



Hidden Physics Models



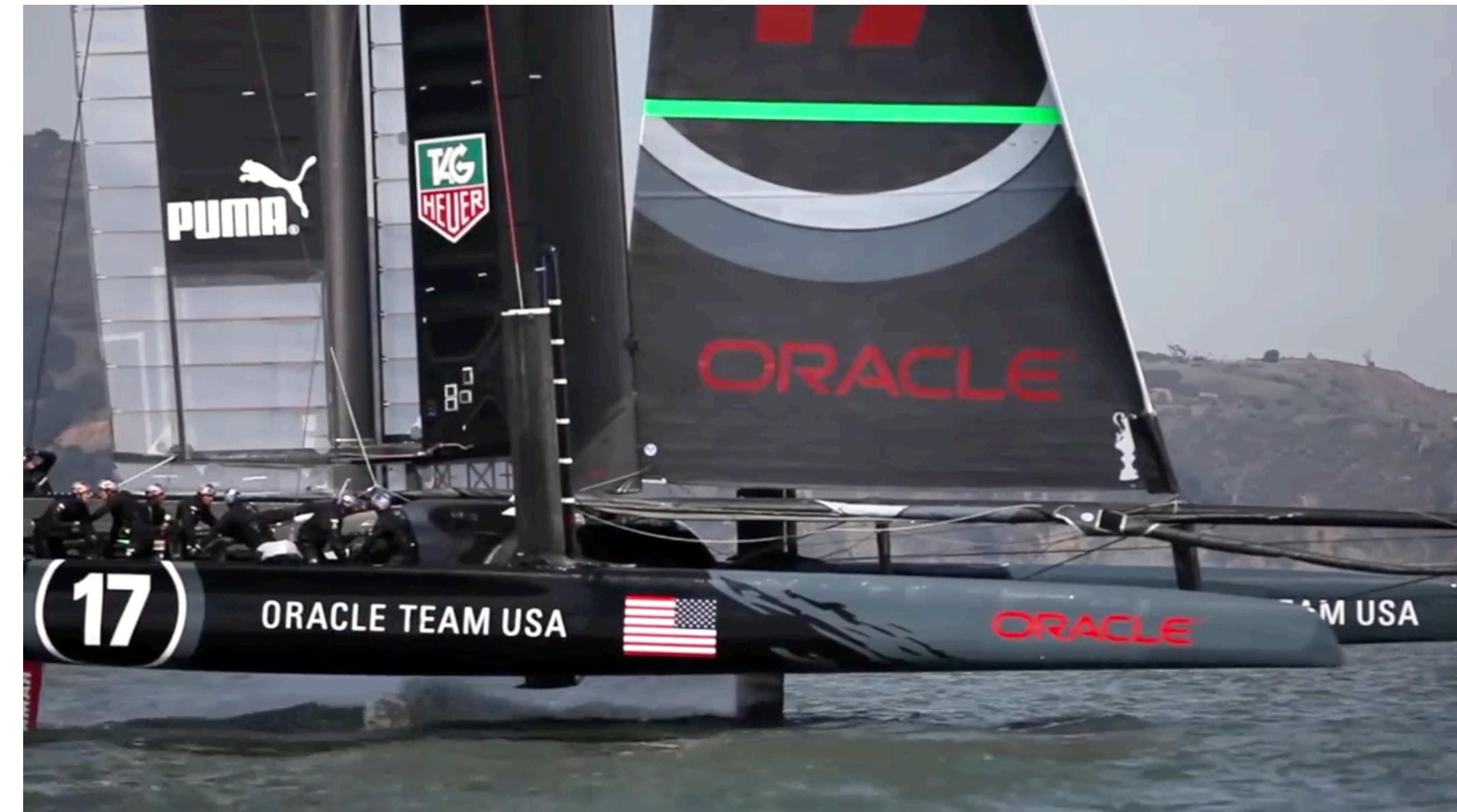
Maziar Raissi

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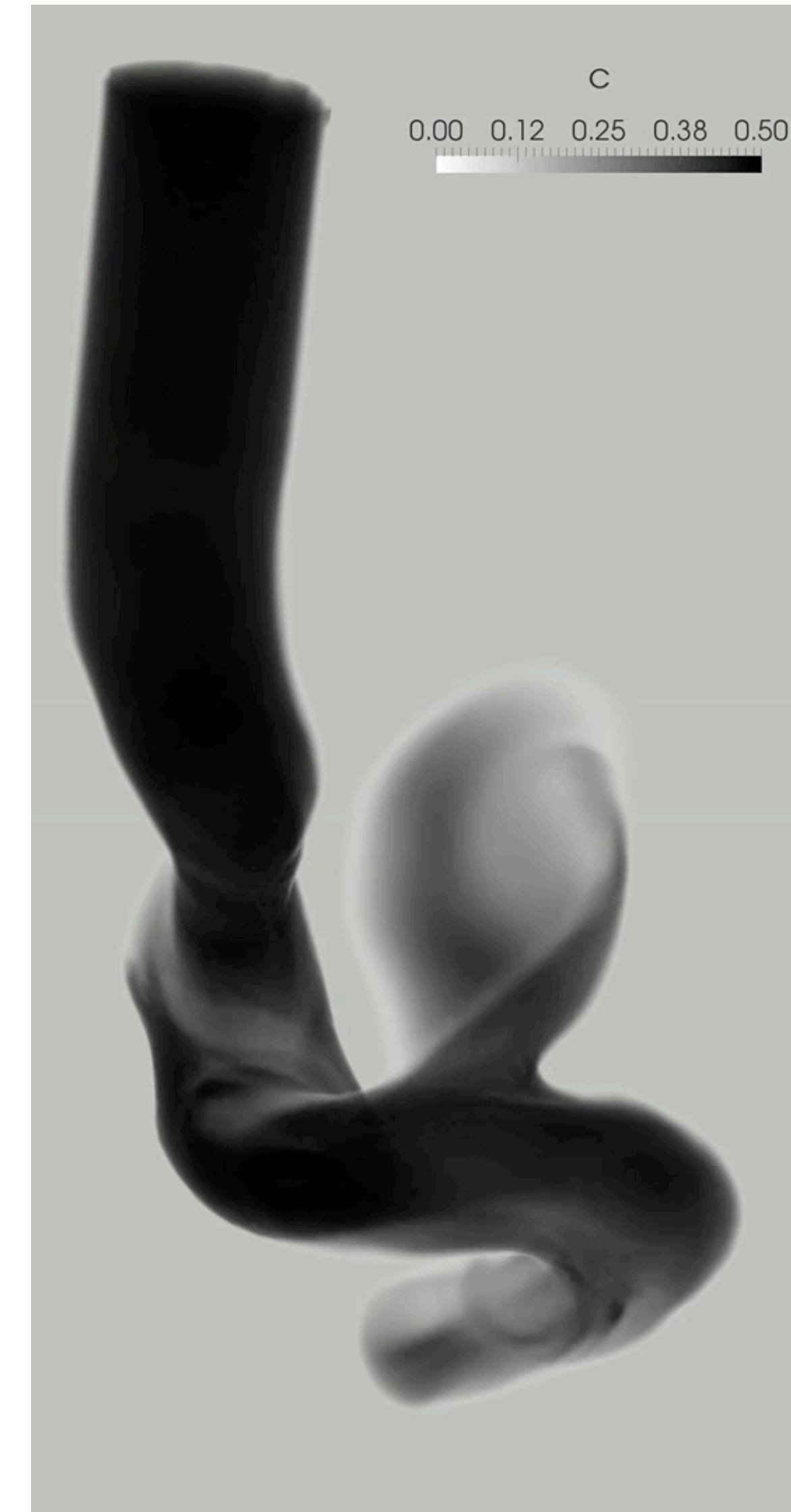
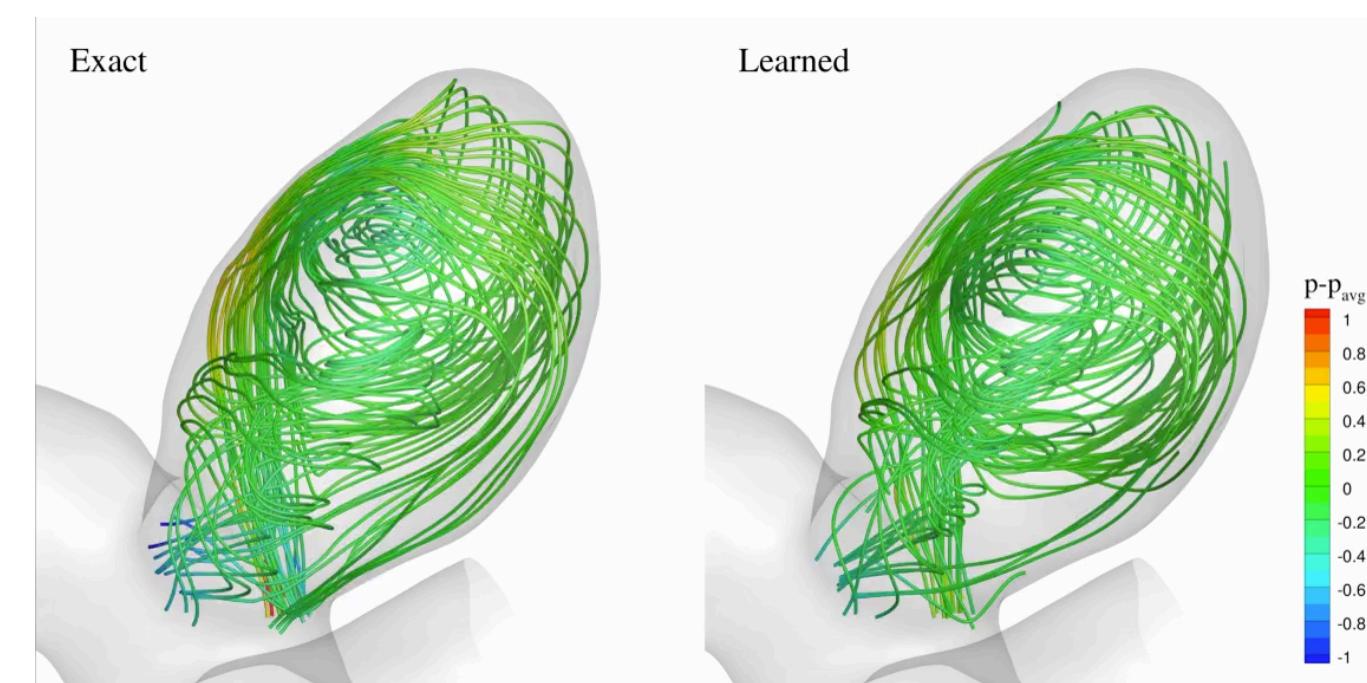


The ORACLE TEAM USA crew flying their AC72 "17" on foils.

Senior Software Engineer

NVIDIA

mraissi@nvidia.com





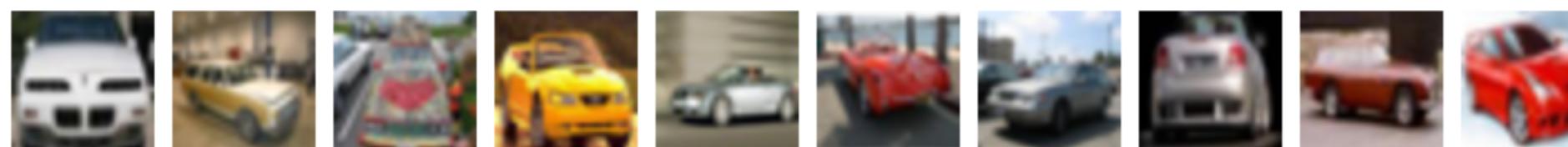
Machine/Deep Learning



airplane



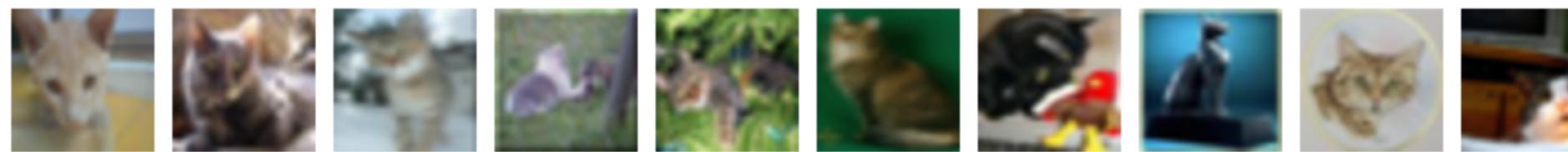
automobile



bird



cat



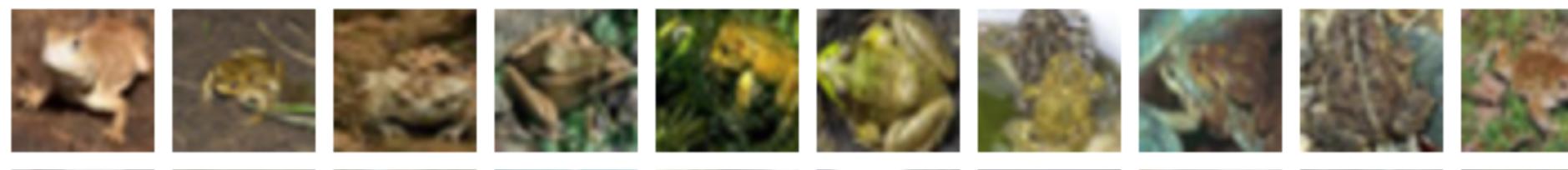
deer



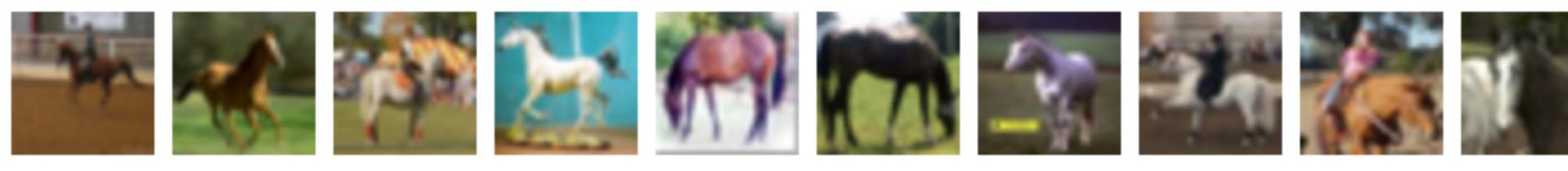
dog



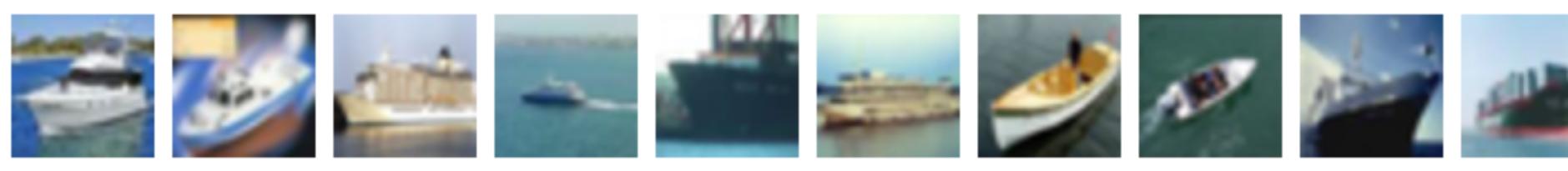
frog



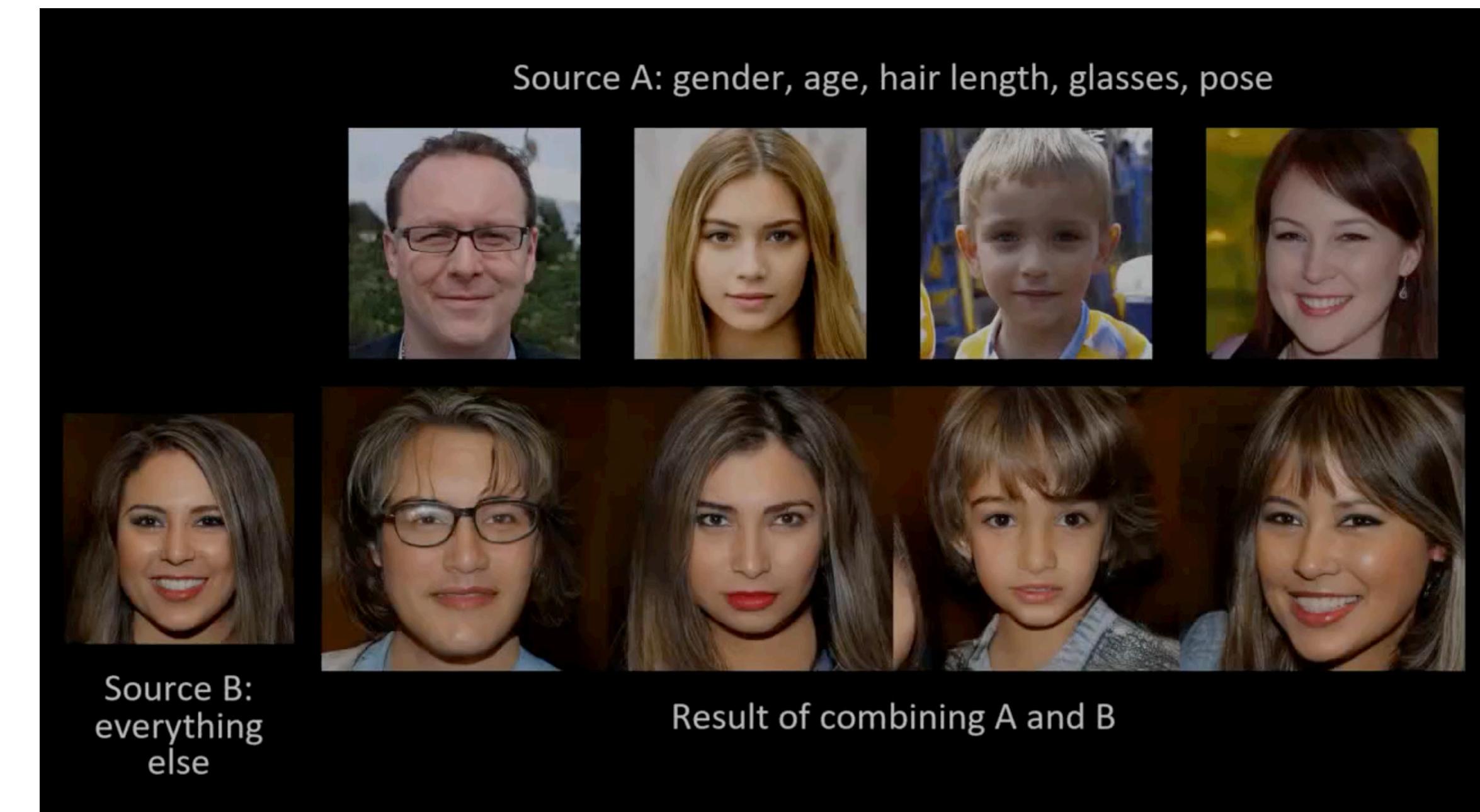
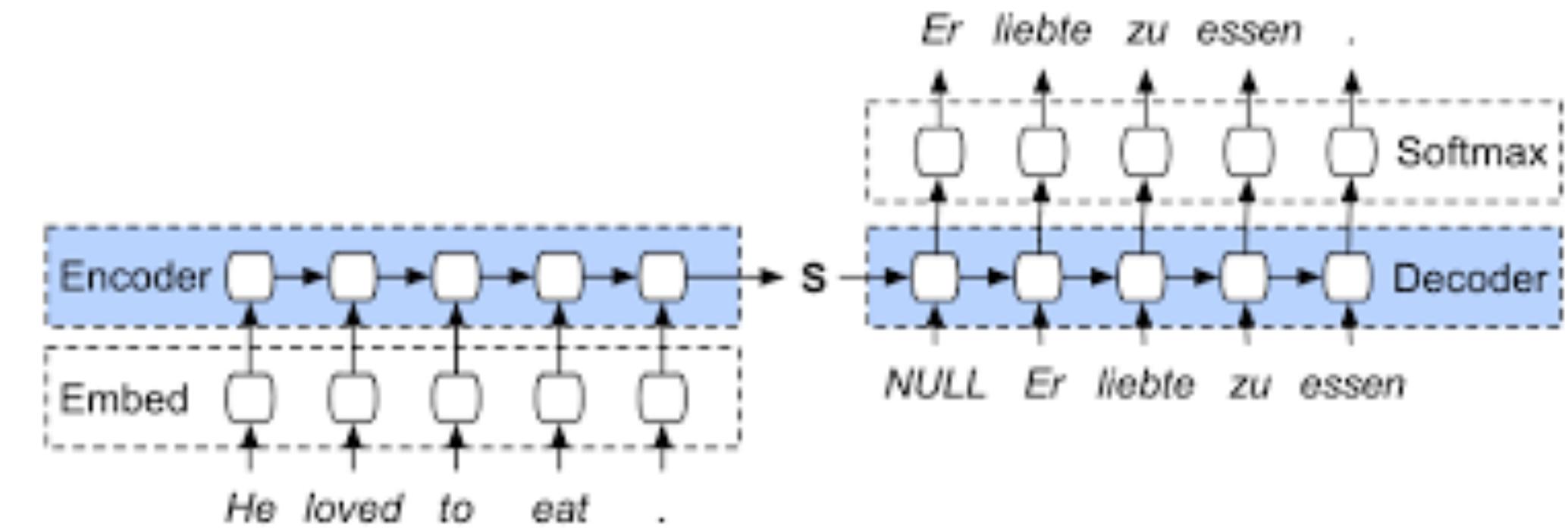
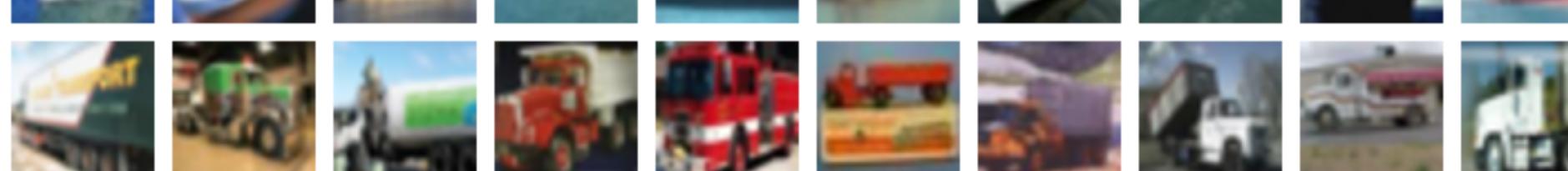
horse



ship

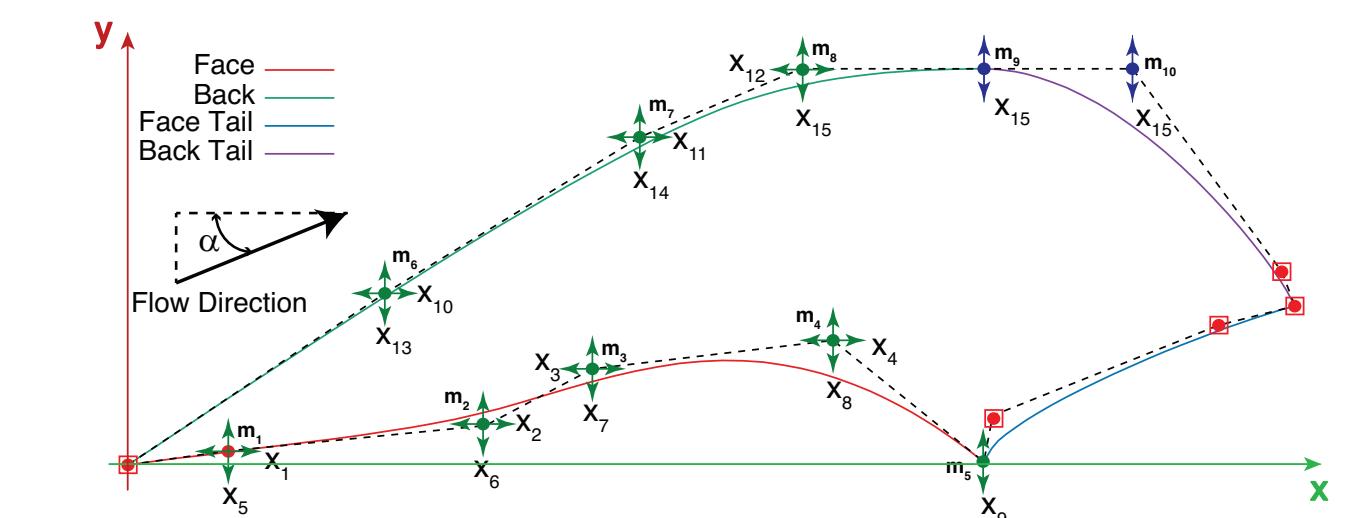
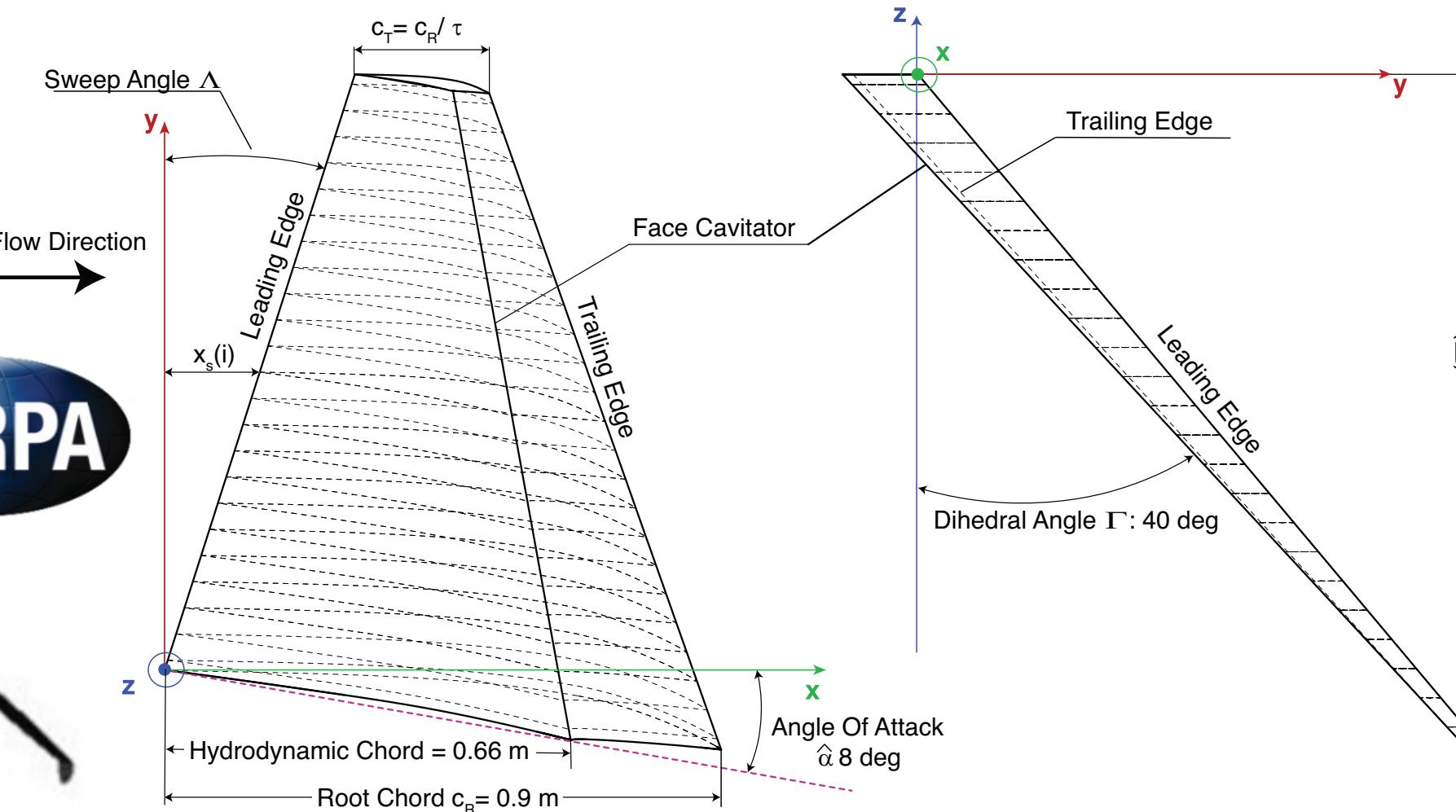
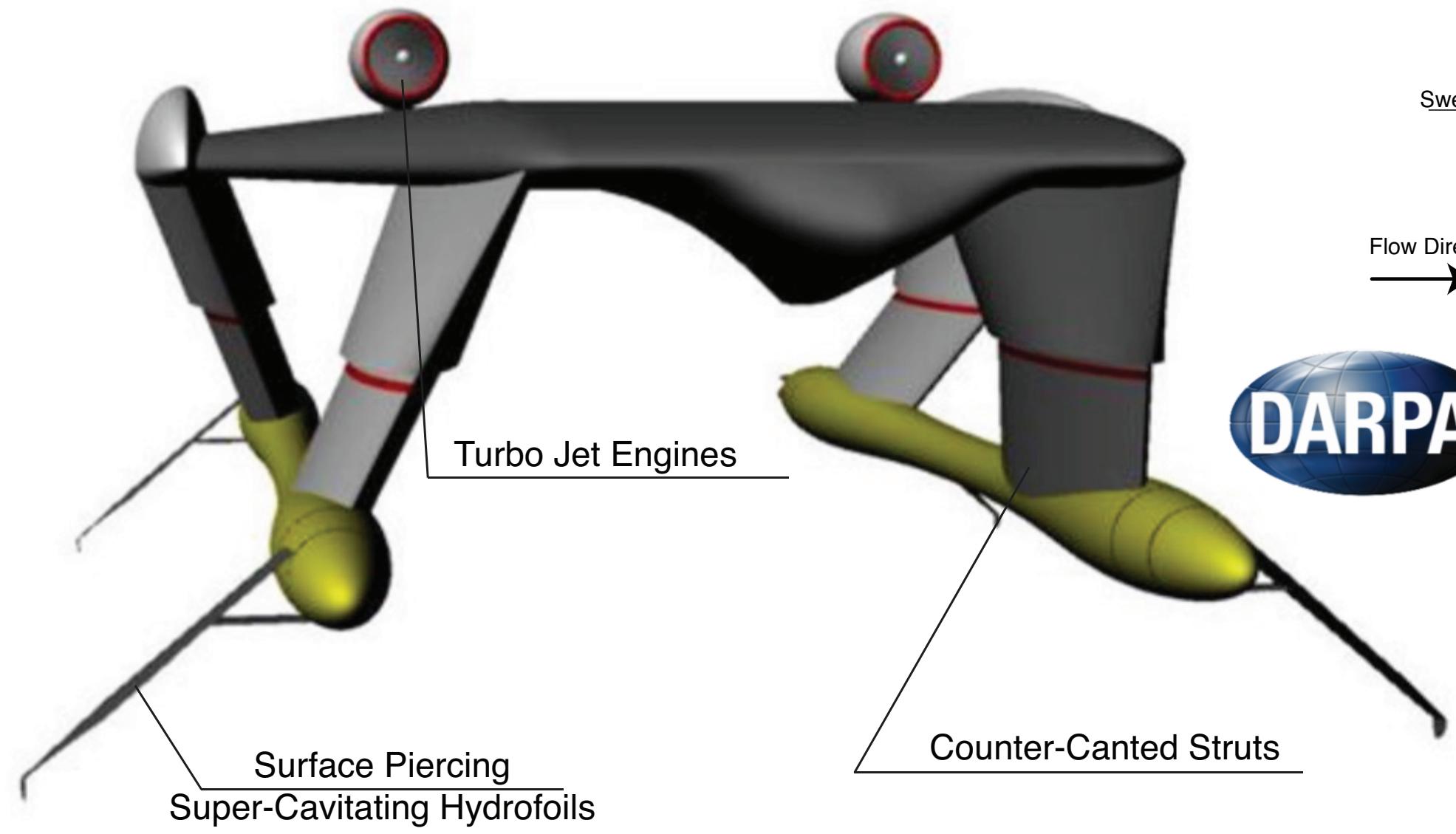


