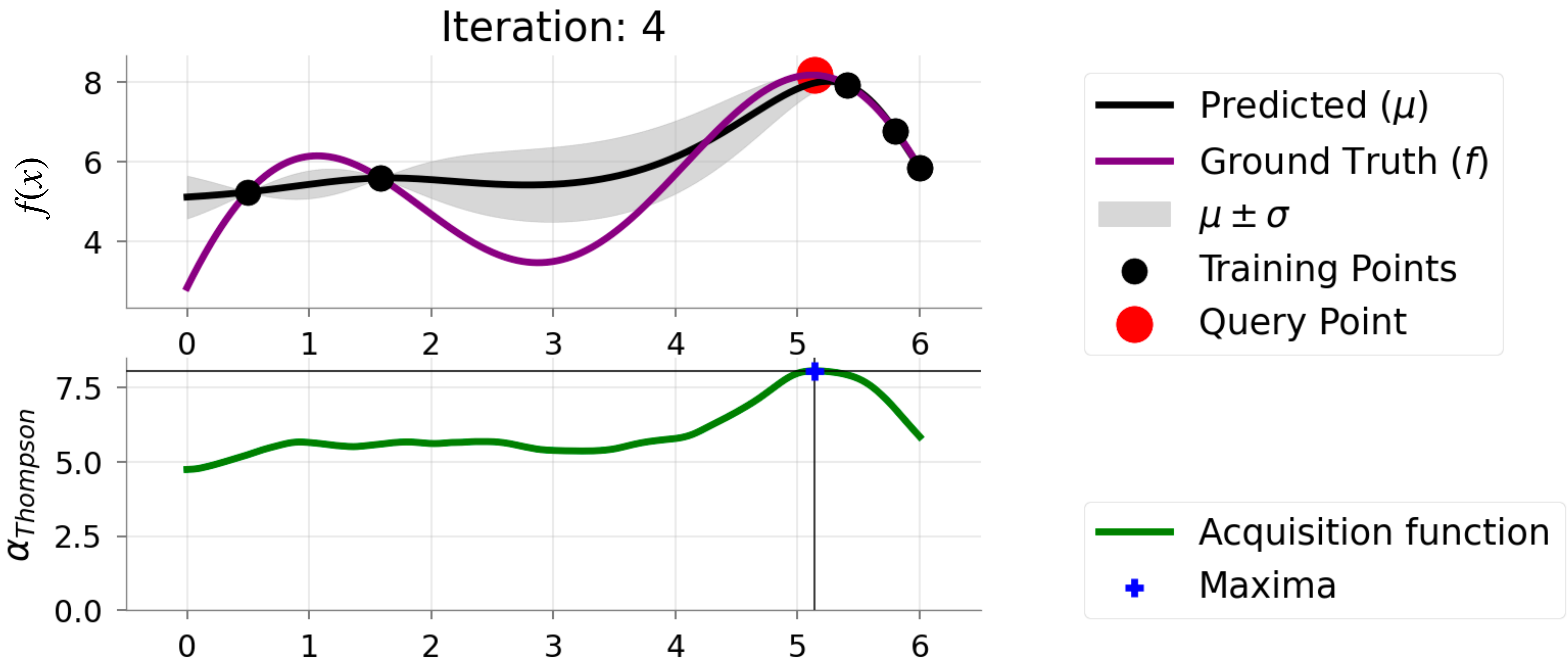

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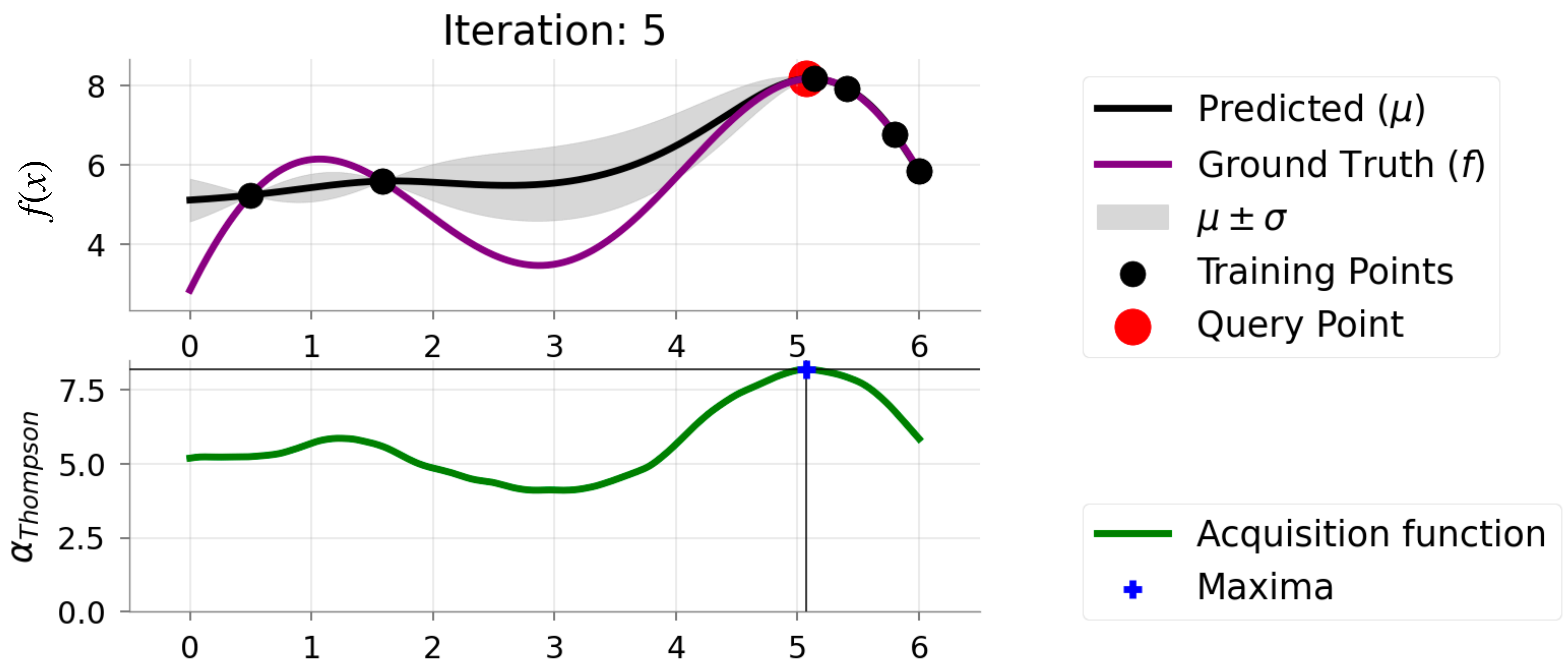

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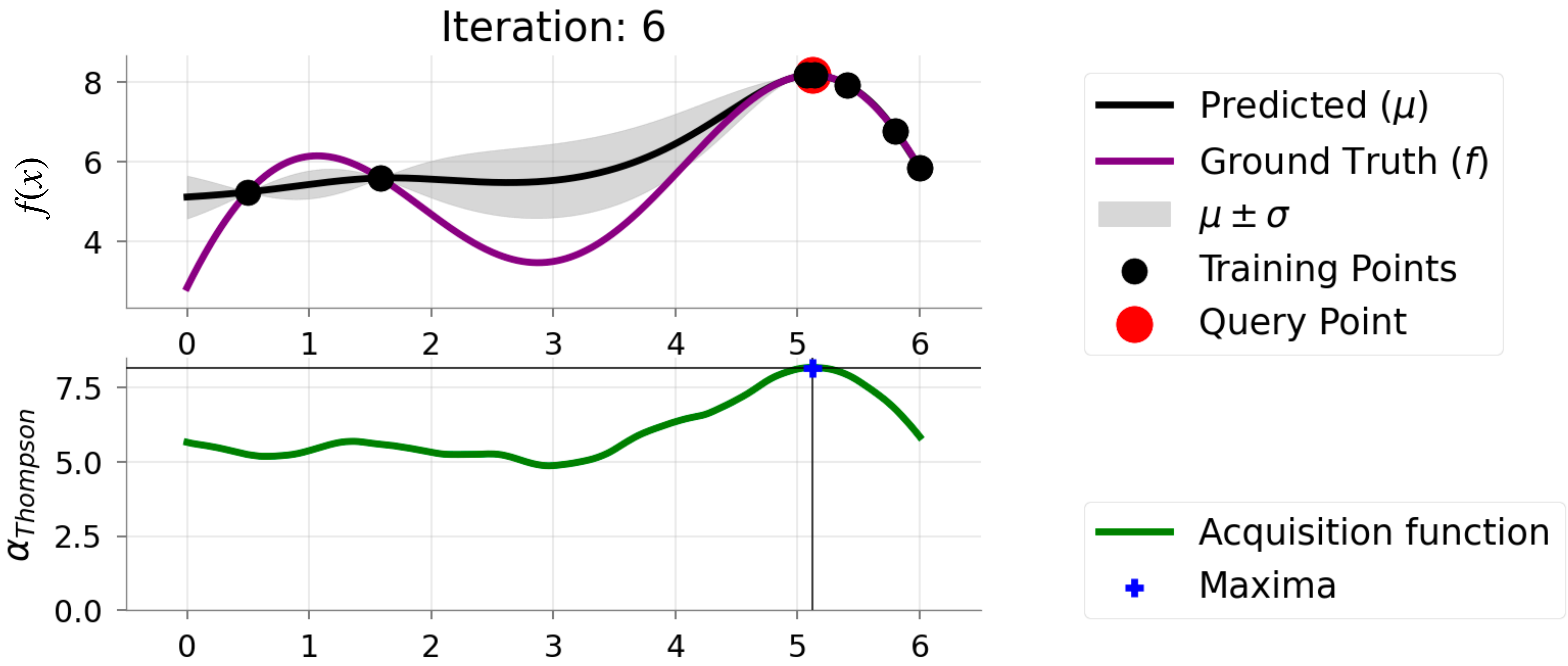

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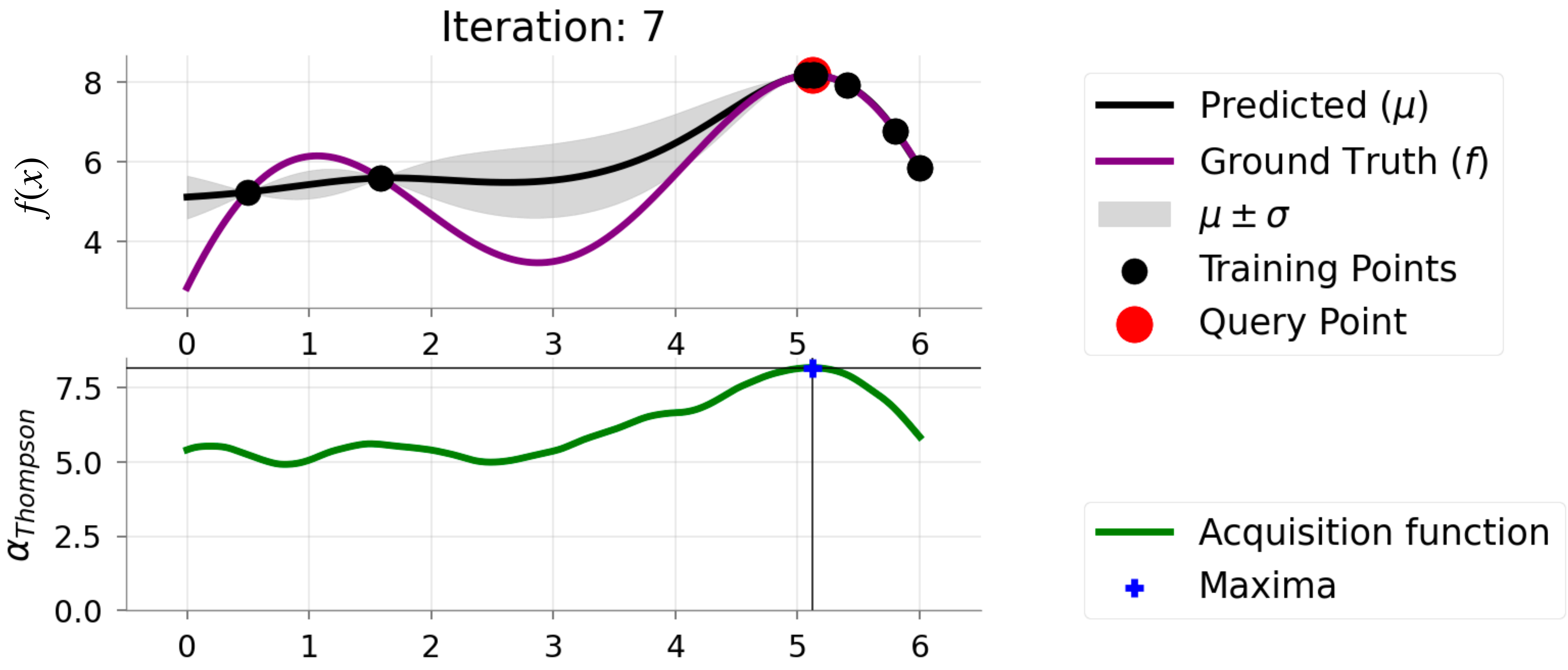

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Computational Considerations

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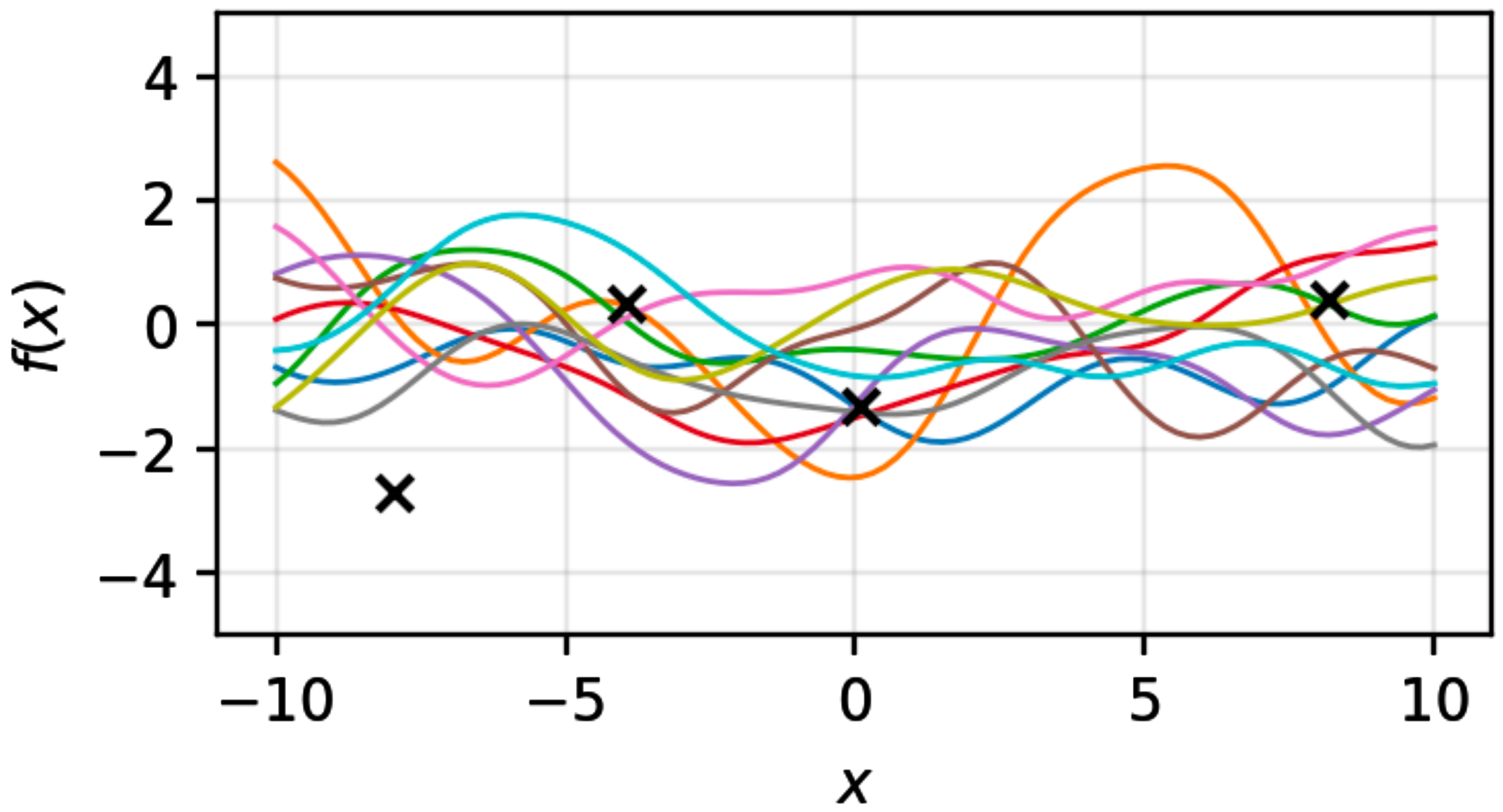

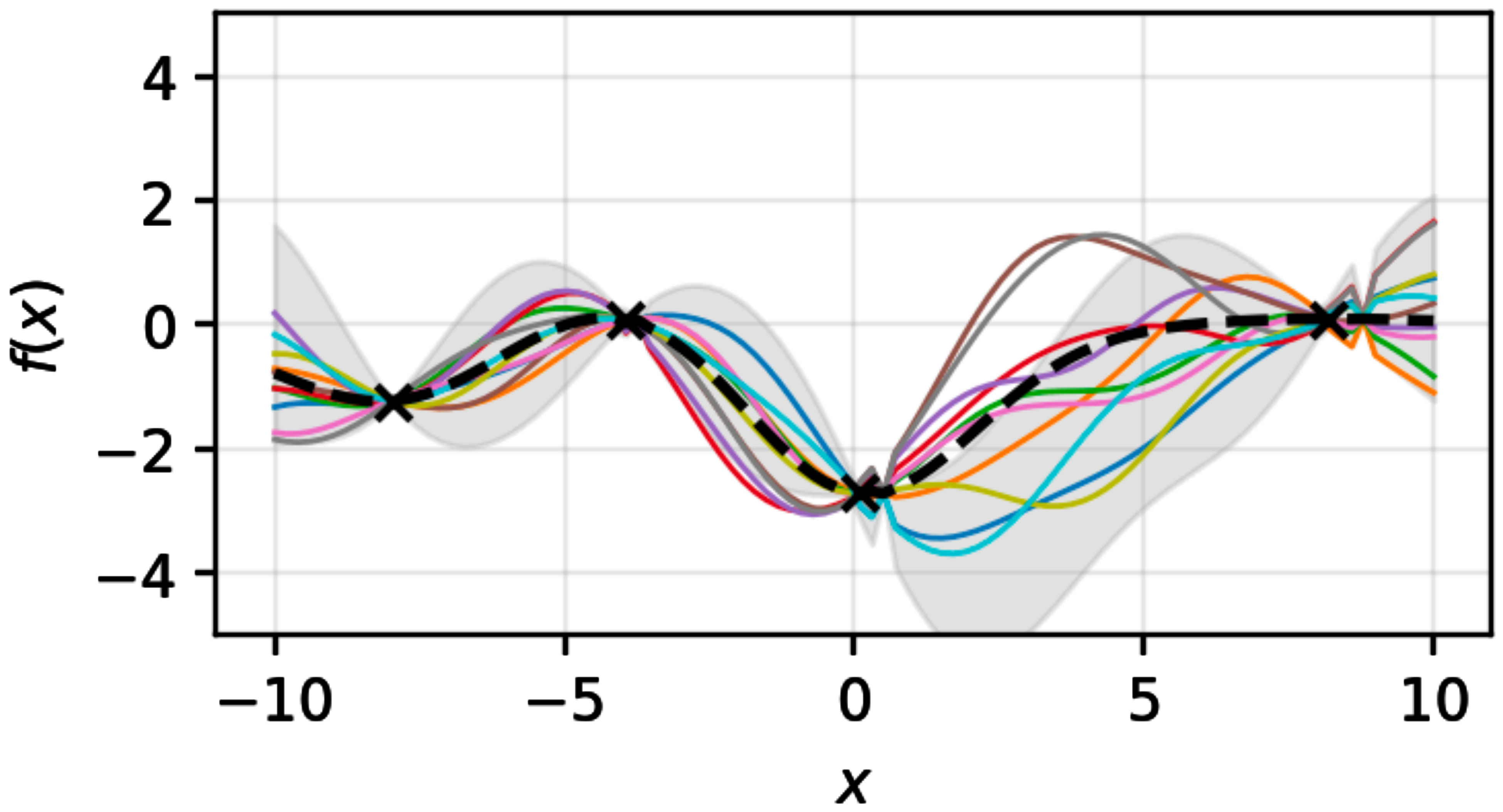

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Predictive Mean

$\mathcal{O}(n^3)$

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Uncertainty Estimate

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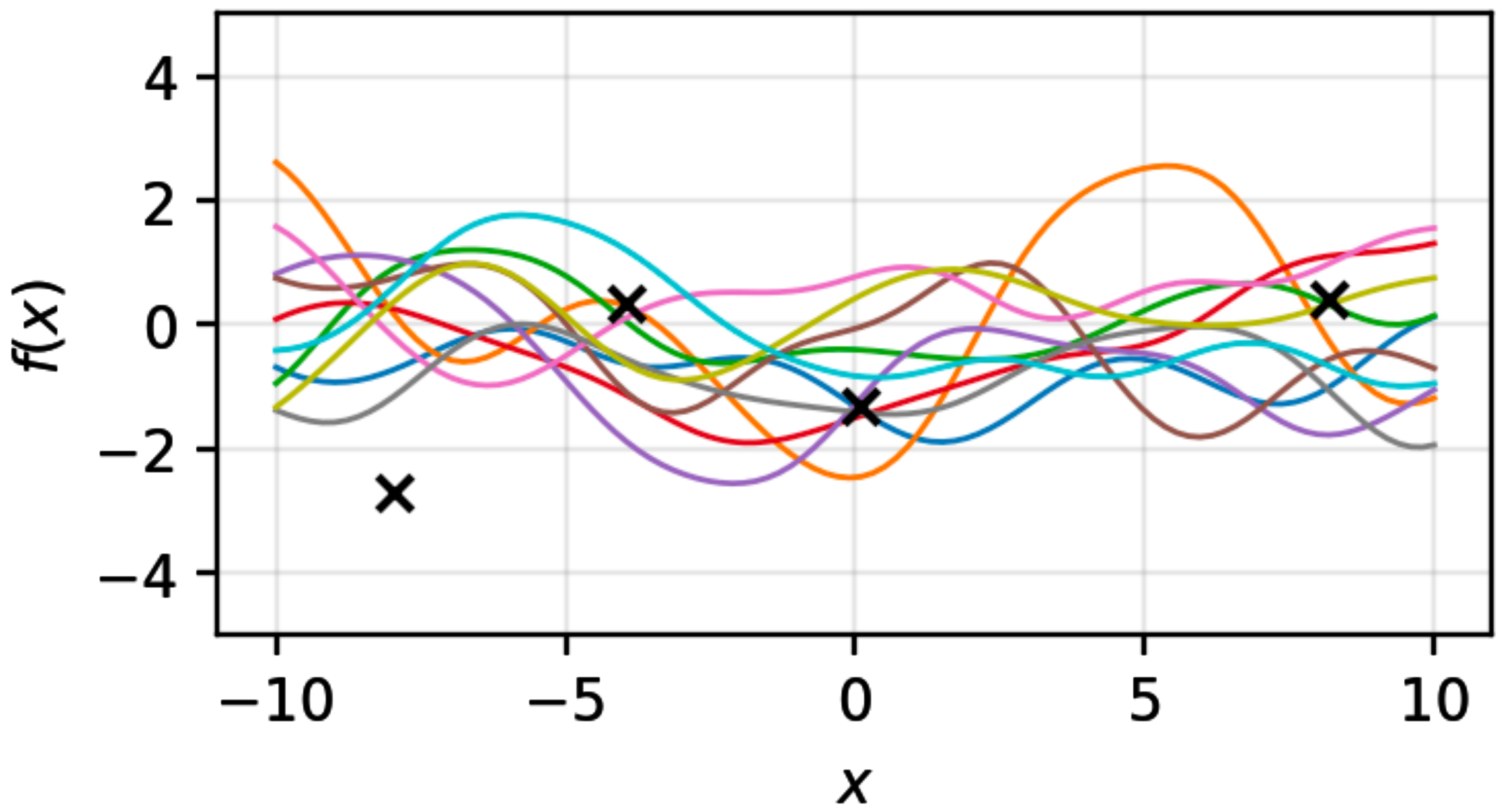

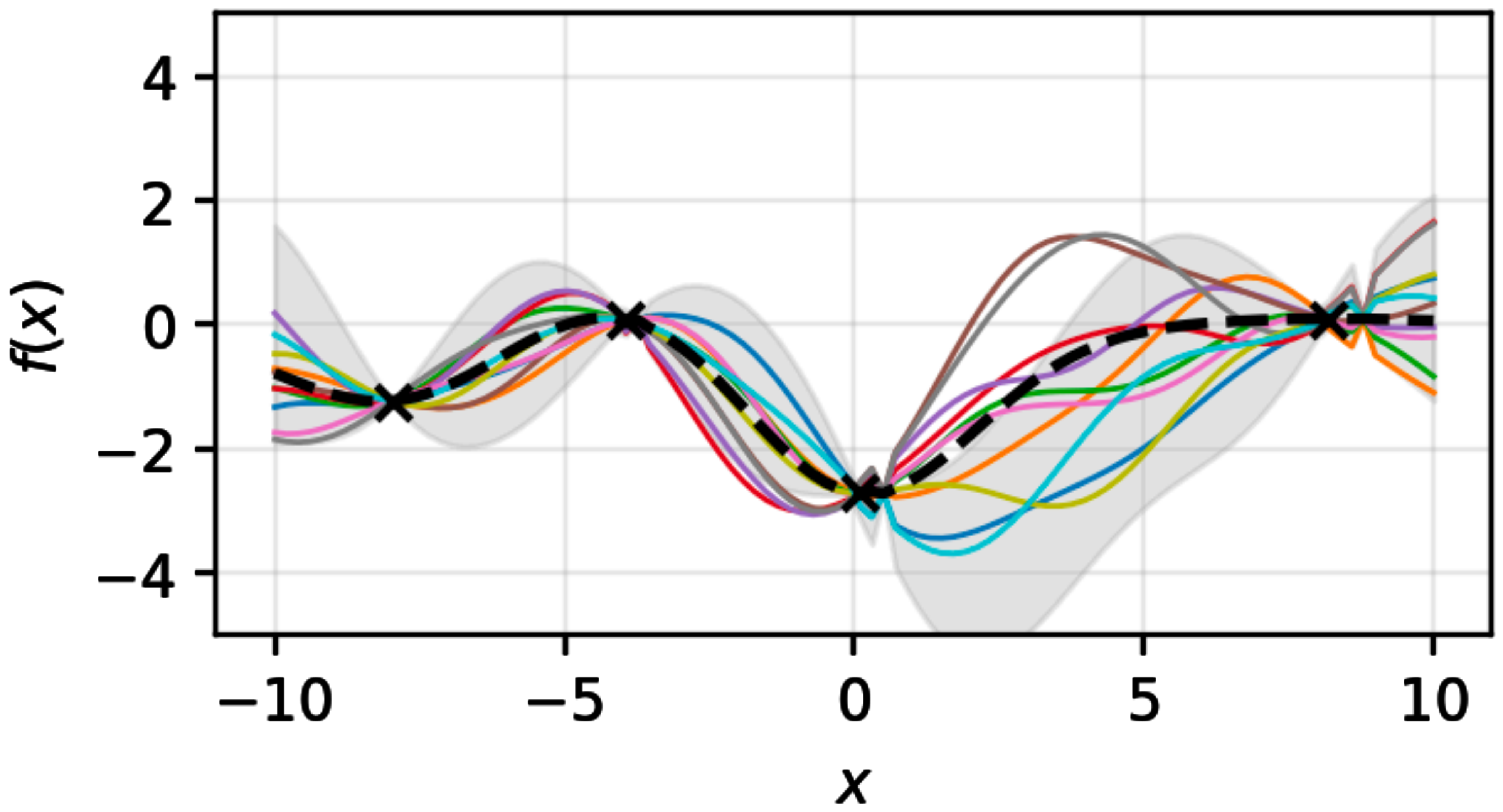

Variational Gaussian Processes

Idea: Kernel matrix can be approximated as $K_{nn} \approx UQU^T$ where $Q \in \mathbb{R}^{m \times m}$