truck

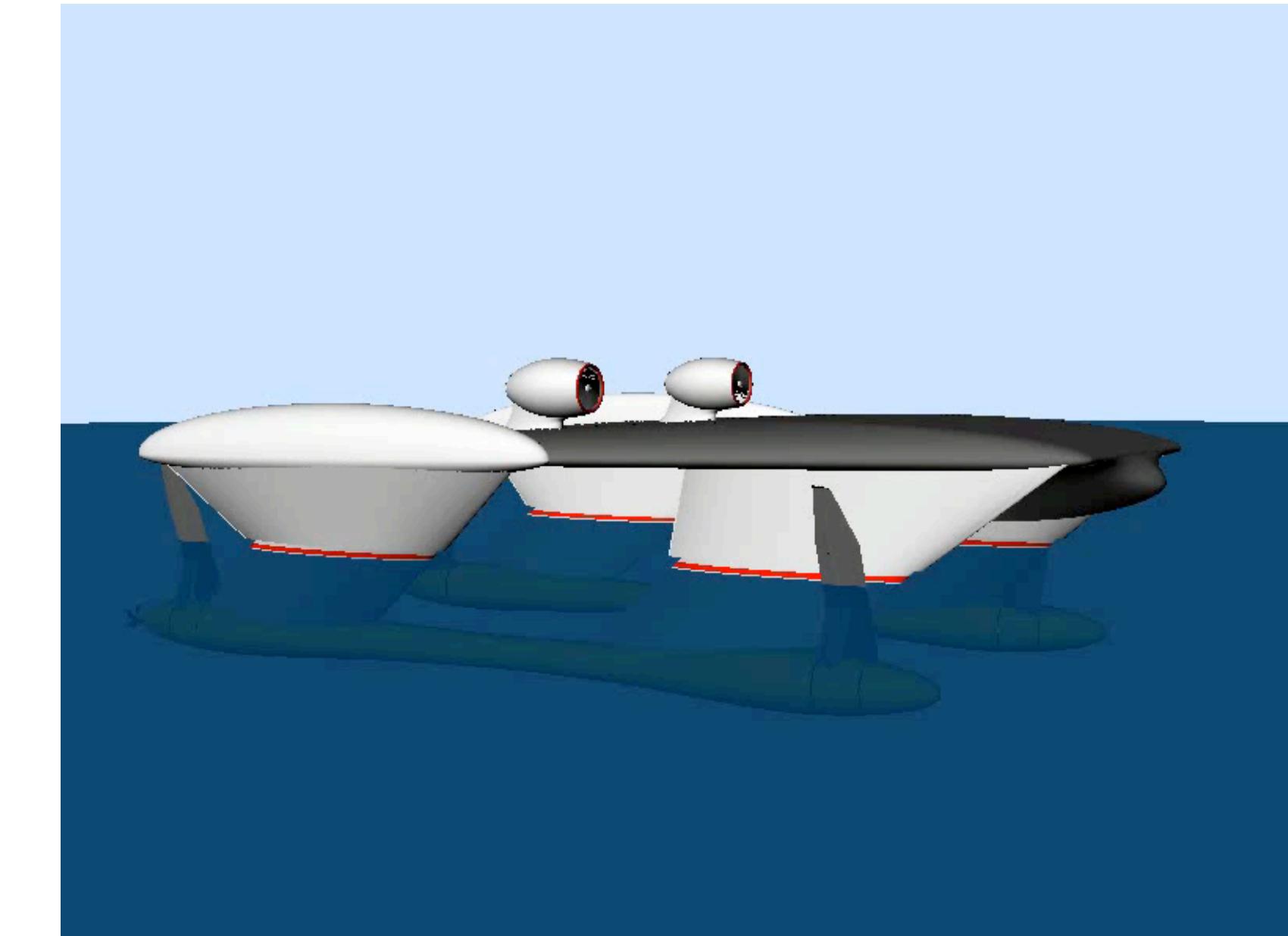
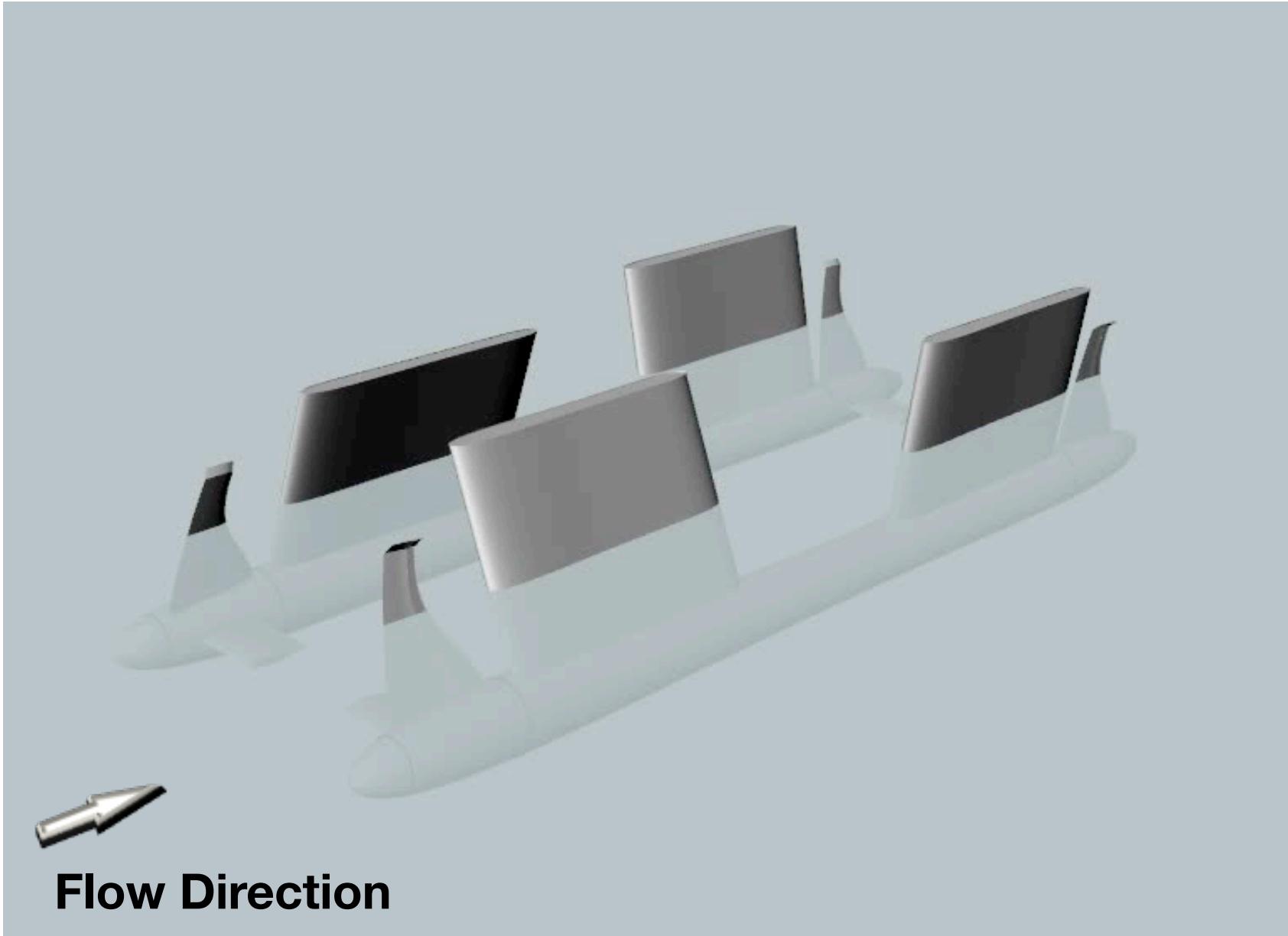




Design Optimization



lift/drag





Gaussian Process Regression



$$\left. \begin{aligned} y_i &= f(x_i) + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, N \\ \mathbf{y} &= f(\mathbf{x}) + \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I}) \end{aligned} \right\} \text{Data}$$

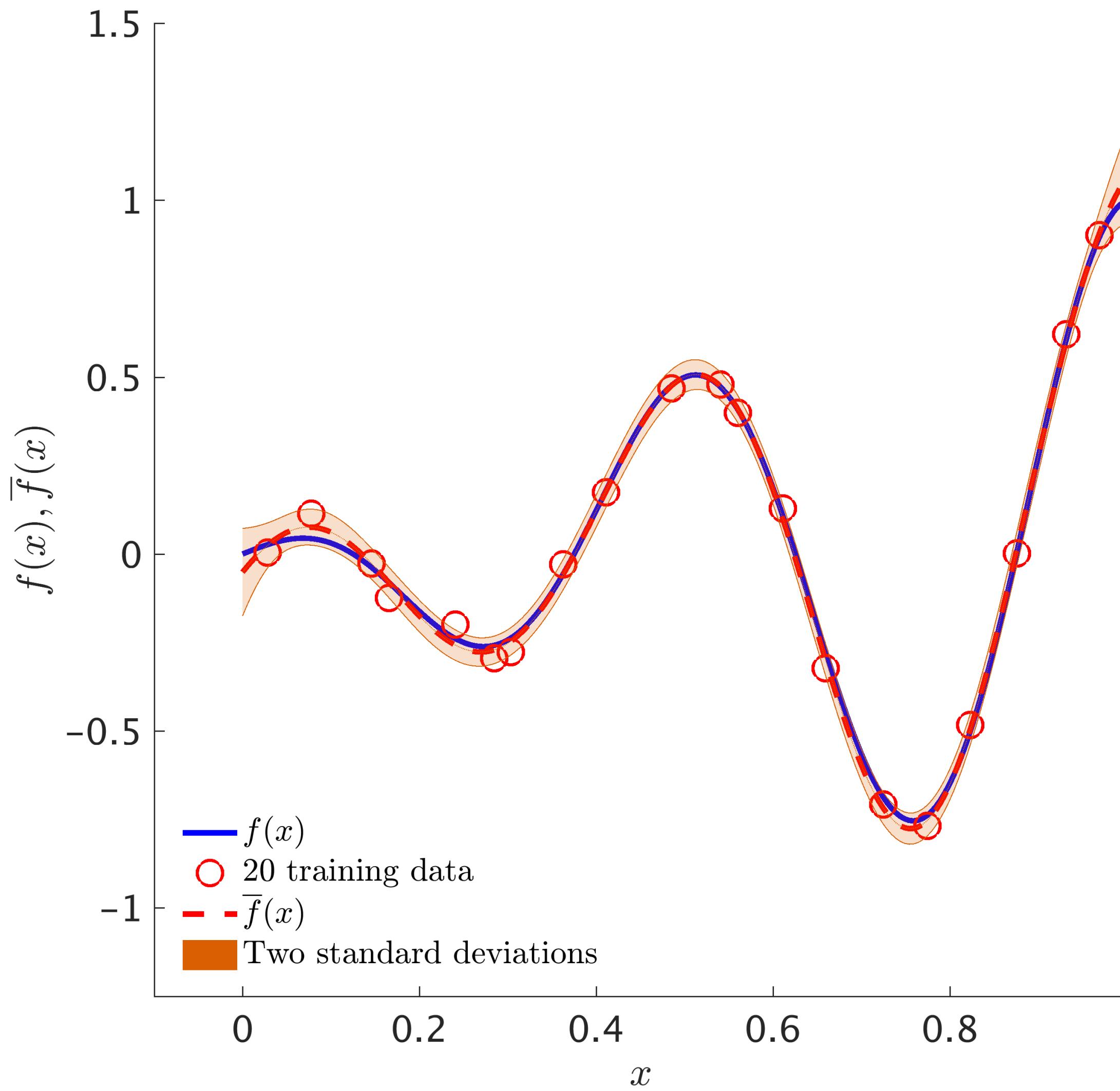
$$\left. \begin{aligned} \mathbf{y} &\sim \mathcal{N}(\mathbf{0}, \mathbf{K}), \quad \mathbf{K} = k(\mathbf{x}, \mathbf{x}; \theta) + \sigma^2 \mathbf{I} \\ \min_{\theta, \sigma} & \mathbf{y}' \mathbf{K}^{-1} \mathbf{y} + \log |\mathbf{K}| \end{aligned} \right\} \text{Training}$$

$$\left. \begin{aligned} f(x) &\sim \mathcal{GP}(0, k(x, x'; \theta)) \\ \begin{bmatrix} f(x) \\ f(x') \end{bmatrix} &\sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} k(x, x; \theta) & k(x, x'; \theta) \\ k(x', x; \theta) & k(x', x'; \theta) \end{bmatrix}\right) \\ k(x, x'; \gamma, \omega) &= \gamma^2 \exp(-0.5 \omega^2 (x - x')^2) \end{aligned} \right\} \text{Prior}$$

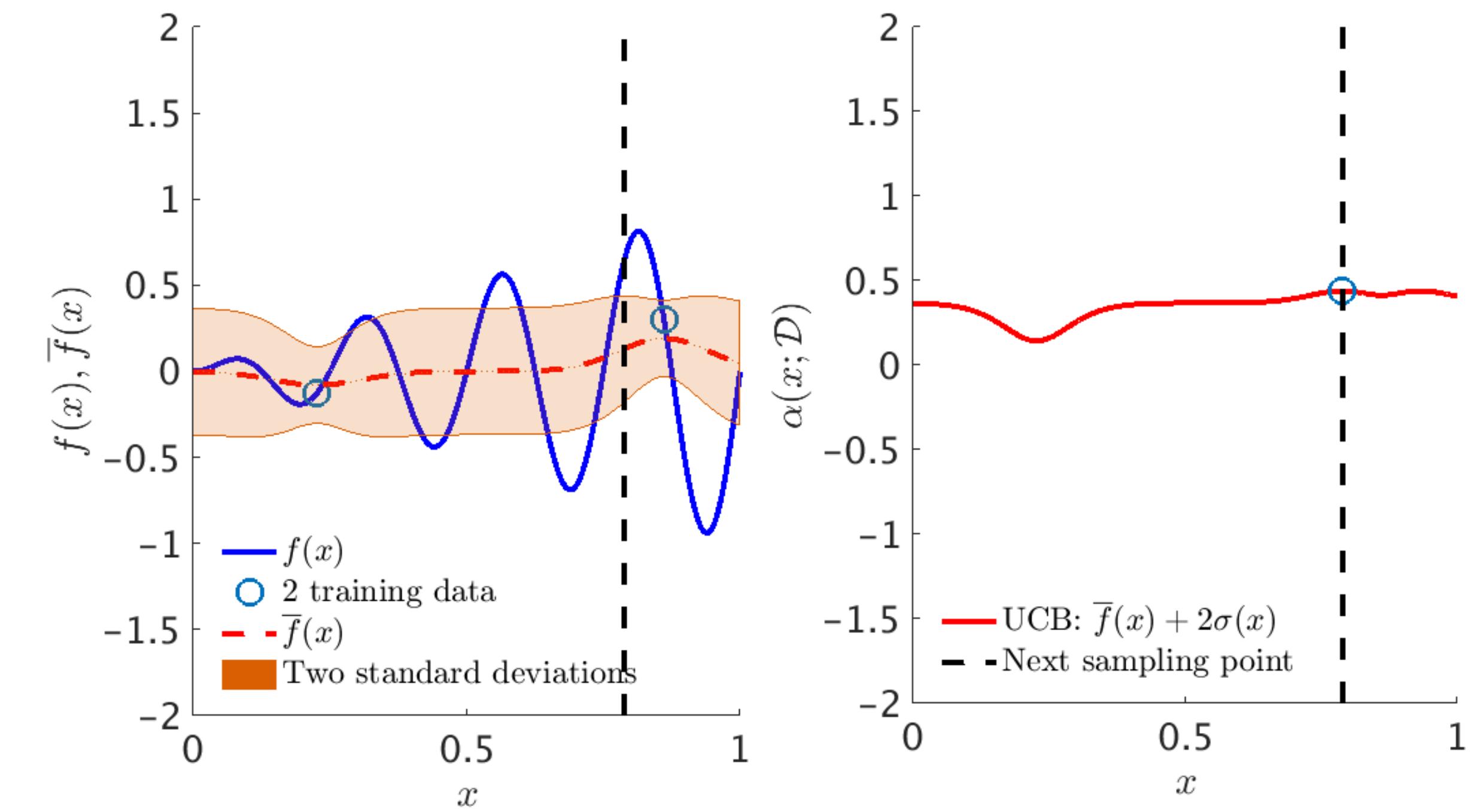
$$\left. \begin{aligned} \begin{bmatrix} f(x^*) \\ \mathbf{y} \end{bmatrix} &\sim \mathcal{N}\left(\begin{bmatrix} 0 \\ \mathbf{0} \end{bmatrix}, \begin{bmatrix} k(x^*, x^*) & k(x^*, \mathbf{x}) \\ k(\mathbf{x}, x^*) & \mathbf{K} \end{bmatrix}\right) \\ f(x^*) | \mathbf{x}, \mathbf{y} &\sim \mathcal{N}(m(x^*), S(x^*, x^*)) \\ m(x^*) &= k(x^*, \mathbf{x}) \mathbf{K}^{-1} \mathbf{y} \\ S(x^*, x^*) &= k(x^*, x^*) - k(x^*, \mathbf{x}) \mathbf{K}^{-1} k(\mathbf{x}, x^*) \end{aligned} \right\} \text{Prediction}$$



Gaussian Process Regression



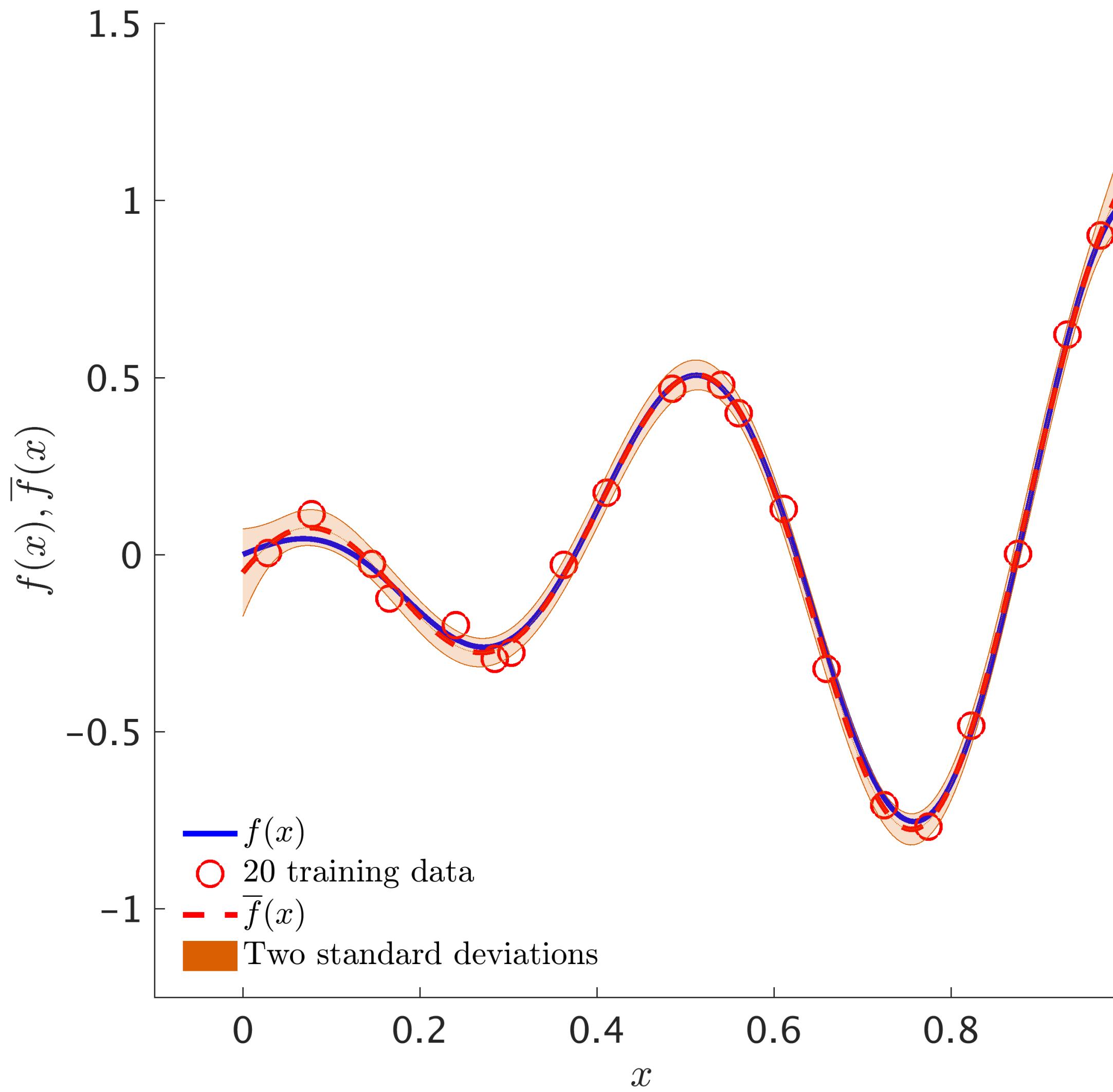
Bayesian Optimization



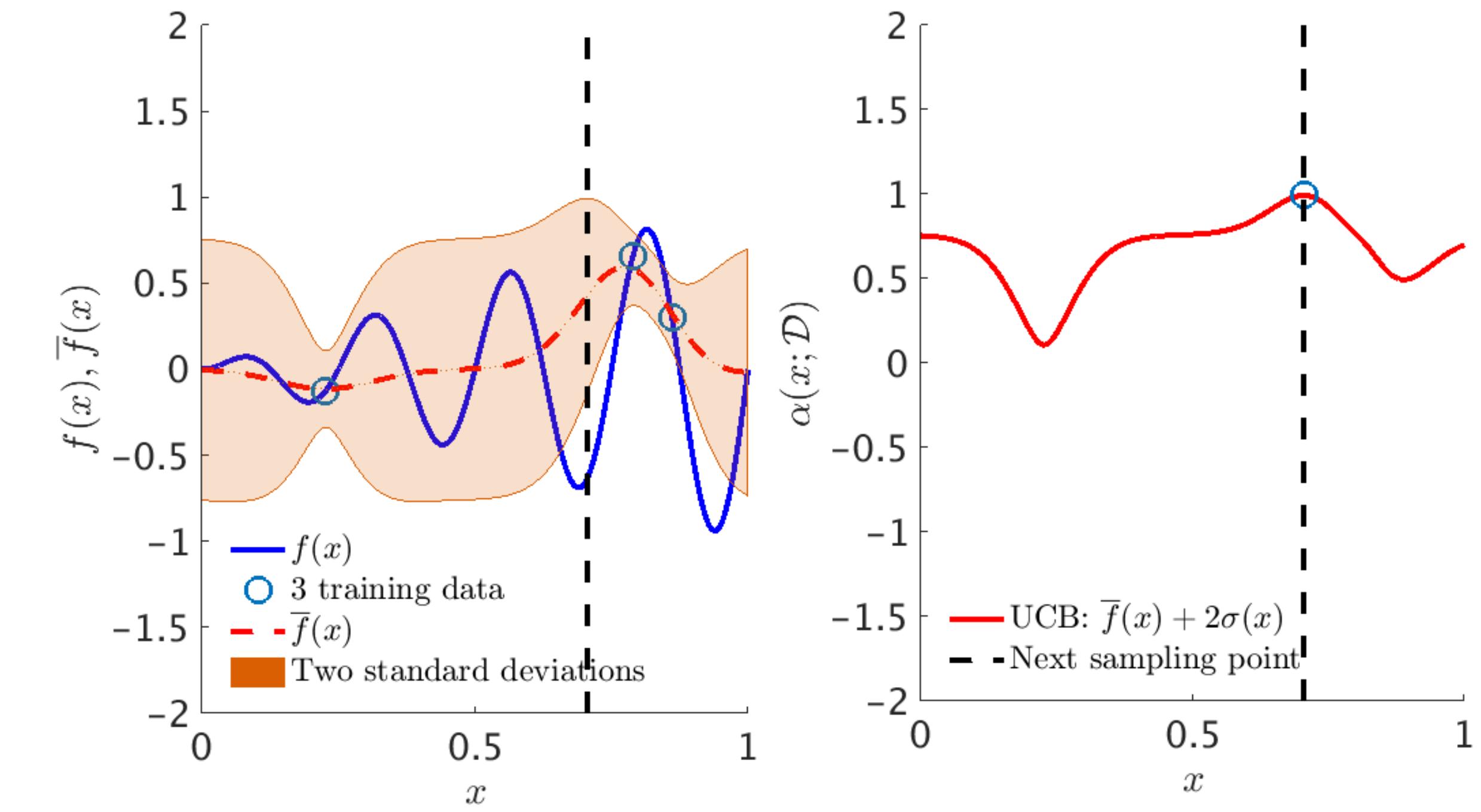
Shahriari, Bobak, et al. "Taking the human out of the loop: A review of bayesian optimization." *Proceedings of the IEEE* 104.1 (2016): 148-175.



Gaussian Process Regression



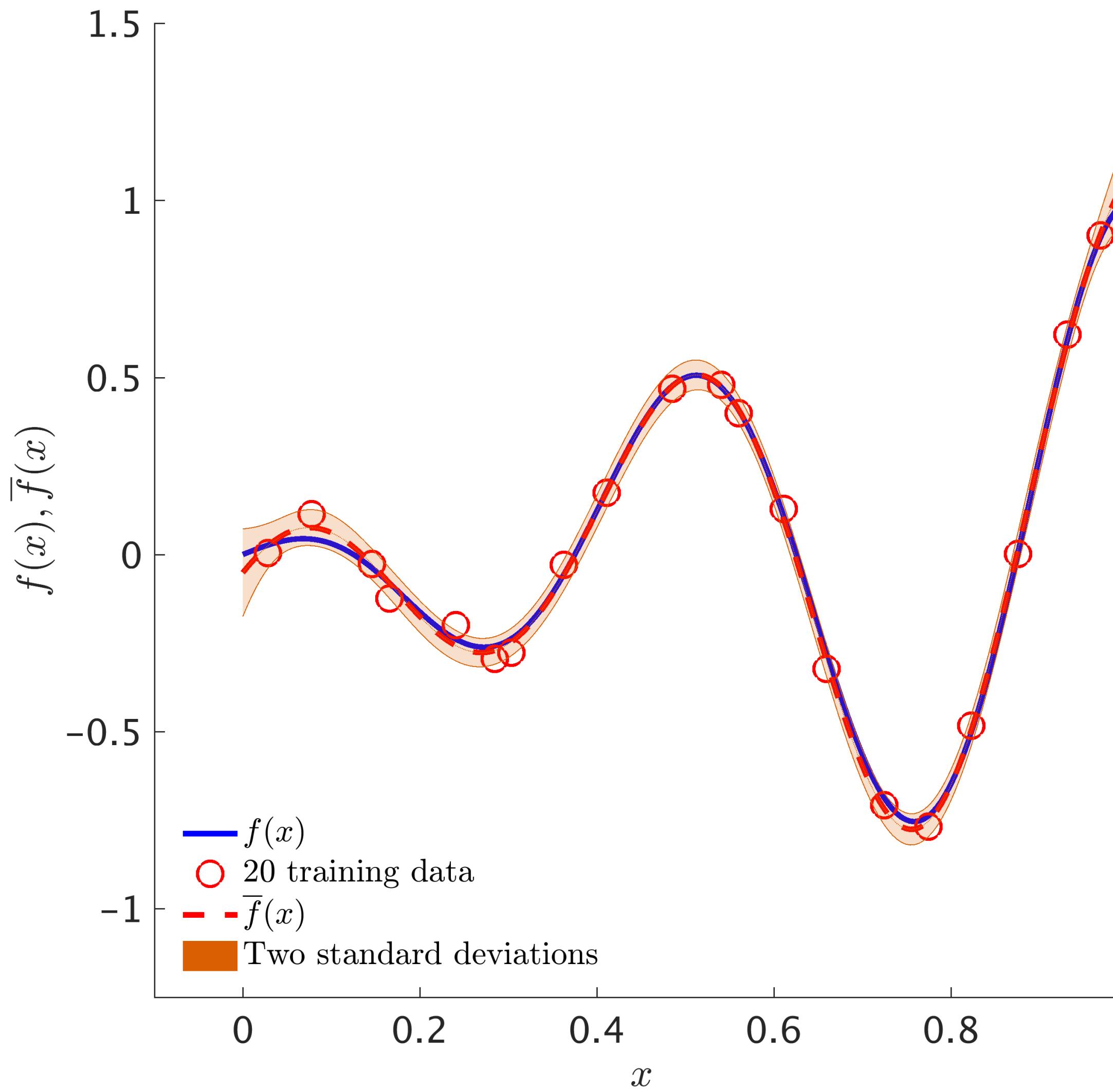
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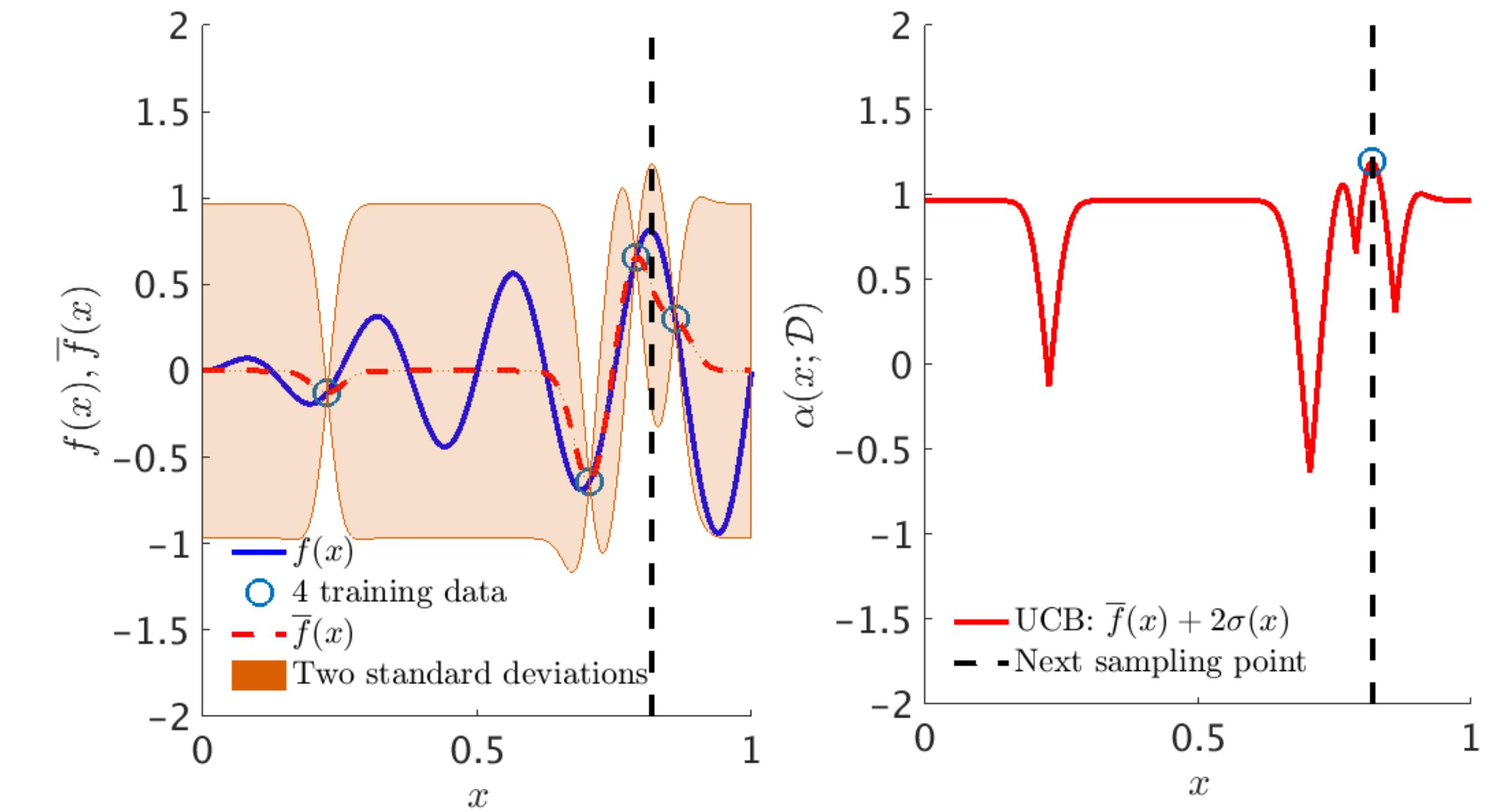
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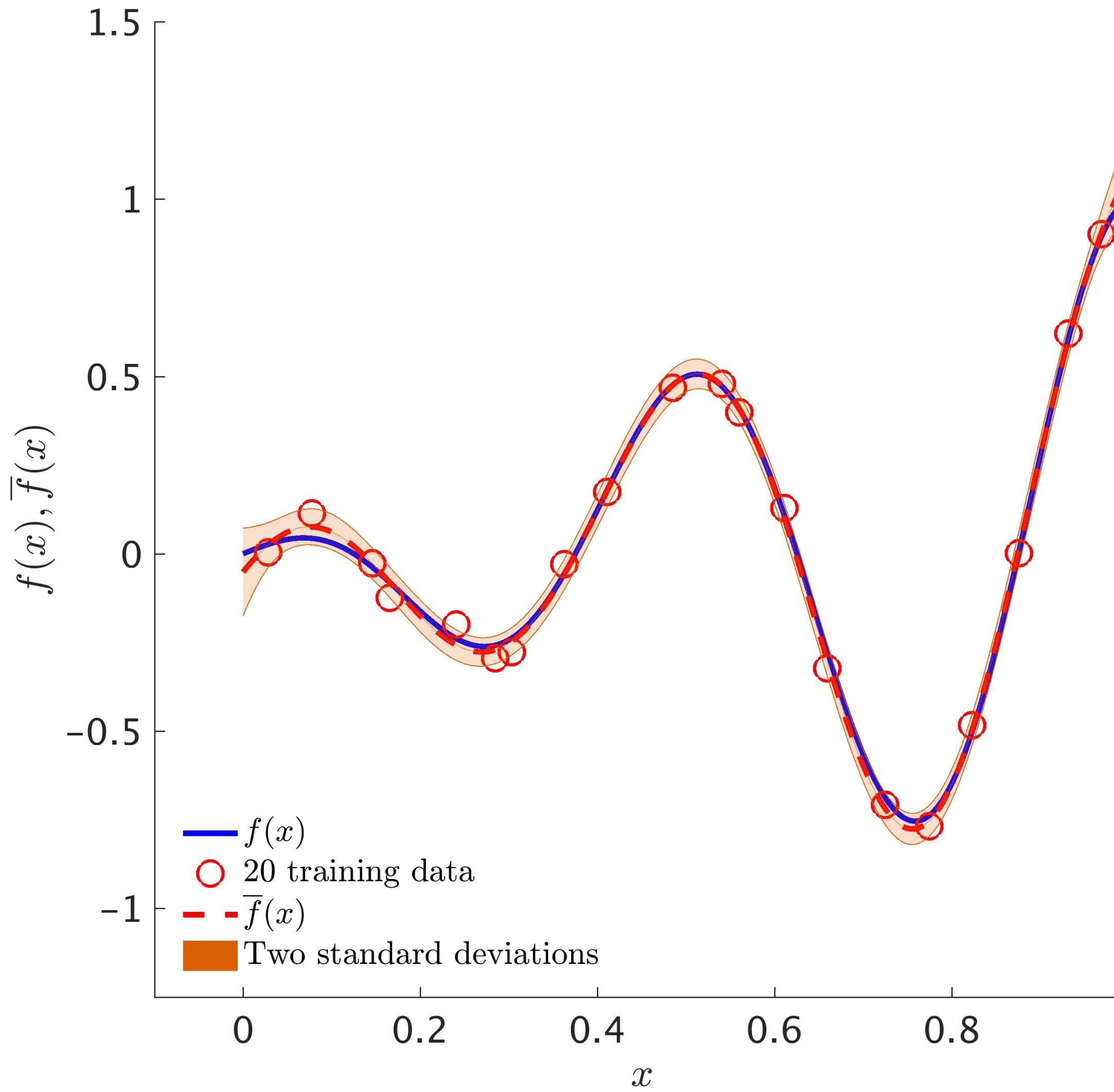
Bayesian Optimization



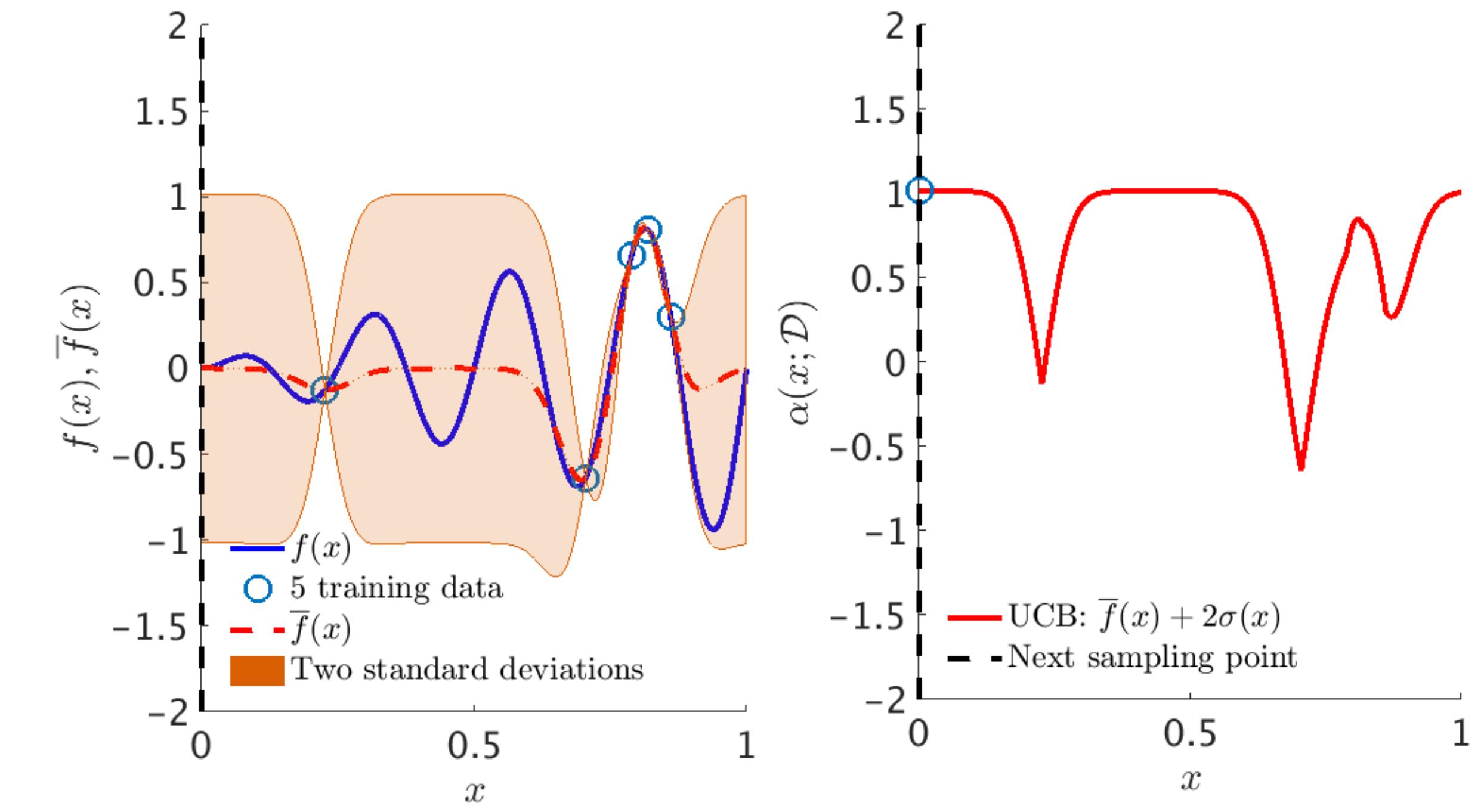
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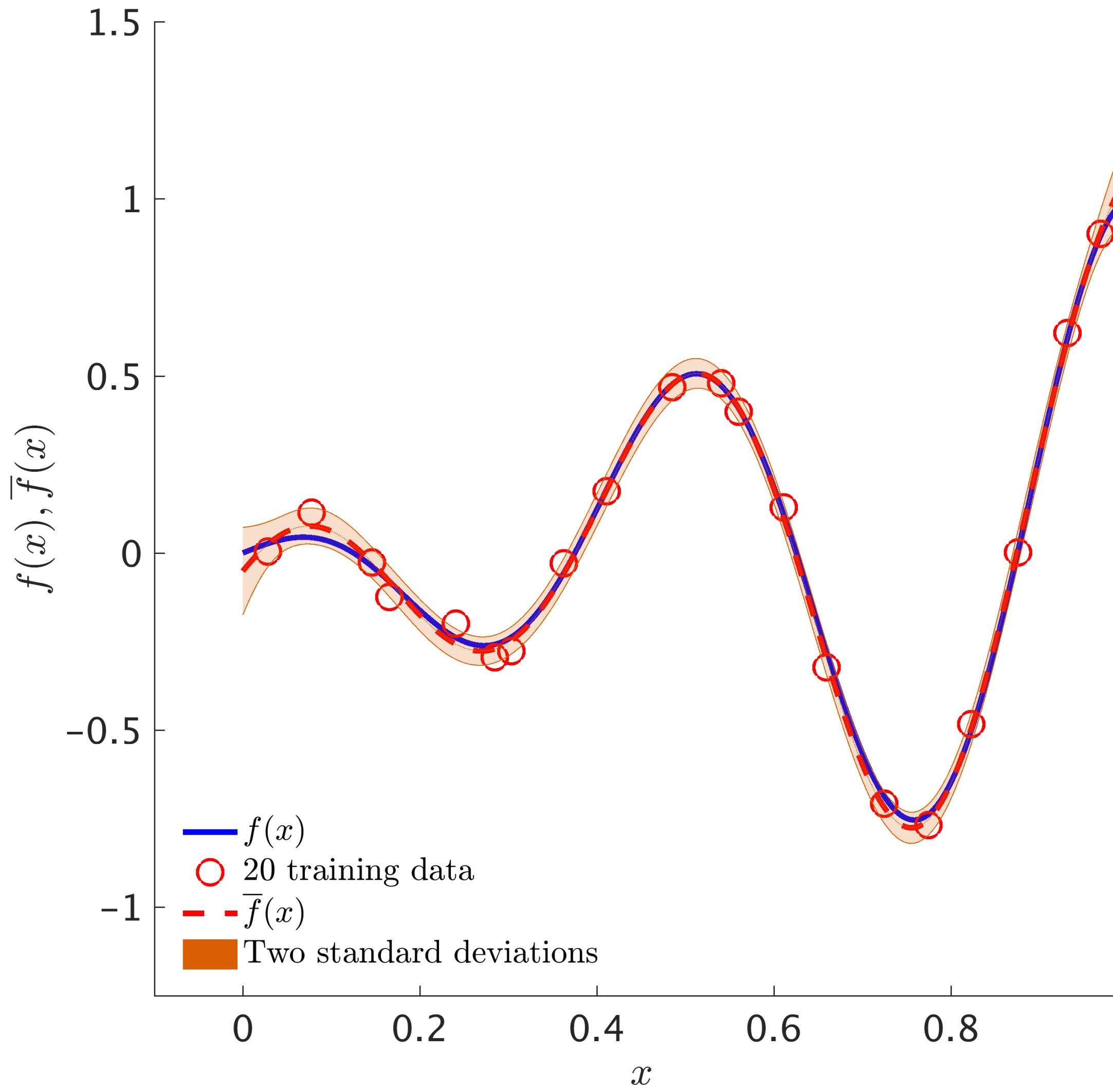
Bayesian Optimization