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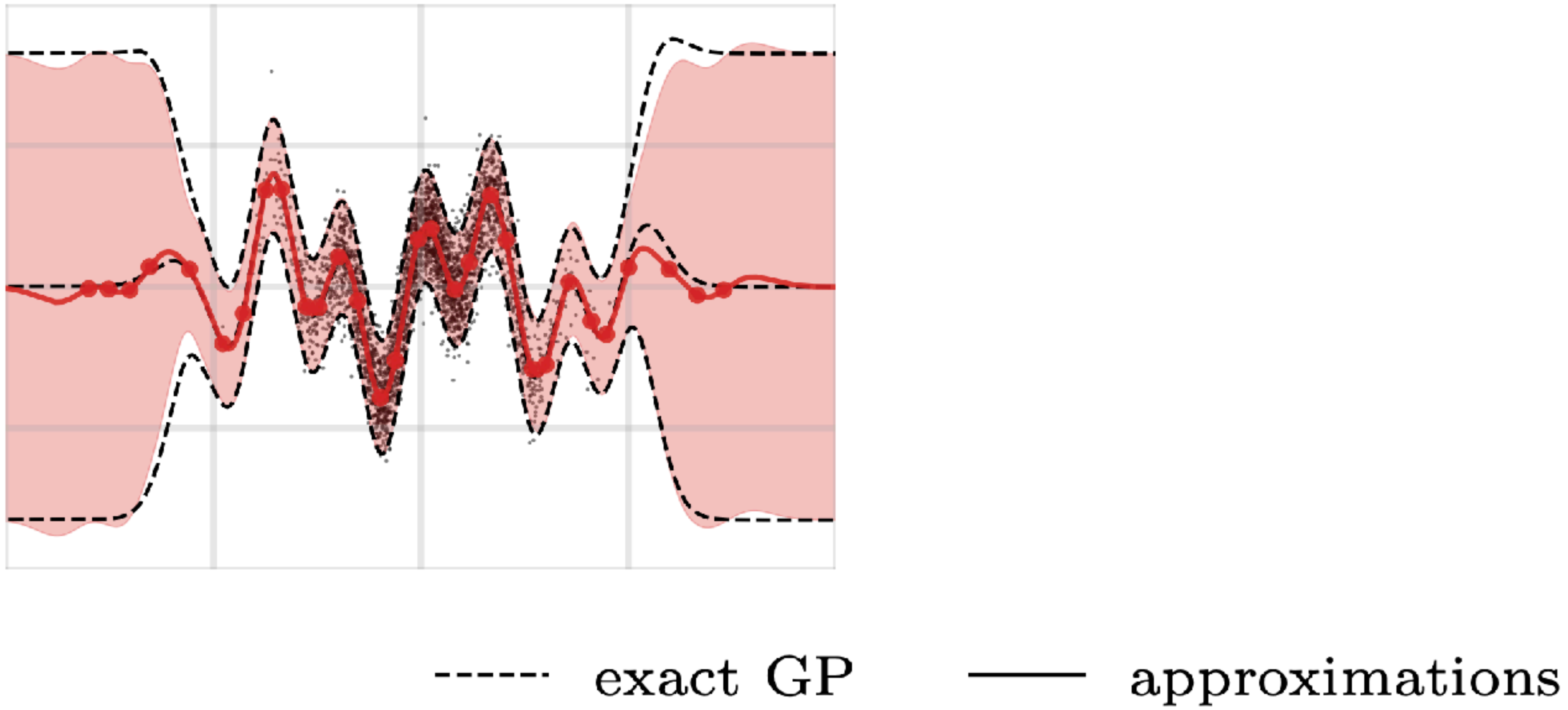
Infill Asymptotics



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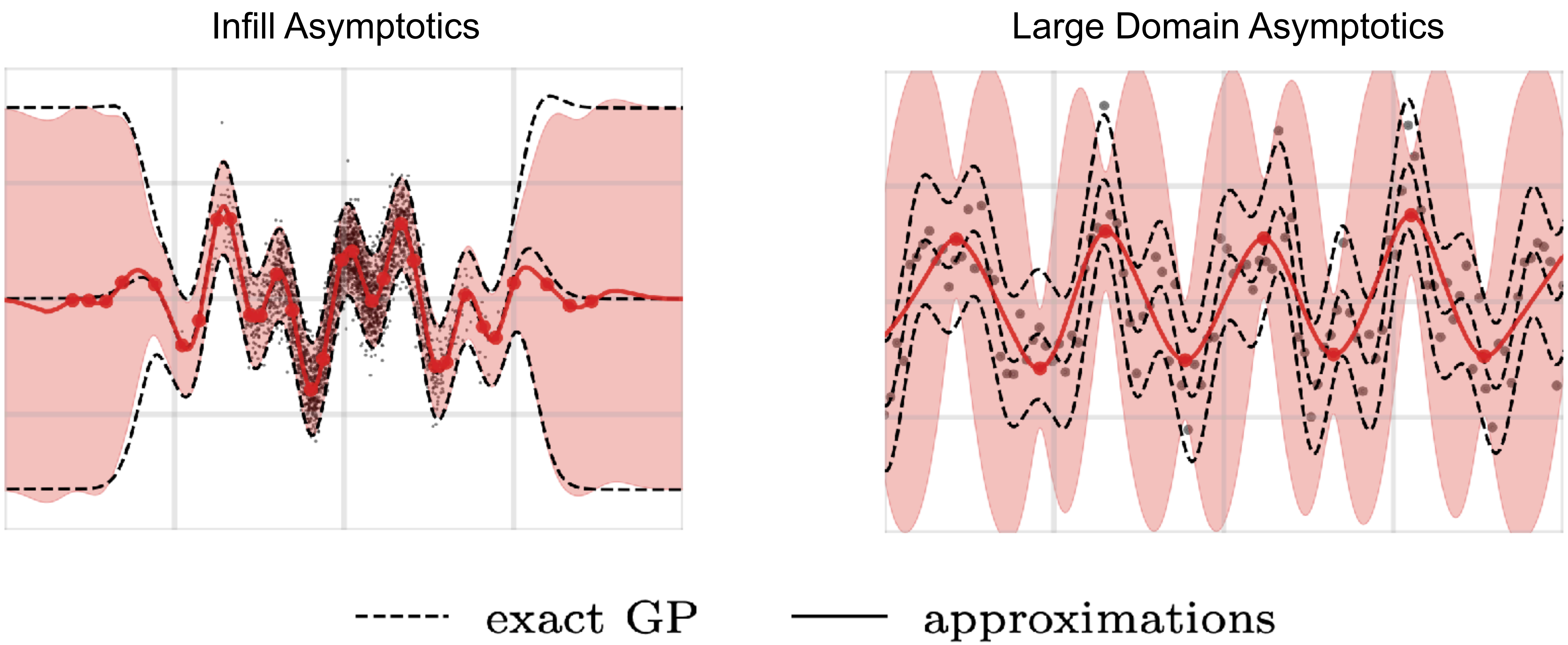

Conjugate Gradients

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Algorithm converges in at most n steps but, in practise, for some tolerance ϵ

$$O\left(\sqrt{\mathrm{cond}(K + \sigma^2 I)}\ \log \frac{\mathrm{cond}(K_{nn} + \sigma^2 I)\|b\|}{\epsilon}\right) \qquad \mathrm{cond}(K_{nn} + \sigma^2 I) = \frac{\lambda_{\mathrm{max}}(K_{nn} + \sigma^2 I)}{\lambda_{\mathrm{min}}(K_{nn} + \sigma^2 I)}$$

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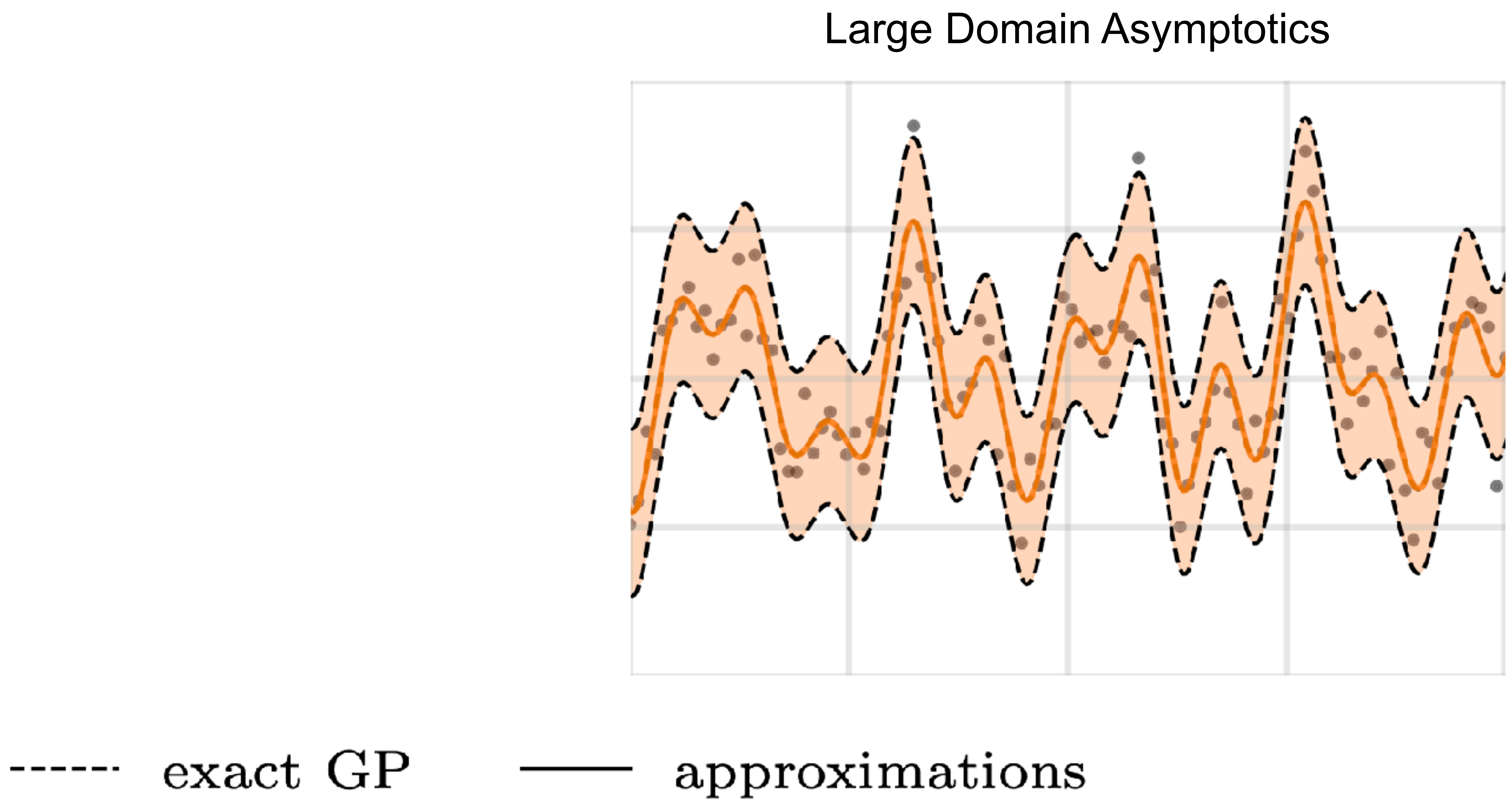

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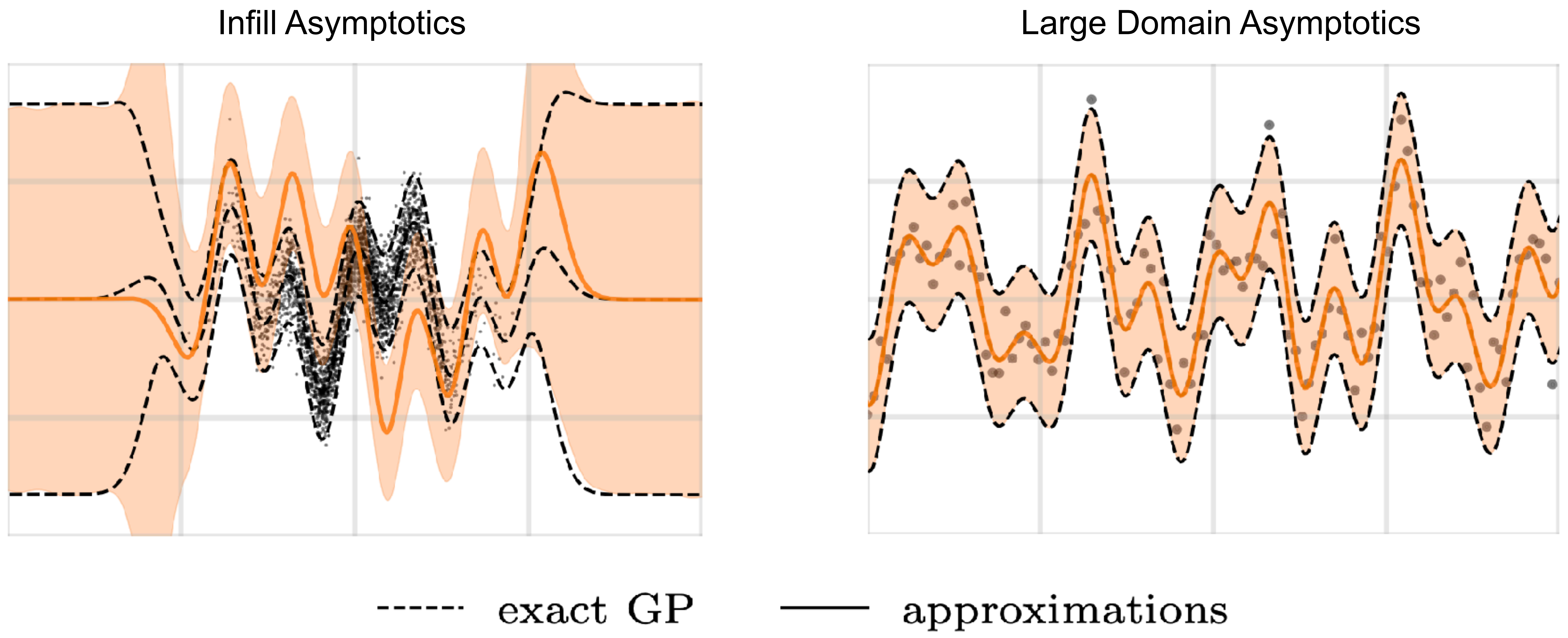
Issue: redundant data creates rank deficiency in K_{xx}



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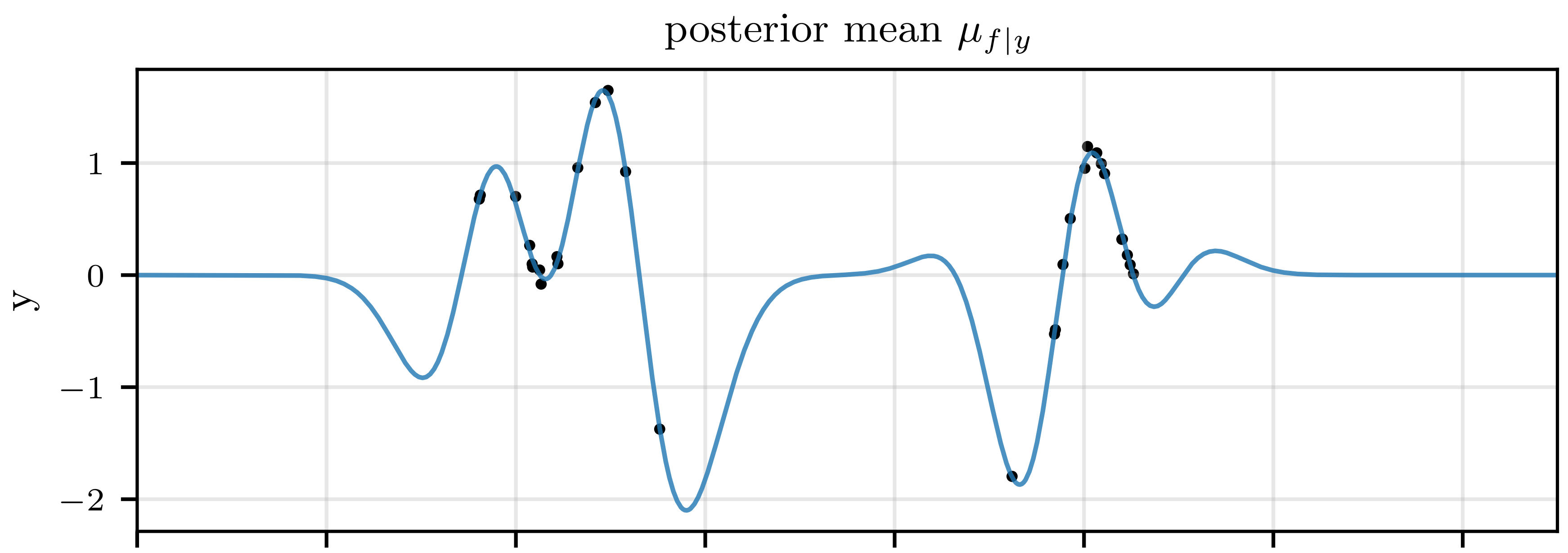

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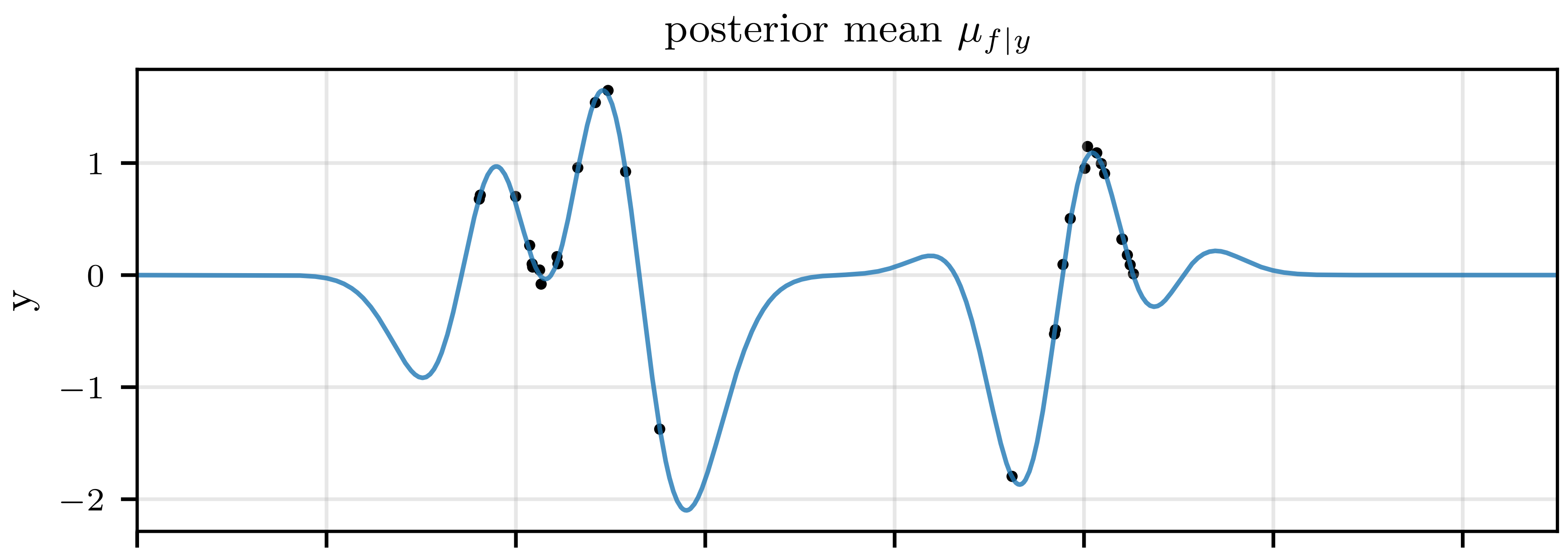

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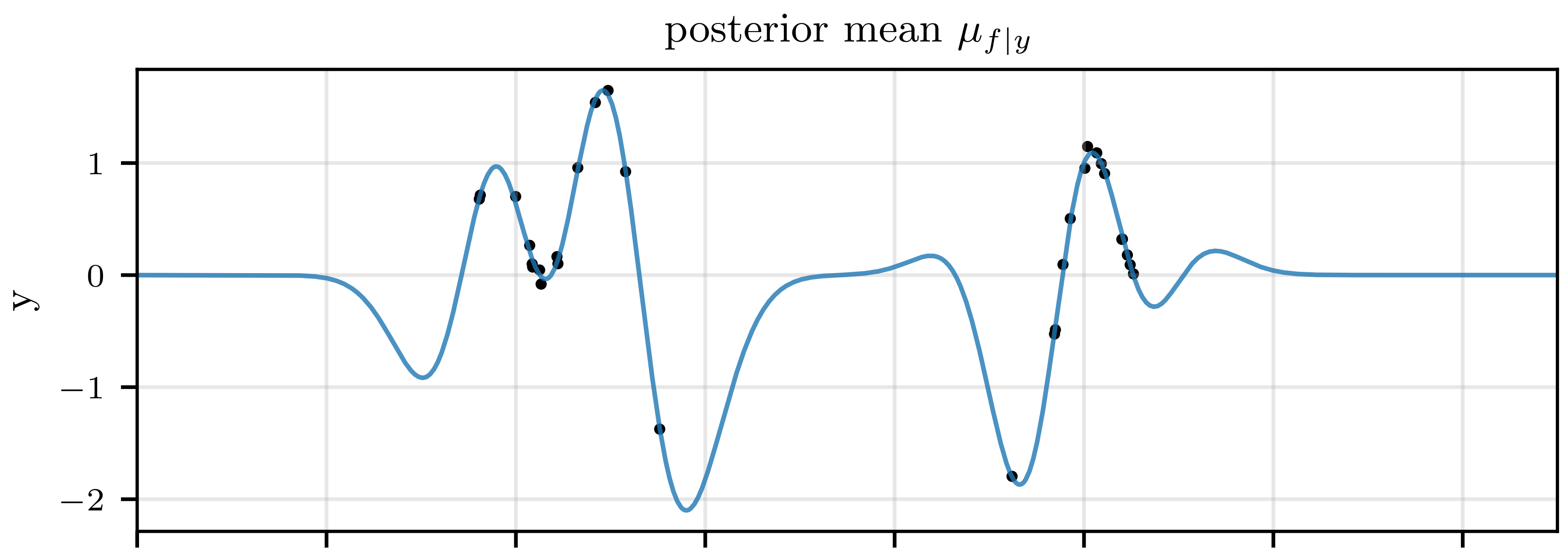

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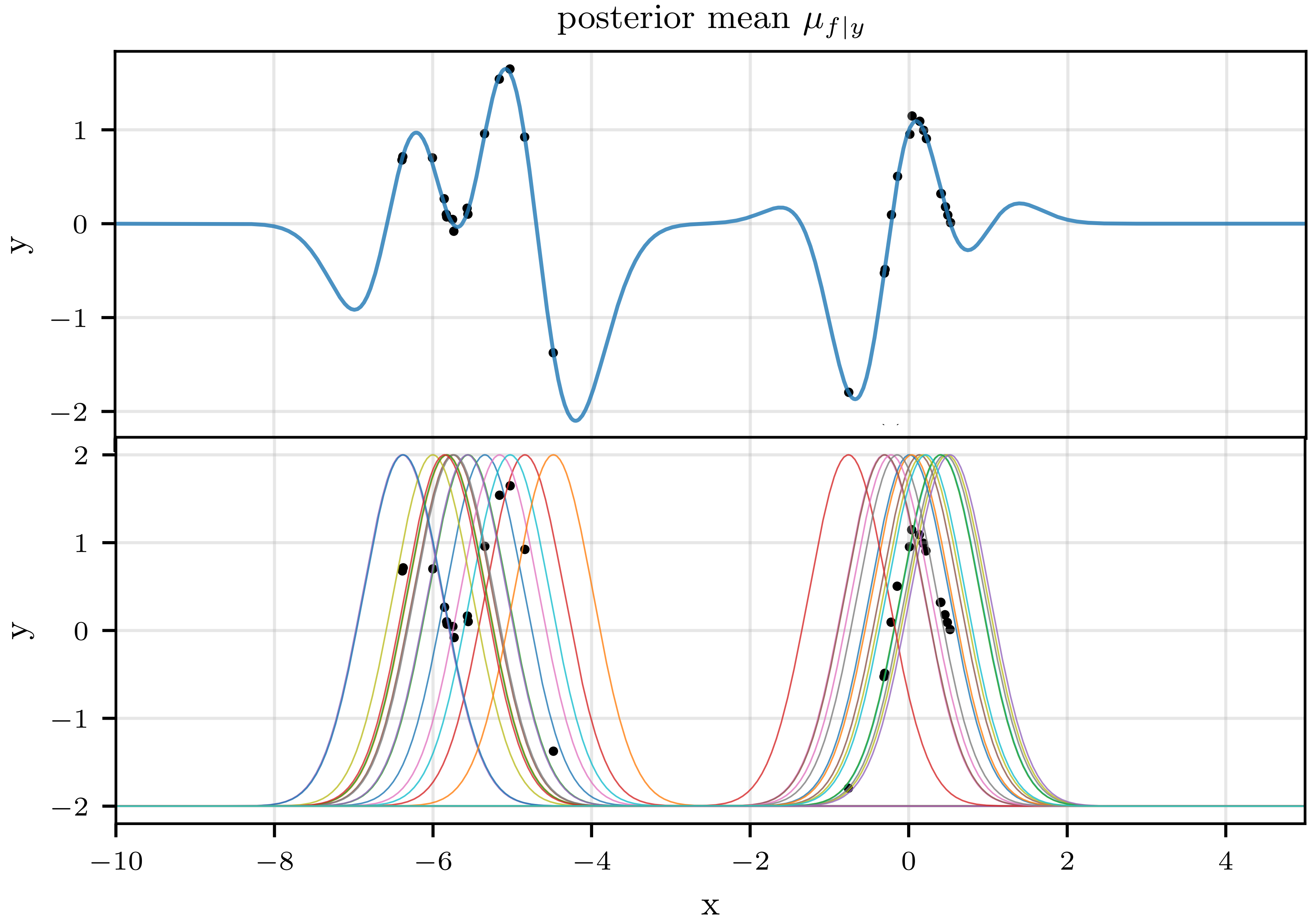