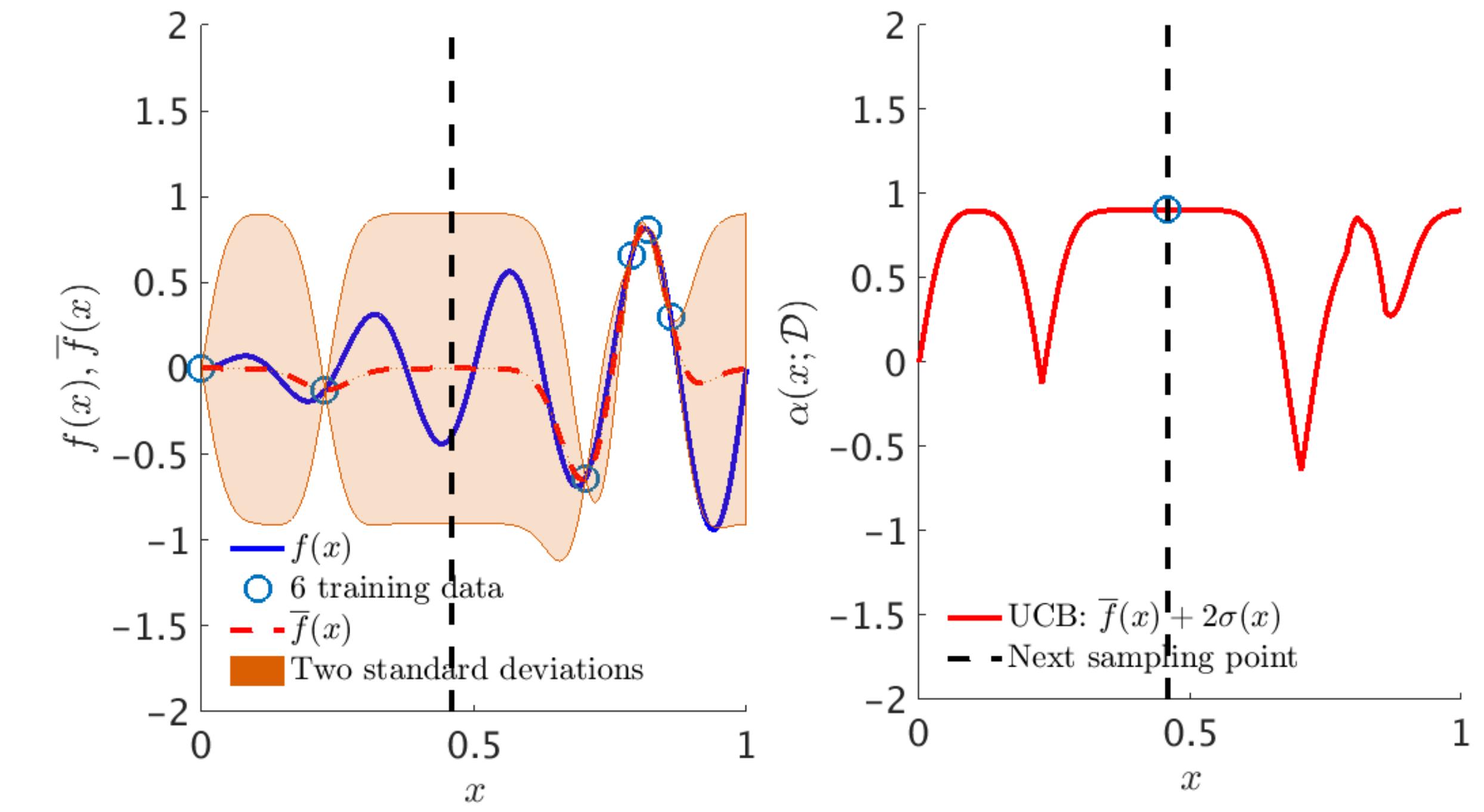
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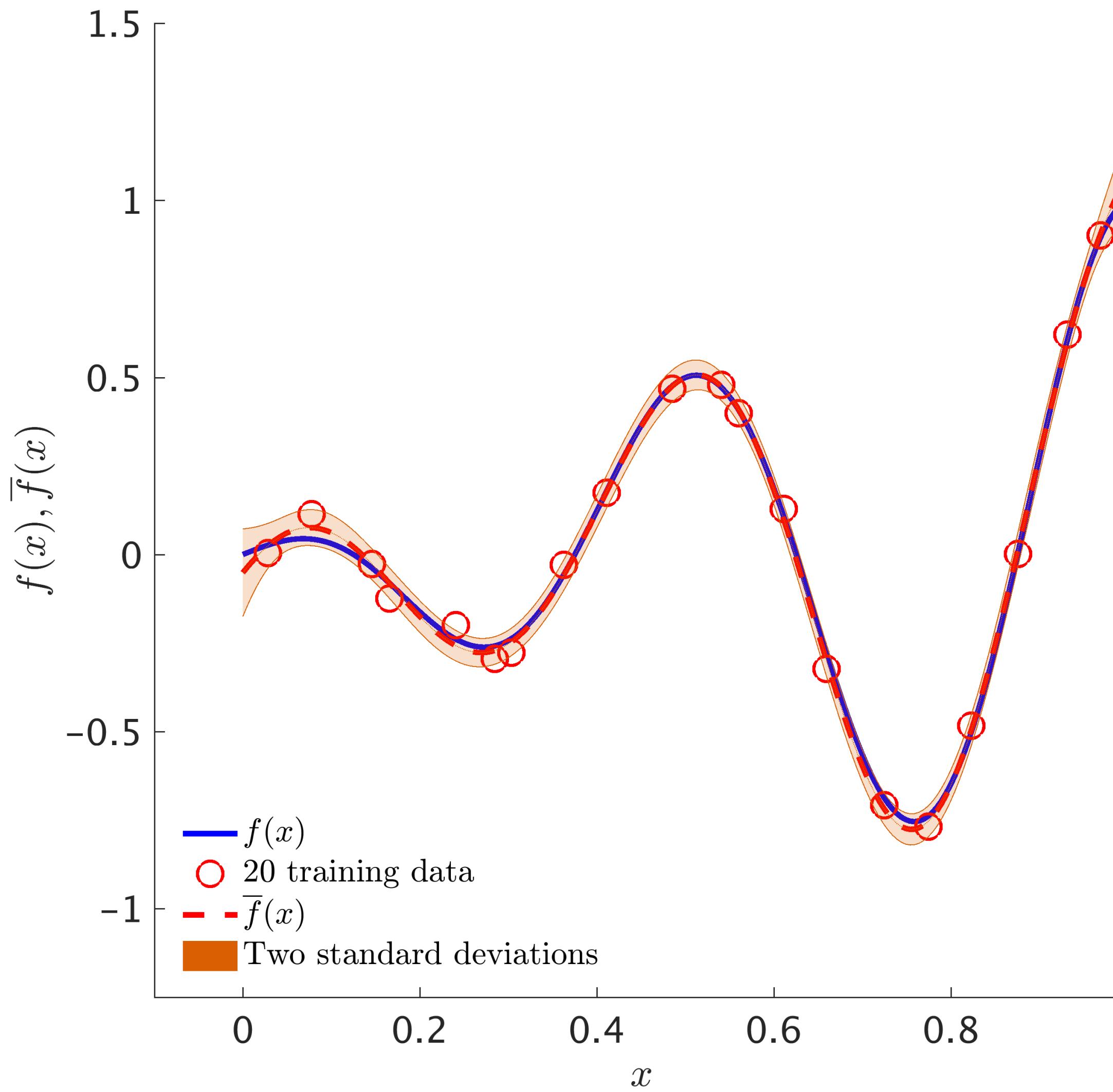
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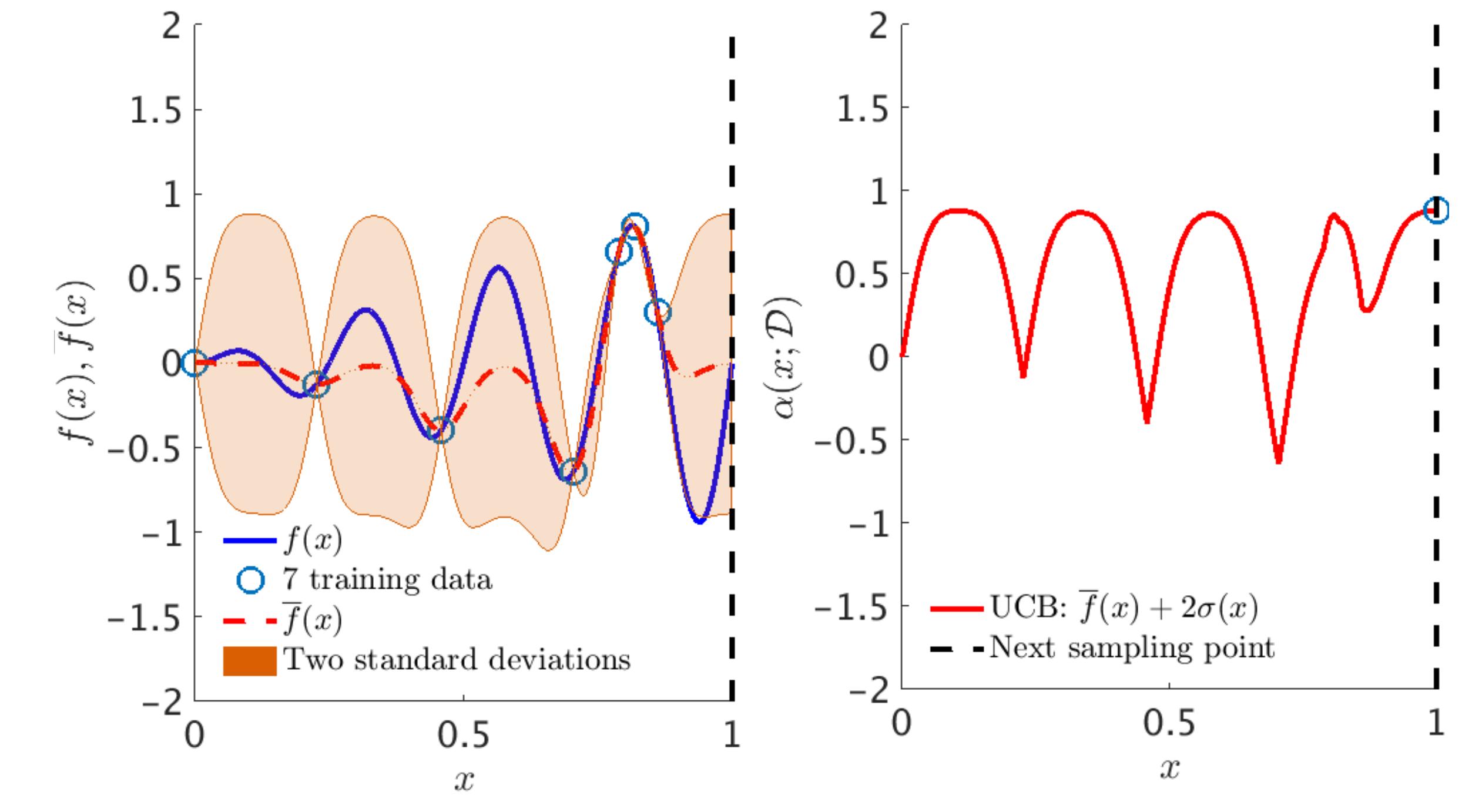
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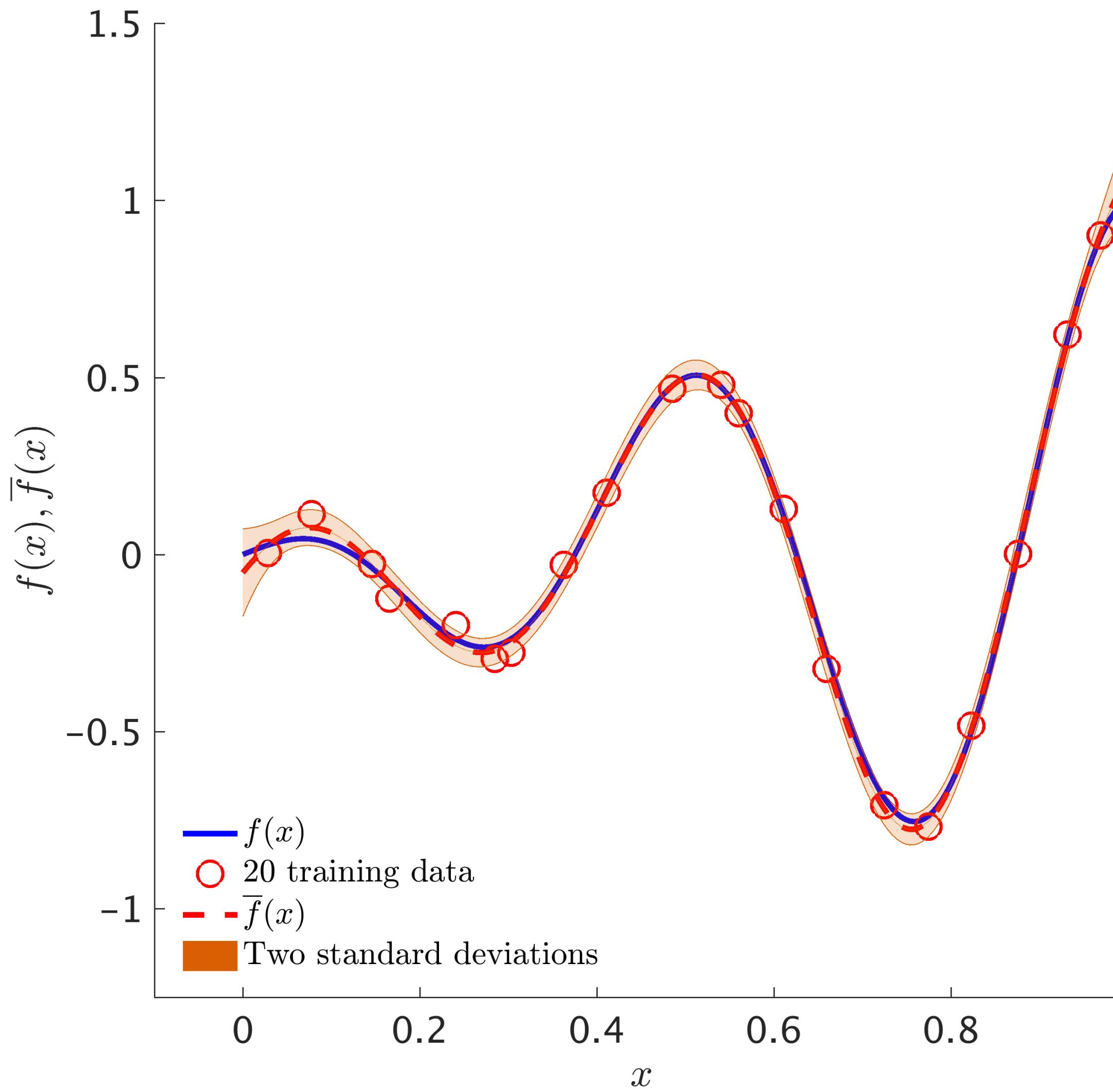
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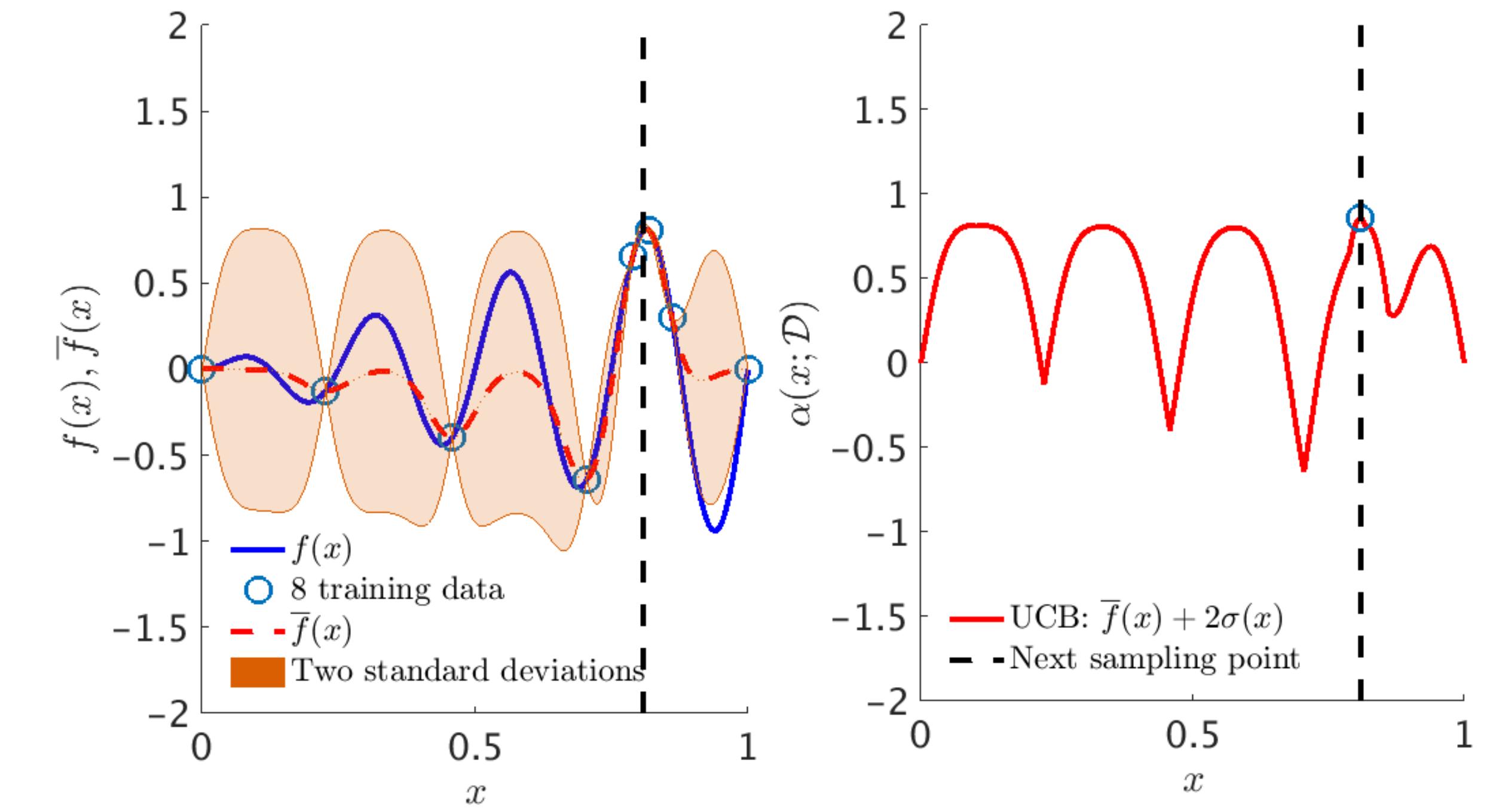
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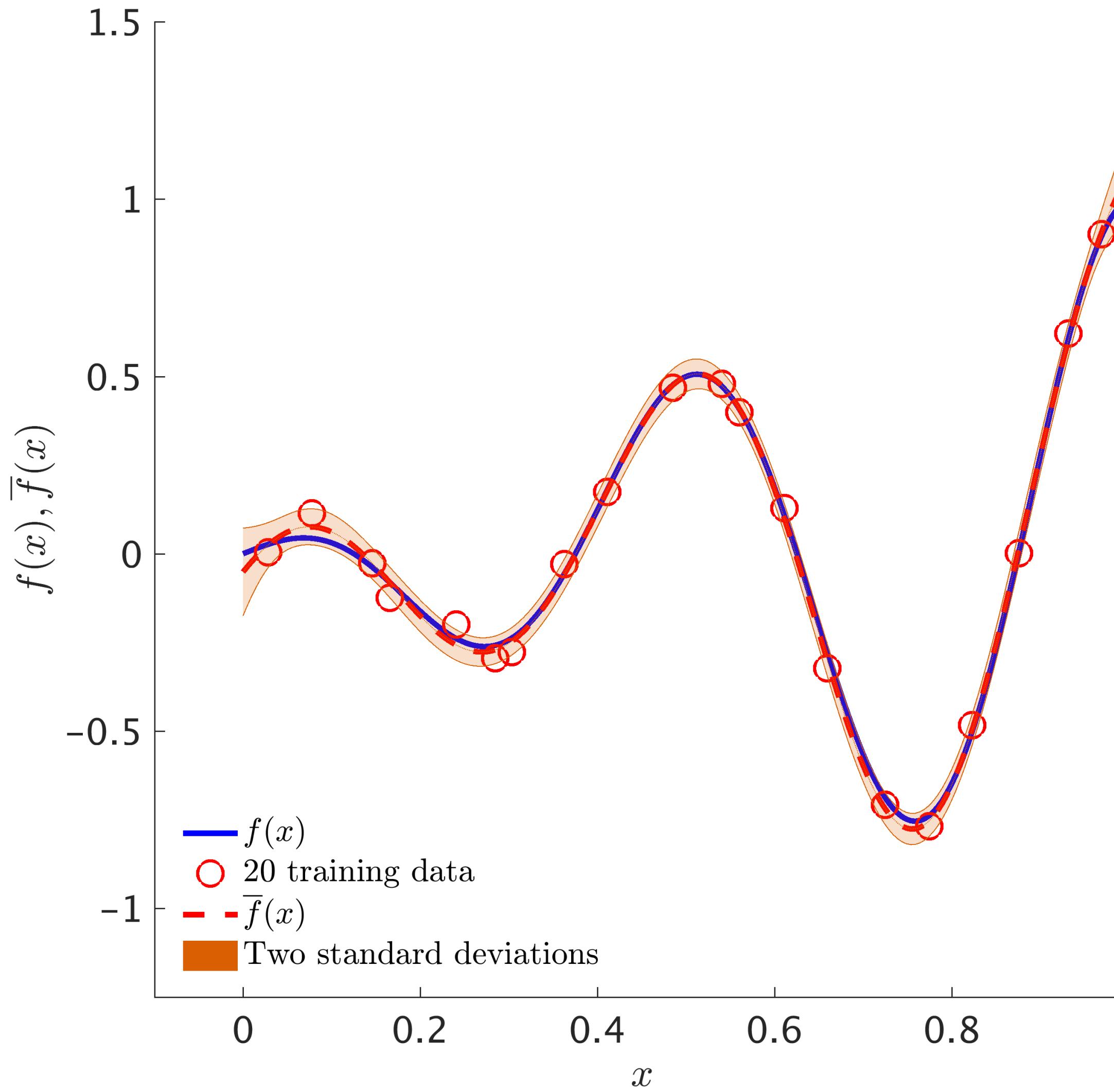
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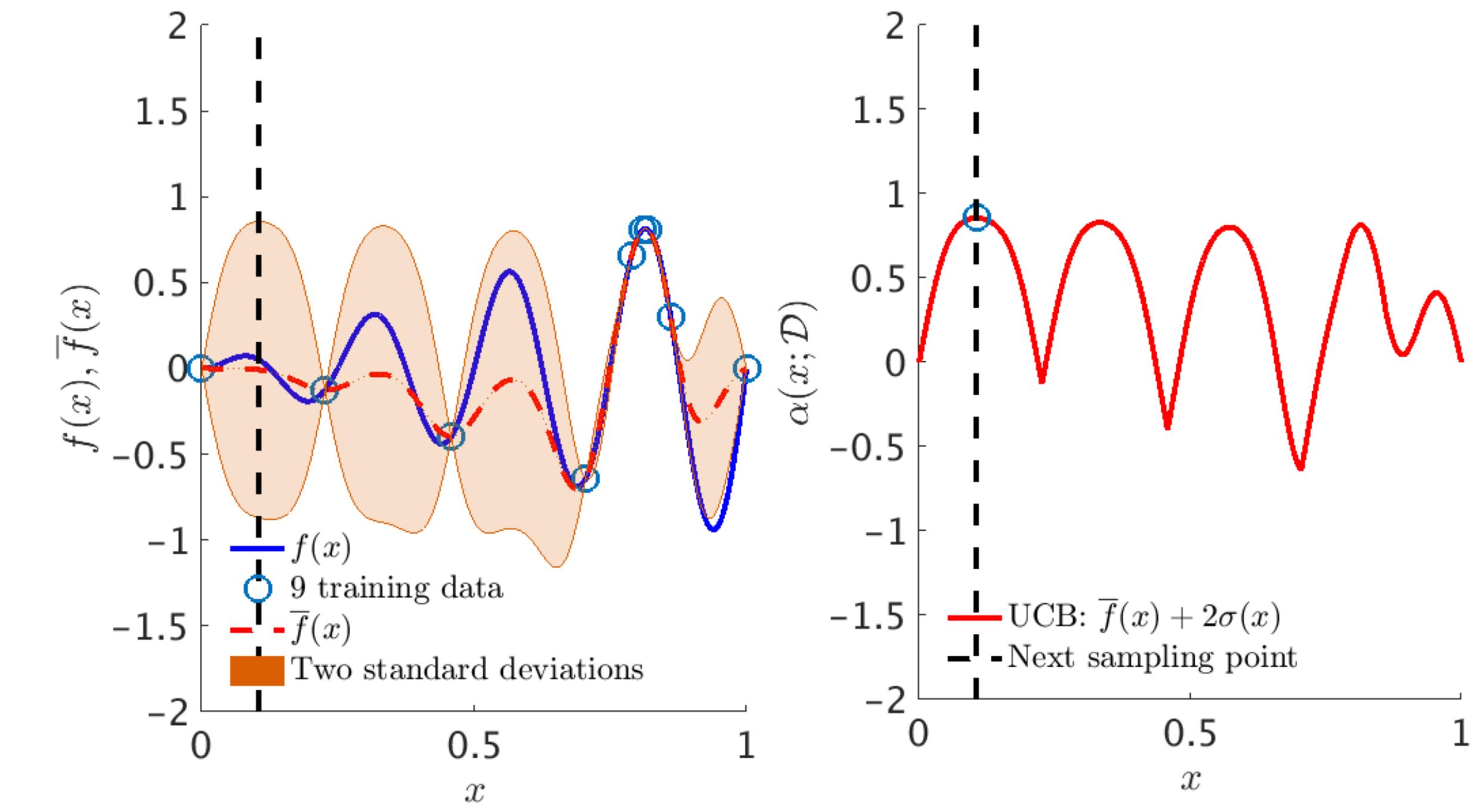
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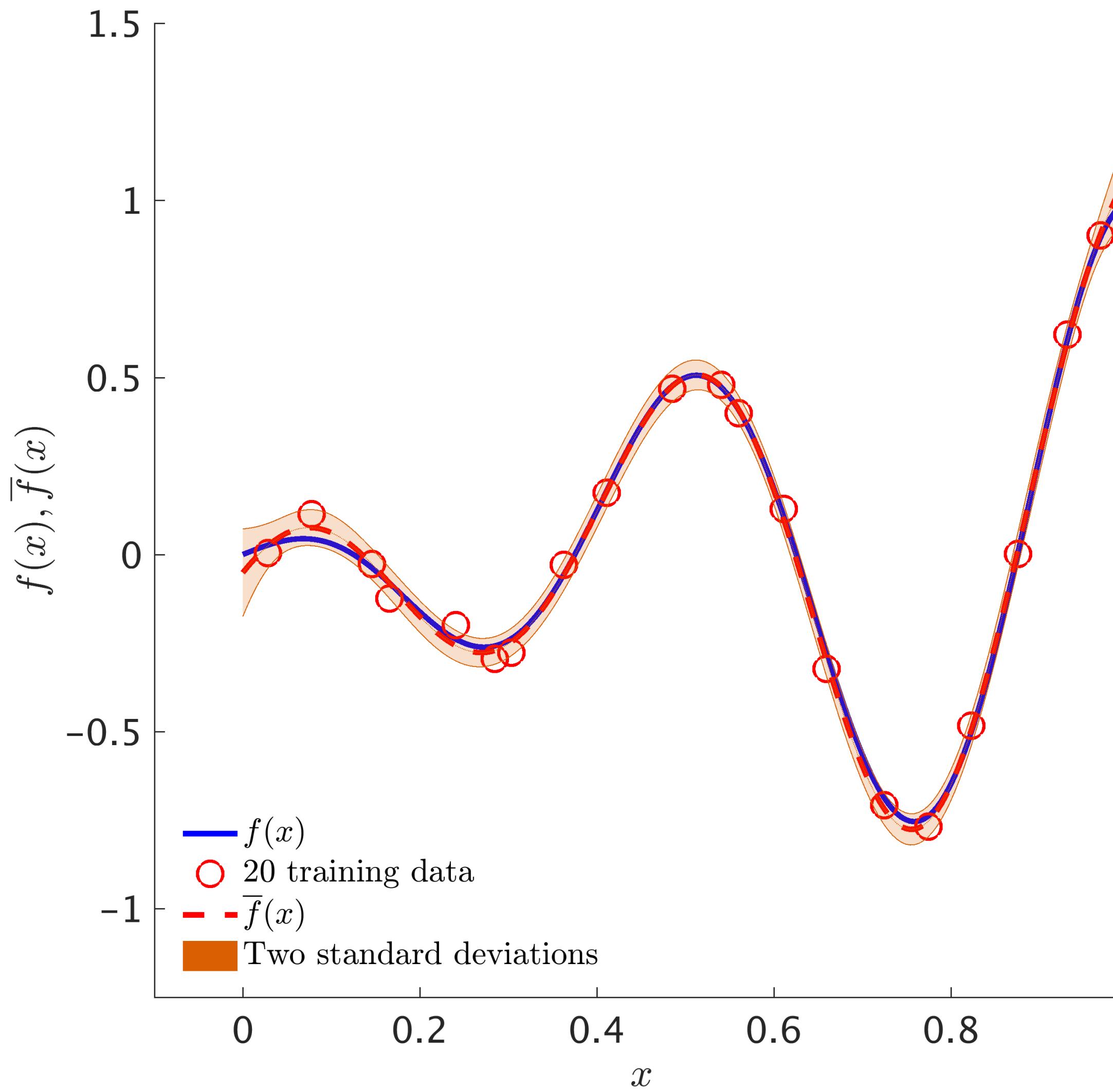
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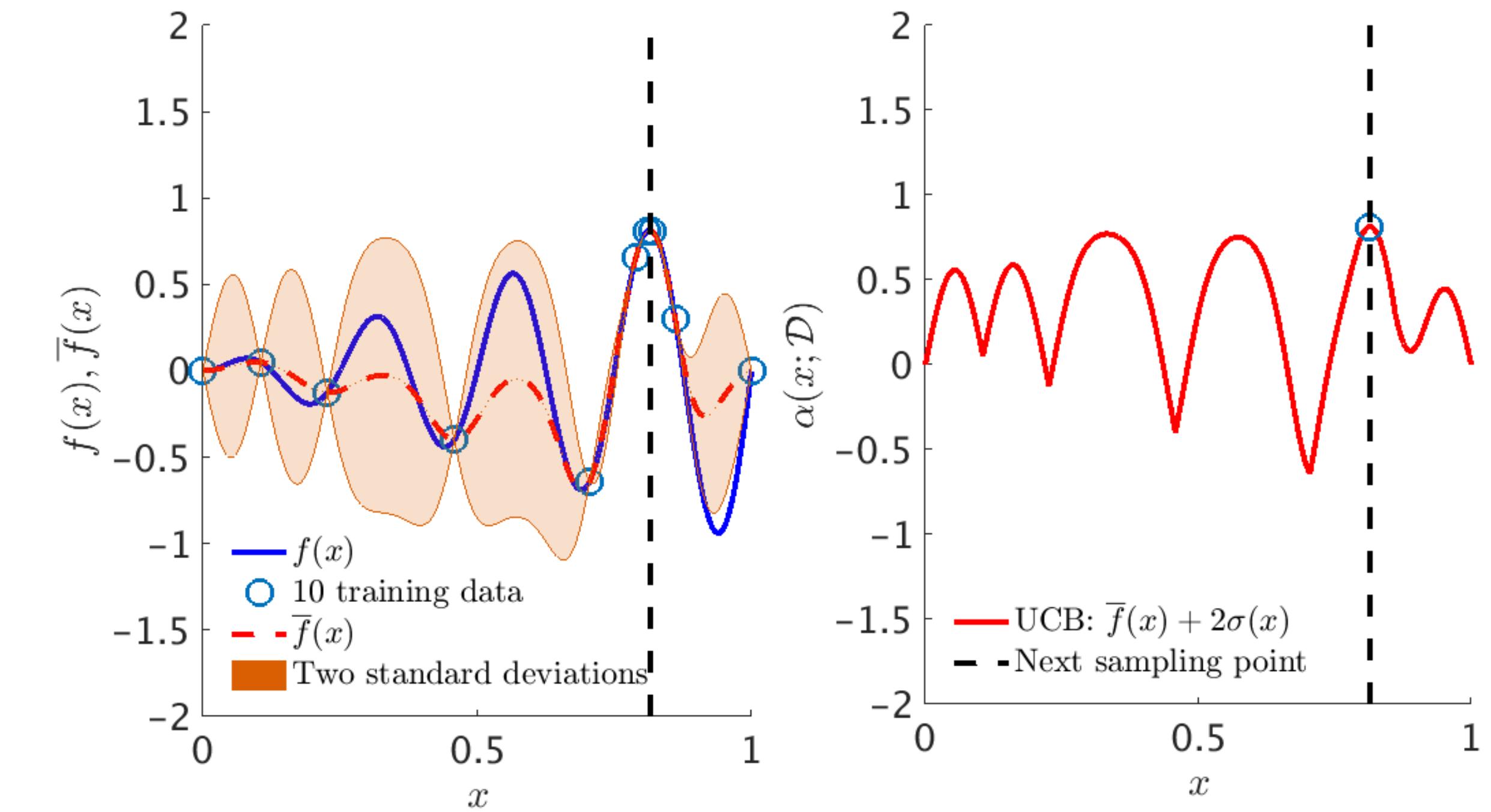
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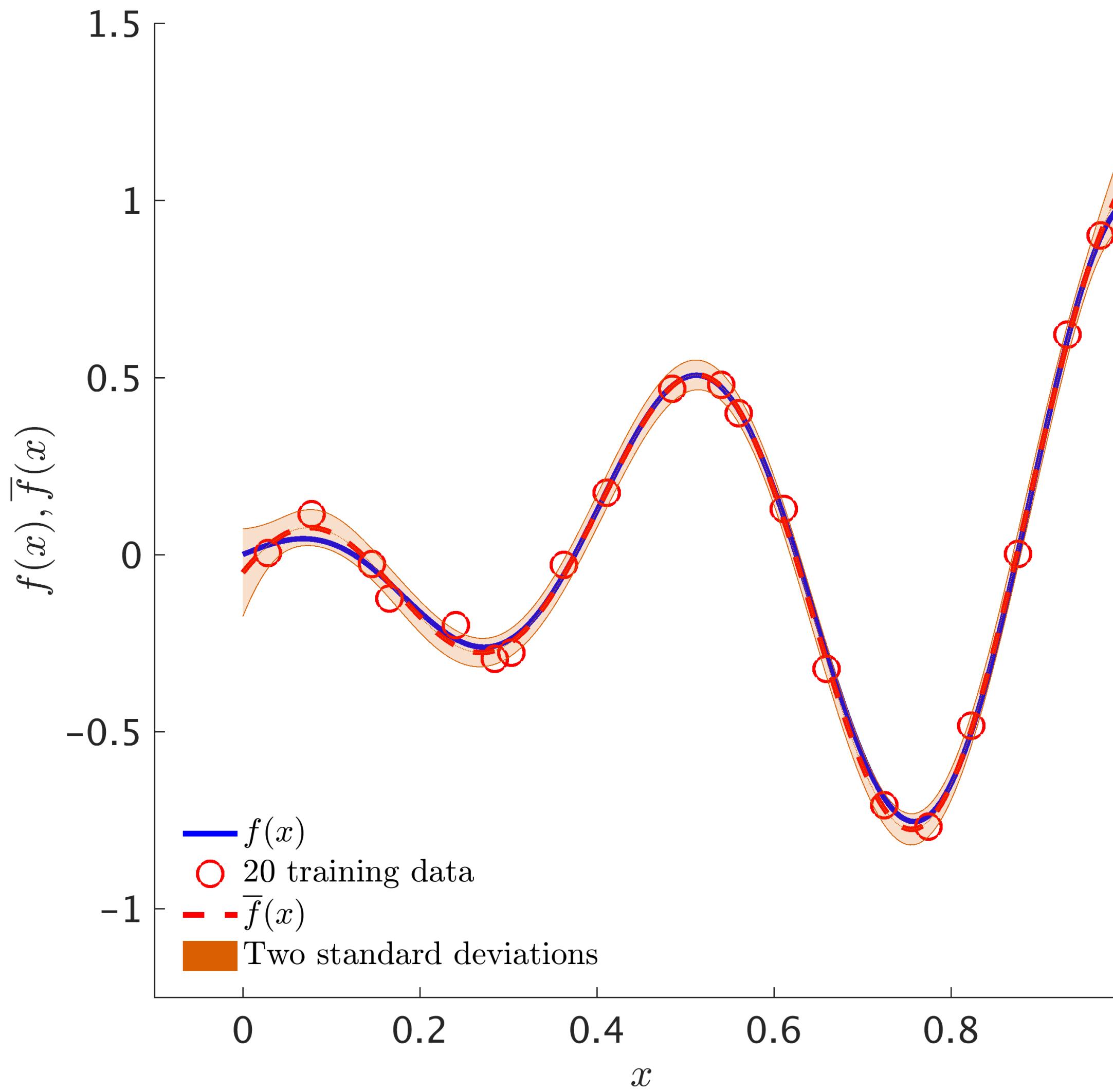
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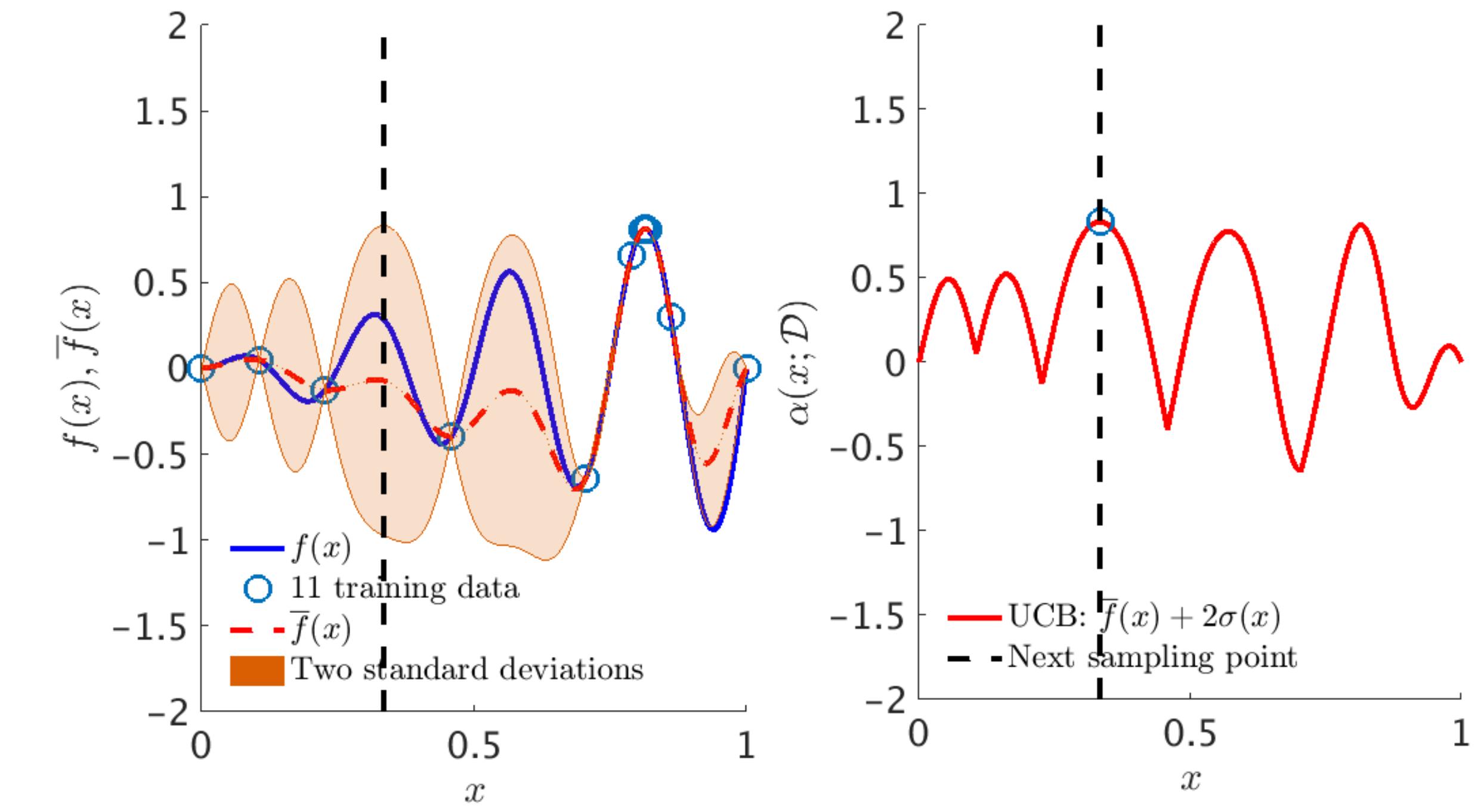
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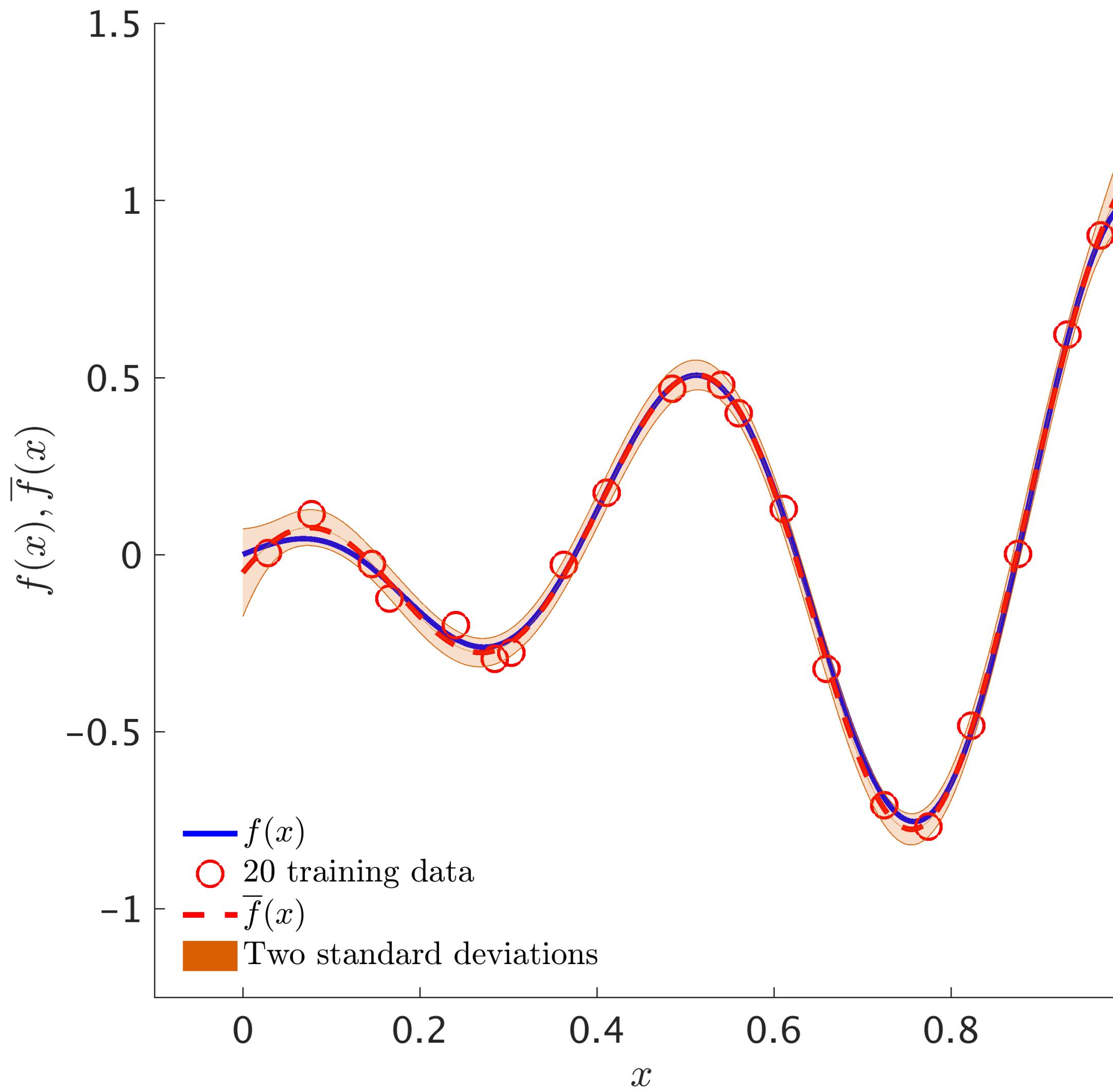
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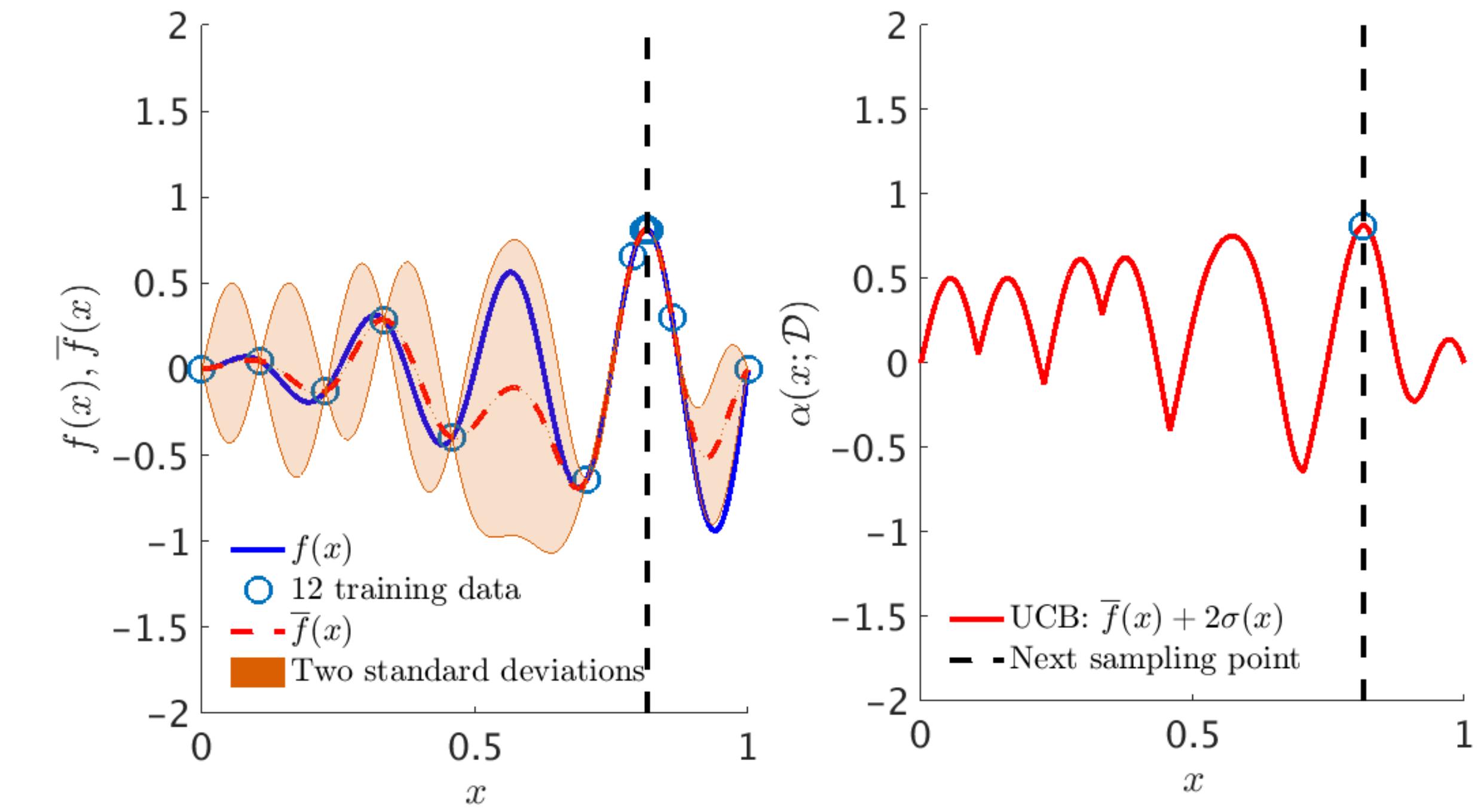
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Gaussian Process Regression