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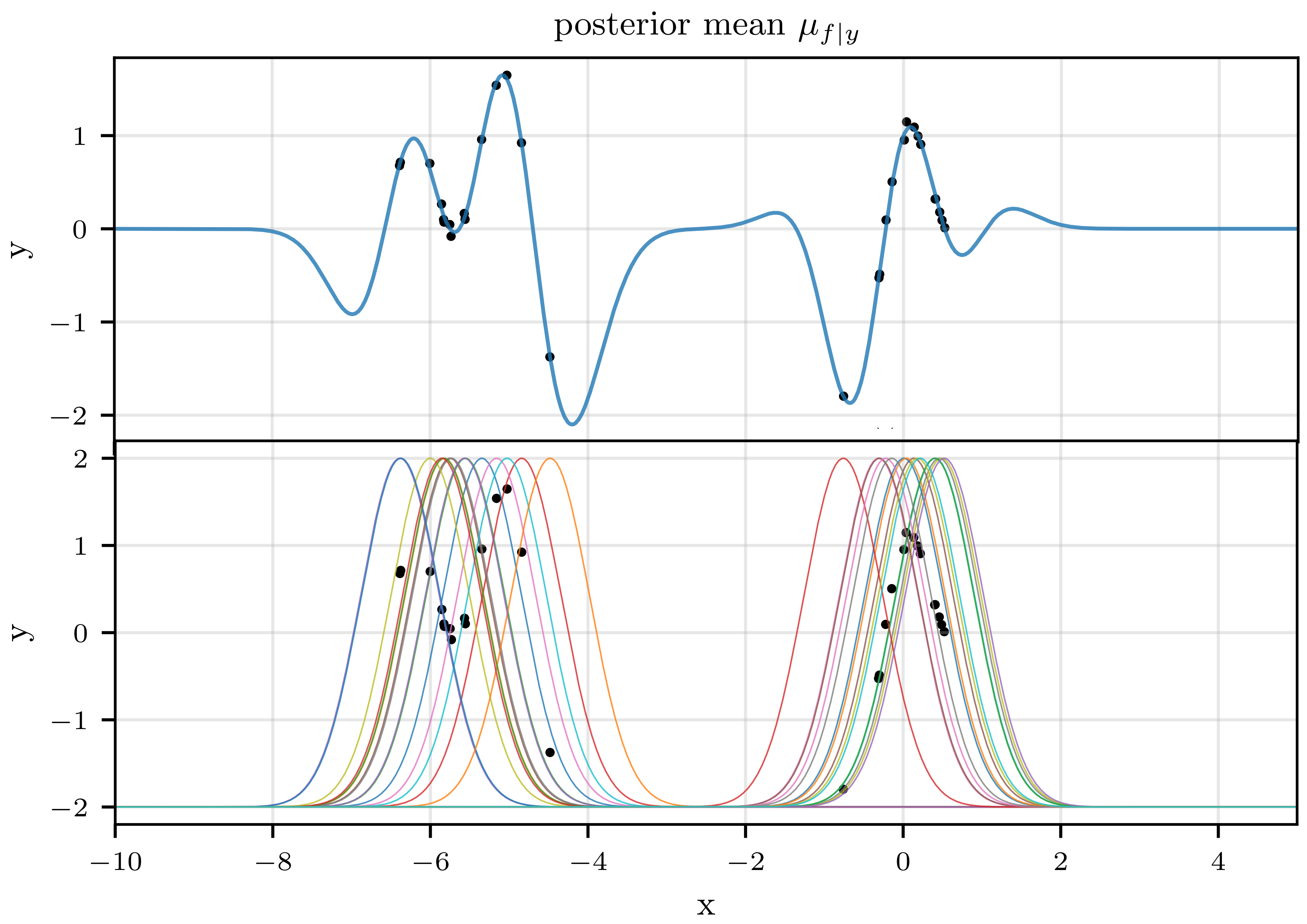

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[1] Lin, JA*, Padhy, S.*, Antorán, J.,*, ... and Hernández-Lobato, J.M., 2022. Sampling from Gaussian Process Posteriors using Stochastic Gradient Descent. ***NeurIPS 2023***

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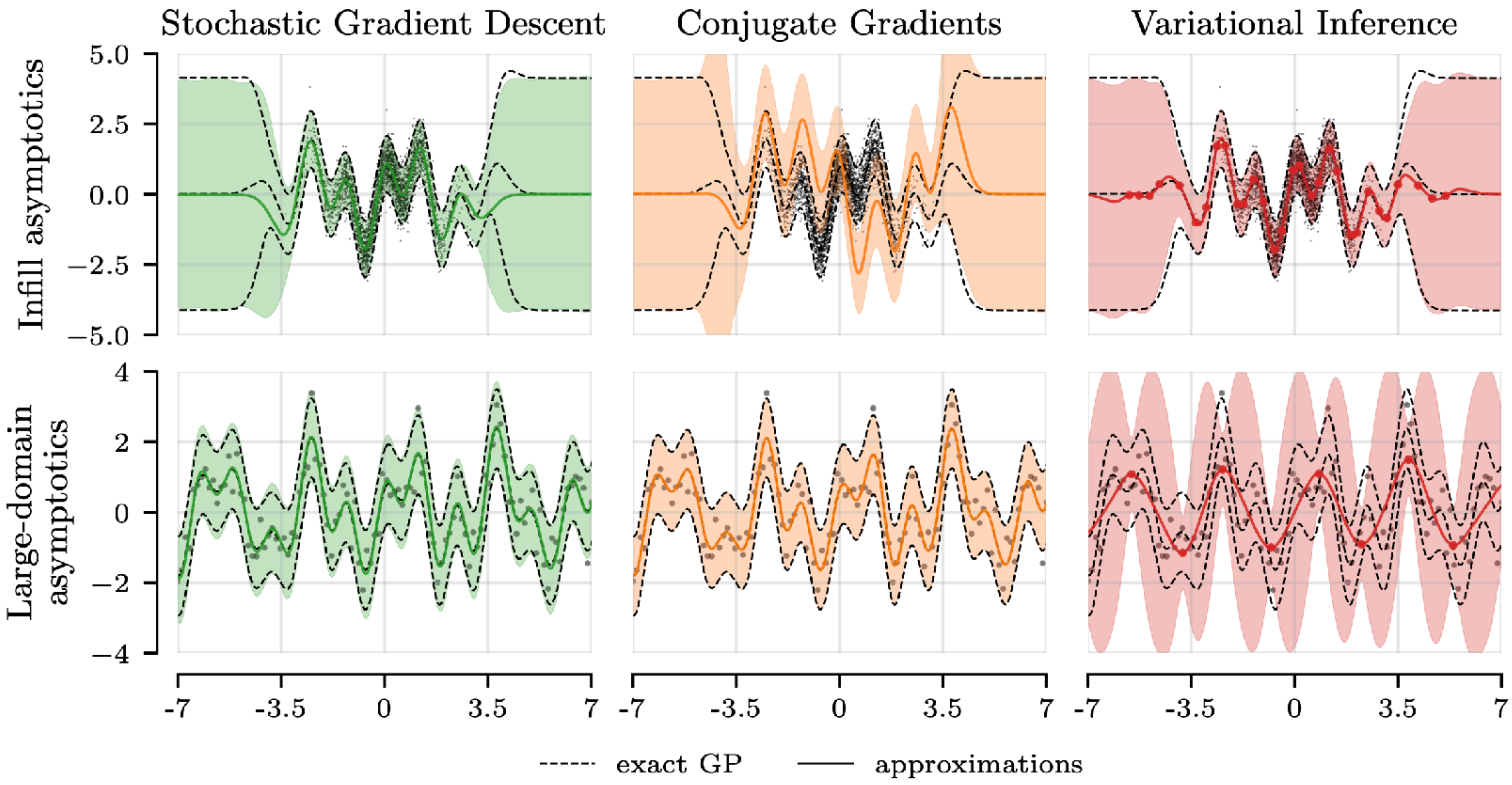
SGD works better on most cases



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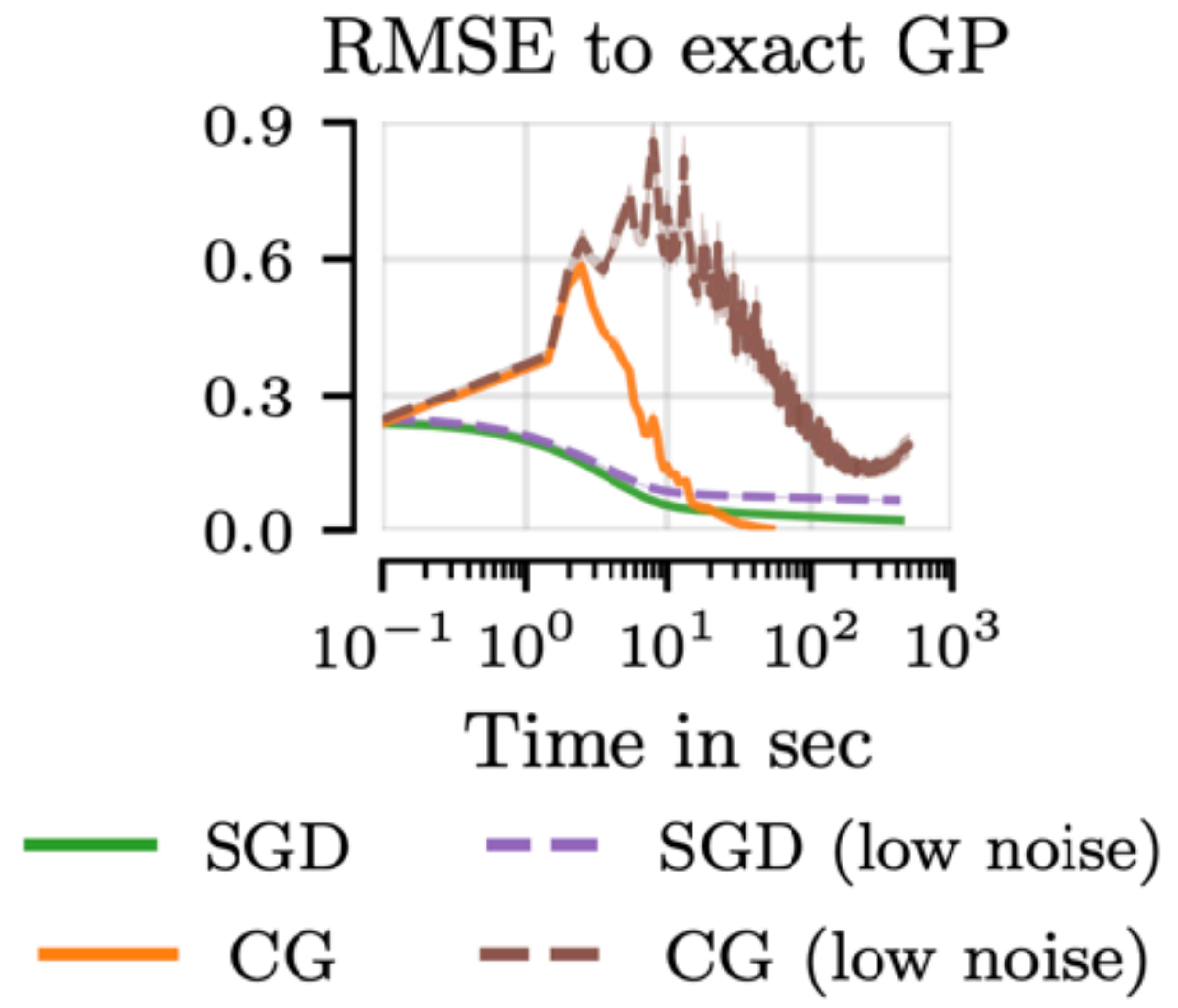

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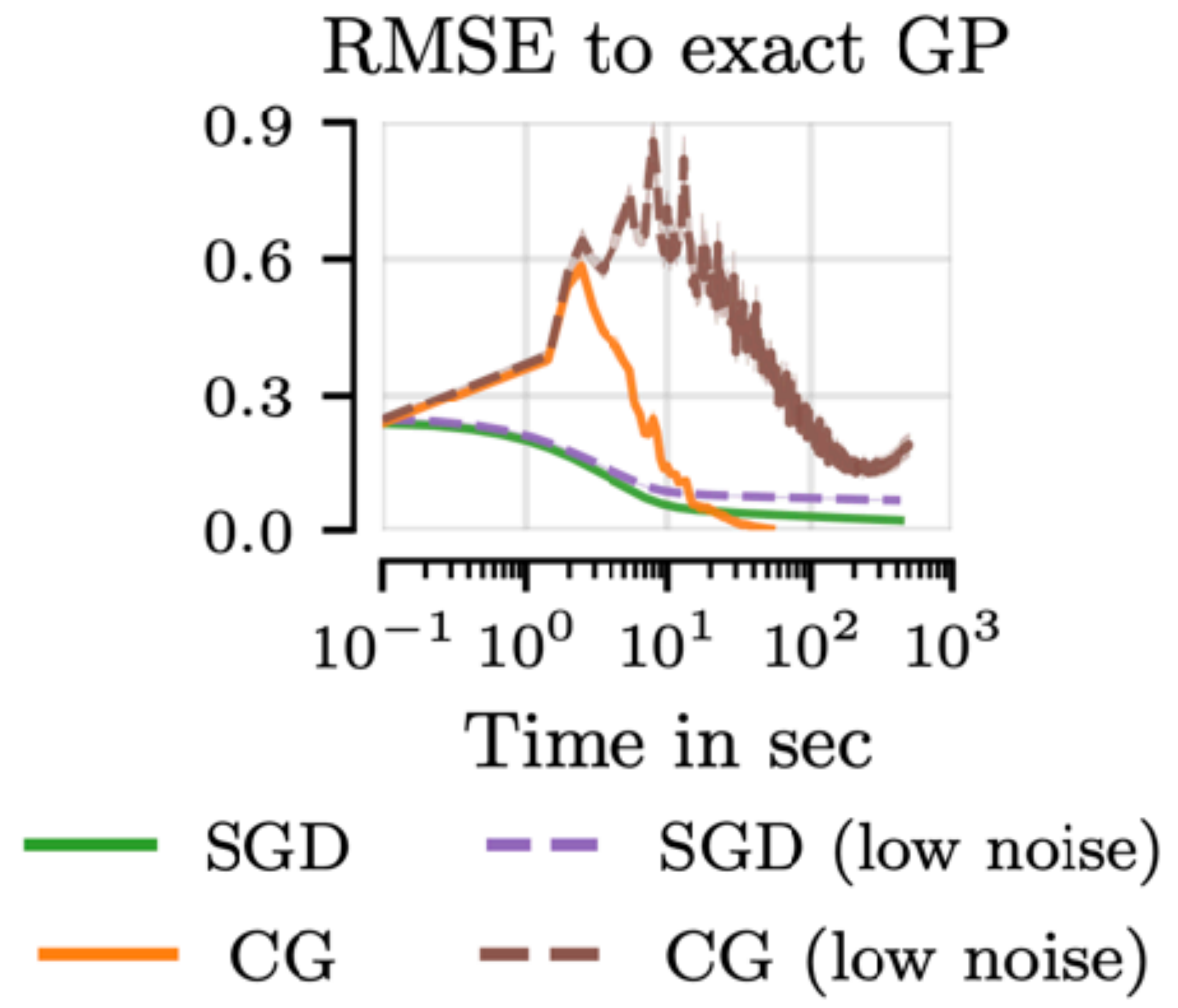
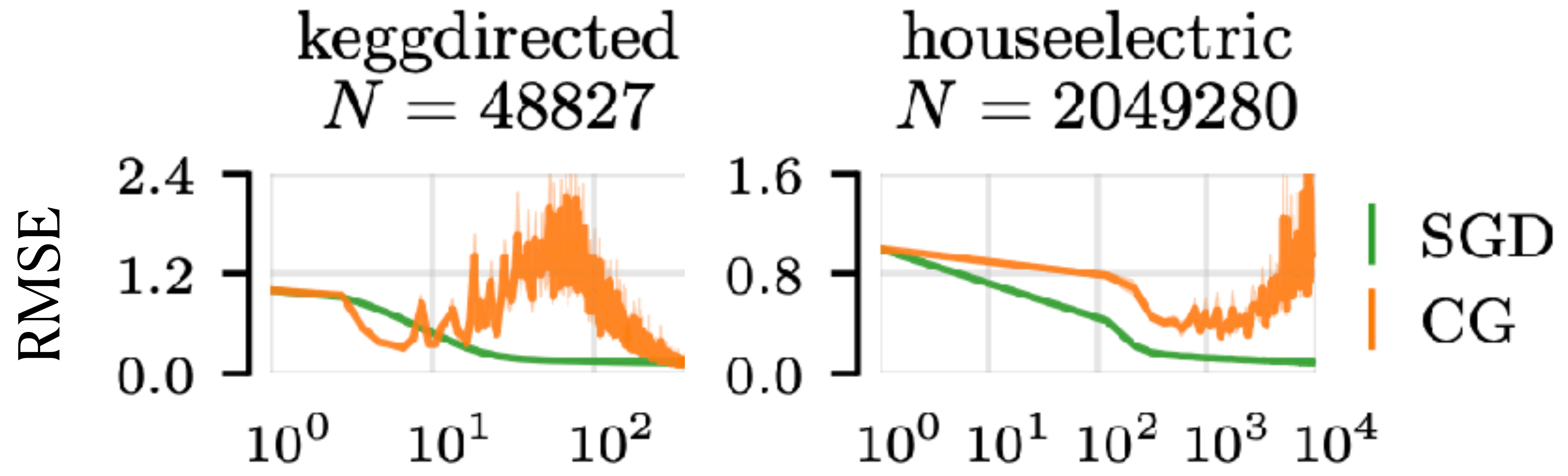
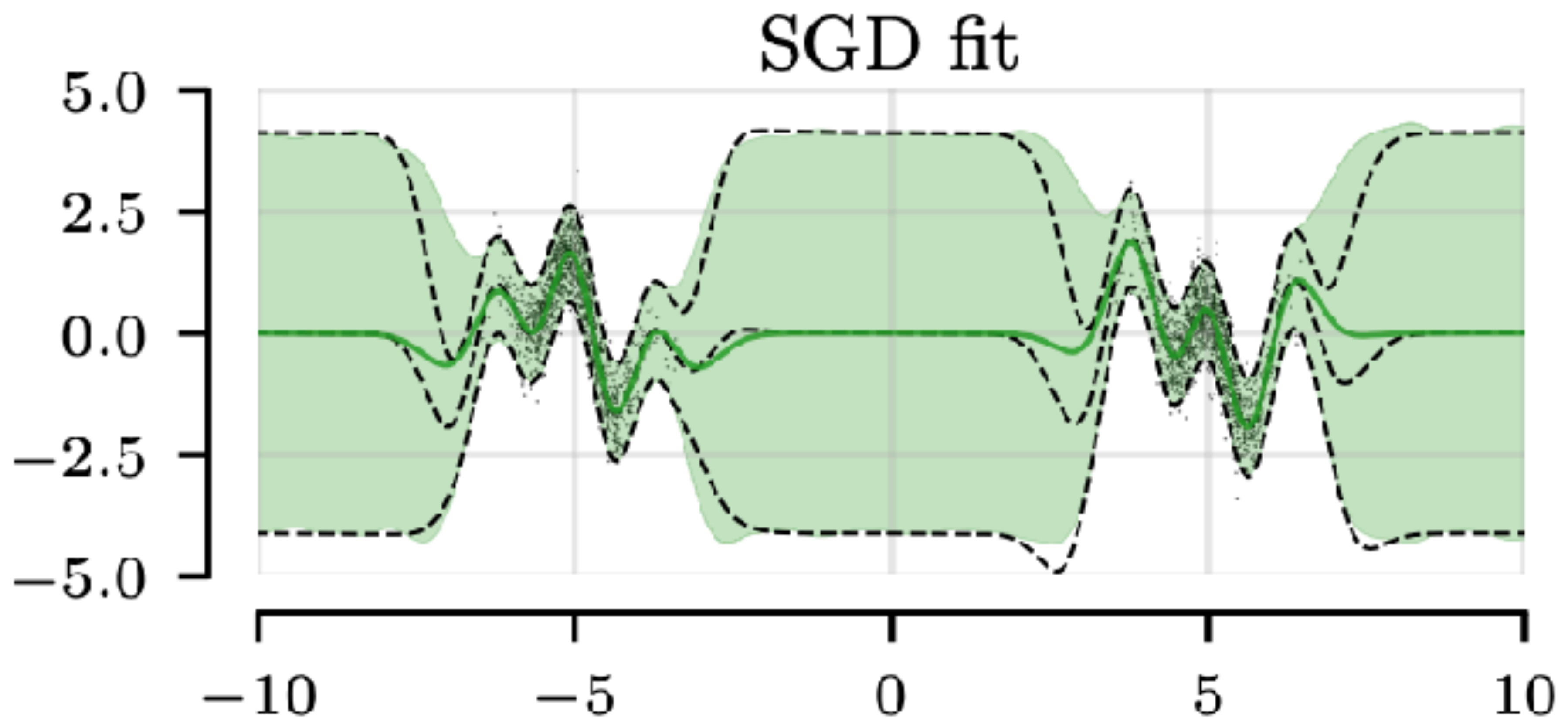




Spectral Analysis of SGD Behaviour



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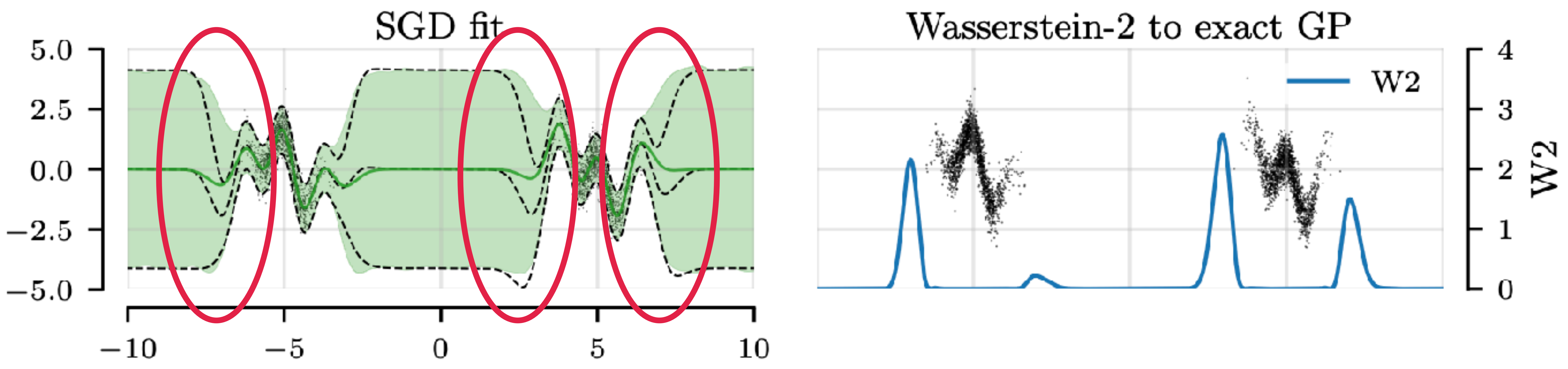

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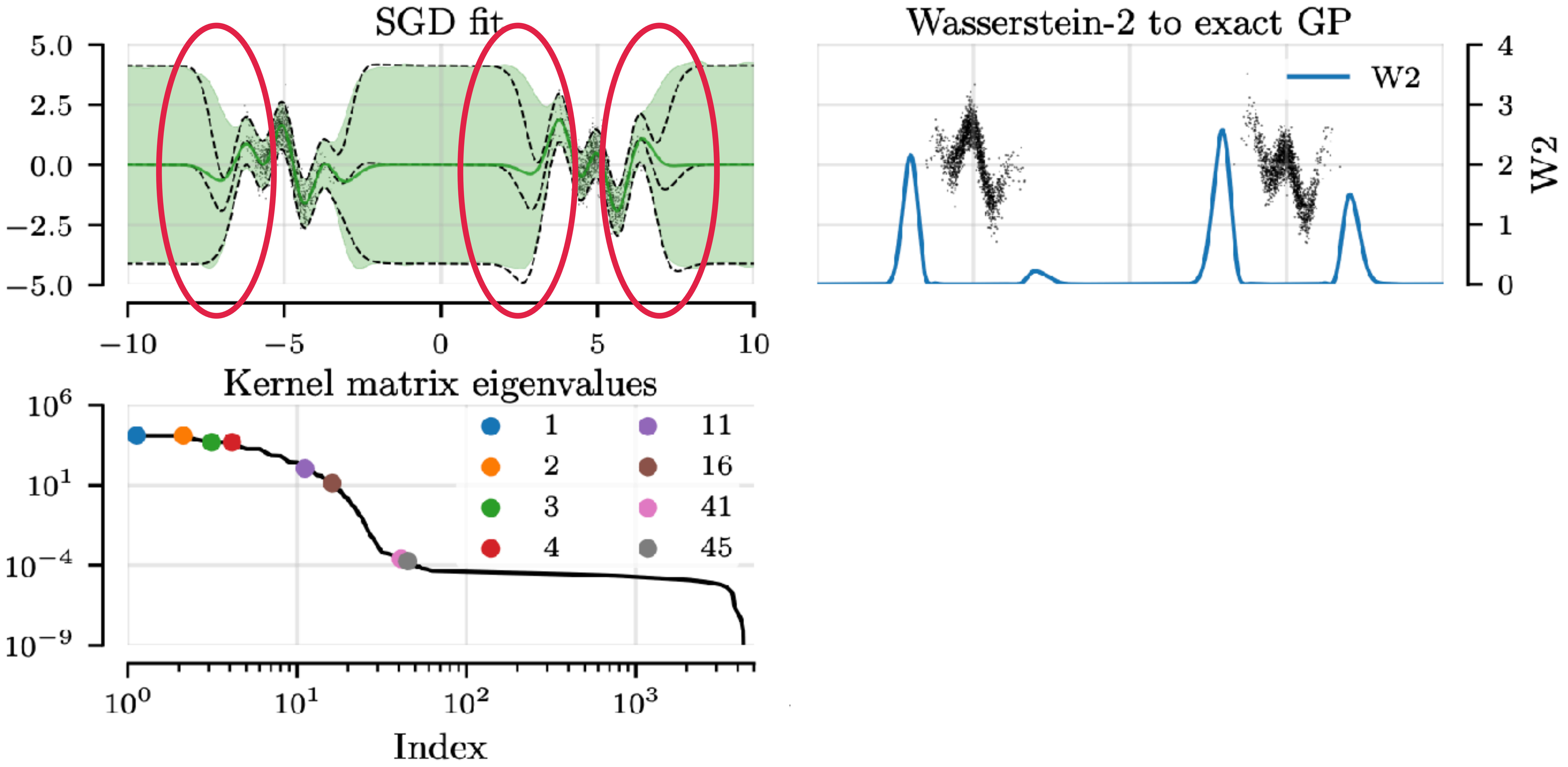