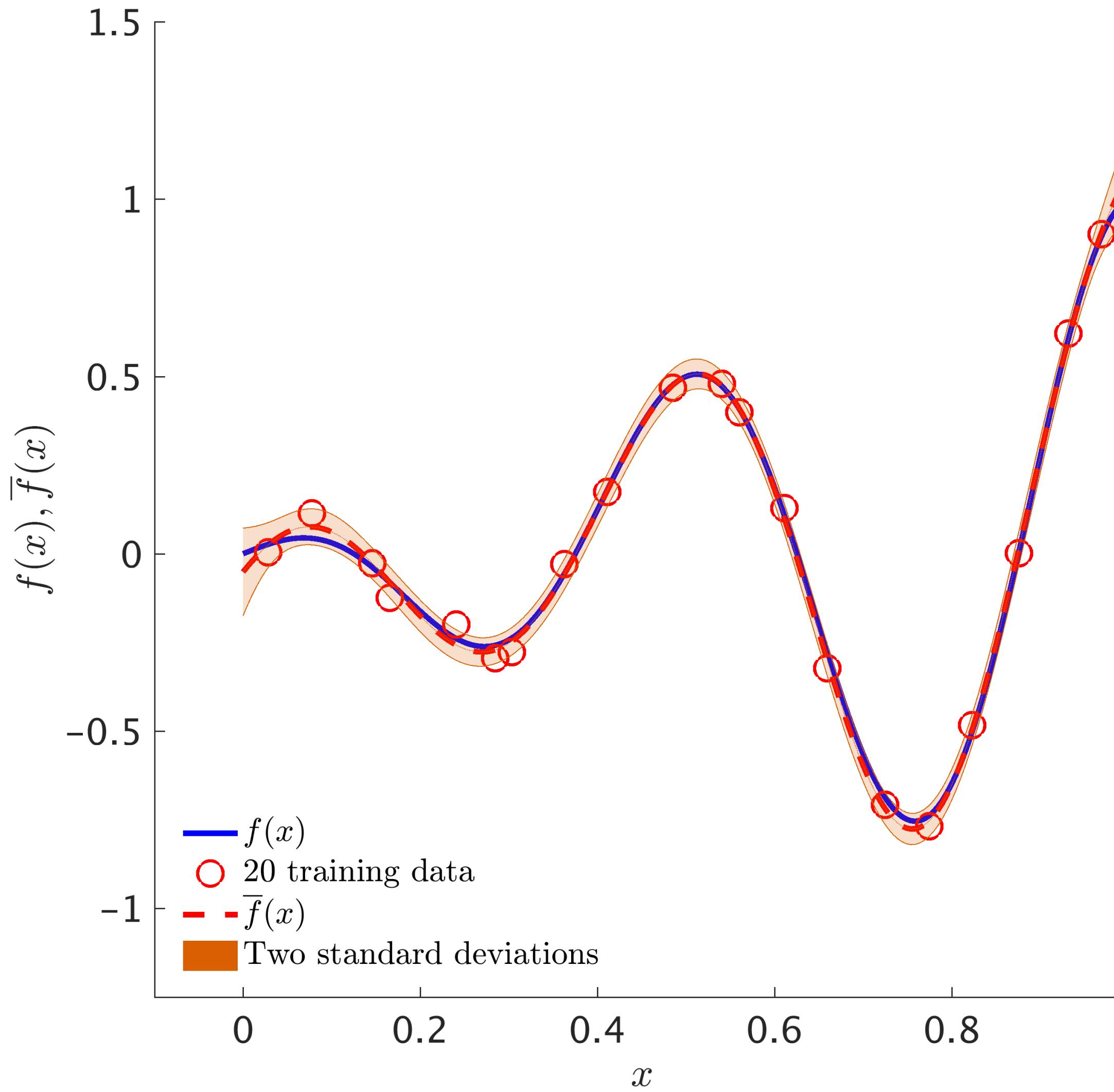
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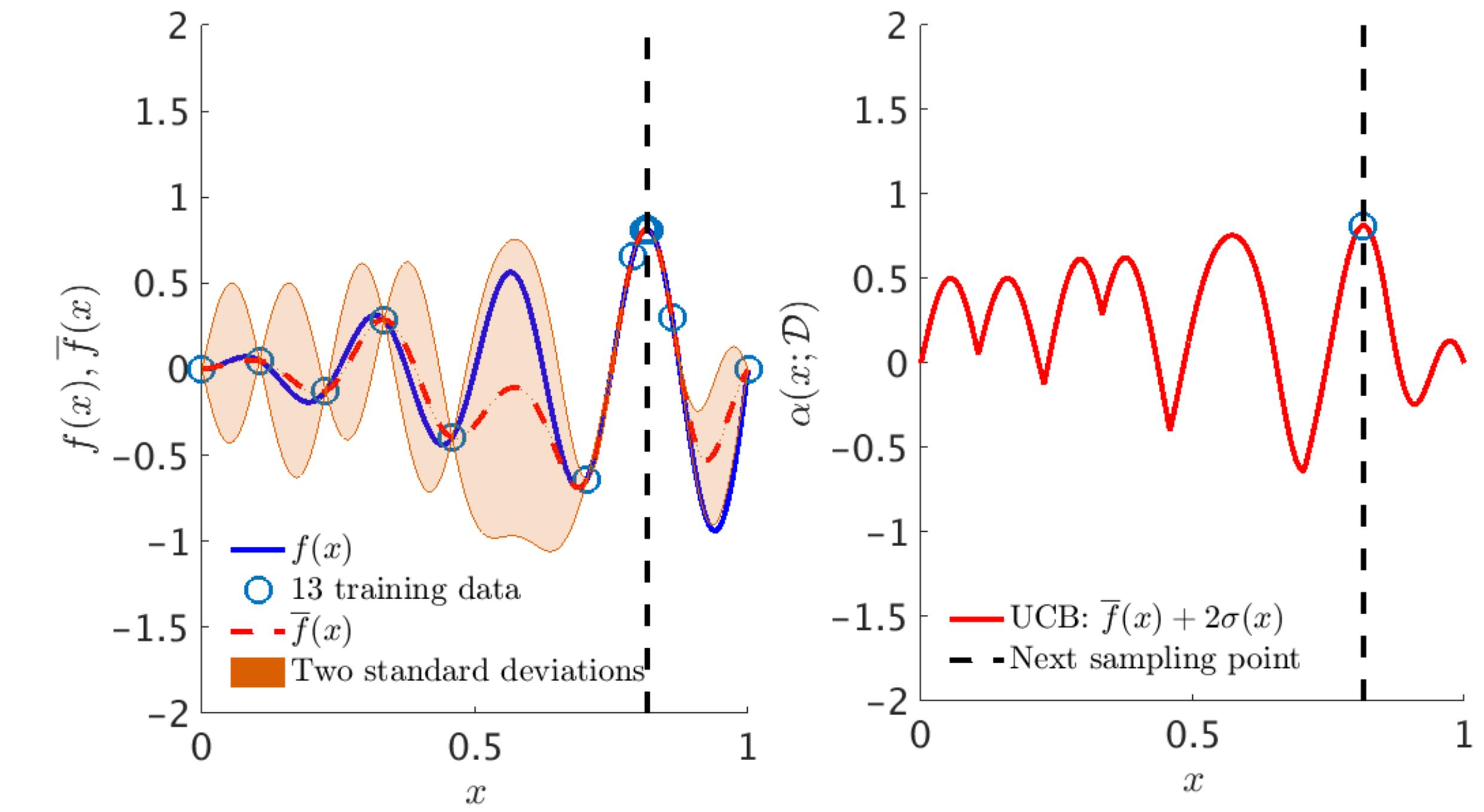
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Gaussian Process Regression



Bayesian Optimization



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Multi-fidelity Modeling



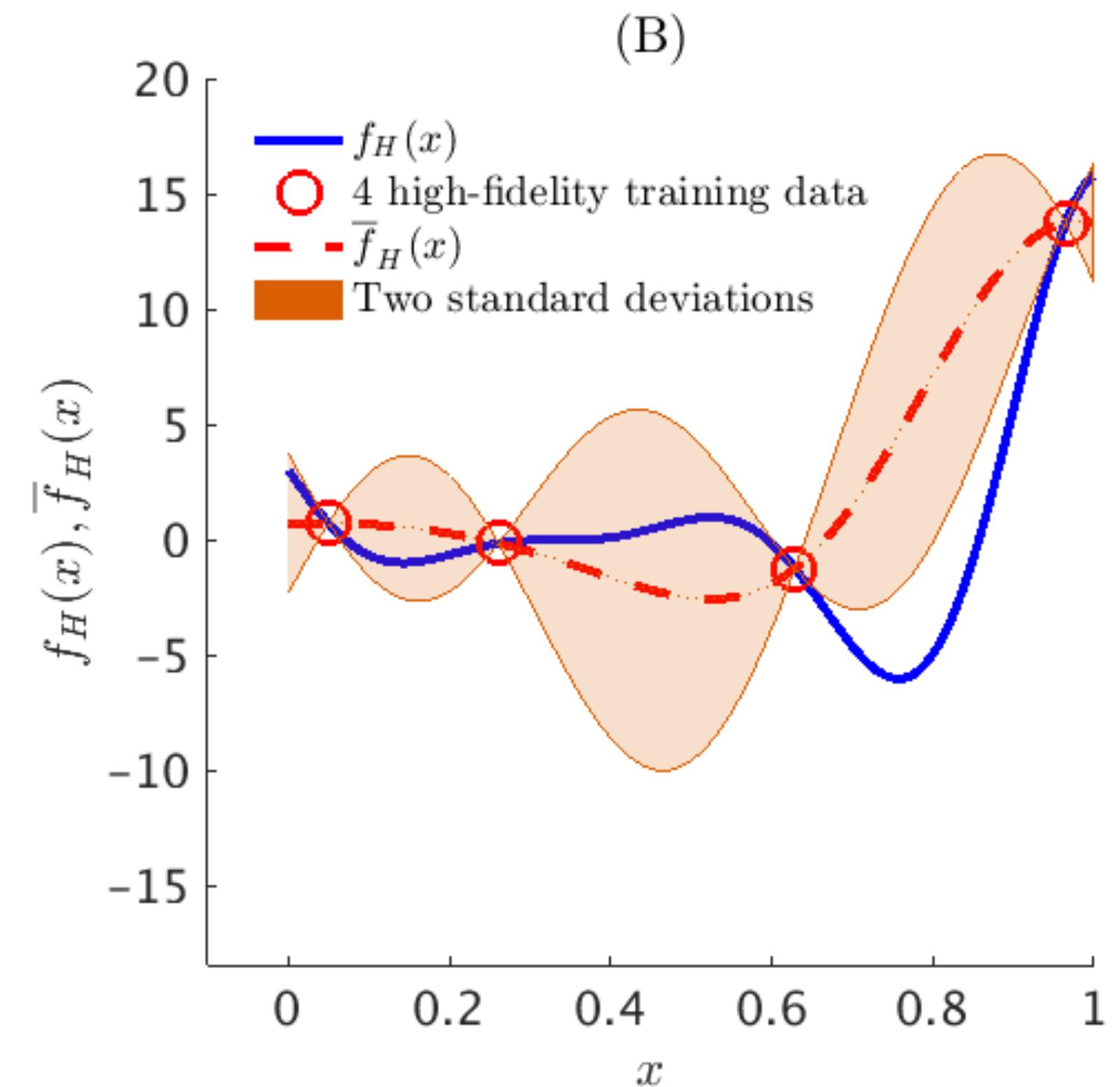
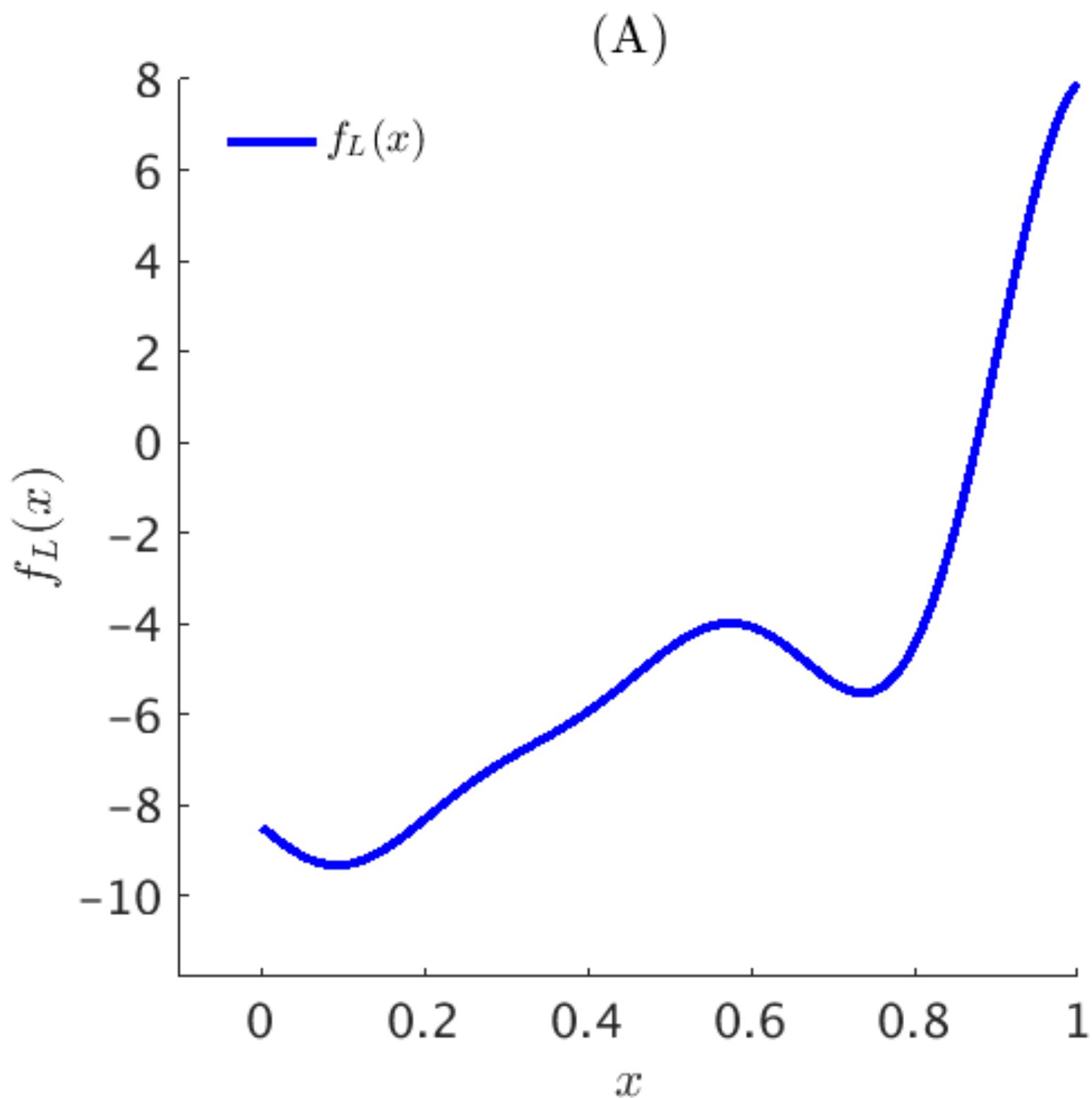
$$f_H(x) = \rho f_L(x) + \delta(x),$$

$$f_L(x) \sim \mathcal{GP}(0, k_1(x, x'; \theta_1)),$$

$$\delta(x) \sim \mathcal{GP}(0, k_2(x, x'; \theta_2)).$$

$$\begin{bmatrix} f_H \\ f_L \end{bmatrix} \sim \mathcal{GP}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} k_{HH} & k_{HL} \\ k_{LH} & k_{LL} \end{bmatrix}\right),$$