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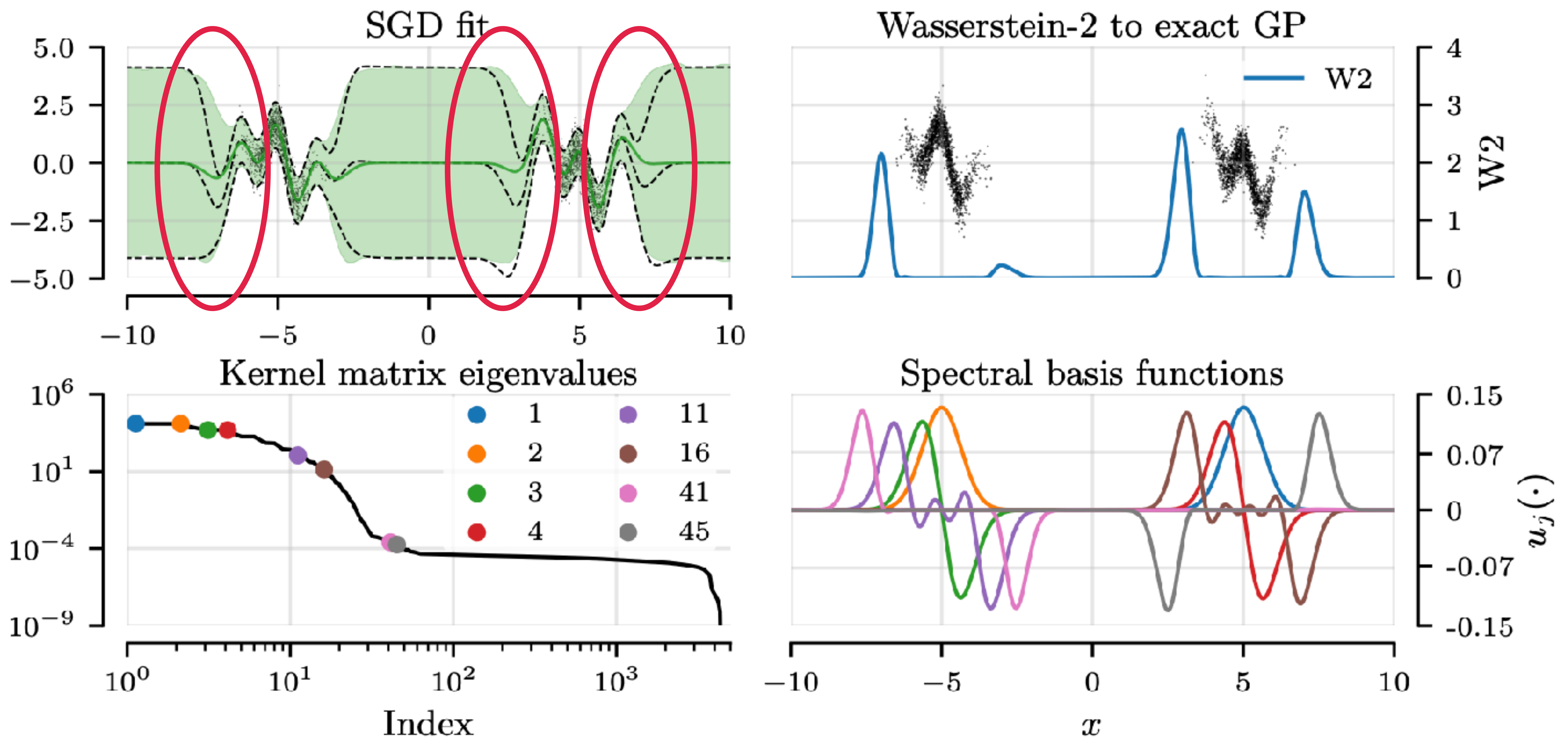

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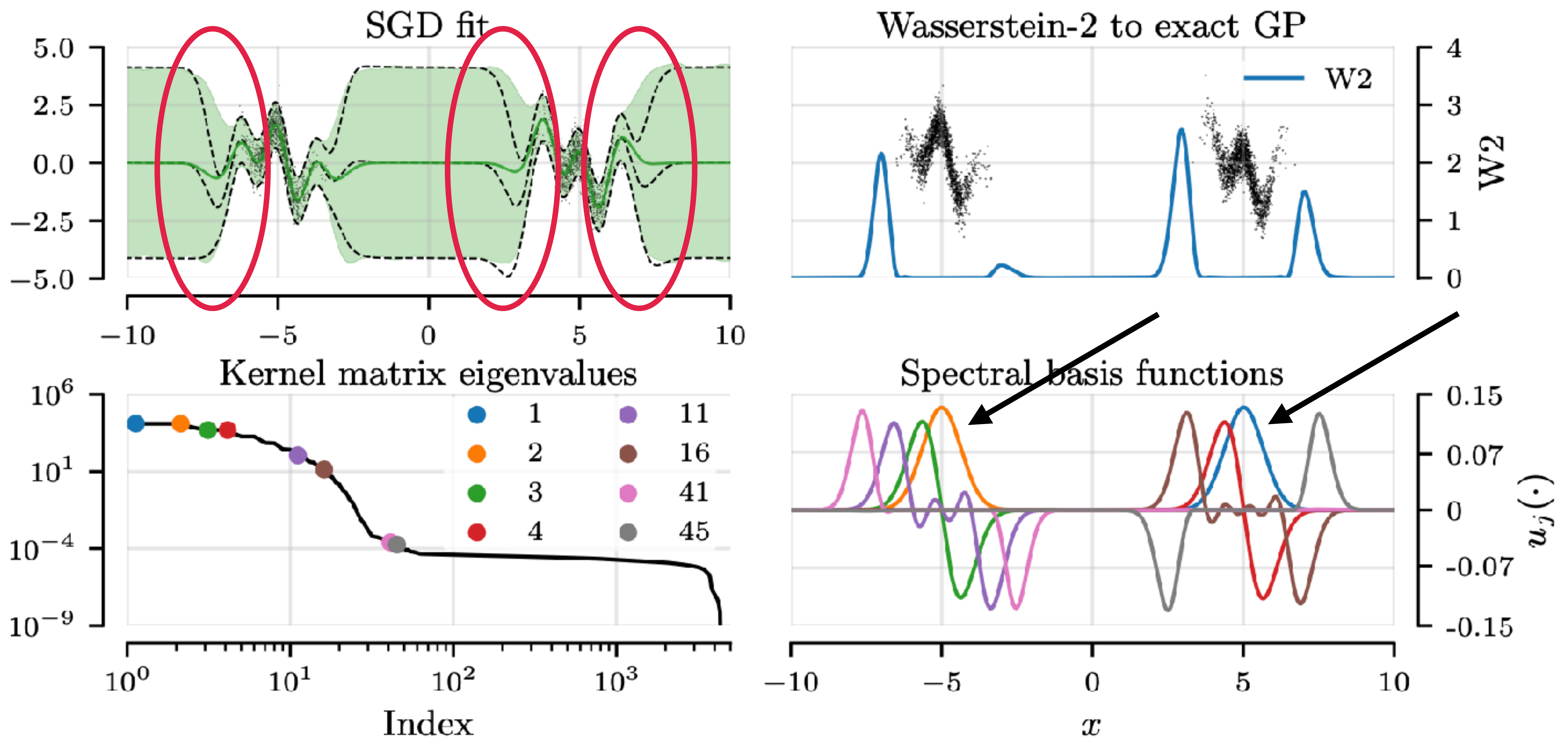

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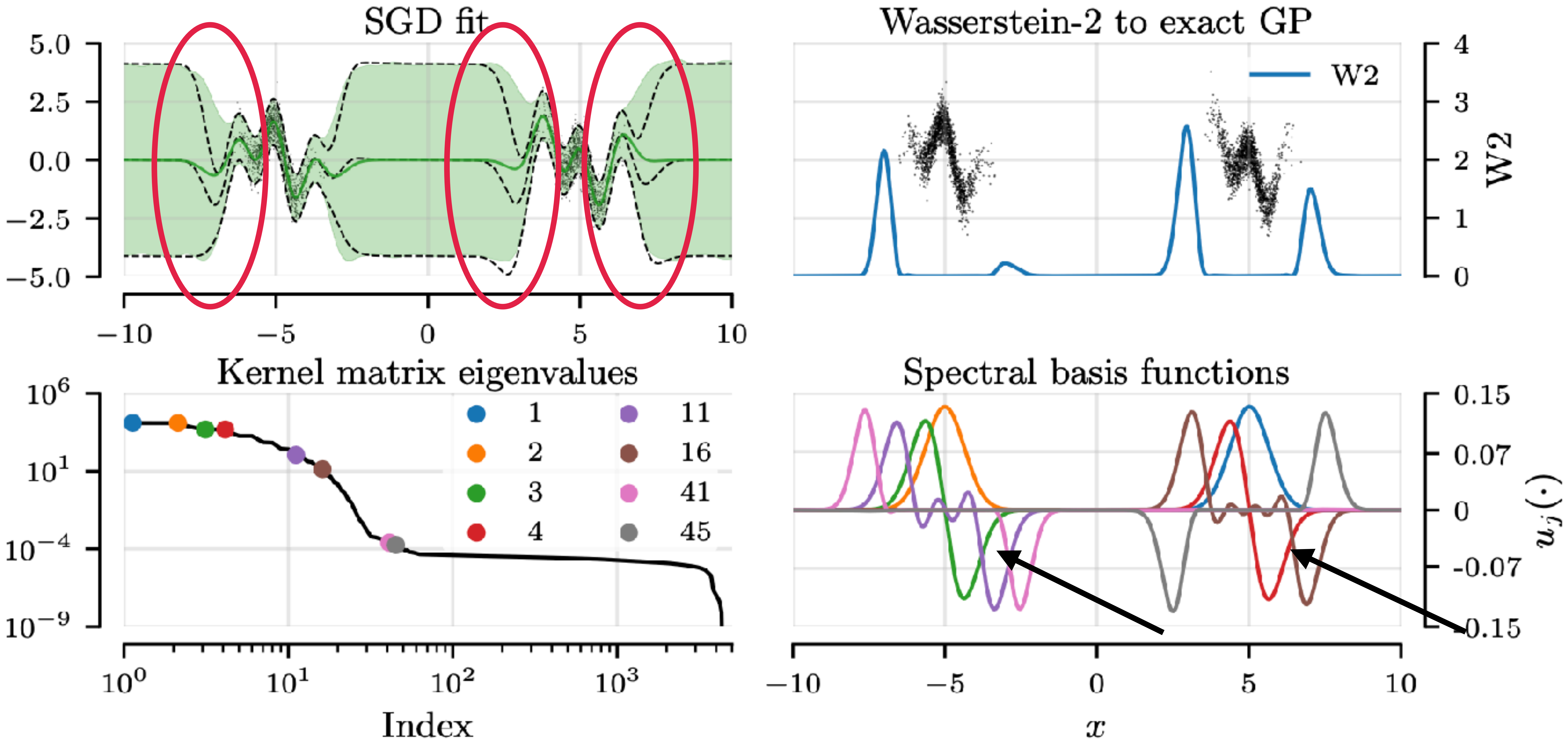

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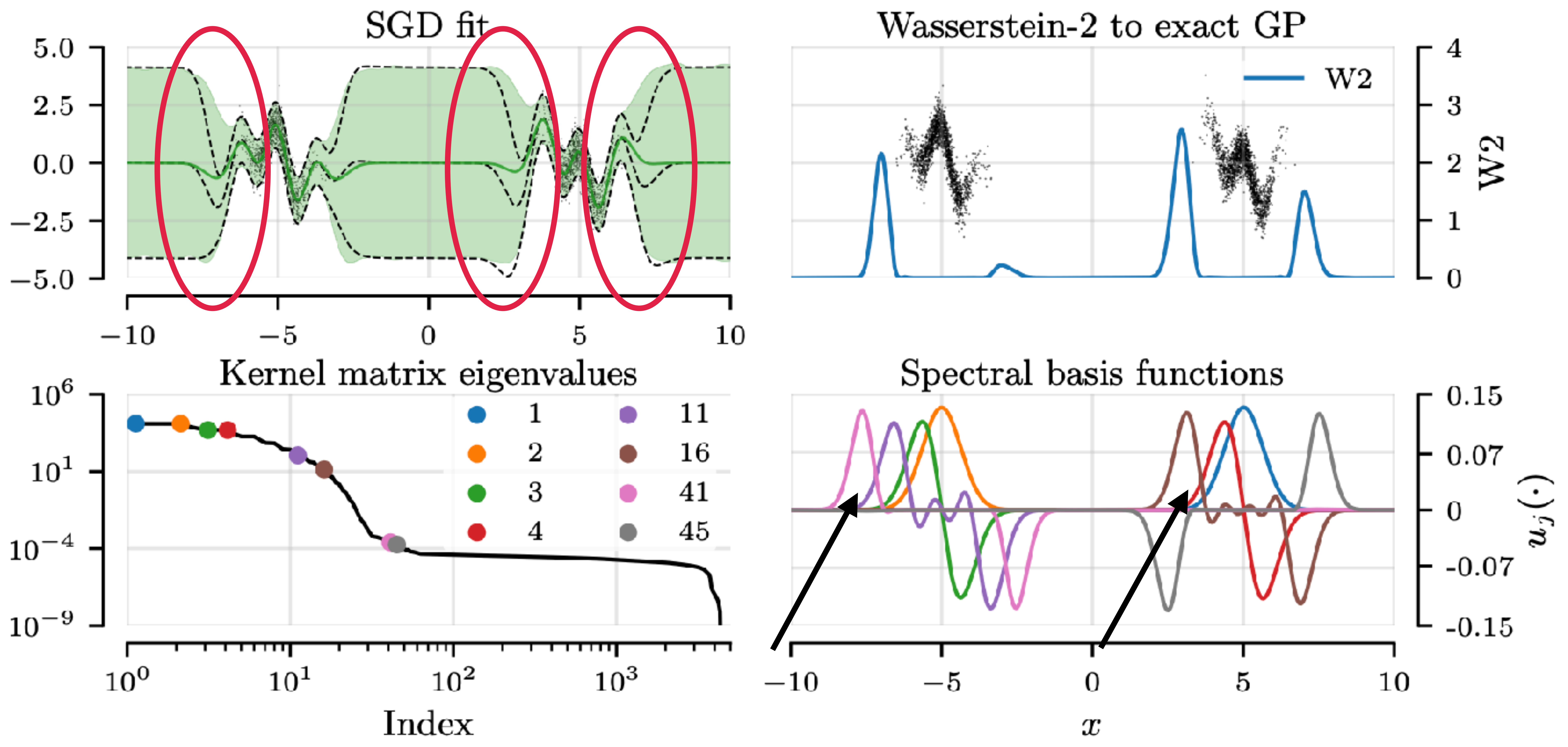

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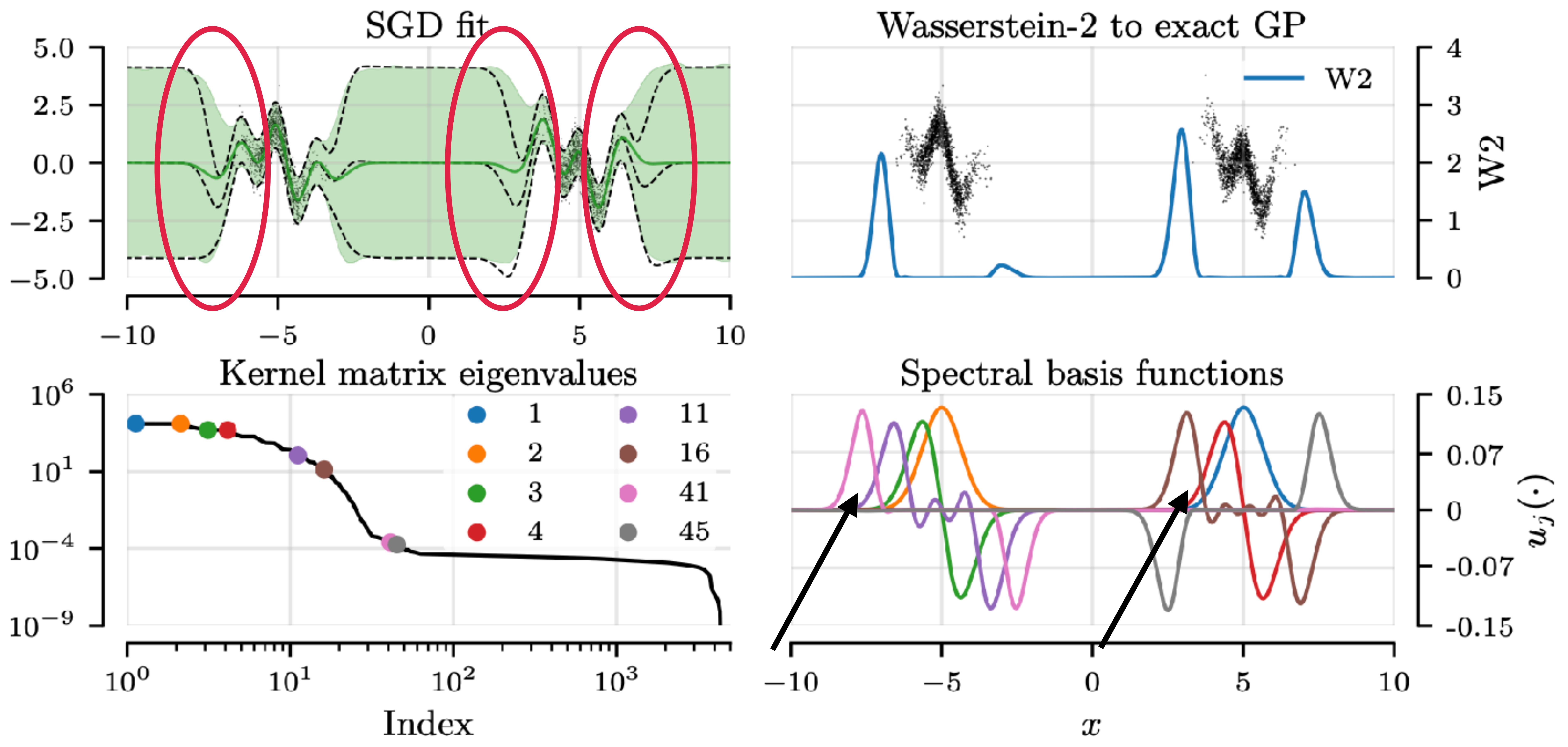

$$\left\| \operatorname{proj}_{u_i} \mu_{f|\mathbf{y}} - \operatorname{proj}_{u_i} \mu_{\mathrm{SGD}} \right\|_{H_k} \leq \frac{4G+1}{\eta} \sqrt{\frac{\log \frac{N}{\delta}}{t\lambda_i}}$$

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  - **Can we do better?**

A Path to More Efficient Sampling [1]

- Let us take another look at multivariate Gaussian distributions (ignore noise)

$$\left[\begin{pmatrix} f(X_*) \\ f(X) \end{pmatrix}\right] \sim \mathcal{N}\left(0, \left[\begin{pmatrix} k(X_*, X_*) & k(X_*, X) \\ k(X_*, X)^\top & k(X, X) \end{pmatrix}\right]\right)$$

[1] Wilson, J.T., Borovitskiy, V., Terenin, A., Mostowsky, P. and Deisenroth, M.P., 2021. Pathwise conditioning of gaussian processes. *The Journal of Machine Learning Research*, *22*(1), pp.4741-4787.

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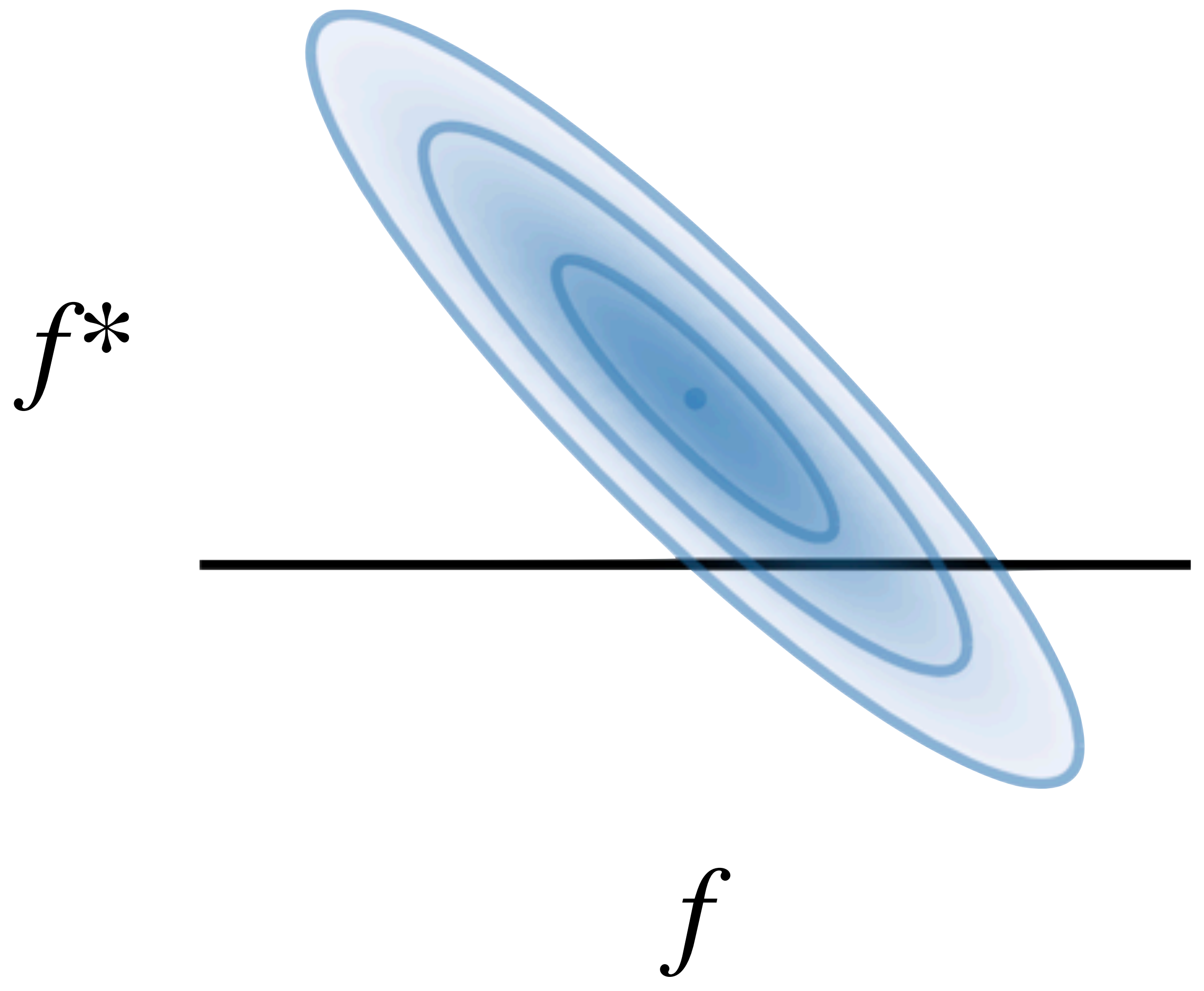

[1] Wilson, J.T., Borovitskiy, V., <u>Terenin, A.</u>, Mostowsky, P. and Deisenroth, M.P., 2021. Pathwise conditioning of gaussian processes. *The Journal of Machine Learning Research*, *22*(1), pp.4741-4787.