$$k_{HL}(x, x'; \theta_1, \rho) = \rho k_1(x, x'; \theta_1).$$





Multi-fidelity Modeling



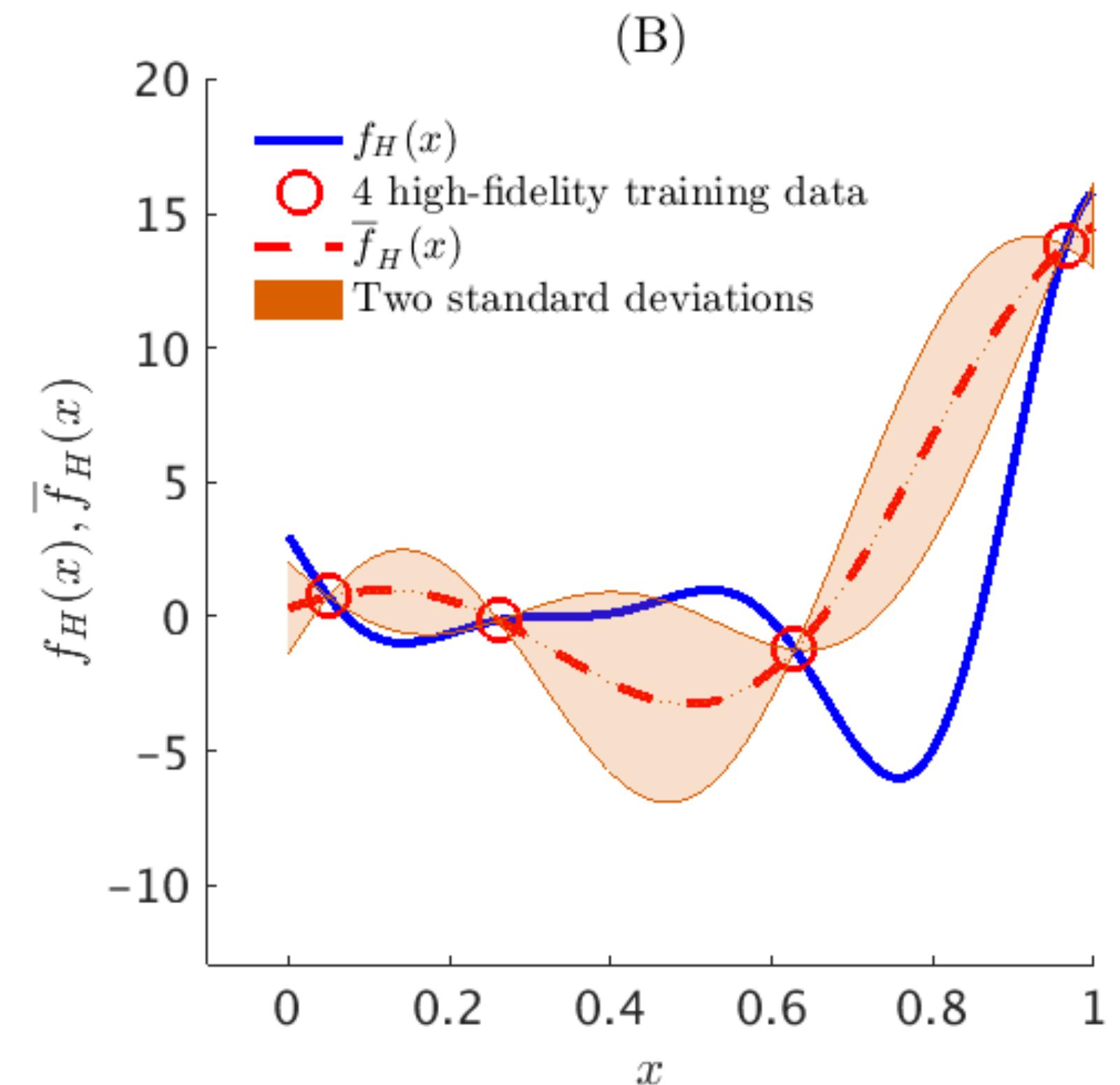
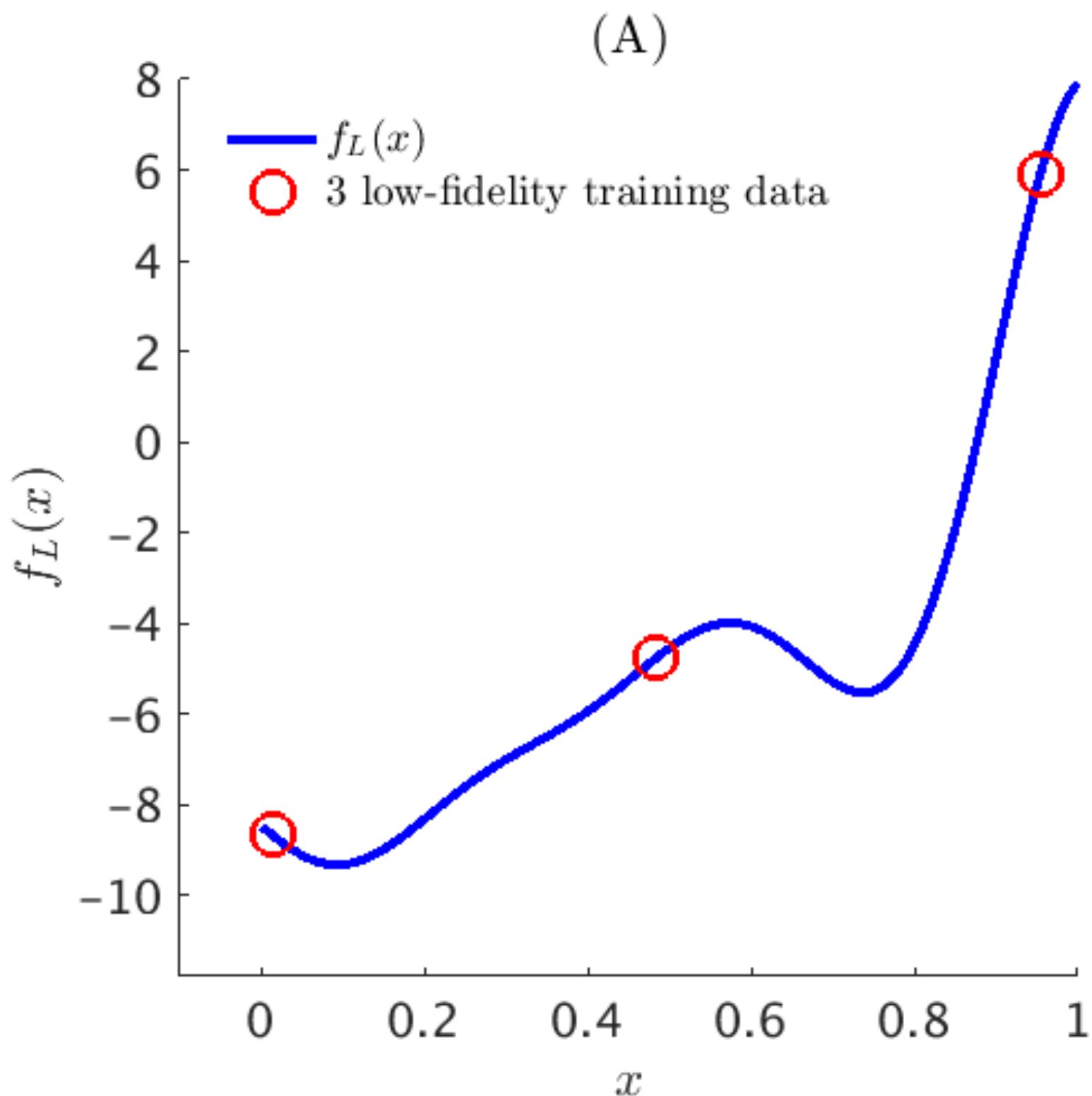
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Multi-fidelity Modeling



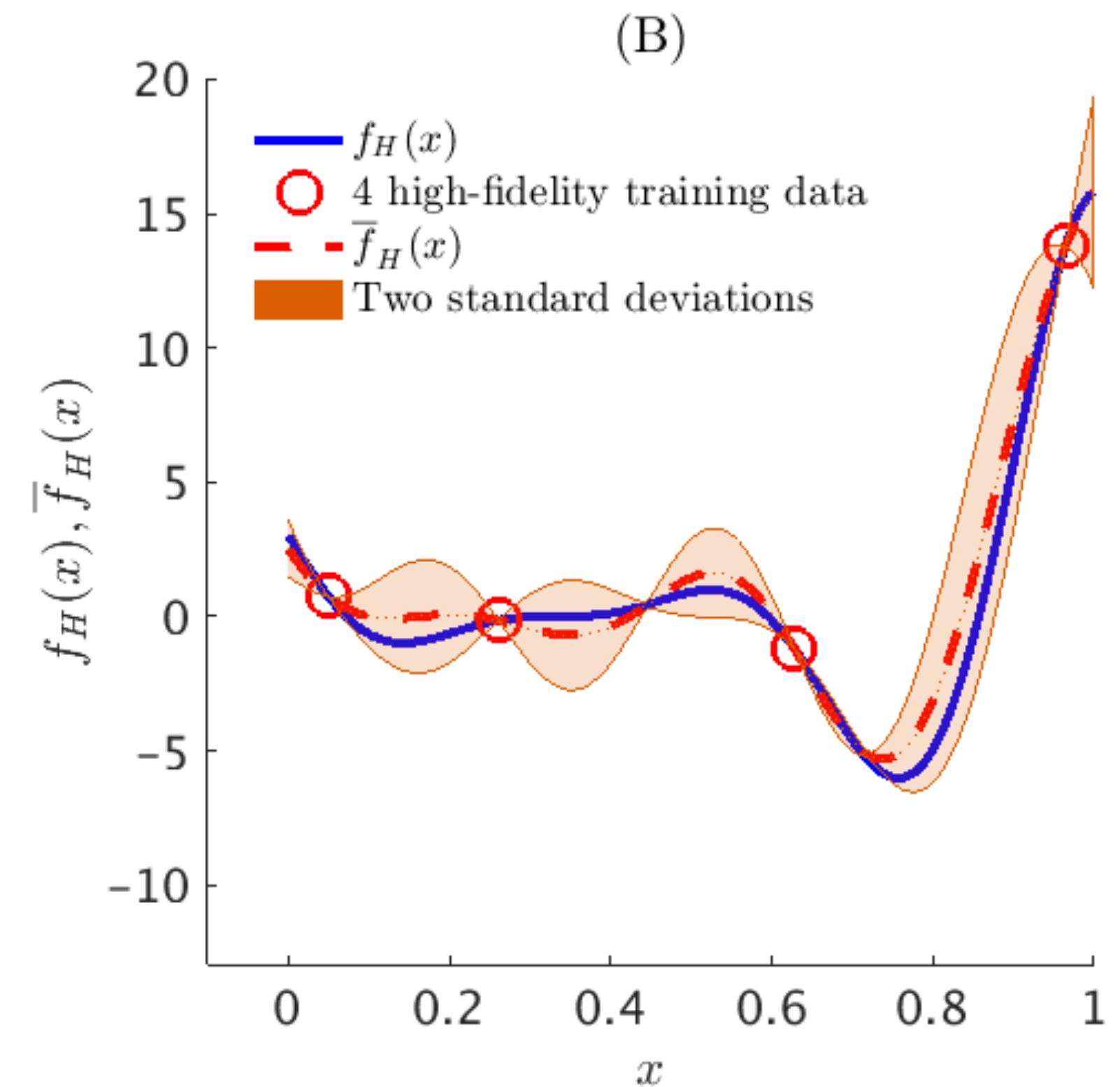
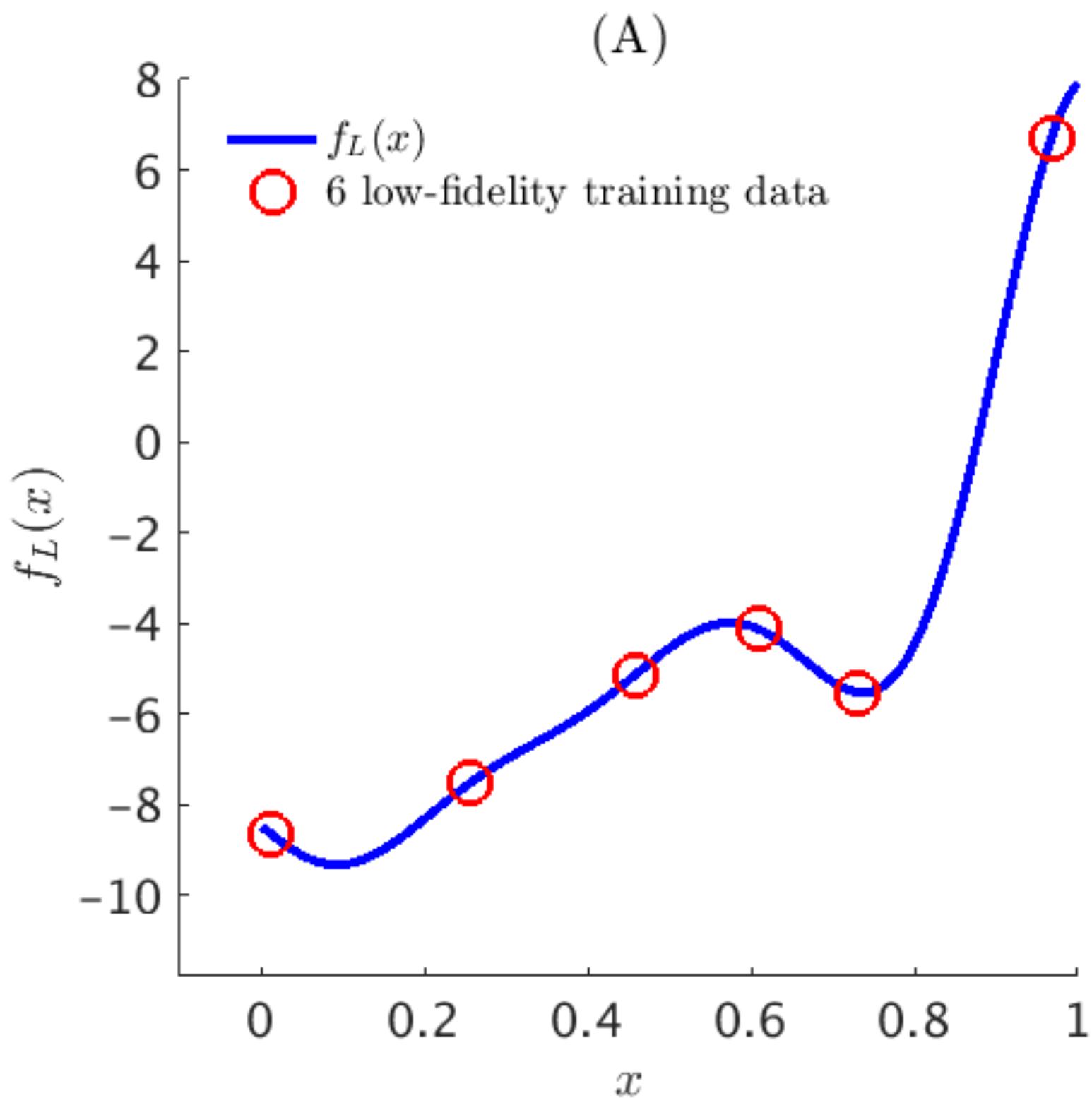
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Multi-fidelity Modeling



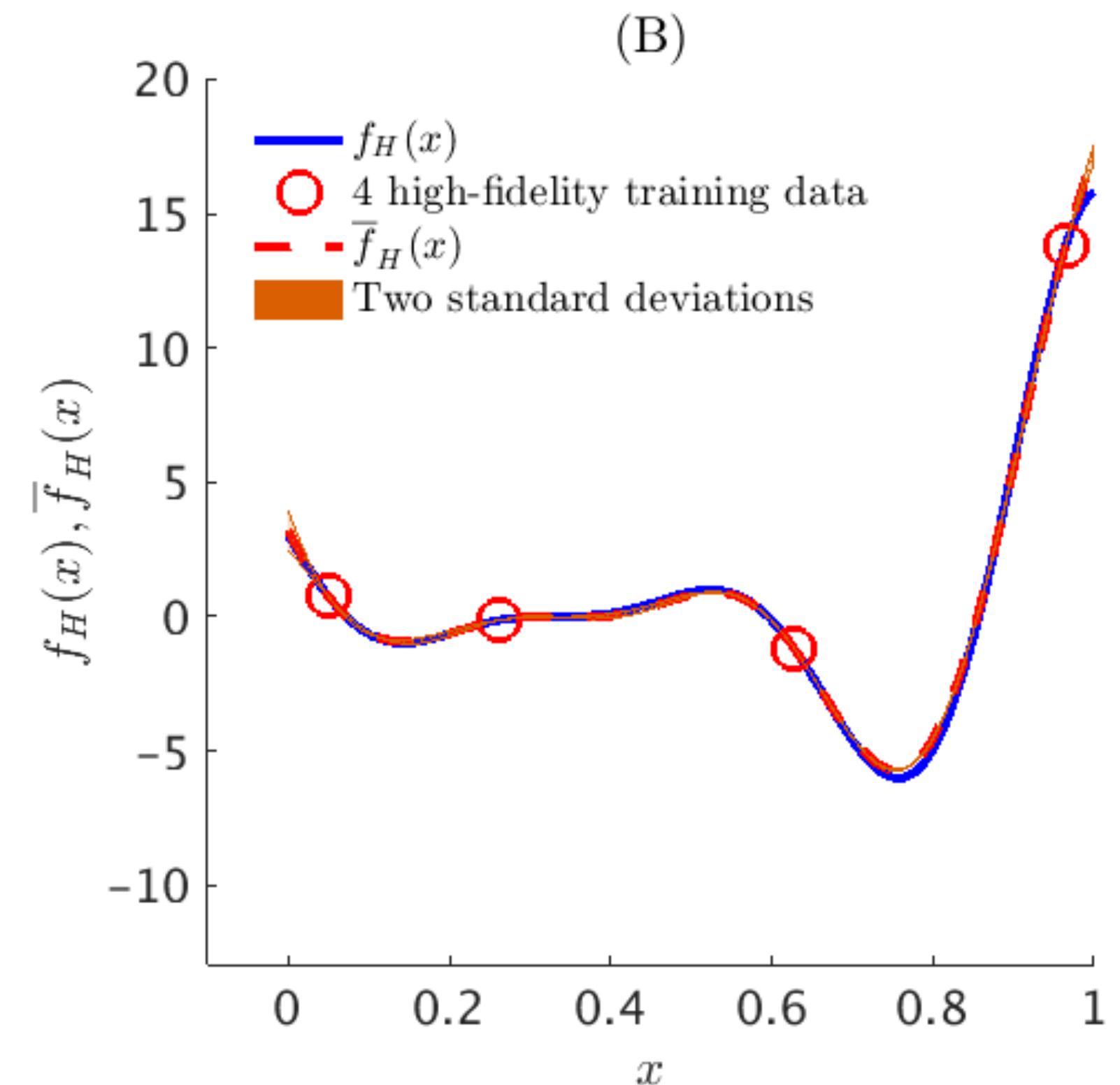
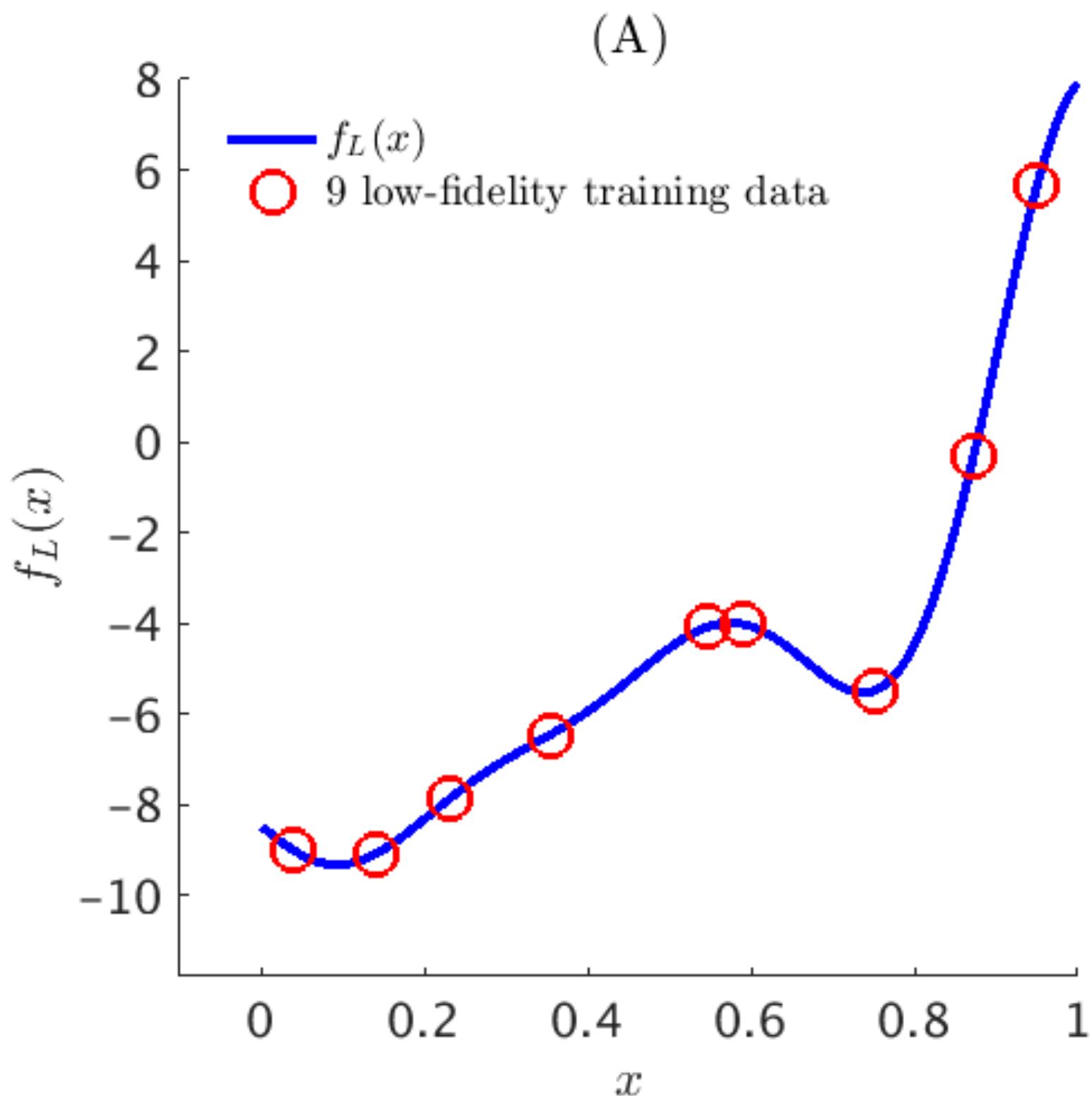
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Multi-fidelity Modeling



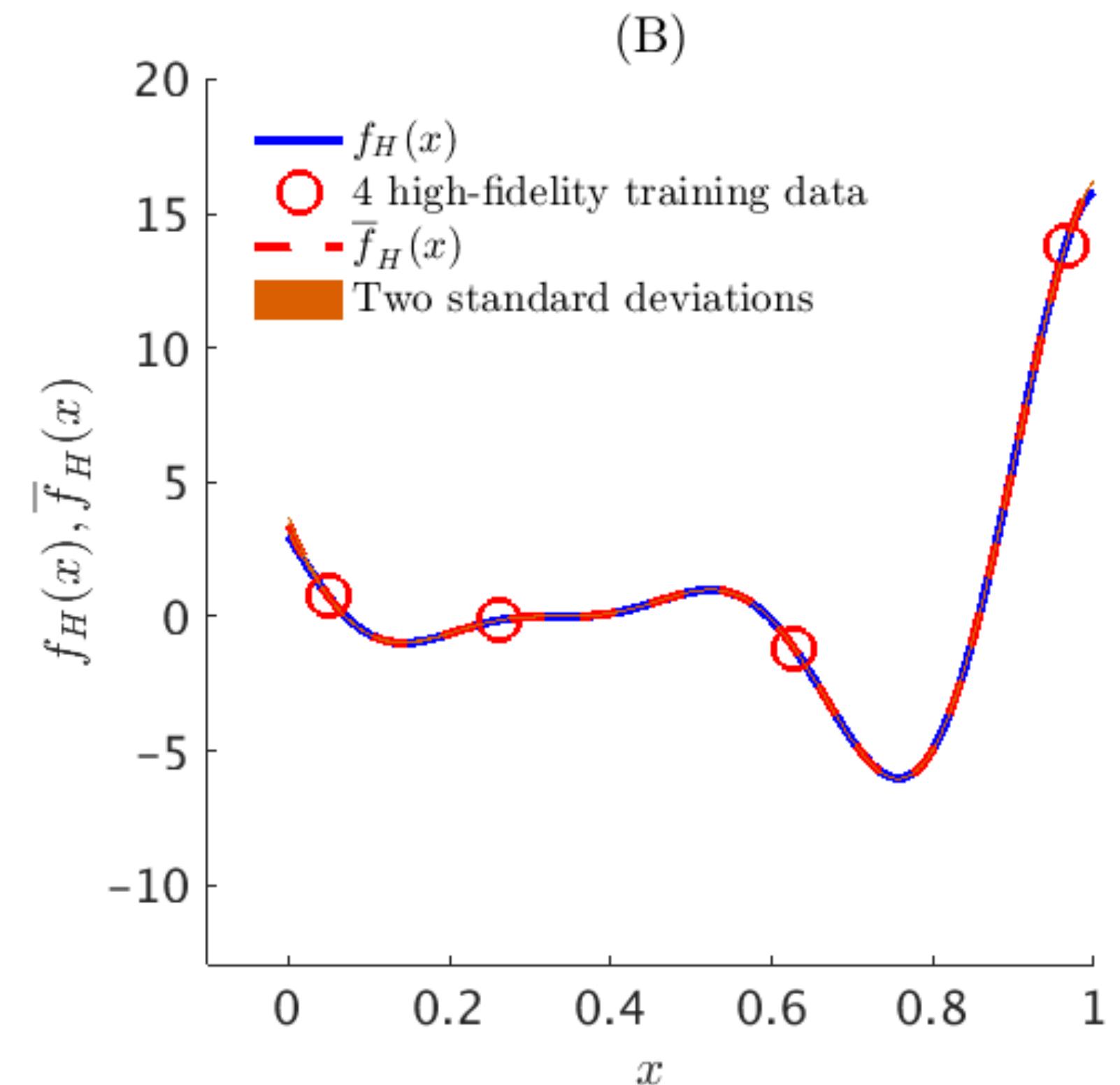
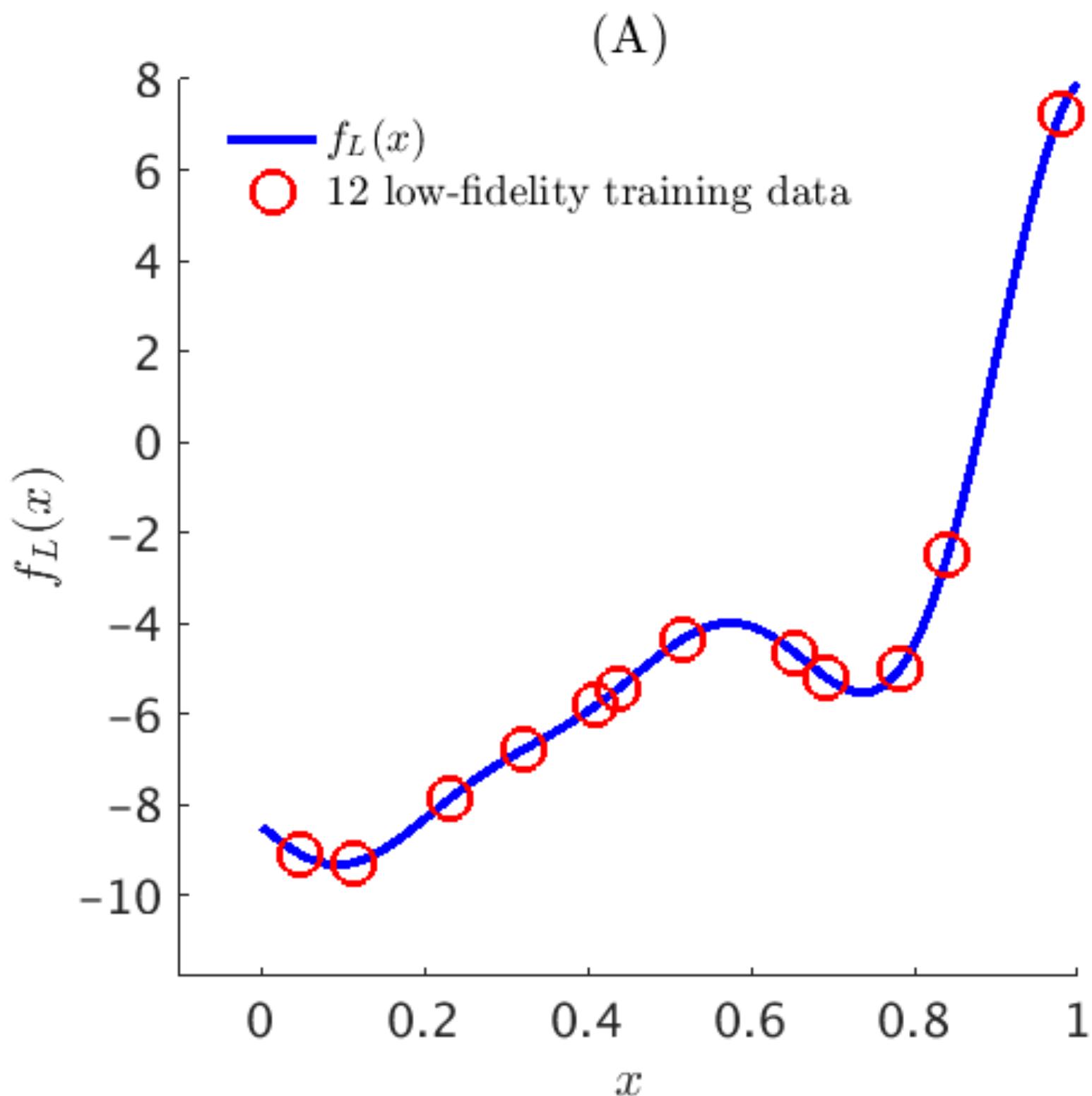
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Multi-fidelity Modeling