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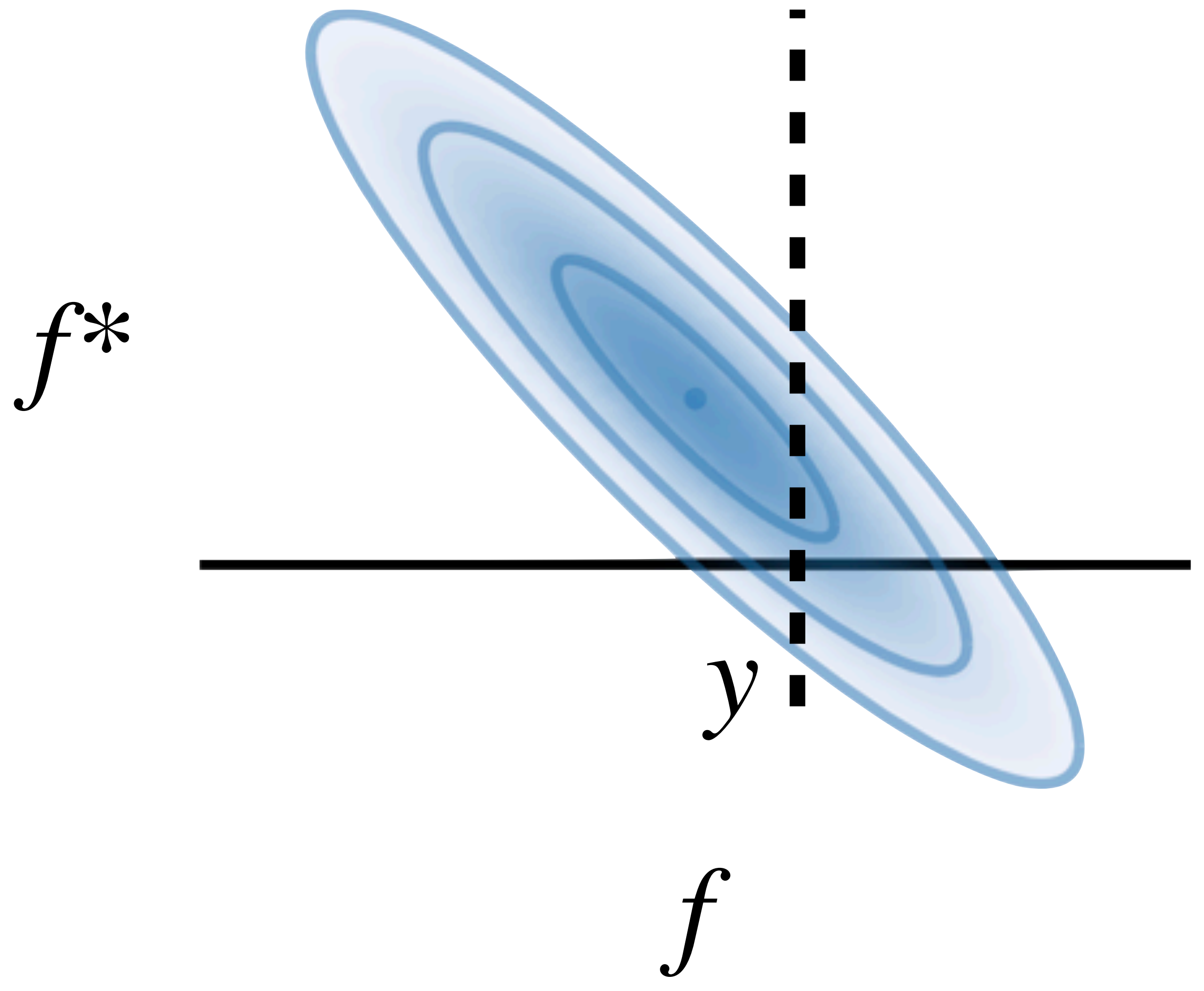

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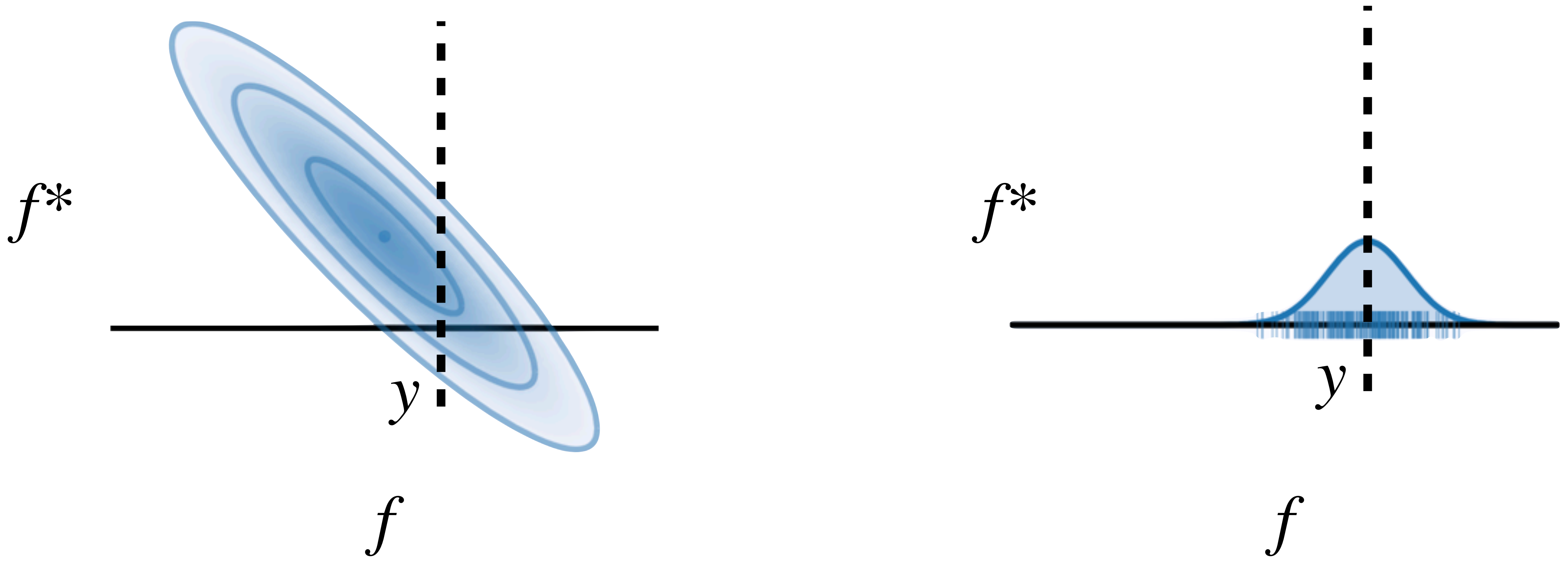

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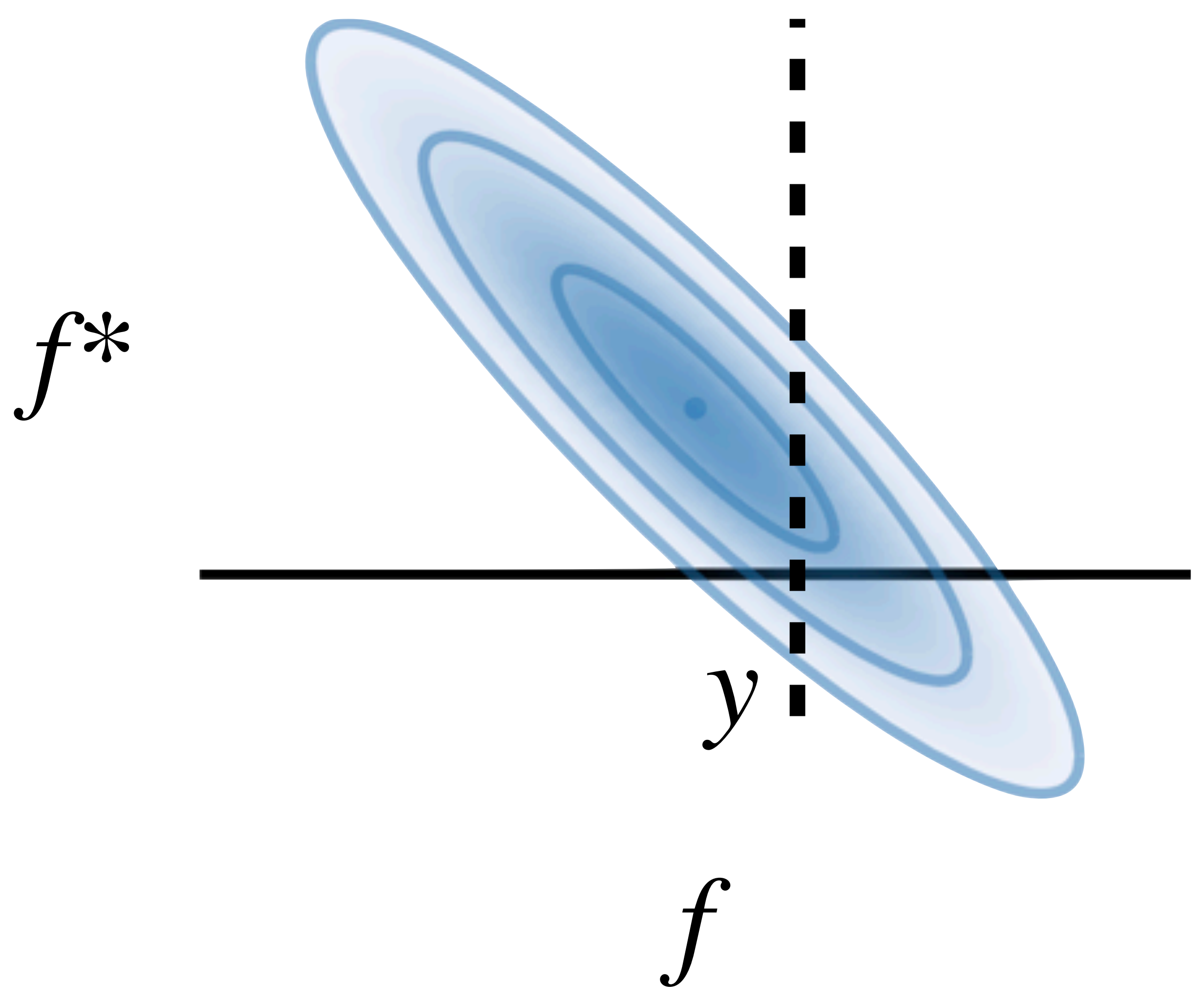

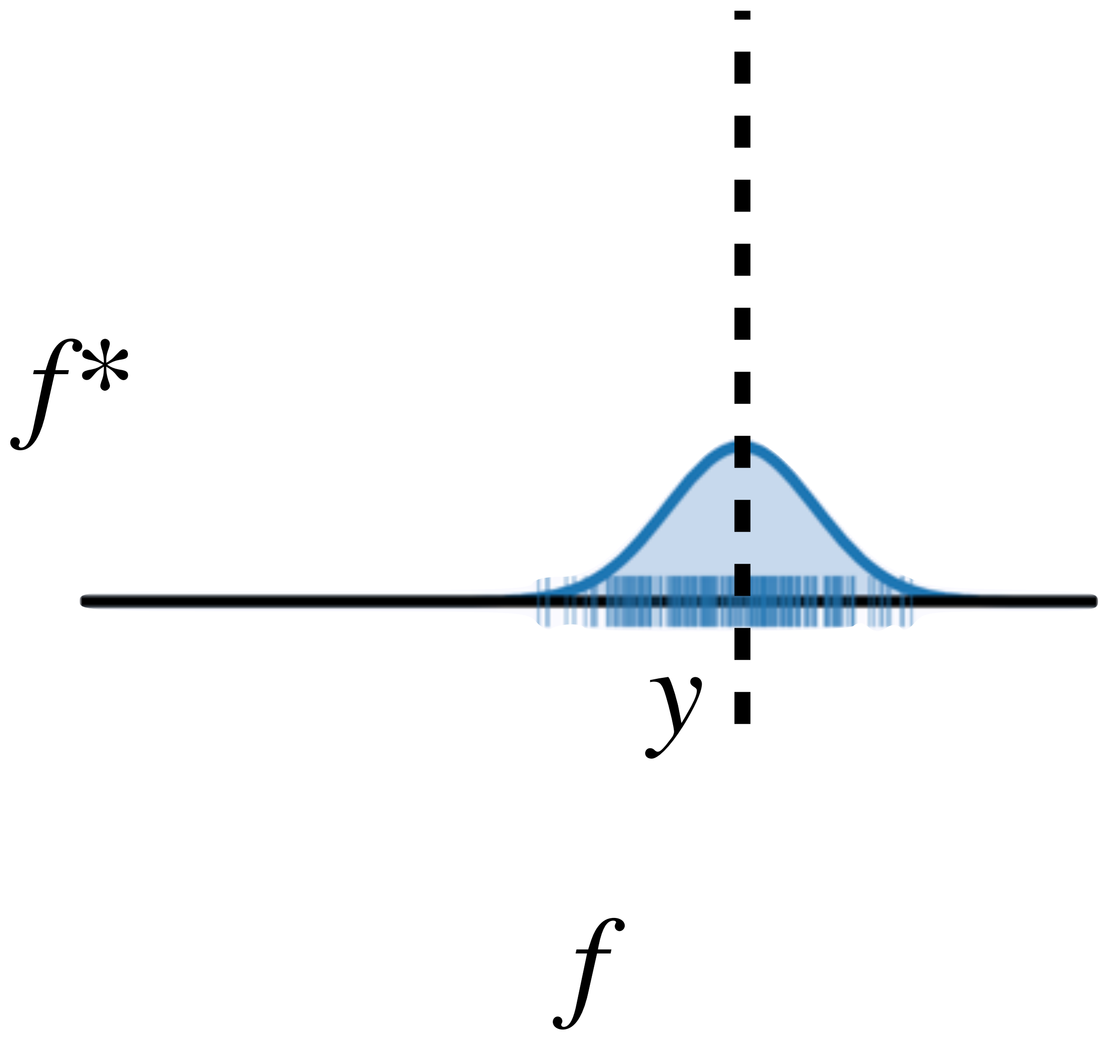

Distributional View

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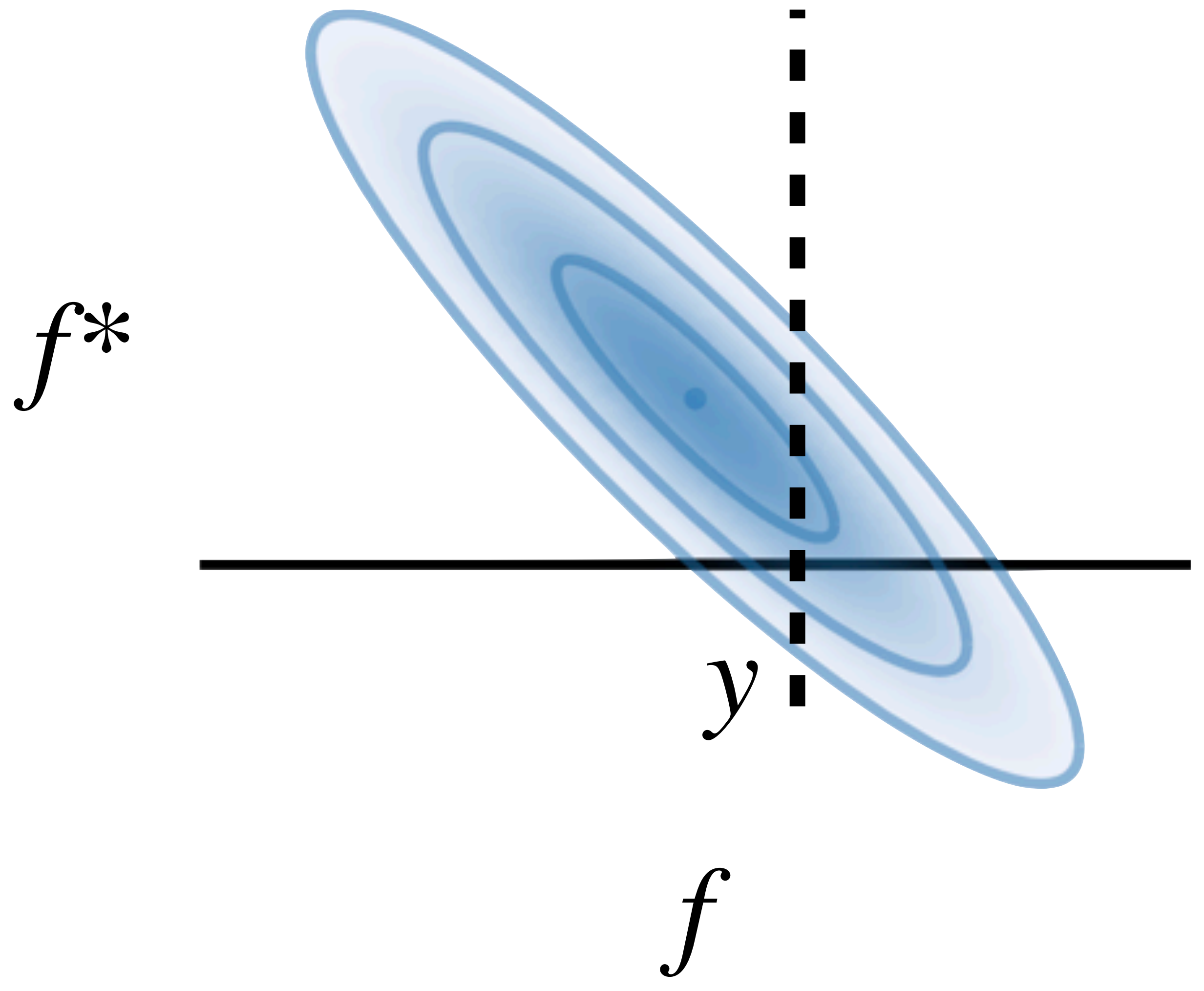

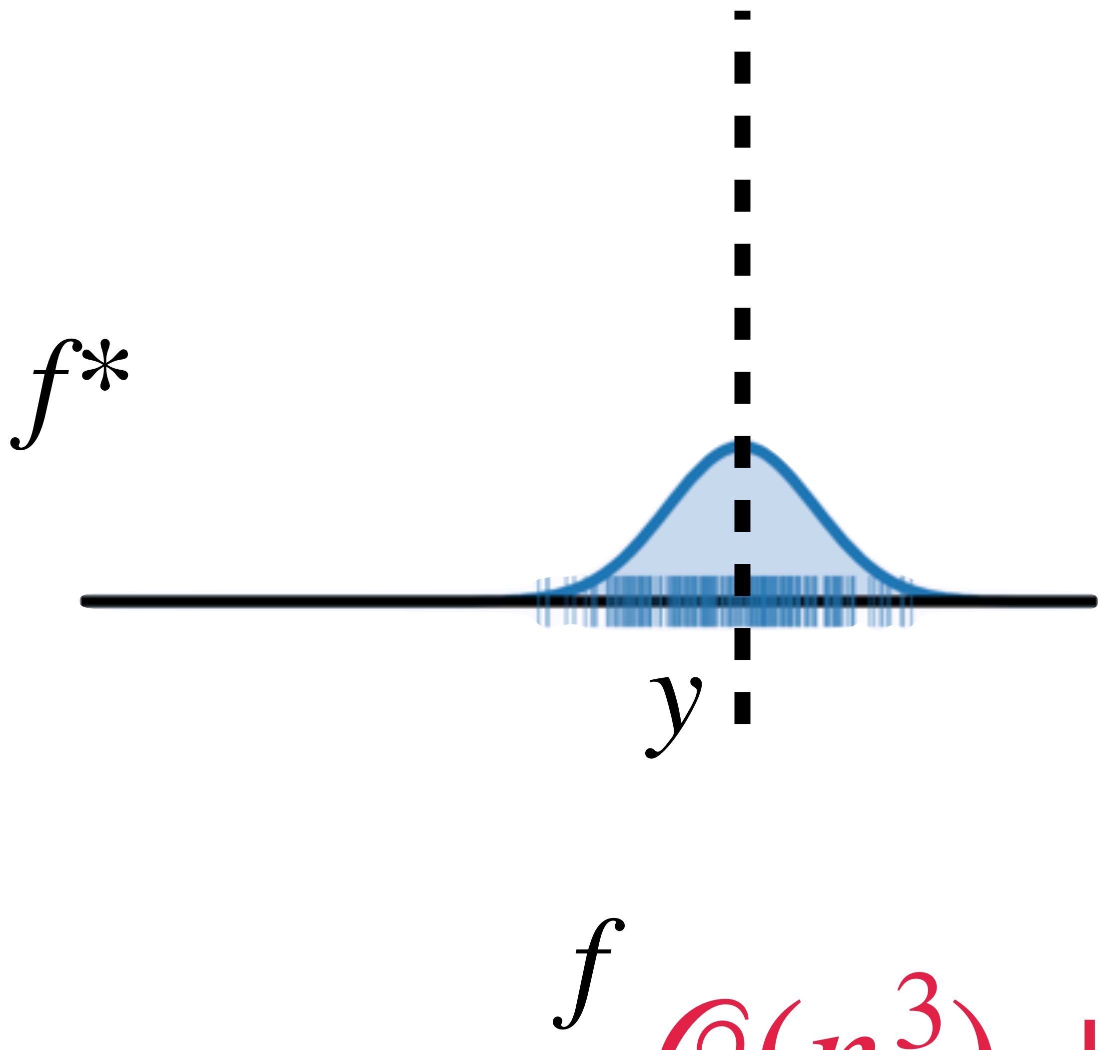

Distributional View

$\mathcal{O}(n^3) + \mathcal{O}(n^{*3})$

$$p(f^* \mid f = y) = \mathcal{N}(K_{*n}K_{nn}^{-1}y, K_{**} - K_{*n}K_{nn}^{-1}K_{n*})$$

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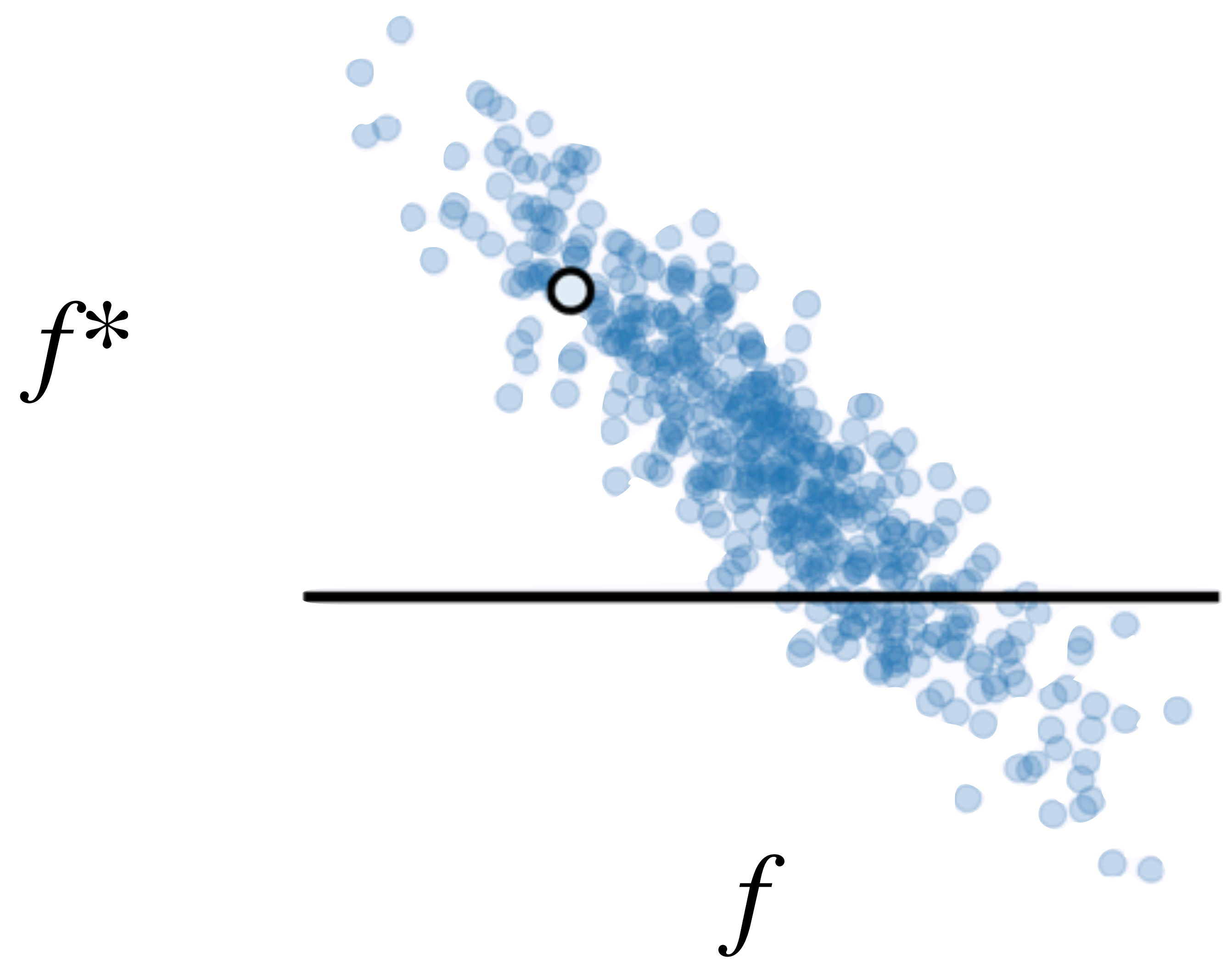
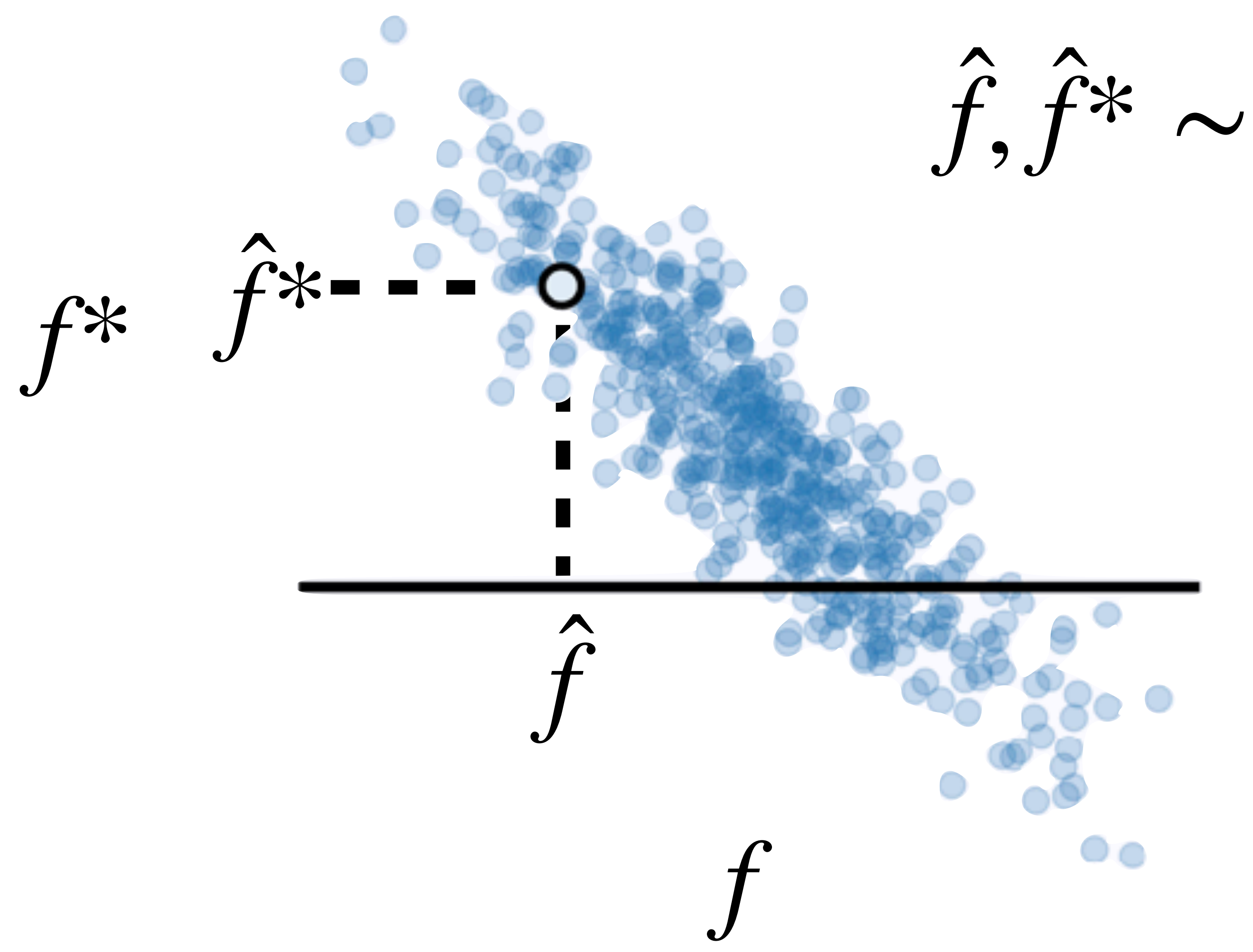
Sample from the Posterior



Sample from the Posterior

$$\hat{f}, \hat{f}^* \sim p(f, f^*)$$



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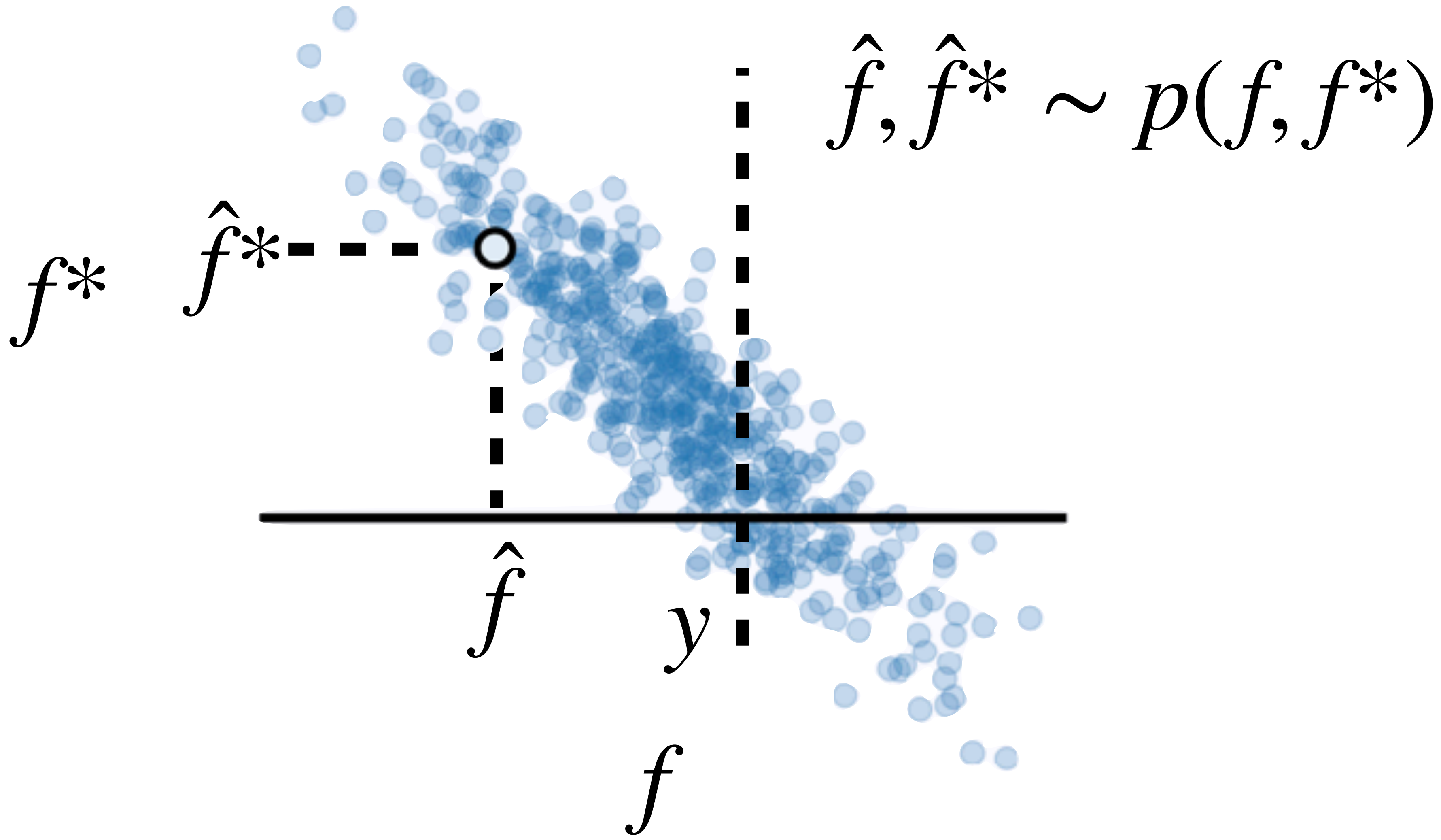

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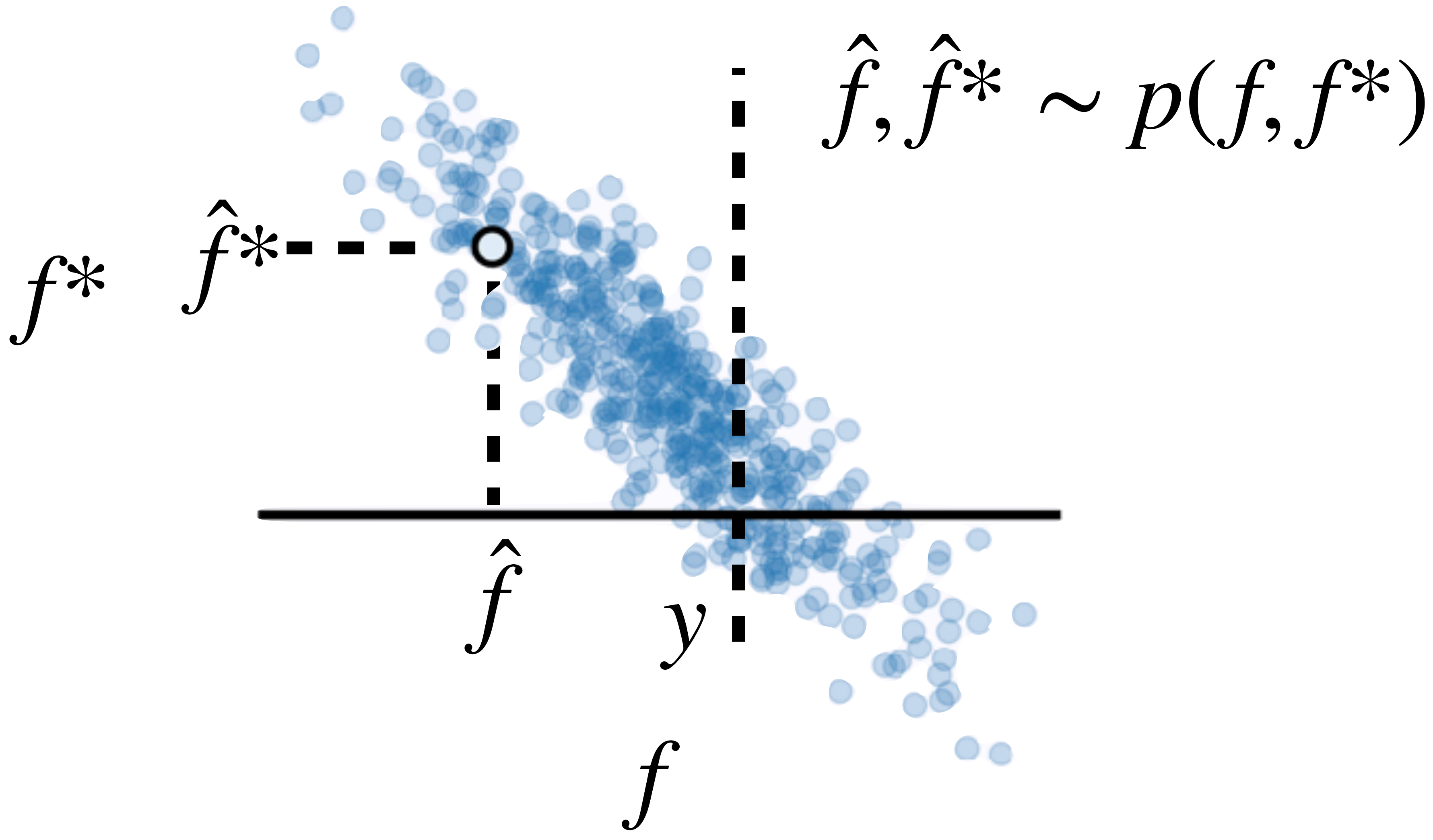

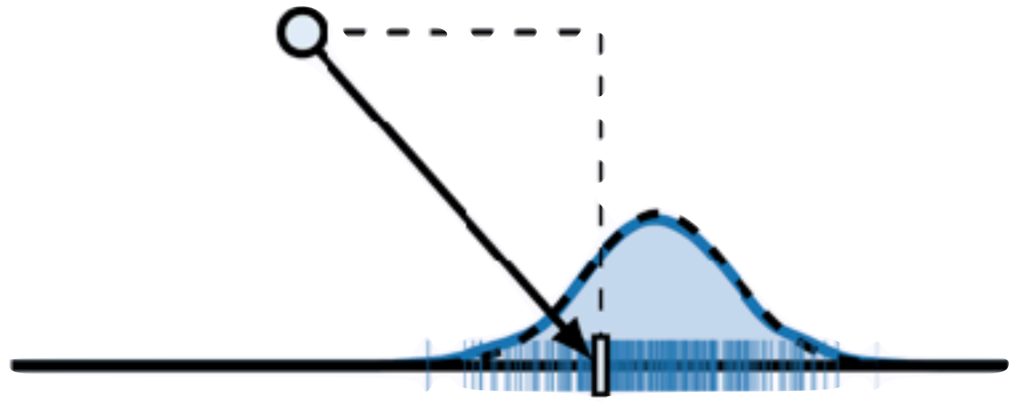

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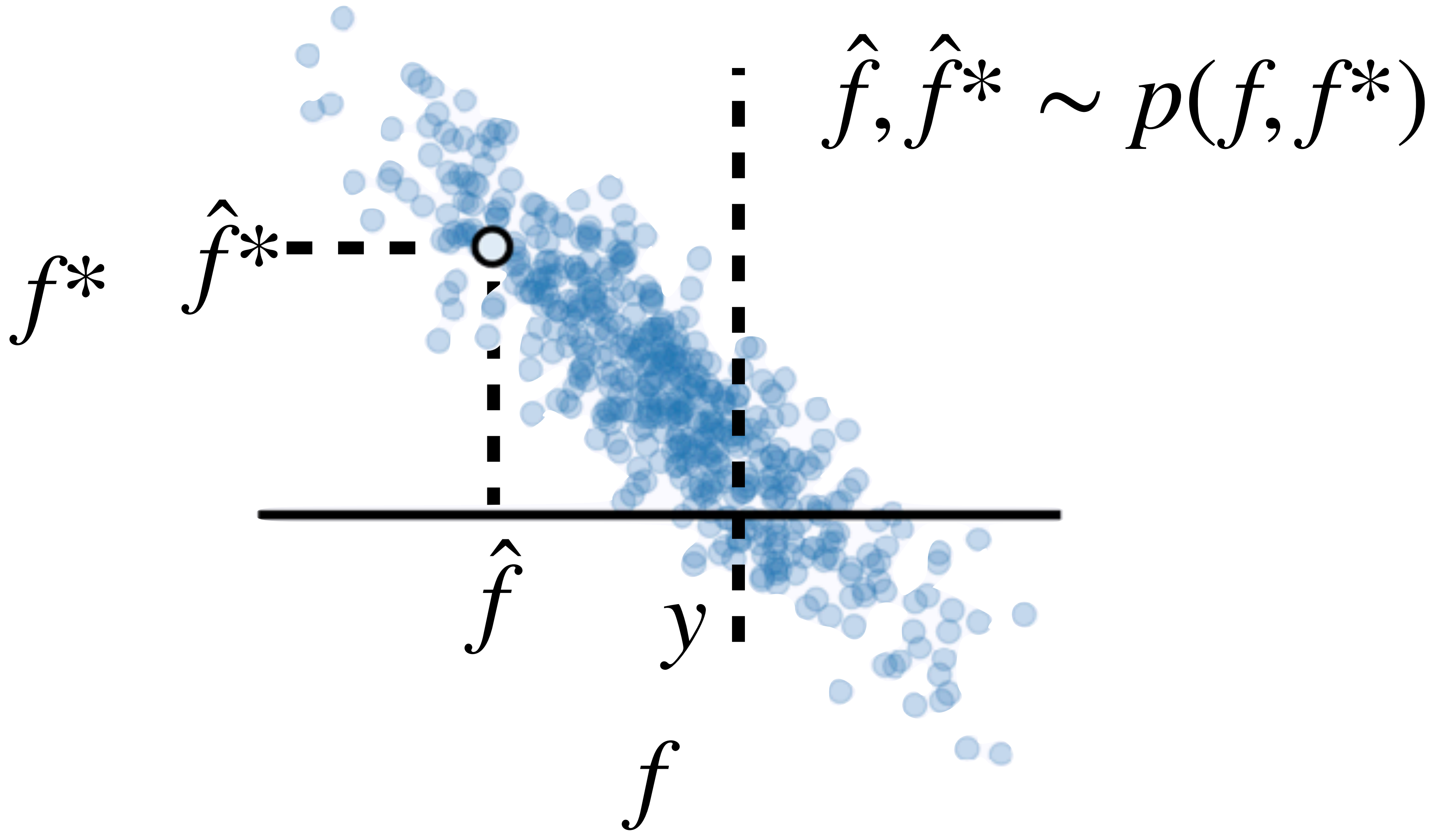
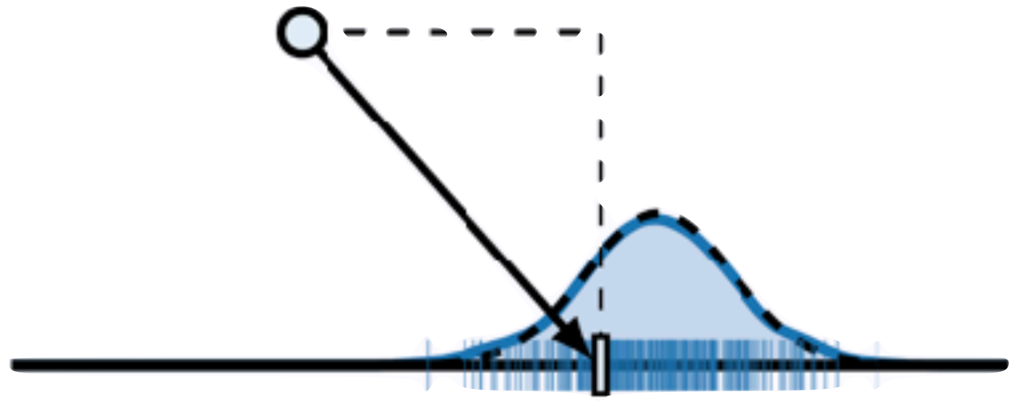
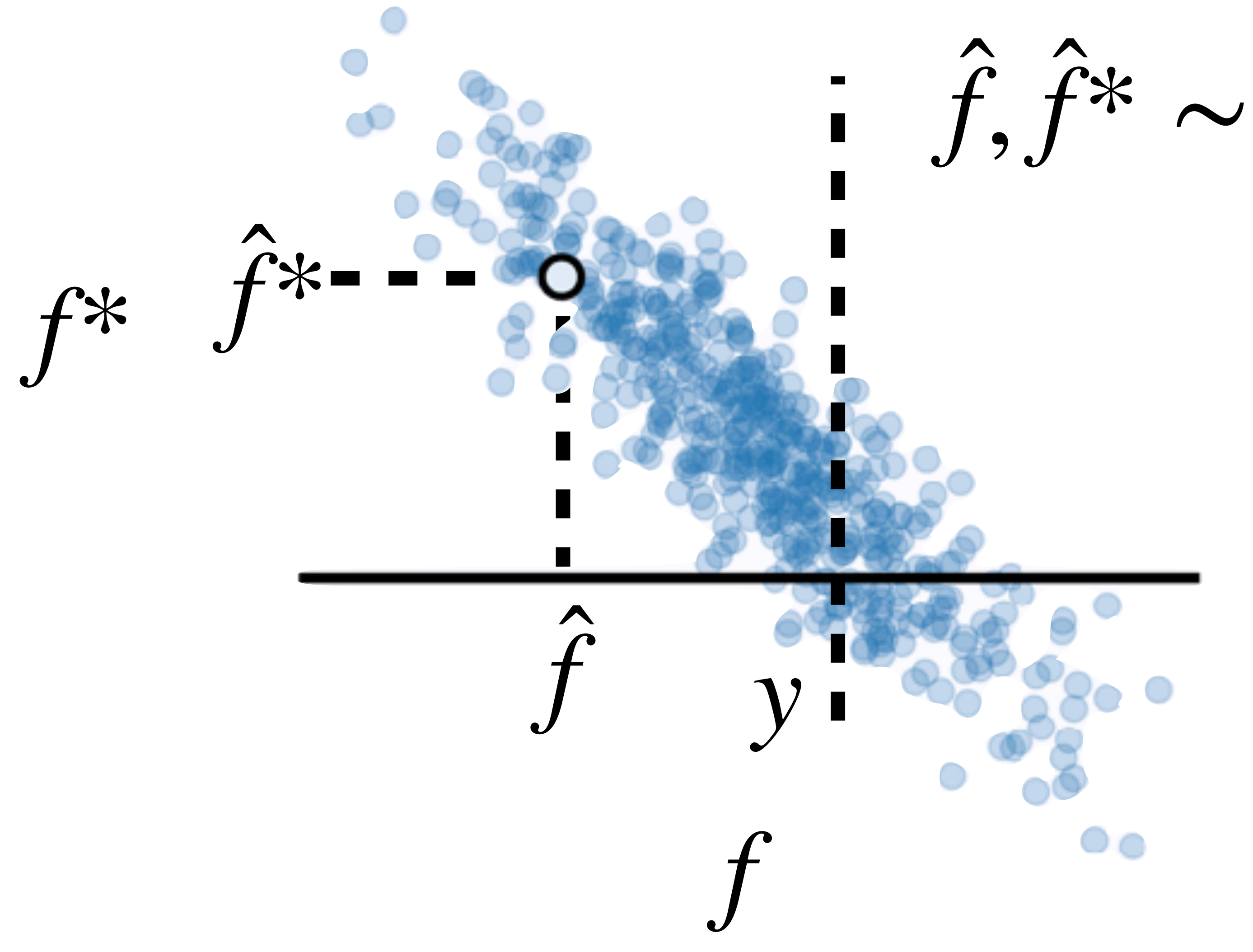


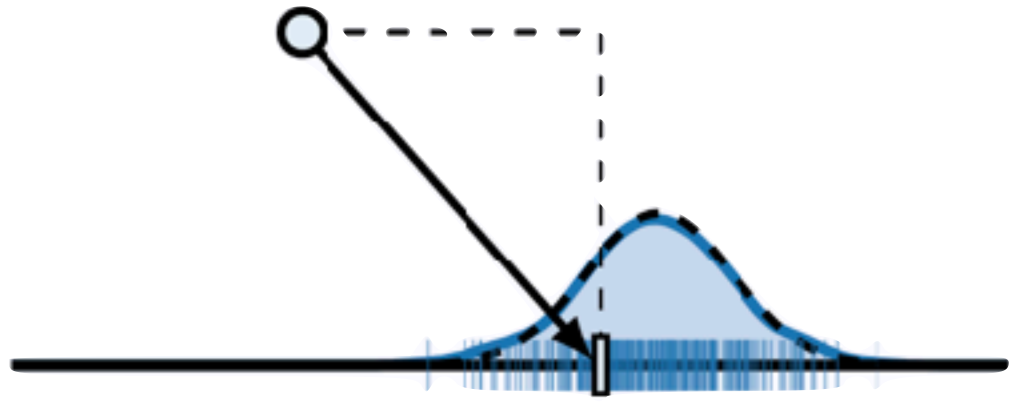


$$(\hat{f}^* \mid \hat{f} = y) = \hat{f}^* + K_{*n} K_{nn}^{-1} (y - \hat{f})$$

(Matheron's Rule)

Sample from the Posterior





Individual Sample View

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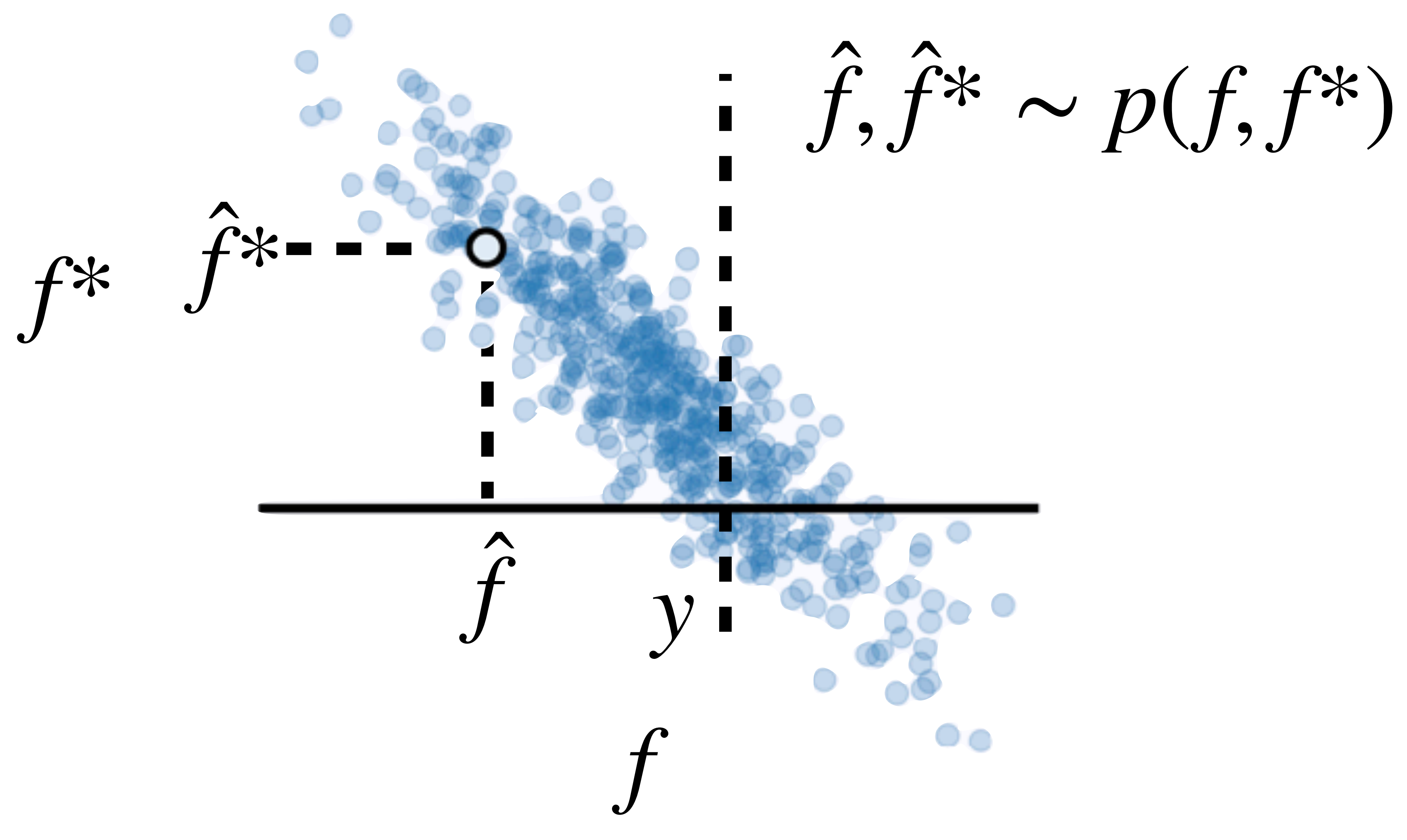

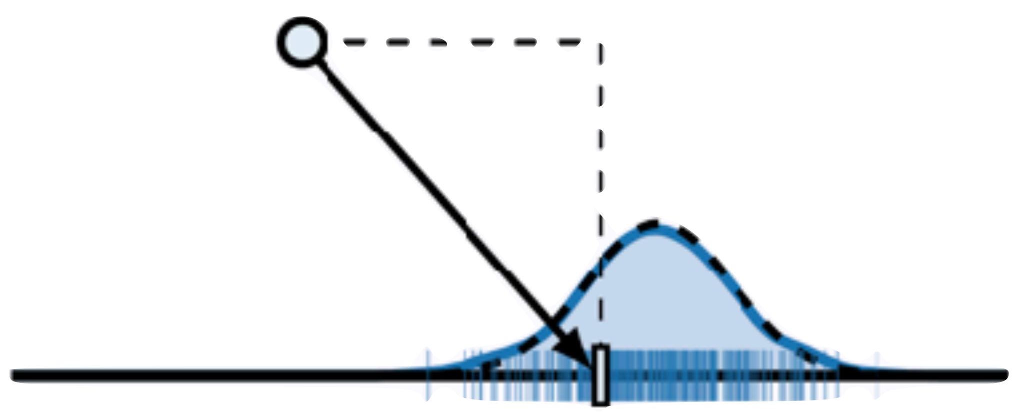

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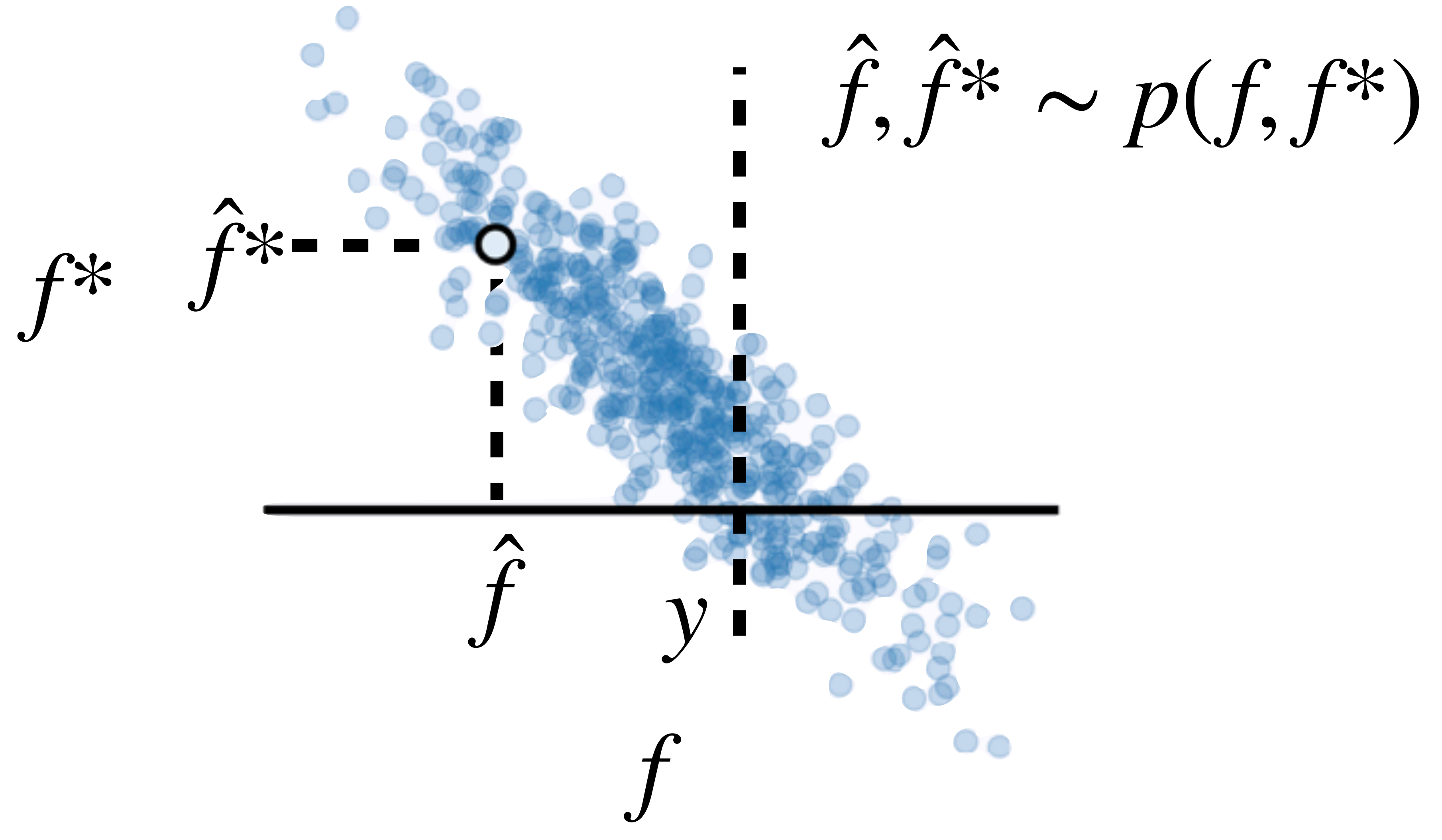