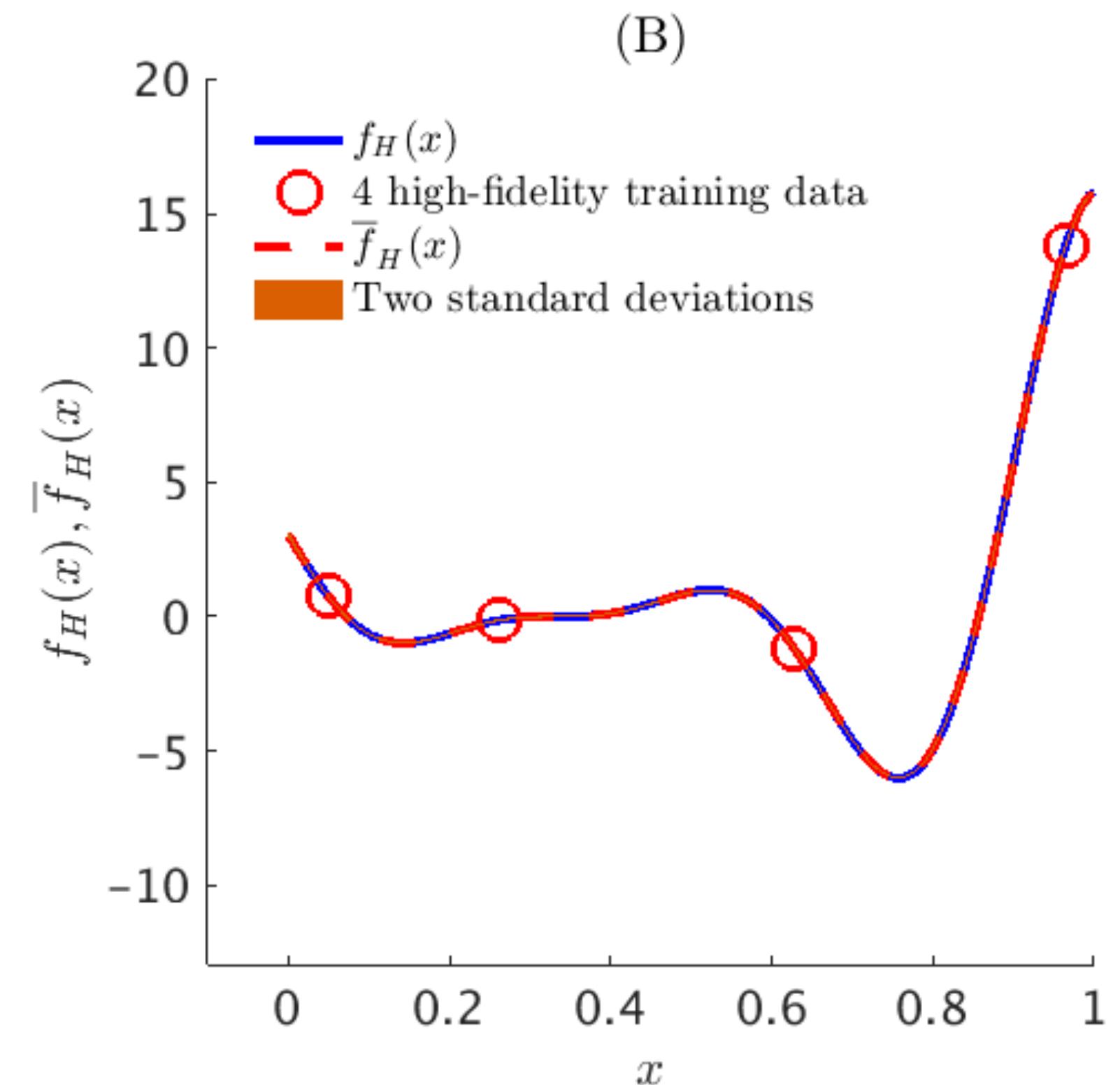
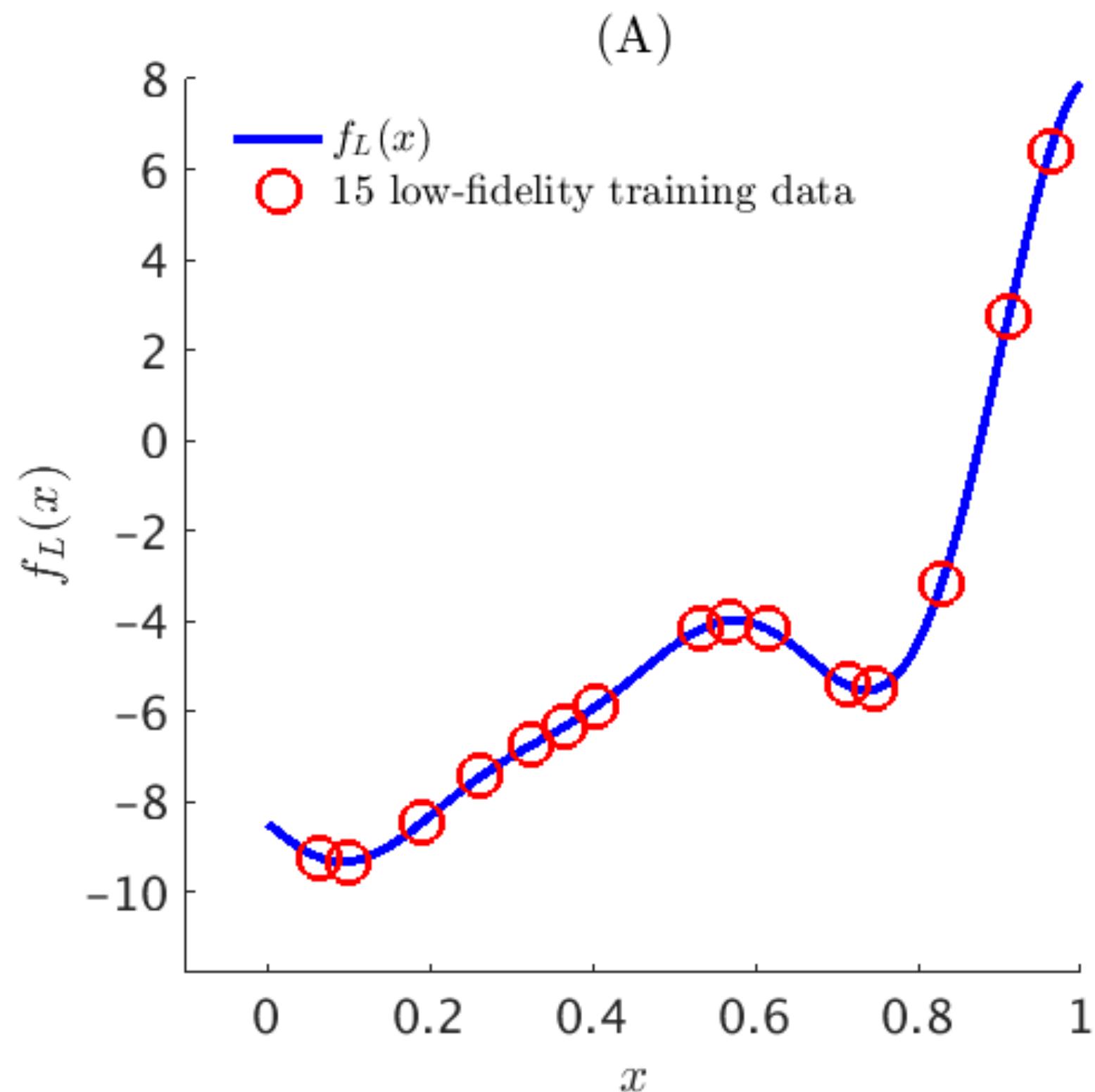
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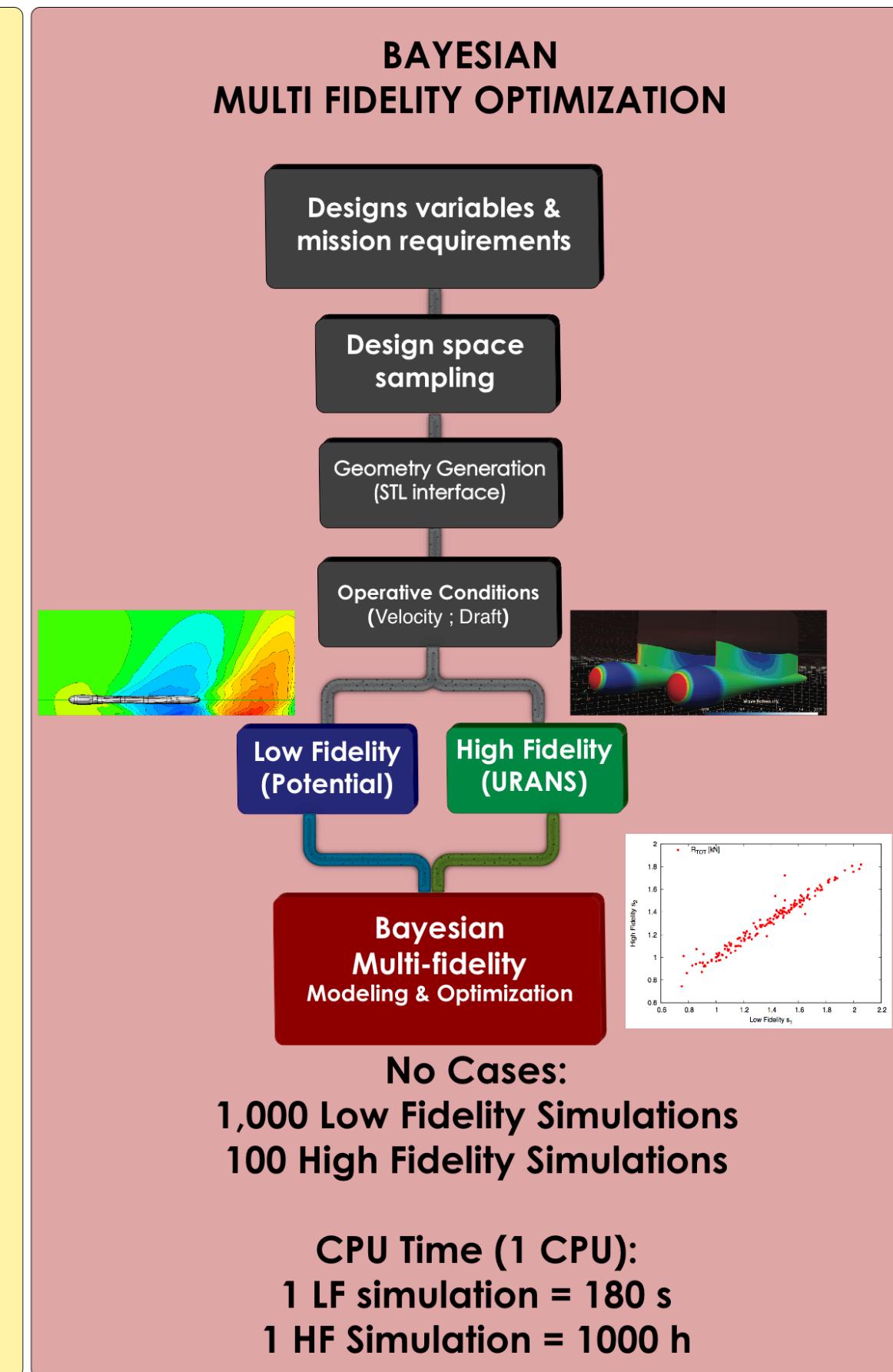
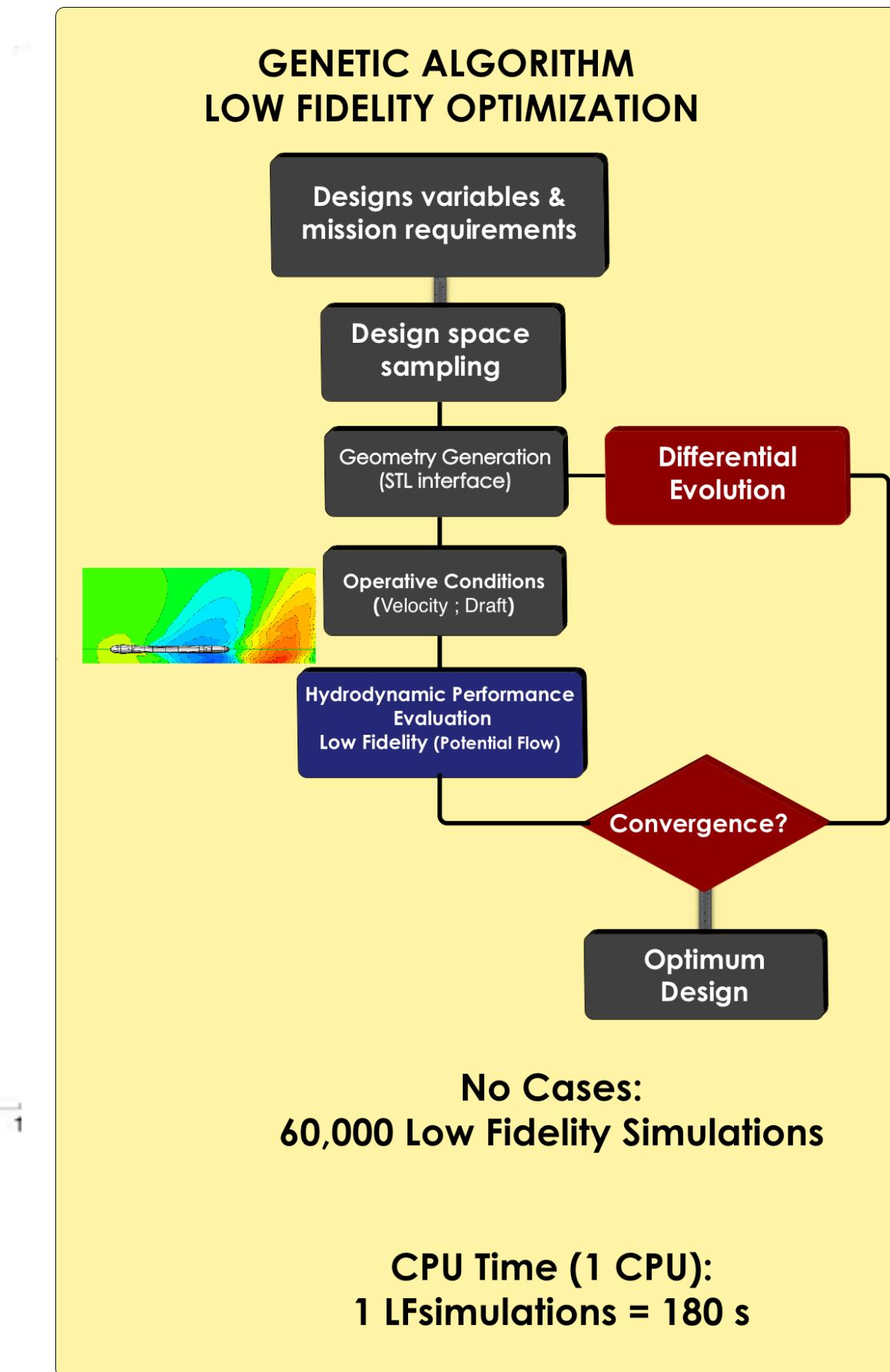
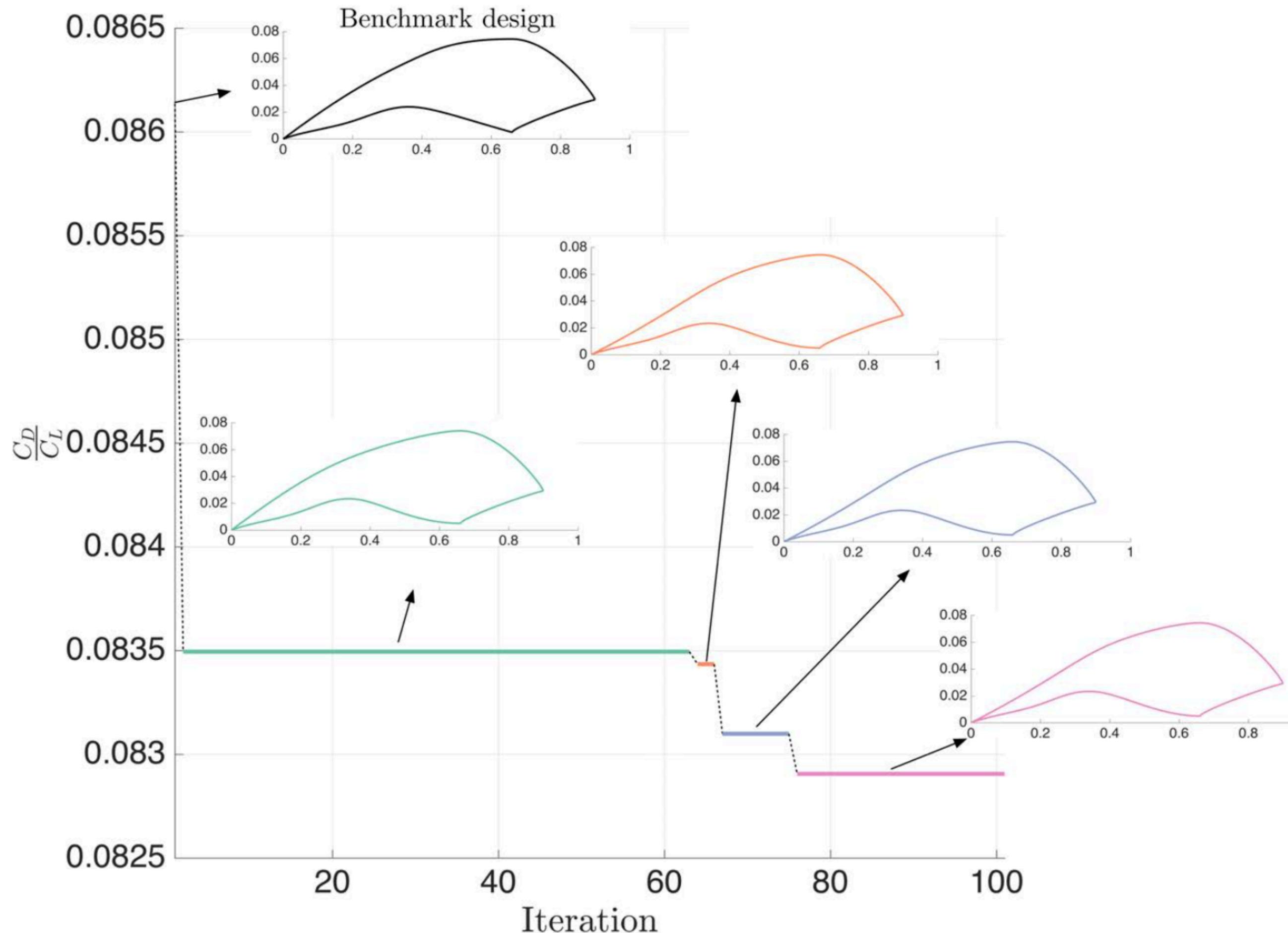




Multi-fidelity Bayesian Optimization



The multi-fidelity framework leads to 30% improvement in performance.





Numerical Gaussian Processes



$$u_t + uu_x - (0.01/\pi)u_{xx} = 0$$

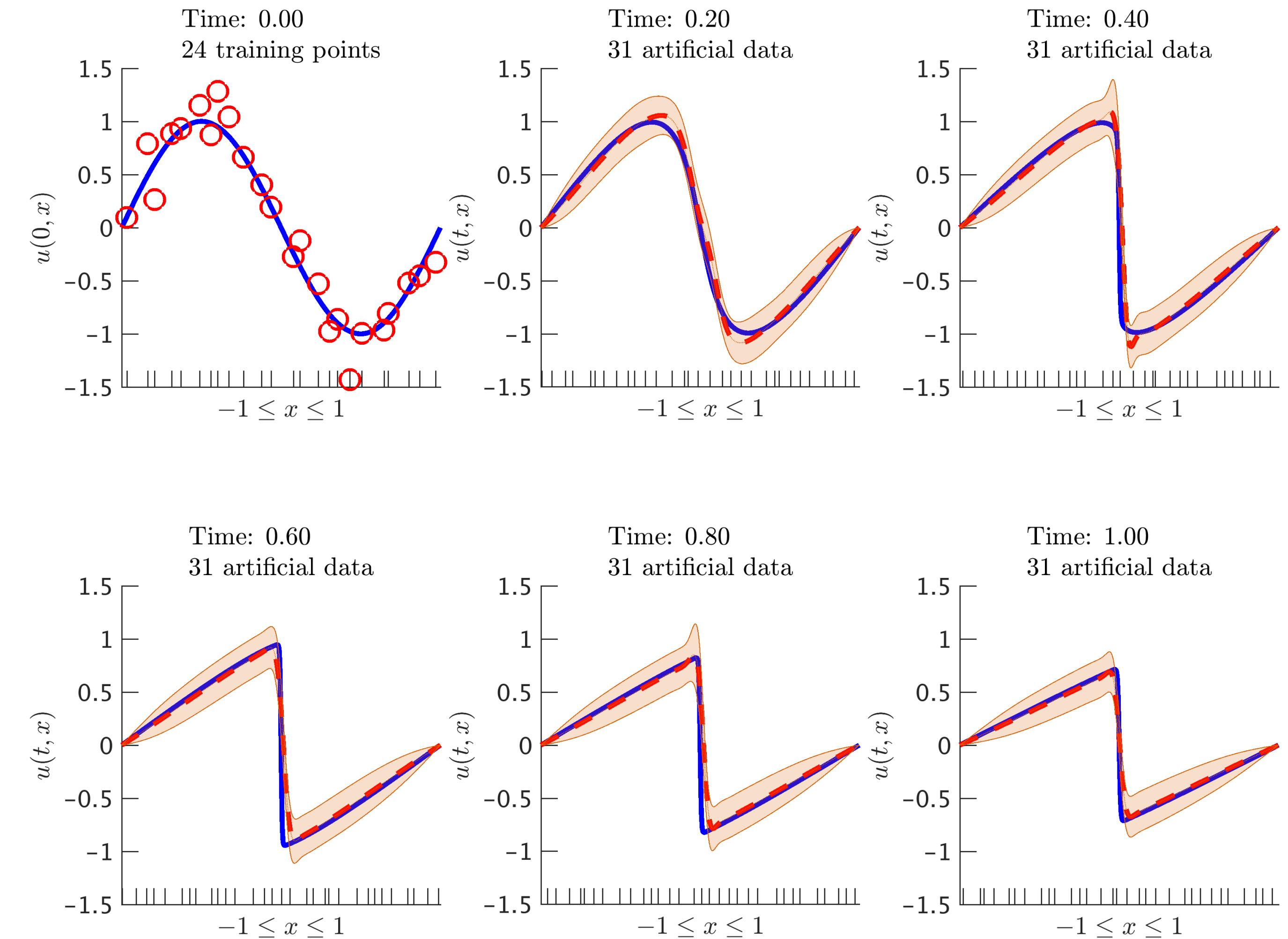
$$u^n + \Delta t (u^{n-1}u_x^n - (0.01/\pi)u_{xx}^n) = u^{n-1}$$

$$u^n \sim \mathcal{GP}(0, k(x, x'; \theta))$$

$$\begin{bmatrix} u^n \\ u^{n-1} \end{bmatrix} \sim \mathcal{GP}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} k^{n,n} & k^{n,n-1} \\ k^{n-1,n} & k^{n-1,n-1} \end{bmatrix}\right)$$

$$k^{n-1,n} = k + \Delta t (u^{n-1}k_x - (0.01/\pi)k_{xx})$$

Physics Informed Prior





Numerical Gaussian Processes



$$\begin{bmatrix} \mathbf{u}^n \\ \mathbf{u}^{n-1} \end{bmatrix} \sim \mathcal{N}(0, \mathbf{K})$$

$$\mathbf{K} = \begin{bmatrix} k^{n,n}(\mathbf{x}^n, \mathbf{x}^n; \theta) + \sigma_n^2 \mathbf{I} & k^{n,n-1}(\mathbf{x}^n, \mathbf{x}^{n-1}; \theta) \\ k^{n-1,n}(\mathbf{x}^{n-1}, \mathbf{x}^n; \theta) & k^{n,n-1}(\mathbf{x}^{n-1}, \mathbf{x}^{n-1}; \theta) + \sigma_{n-1}^2 \mathbf{I} \end{bmatrix}$$

$$\min_{\theta, \sigma_n, \sigma_{n-1}} \left[\begin{bmatrix} \mathbf{u}^n \\ \mathbf{u}^{n-1} \end{bmatrix}^T \mathbf{K}^{-1} \begin{bmatrix} \mathbf{u}^n \\ \mathbf{u}^{n-1} \end{bmatrix} + \log |\mathbf{K}| \right]$$

$$u^n(x^*) \mid \mathbf{u}^n \sim \mathcal{N}(m^n(x^*), S^{n,n}(x^*, x^*))$$

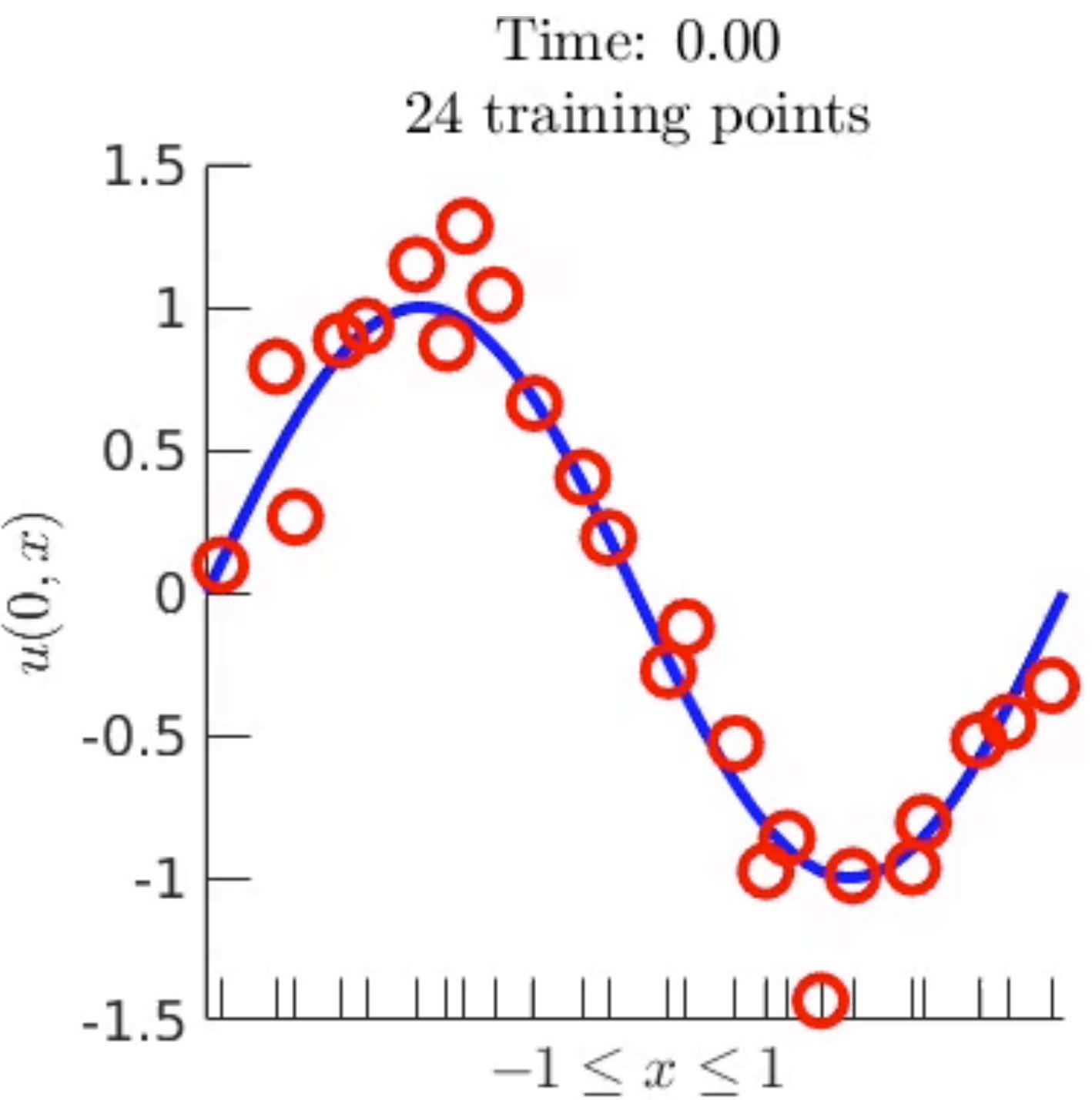
$$m^n(x^*) = \mathbf{q}^T \mathbf{K}^{-1} \begin{bmatrix} \mathbf{u}^n \\ \mathbf{m}^{n-1} \end{bmatrix}$$

$$\mathbf{q}^T = [k^{n,n}(x^n, \mathbf{x}^n) \quad k^{n,n-1}(x^n, \mathbf{x}^{n-1})]$$

$$S^{n,n}(x^*, x^*) = k^{n,n}(x^*, x^*) - \mathbf{q}^T \mathbf{K}^{-1} \mathbf{q} + \boxed{\mathbf{q}^T \mathbf{K}^{-1} \begin{bmatrix} 0 & 0 \\ 0 & \mathbf{S}^{n-1,n-1} \end{bmatrix} \mathbf{K}^{-1} \mathbf{q}}$$