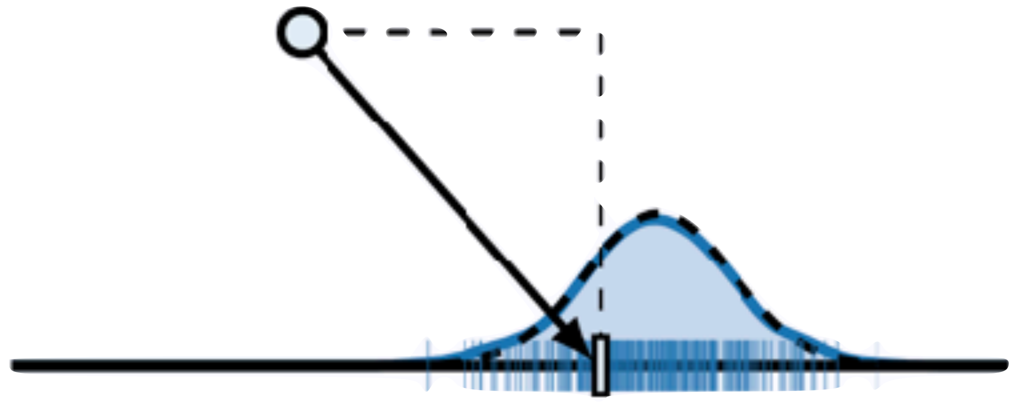

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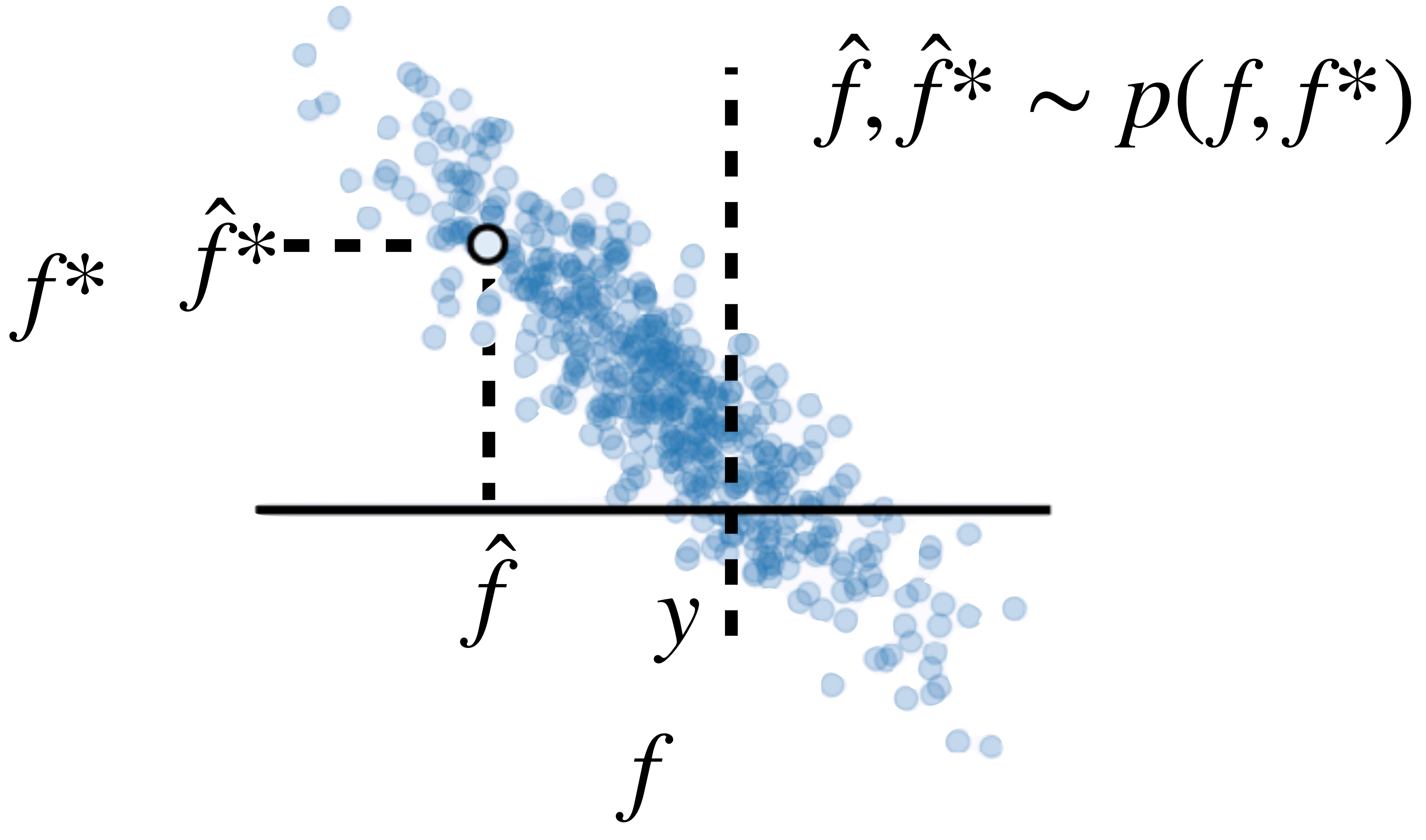
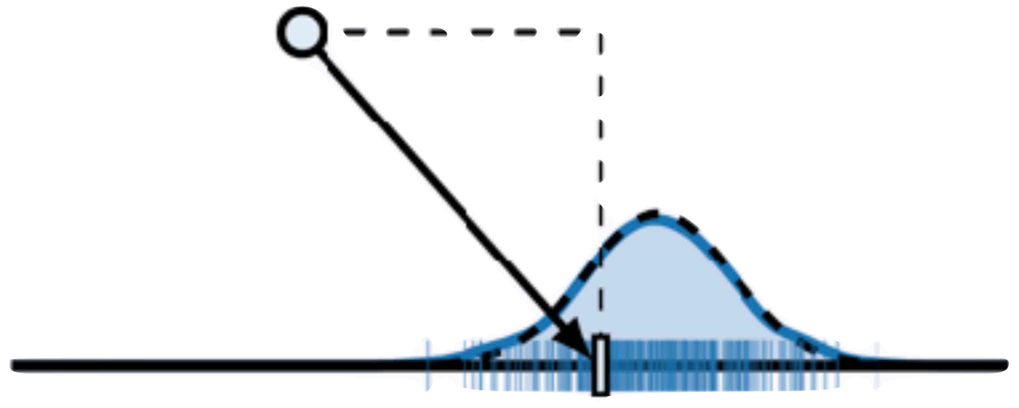
Sample from the Posterior





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$$\downarrow$$

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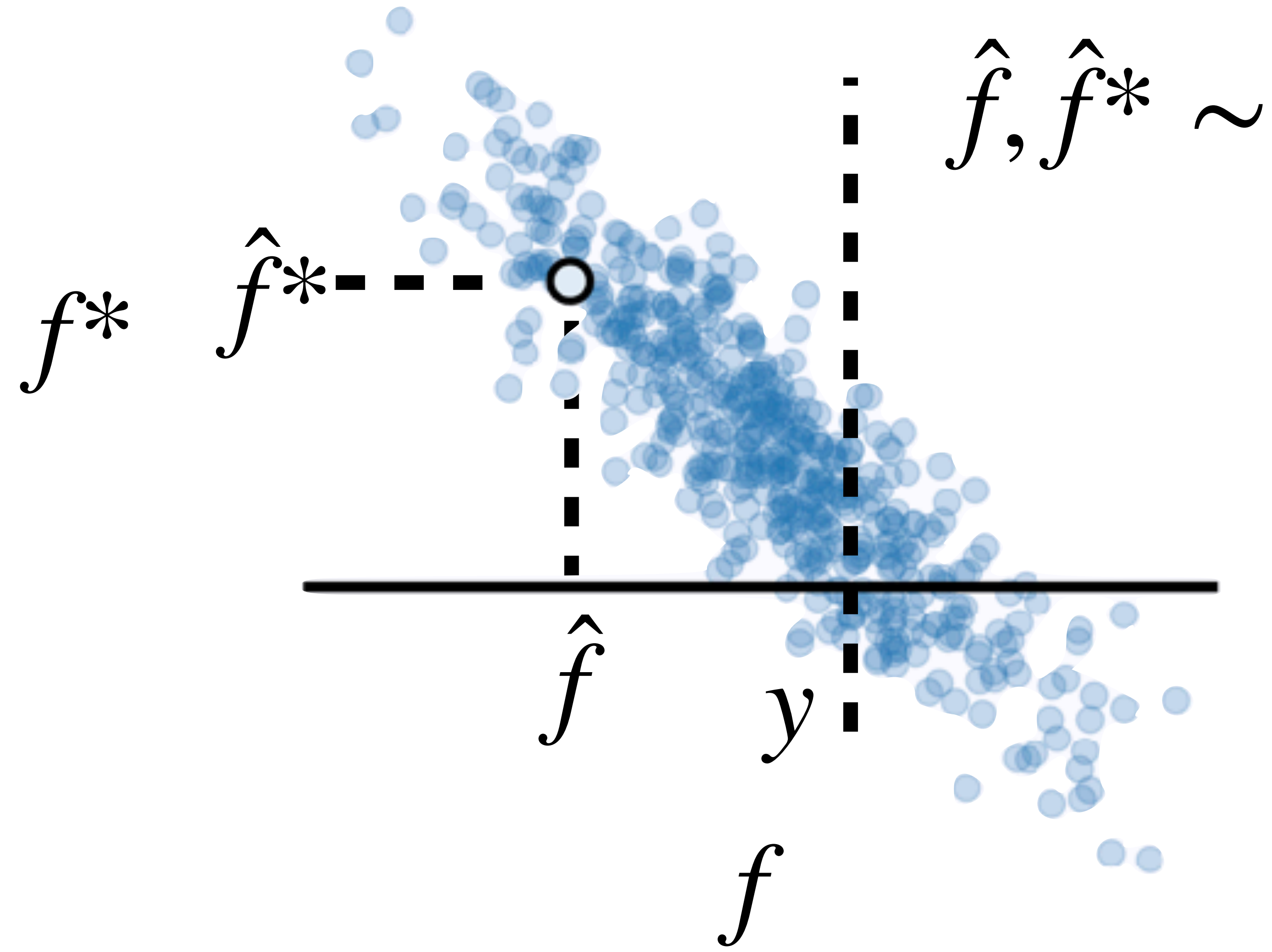

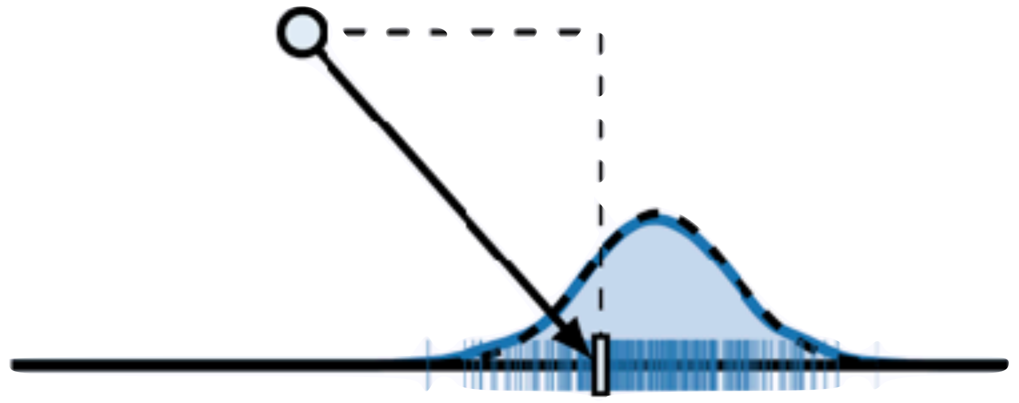

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$\mathcal{O}(n^3)$

Sample from the Posterior

$(f \mid \boldsymbol{y})(\,\cdot\,) =$

Sample from the Posterior

$$(f \mid \boldsymbol{y})(\,\cdot\,) = f(\,\cdot\,)$$

Sample from the Posterior

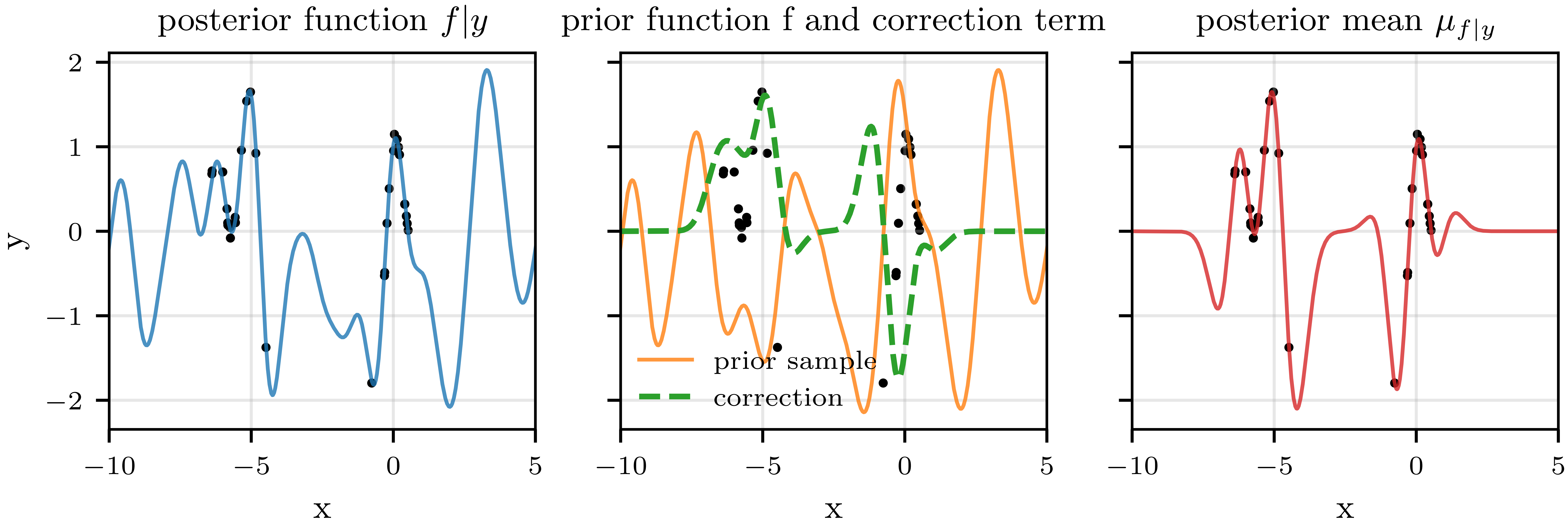
$$(f \mid \boldsymbol{y})(\,\cdot\,) = \; f(\,\cdot\,) \qquad \underbrace{+K_{(\cdot)n}\left(K_{nn} + \sigma^2 I\right)^{-1} y}_{\text{mean } \mu_{f\mid\boldsymbol{y}}(\cdot)}$$

Sample from the Posterior

$$(f \mid \boldsymbol{y})(\,\cdot\,) = \; f(\,\cdot\,) \;\; \underbrace{+K_{(\cdot)n}\left(K_{nn} + \sigma^2 I\right)^{-1}(-f(x) + \epsilon)}_{\text{correction term}} \;\; \underbrace{+K_{(\cdot)n}\left(K_{nn} + \sigma^2 I\right)^{-1} y}_{\text{mean } \mu_{f|\mathbf{y}}(\cdot)}$$

Sample from the Posterior

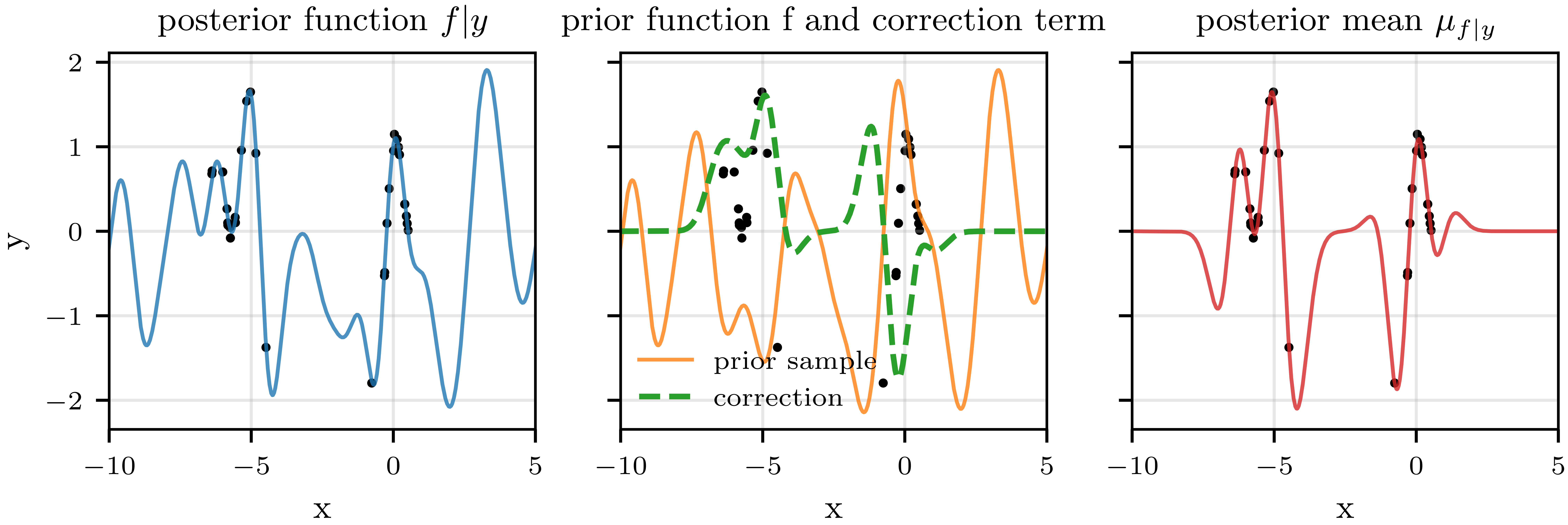
$$(f \mid \boldsymbol{y})(\,\cdot\,) = \; f(\,\cdot\,) \; \underbrace{+K_{(\cdot)n}\left(K_{nn}+\sigma^2 I\right)^{-1}(-f(x)+\epsilon)}_{\text{correction term}} \; \underbrace{+K_{(\cdot)n}\left(K_{nn}+\sigma^2 I\right)^{-1} y}_{\text{mean } \mu_{f|\mathbf{y}}(\cdot)}$$



Sample from the Posterior

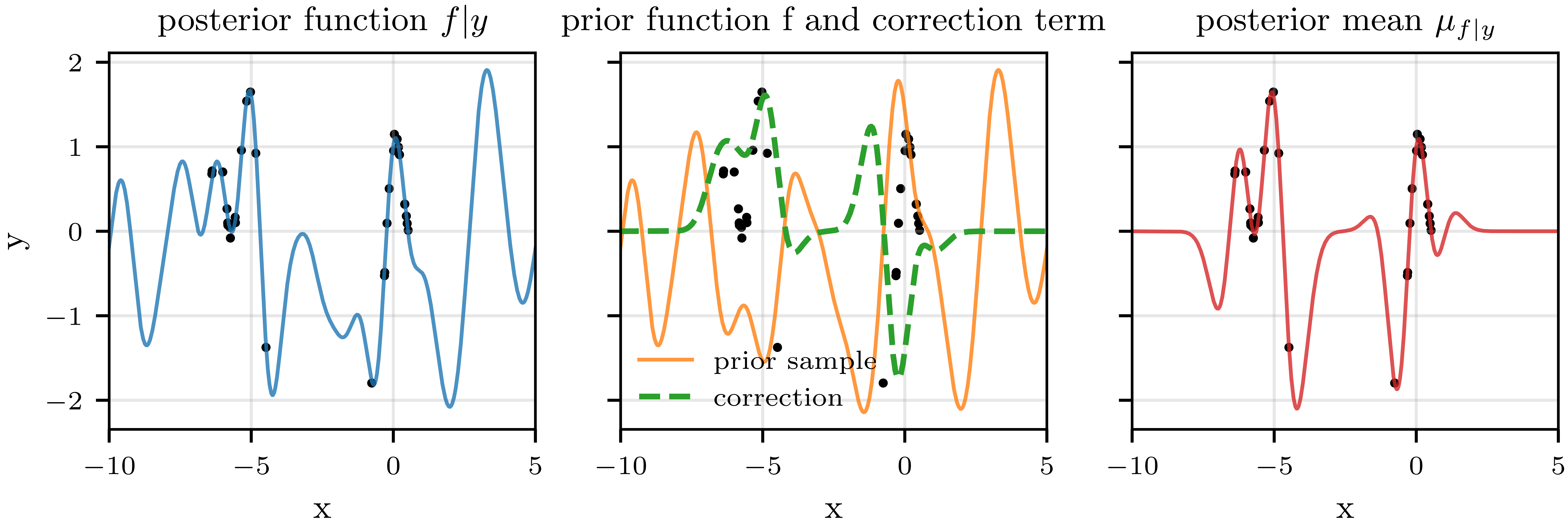
$$(f \mid \boldsymbol{y})(\,\cdot\,) = f(\,\cdot\,) \underbrace{+K_{(\cdot)n}\left(K_{nn}+\sigma^2 I\right)^{-1}(-f(x)+\epsilon)}_{\text{correction term}} \underbrace{+K_{(\cdot)n}\left(K_{nn}+\sigma^2 I\right)^{-1} y}_{\text{mean } \mu_{f|\mathbf{y}}(\cdot)}$$

v^*

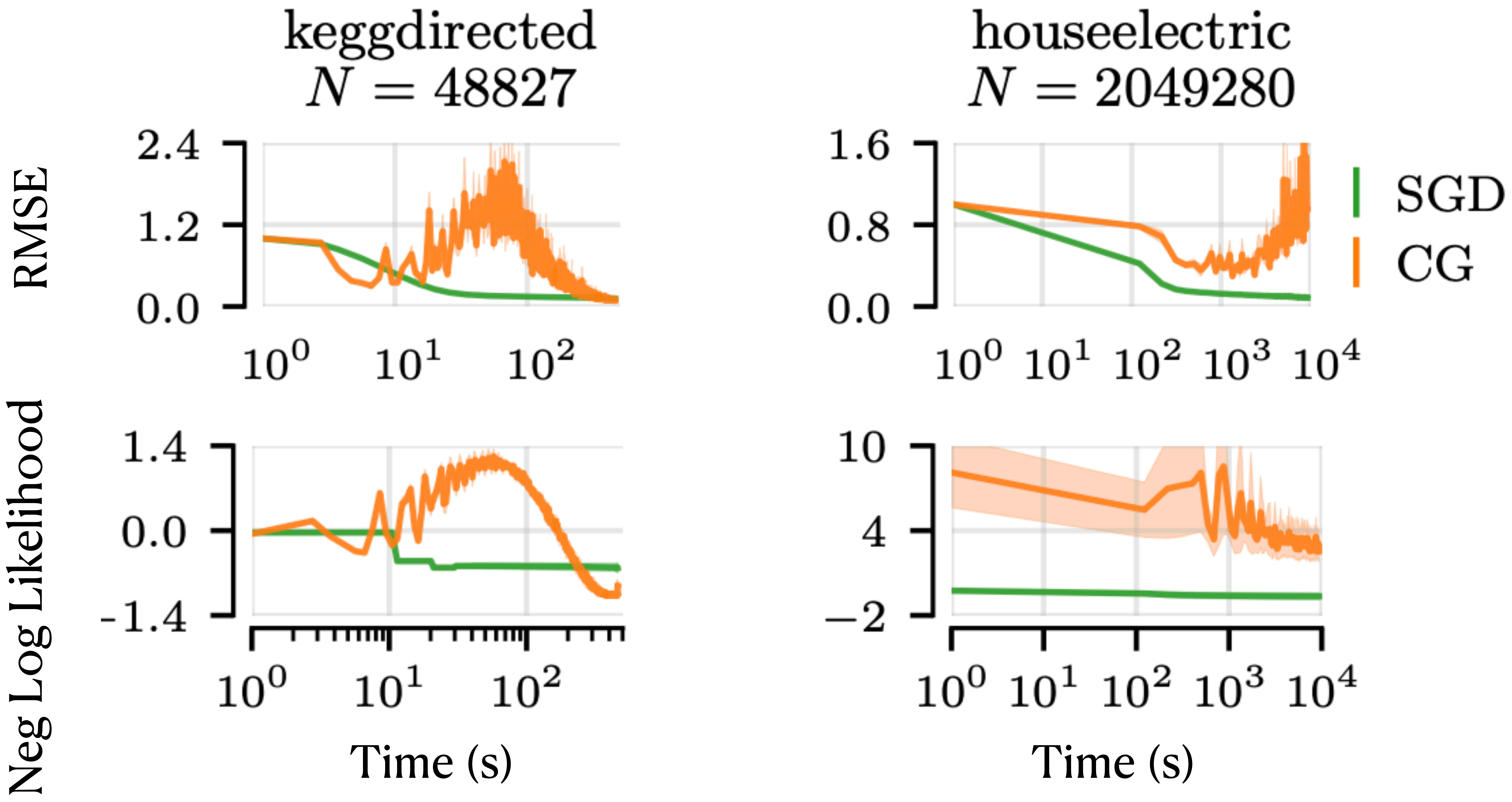


Sample from the Posterior

$$(f \mid \boldsymbol{y})(\cdot) = f(\cdot) \underbrace{+K_{(\cdot)n}\overset{v^*_{\text{sample}}}{\left(K_{nn}+\sigma^2 I\right)^{-1}(-f(x)+\epsilon)}}_{\text{correction term}} \underbrace{+K_{(\cdot)n}\overset{v^*}{\left(K_{nn}+\sigma^2 I\right)^{-1} y}}_{\text{mean } \mu_{f|\mathbf{y}}(\cdot)}$$

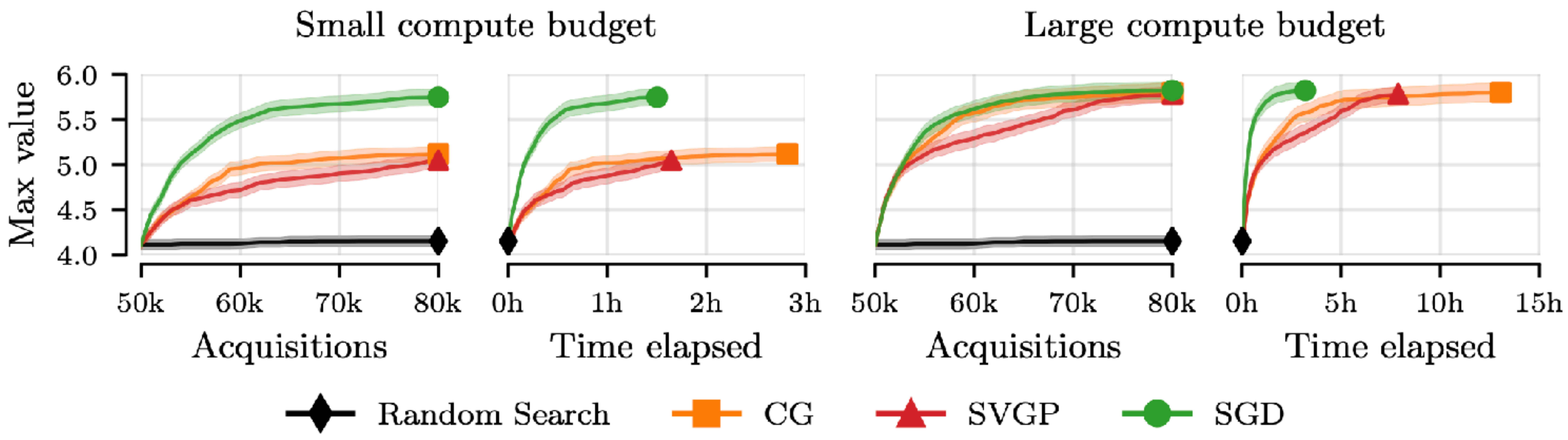


SGD scales much better in uncertainty estimates



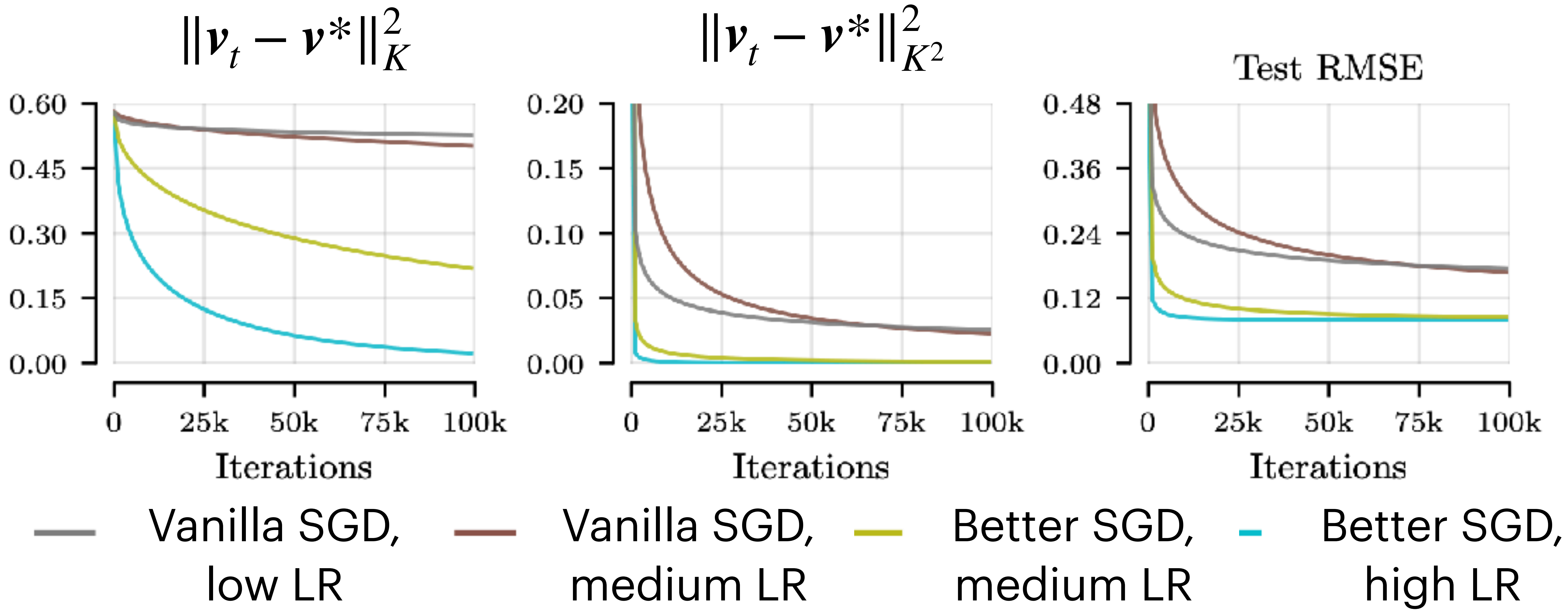
Where can we apply this?

- Sequential Decision Making -> Bayesian Optimisation at a fixed compute budget



Where can we improve this?

- We can derive an SGD objective that is much faster and even better-conditioned



	Data Size	HOUSEELEC 2M
RMSE	SDD*	**0.04 ± 0.00**
	SGD	0.09 ± 0.00
	CG	0.87 ± 0.14
	SVGP	0.12 ± 0.00
Time (min)	SDD*	**47.8 ± 0.02**
	SGD	69.5 ± 0.06
	CG	157 ± 0.01
	SVGP	154 ± 0.12
NLL	SDD*	**-1.46 ± 0.10**
	SGD	-1.09 ± 0.04
	CG	2.07 ± 0.58
	SVGP	-0.61 ± 0.01

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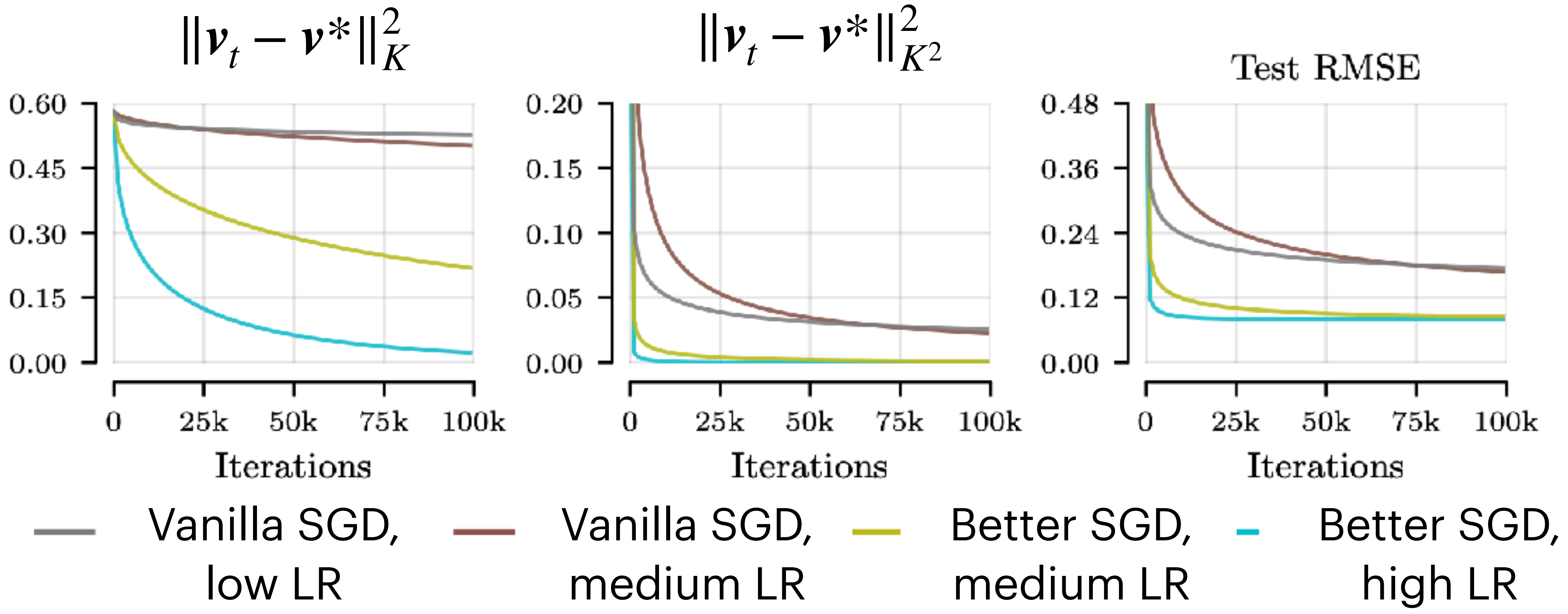

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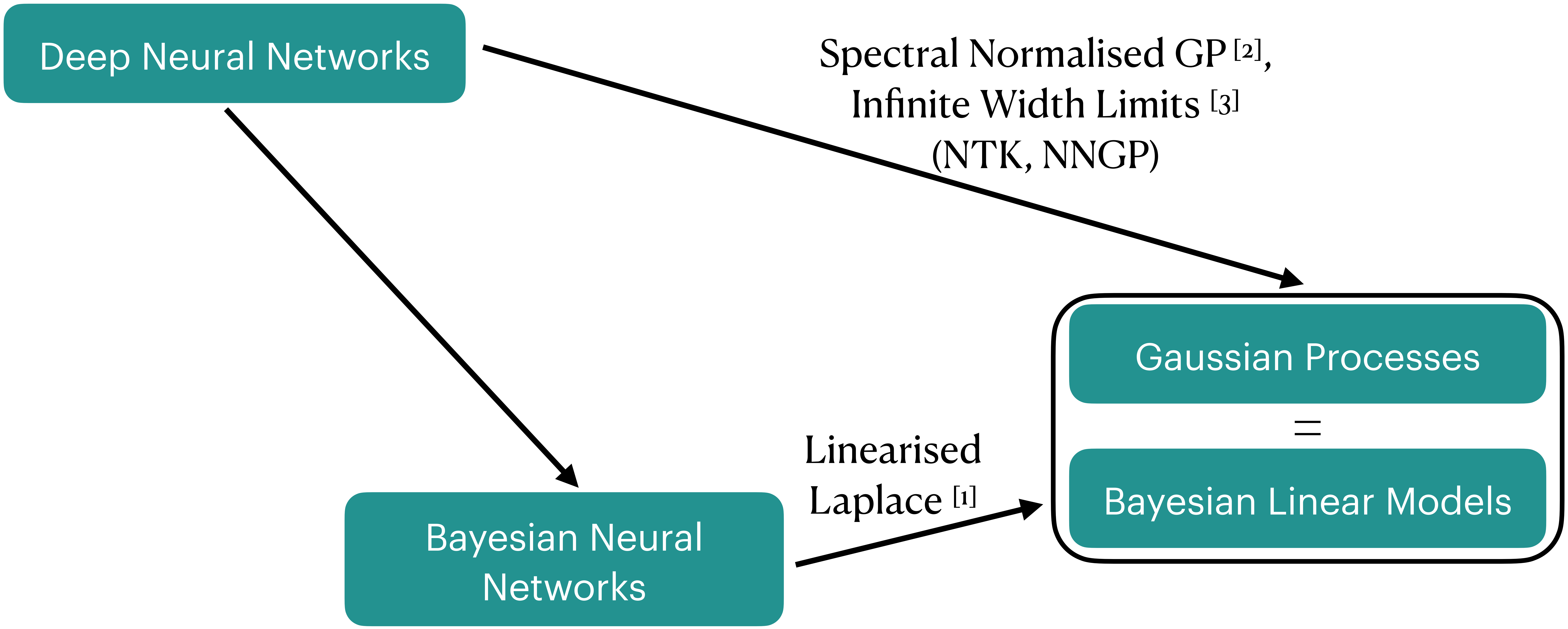
[1] **Padhy, S.***, Lin, J. A.*, Antorán, J.*, Tripp, A., Terenin, A., Szepesvári, C., ... & Janz, D. Stochastic Gradient Descent for Gaussian Processes Done Right. ***ICLR 2024***

How can we apply this to Deep Learning?



[1] **Padhy, S.***, Antorán, J.,*, Barbano, R., Nalisnick, E., ... and Hernández-Lobato, J.M., 2022. Sampling-based inference for large linear models, with application to linearised Laplace. ***ICLR 2023***
[2] **Padhy, S.***, Liu, J. Z.*, Ren, J.*, Lin, Z., Wen, Y., Jerfel, G., ... & Lakshminarayanan, B. A simple approach to improve single-model deep uncertainty via distance-awareness. ***JMLR 2023***
[3] Adlam, B., Lee, J., **Padhy, S.**, Nado, Z. and Snoek, J., 2023. Kernel Regression with Infinite-Width Neural Networks on Millions of Examples. *arXiv preprint*

Uncertainty in Deep NNs

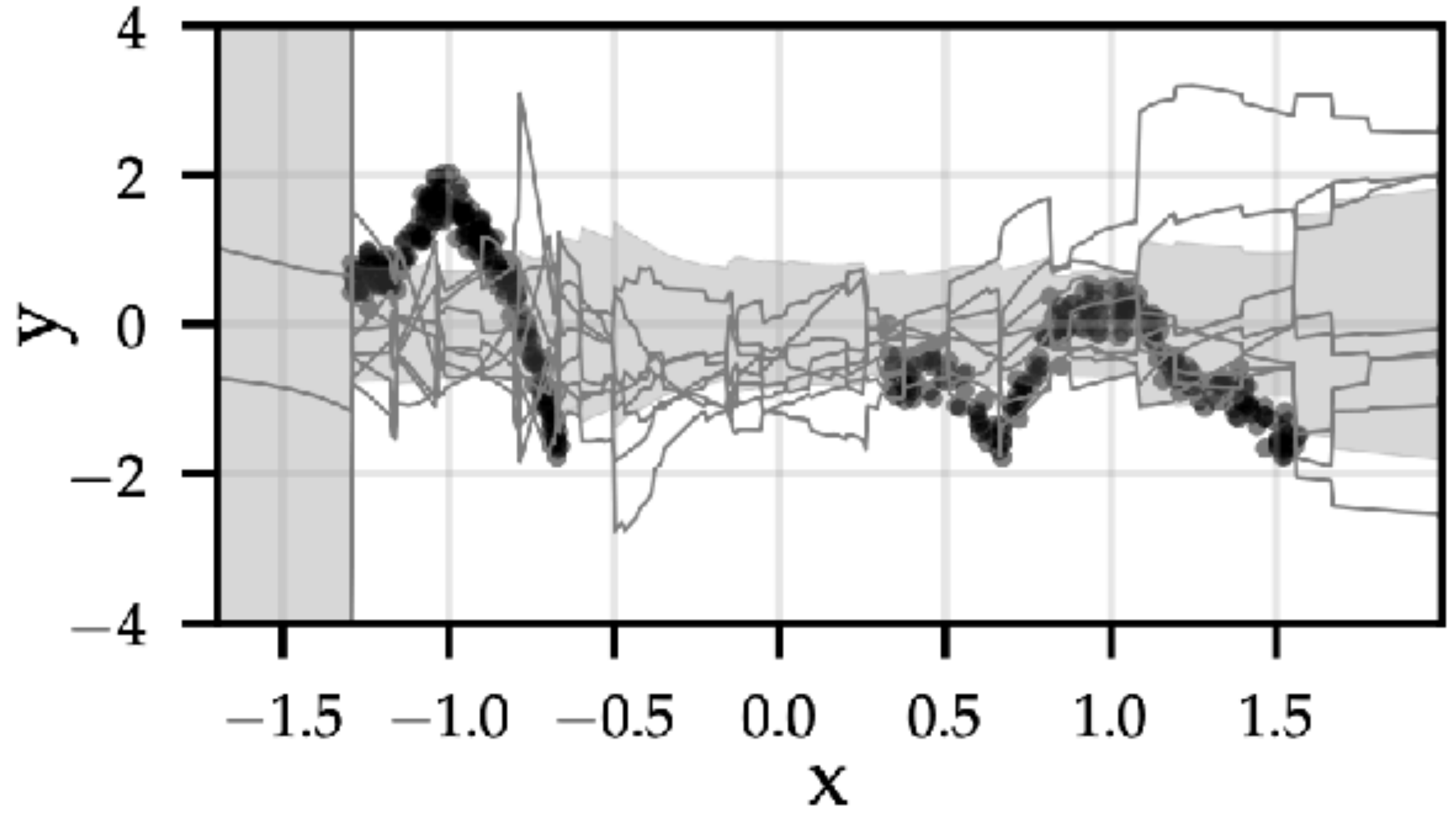
- Given a neural network $f : \mathbb{R}^{d'} \to \mathbb{R}^m$ parameterised by $\theta \in \mathbb{R}^d$
- We estimate uncertainty in $f(x)$ as uncertainty in the tangent **linear** model around MAP $\bar{w}$

$$h(\theta, x) = f(\bar{w}, x) + \nabla_w f(\bar{w}, x)(\theta - \bar{w}), \qquad \theta \sim \mathcal{N}(0,\ A^{-1})$$

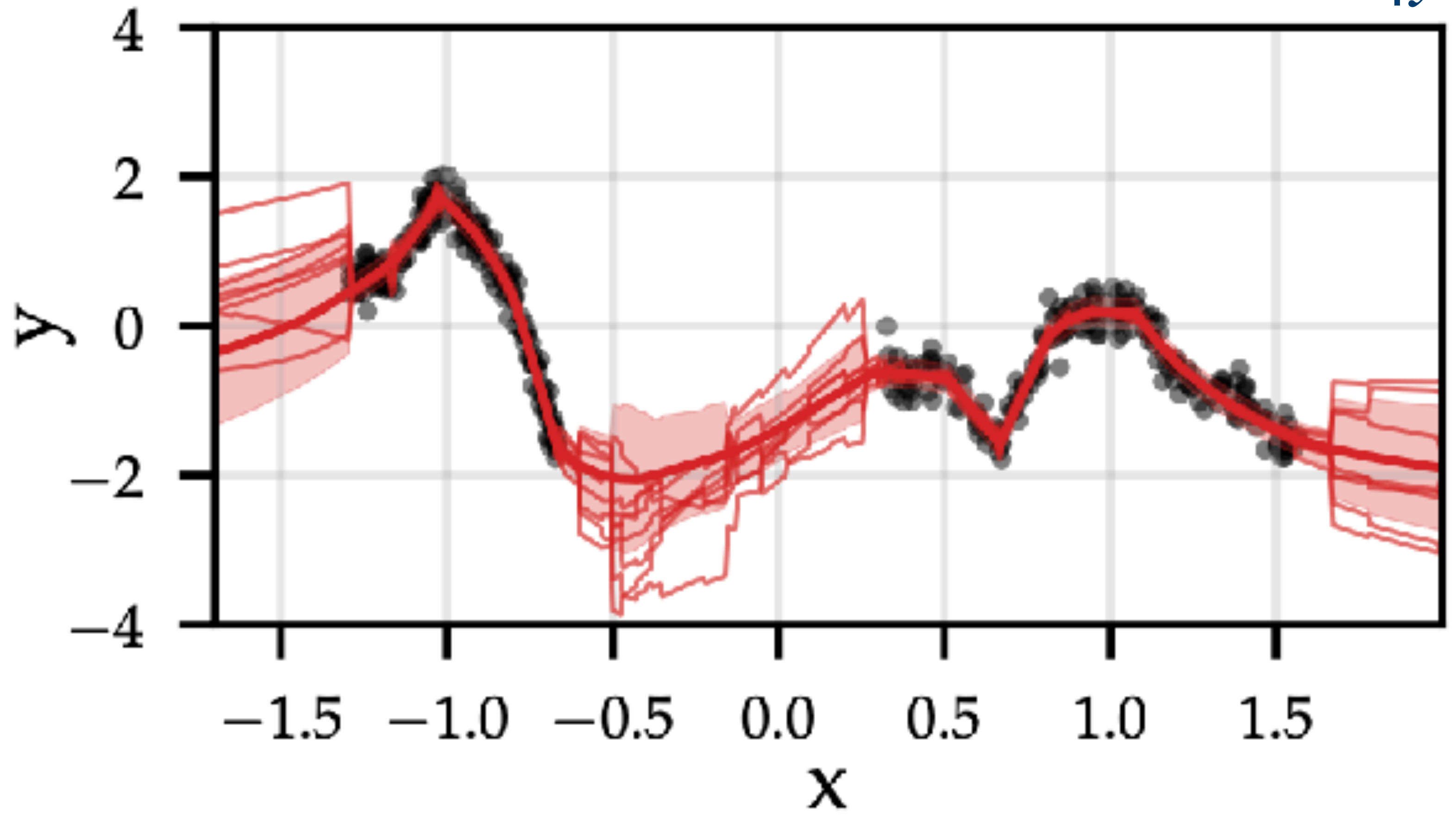
$$h(\theta, x) = \text{MAP solution} + J(x)(\theta - \bar{w})$$

- Turns out $h \sim \mathrm{GP}(0,k)$ where $k(x_i, x_j) = J(x_i)^T A^{-1} J(x_j)$

Prior samples $h \sim GP(0, k)$



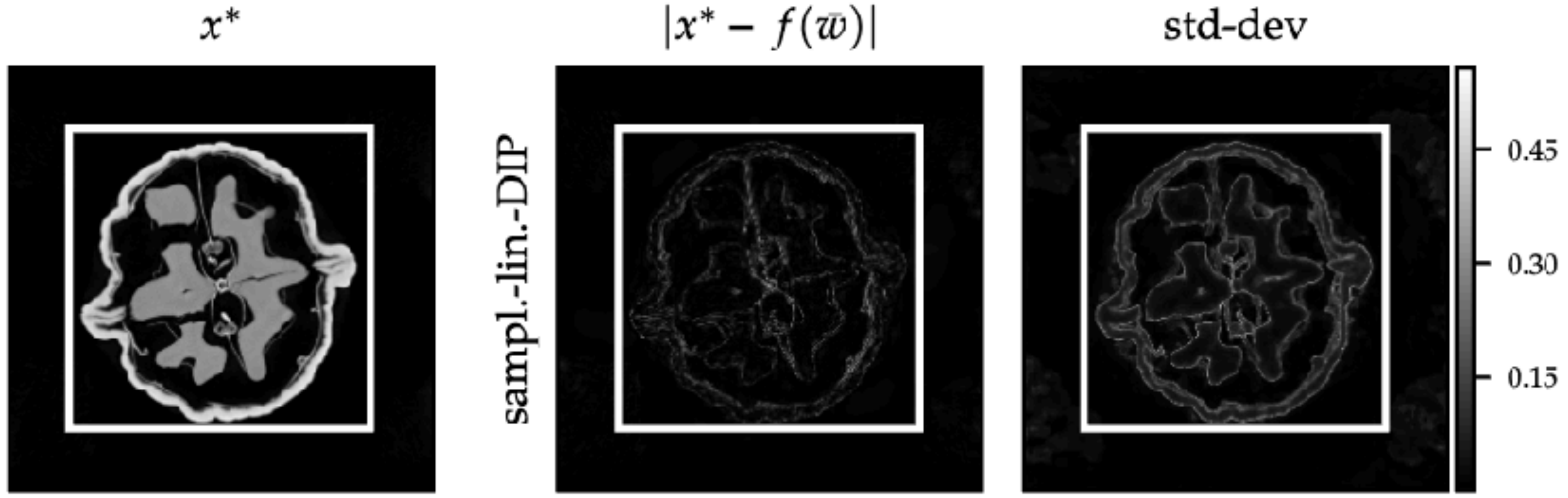
Posterior samples $h \sim GP(\mu_{h|y}, k_{h|y})$



Where can we scale this?

- ImageNet-scale [1] ($nm = 2B, d = 1.5M$)
- 2D Computed Tomography [1] ($m = 13k, d = 3M$)
- Large-scale/ill-conditioned regression [2, 3] ($n = 2M$)

	$m = 7680$			
	LL		wall-clock time (min.)	
Method	marginal	(10×10)	params optim.	prediction
MCDO-UNet	0.028	2.474	0	$3'$
lin.-UNet	2.214	2.601	$1260'$	$196'$
sampl.-lin.-UNet	**2.341**	**2.869**	$12'$	$14'$



	Dataset	HOUSEELEC
	N	2049280
RMSE	SGD	$\mathbf{0.09 \pm 0.00}$
RMSE	CG	0.87 ± 0.14
RMSE	SVGP	0.10 ± 0.02
RMSE †	SGD	$\mathbf{0.09 \pm 0.00}$
RMSE †	CG	0.93 ± 0.19
RMSE †	SVGP	—
Hours	SGD	2.69 ± 0.91
Hours	CG	2.62 ± 0.01
Hours	SVGP	$\mathbf{0.04 \pm 0.00}$

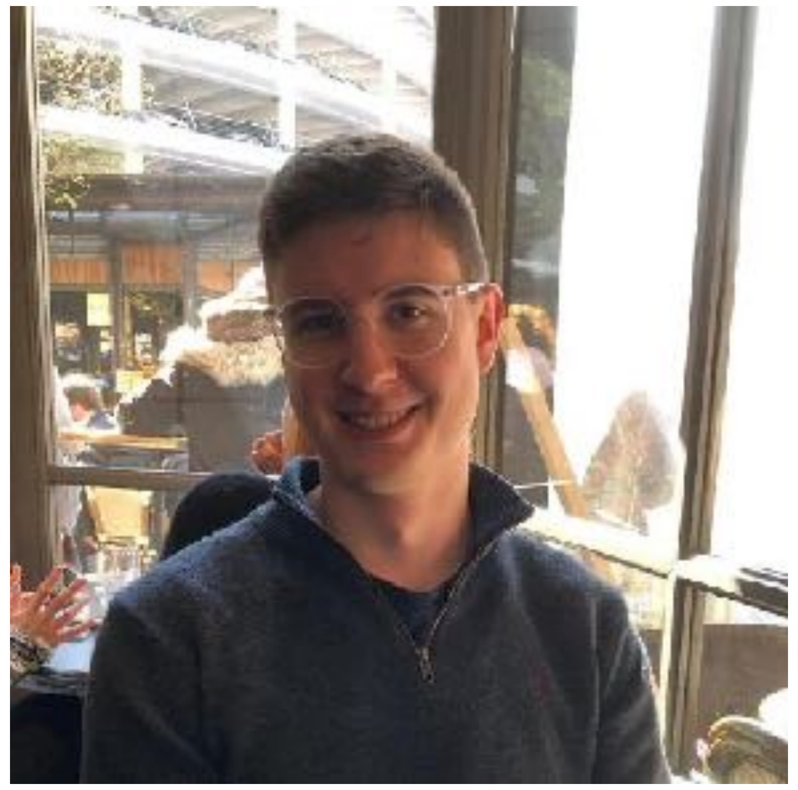
[1] **Padhy, S.***, Antorán, J.,*, Barbano, R., Nalisnick, E., ... and Hernández-Lobato, J.M., 2022. Sampling-based inference for large linear models, with application to linearised Laplace. ***ICLR 2023***

My Collaborators

Andy Lin

Javier Antoran

Riccardo Barbano



Dave Janz

Alex Terenin

Miguel Hernandez-Lobato

Appendix: Linear Models are GPs

$$y_i = \phi(x_i)\theta + \eta_i$$

$$y_i \in \mathbb{R}^m$$

$$\theta \in \mathbb{R}^d$$

$$\phi(x_i) \in \mathbb{R}^{m \times d}$$

$$i \in \{1,\ldots,n\}$$

$$\theta \sim \mathcal{N}(0, A^{-1})$$

$$\eta_i \sim \mathcal{N}(0, B_i^{-1})$$

$$\longrightarrow$$

$$y_i = GP(0, k(\,.\,,\,.\,)) + \eta_i$$

where $K_n n = \Phi^\top A^{-1} \Phi$