Training

Prediction



$$\begin{aligned} \mathbf{u}^n &\sim \mathcal{N}(\mathbf{m}^n, \mathbf{S}^{n,n}) \\ \mathbf{m}^n &= m^n(\mathbf{x}^n) \\ \mathbf{S}^{n,n} &= S^{n,n}(\mathbf{x}^n, \mathbf{x}^n) \end{aligned}$$



Hidden Physics Models



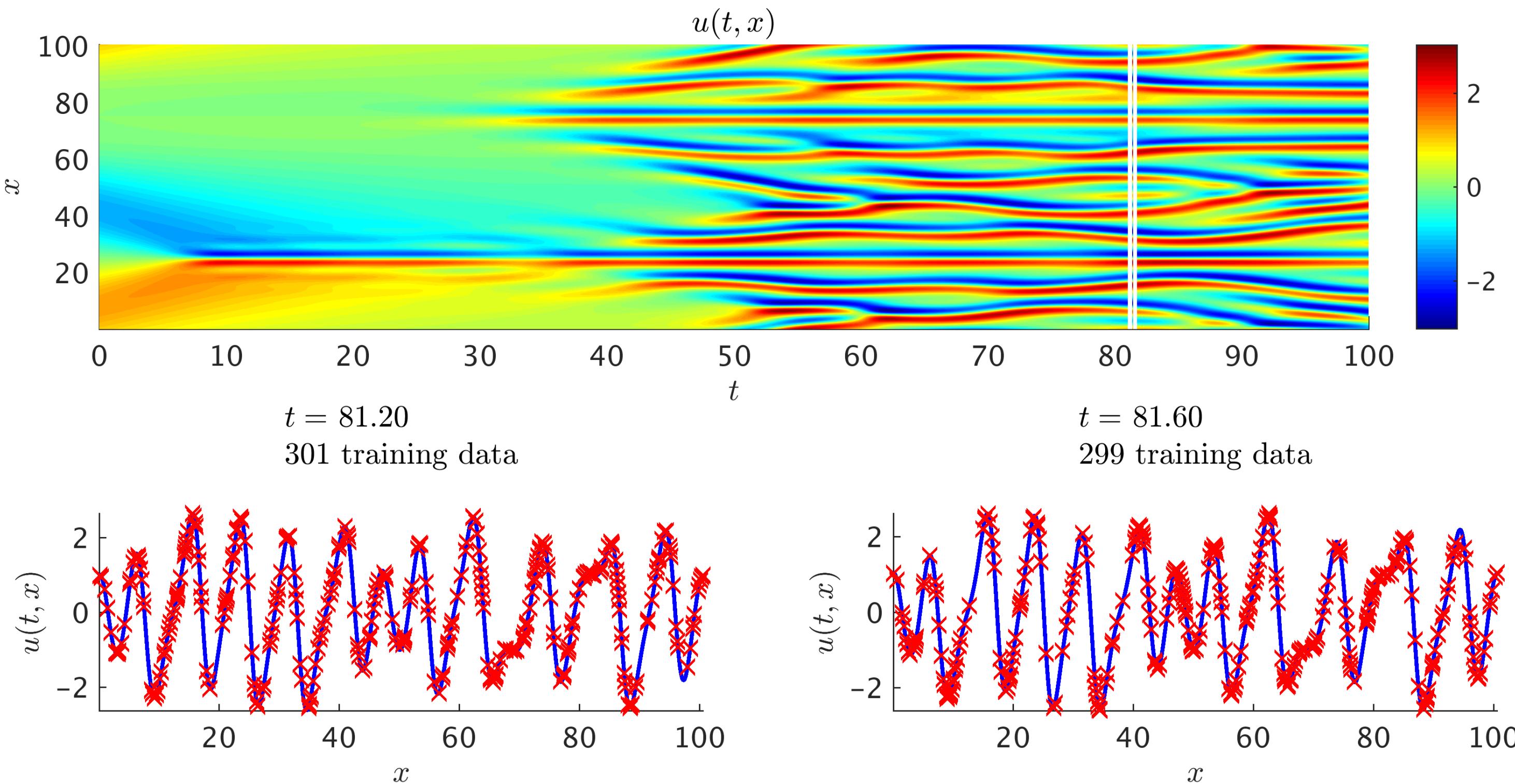
$$u_t + \lambda_1 u u_x + \lambda_2 u_{xx} + \lambda_3 u_{xxxx} = 0$$

$$u^n + \Delta t (\lambda_1 u^{n-1} u_x^n + \lambda_2 u_{xx}^n + \lambda_3 u_{xxxx}^n) = u^{n-1}$$

$$u^n \sim \mathcal{GP}(0, k(x, x'; \theta))$$

$$\begin{bmatrix} u^n \\ u^{n-1} \end{bmatrix} \sim \mathcal{GP}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} k^{n,n} & k^{n,n-1} \\ k^{n-1,n} & k^{n-1,n-1} \end{bmatrix}\right)$$

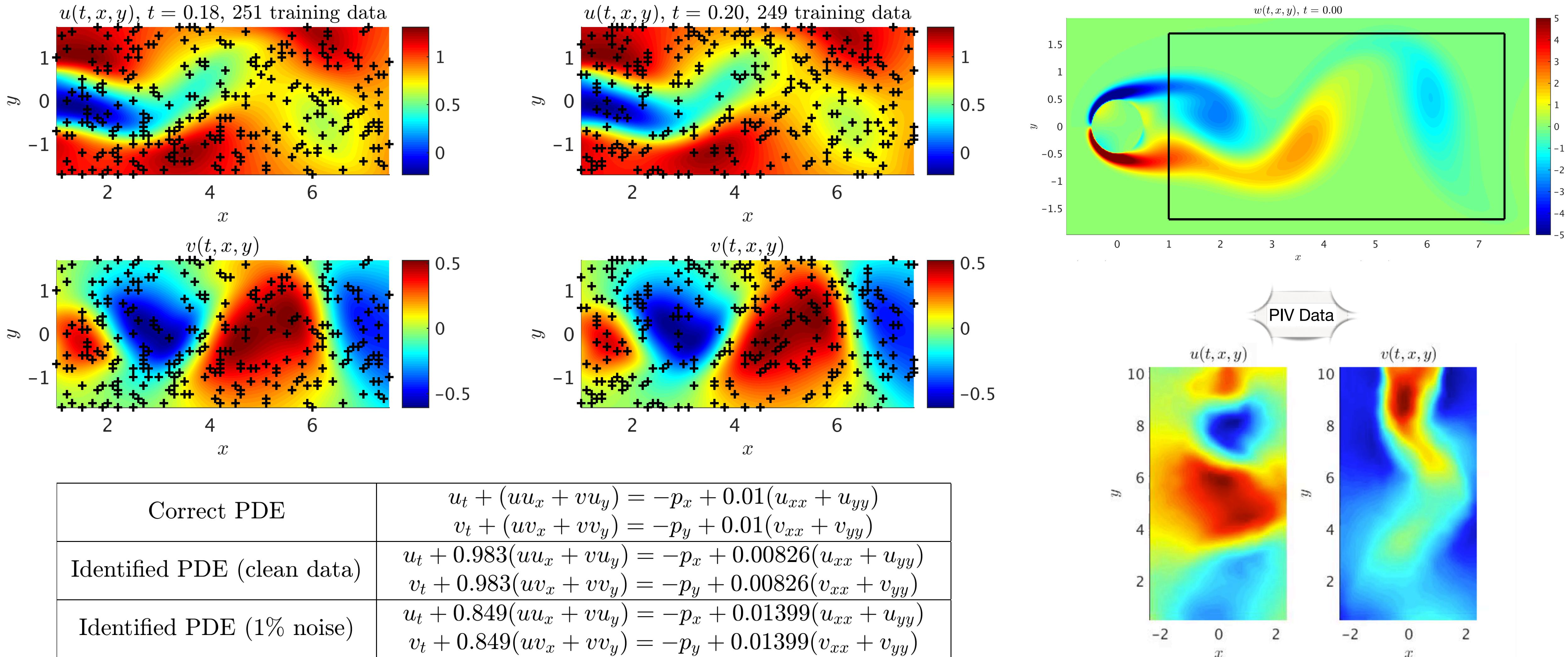
$$k^{n-1,n} = k + \Delta t (\lambda_1 u^{n-1} k_x + \lambda_2 k_{xx} + \lambda_3 k_{xxxx})$$



Correct PDE	$u_t + uu_x + u_{xx} + u_{xxxx} = 0$
Identified PDE (clean data)	$u_t + 0.952uu_x + 1.005u_{xx} + 0.980u_{xxxx} = 0$
Identified PDE (1% noise)	$u_t + 0.908uu_x + 0.951u_{xx} + 0.927u_{xxxx} = 0$

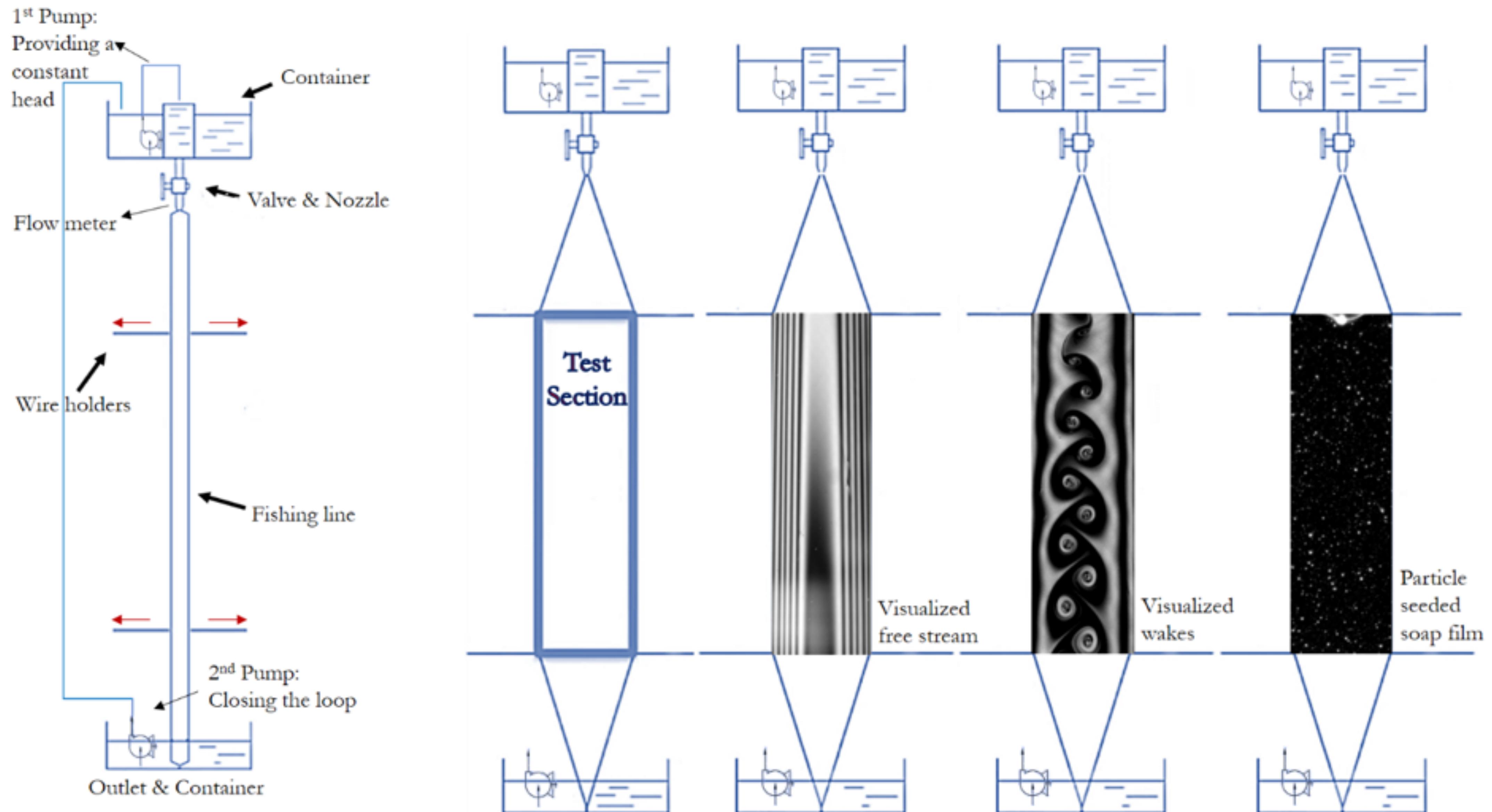


Hidden Physics Models





Hidden Physics Models



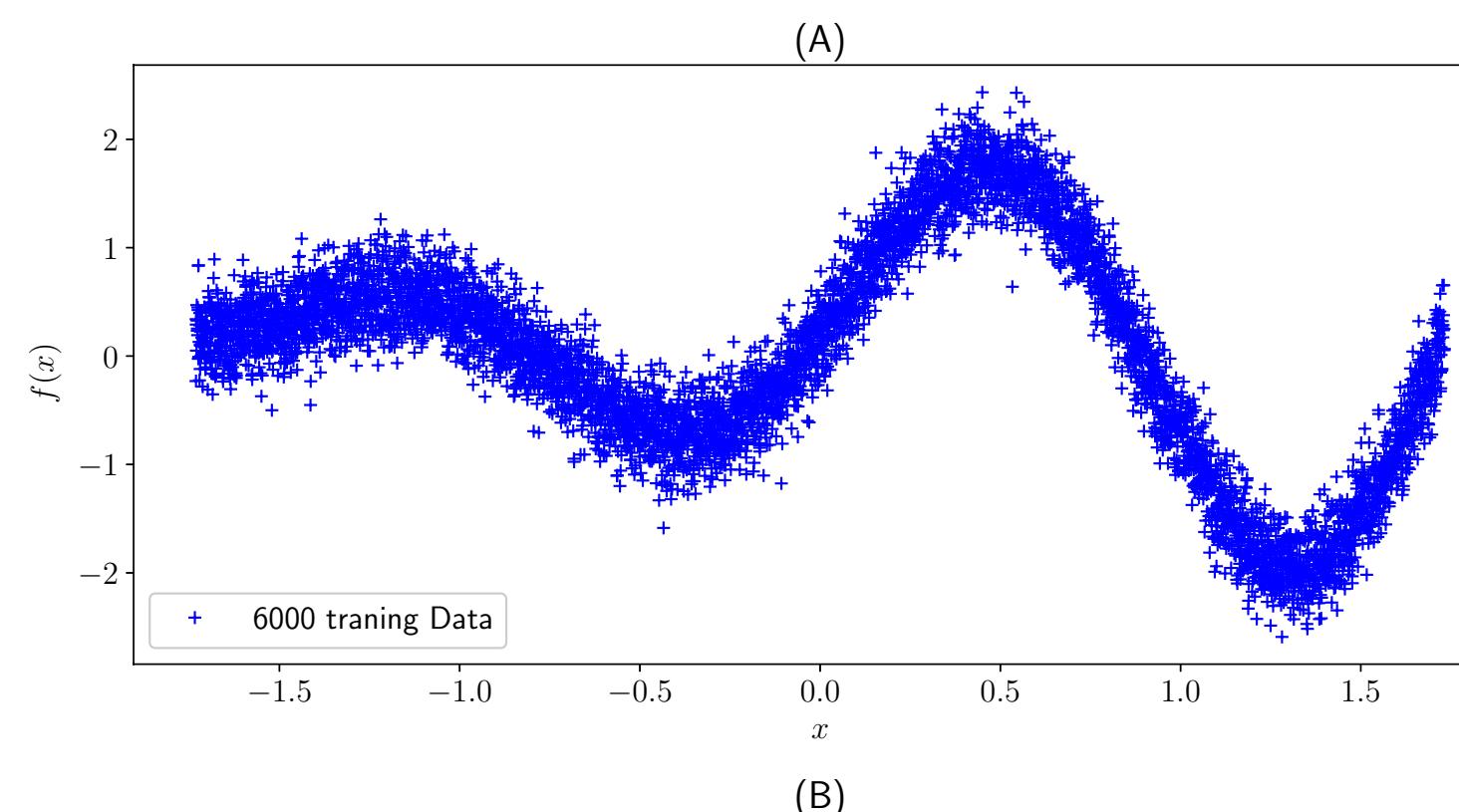


Parametric Gaussian Processes for Big Data



1) Parametric Gaussian process
(producer of the hypothetical data)

2) Classical Gaussian process
(consumer of the hypothetical data)

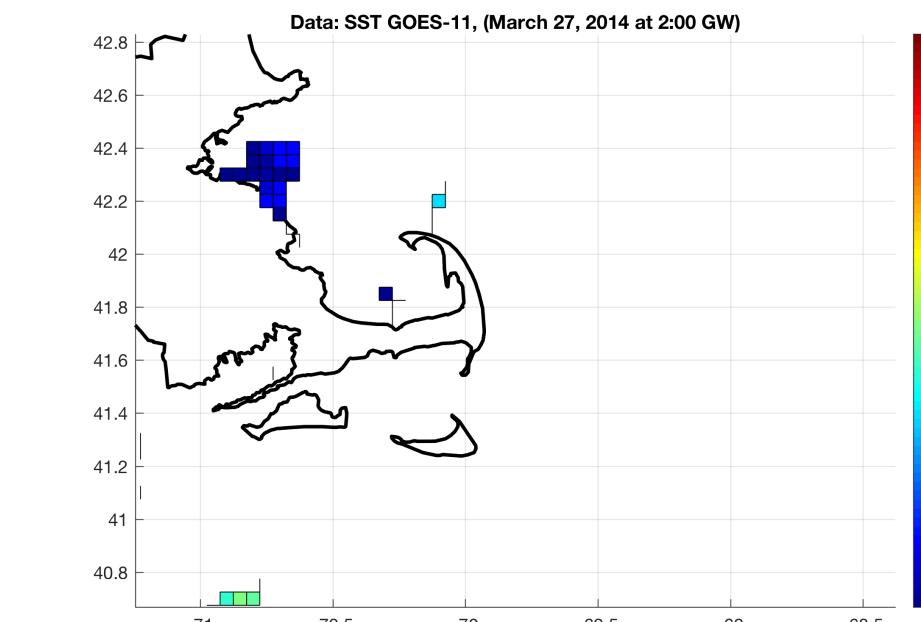


GOES_11
Satellite

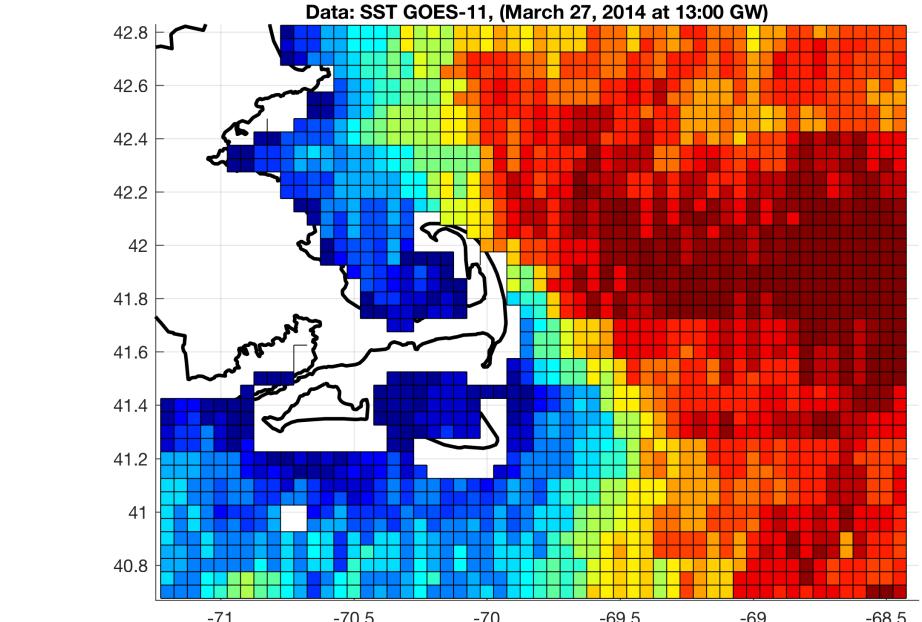
Prediction

Uncertainty
Map

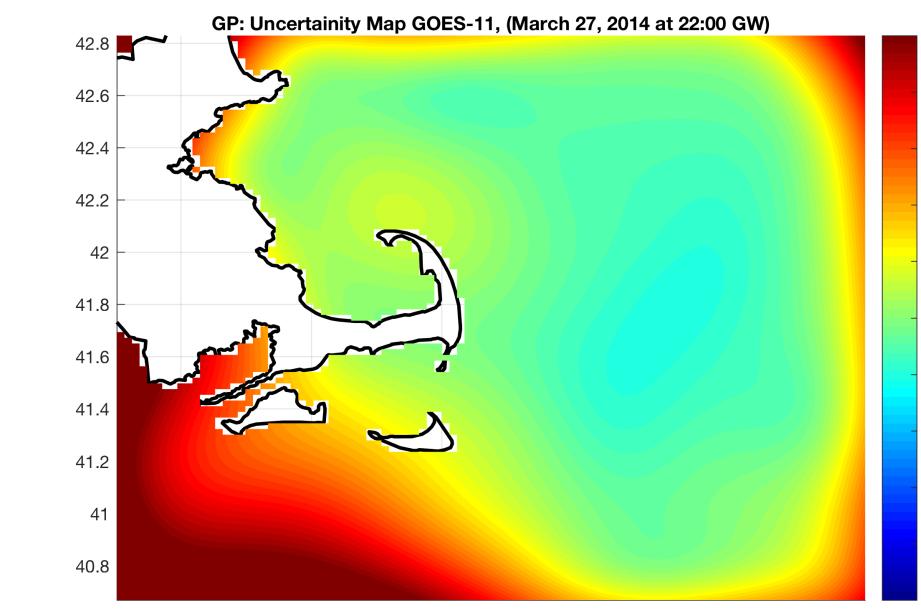
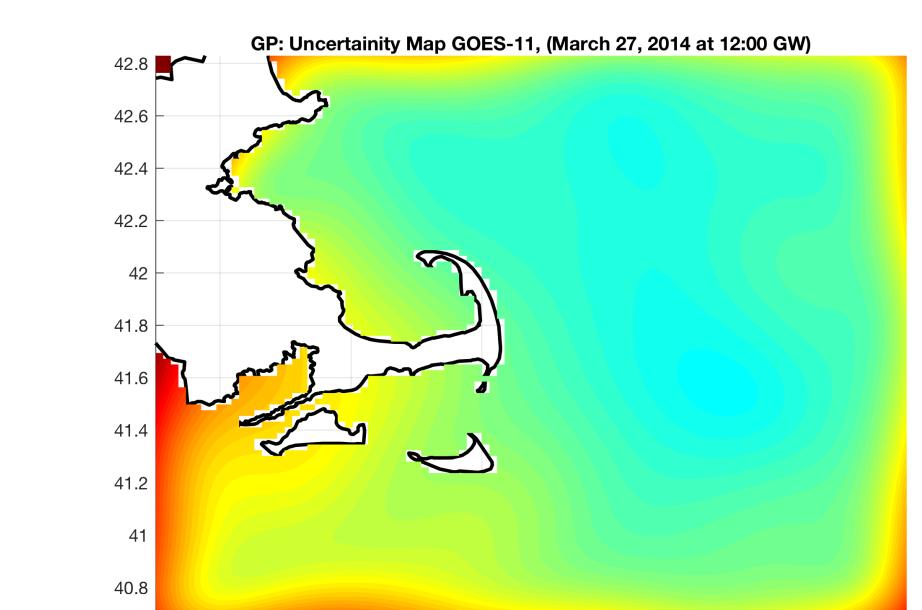
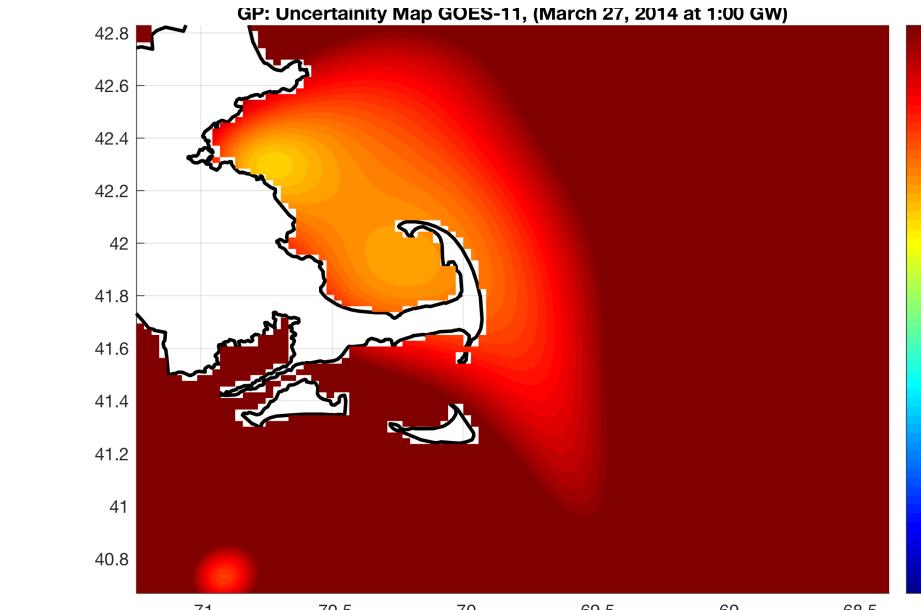
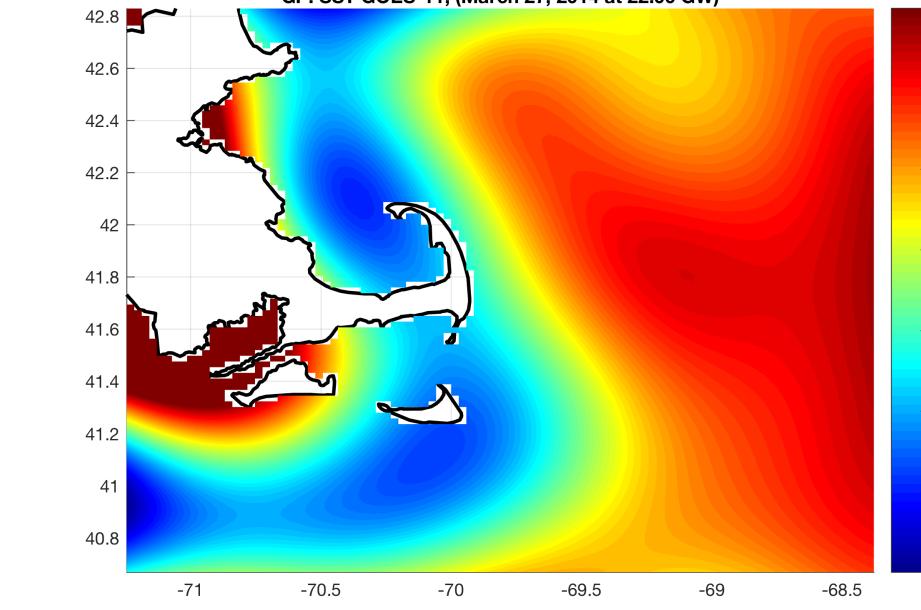
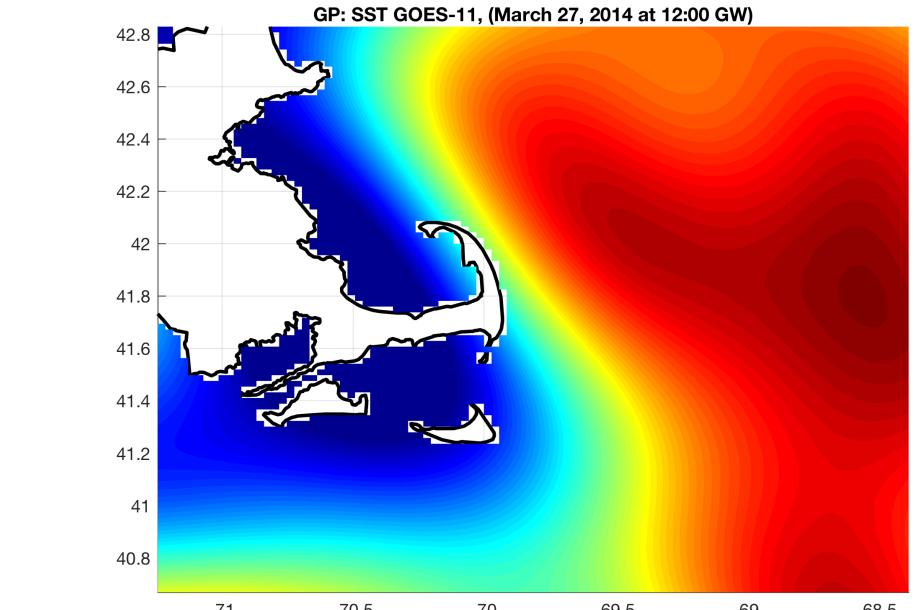
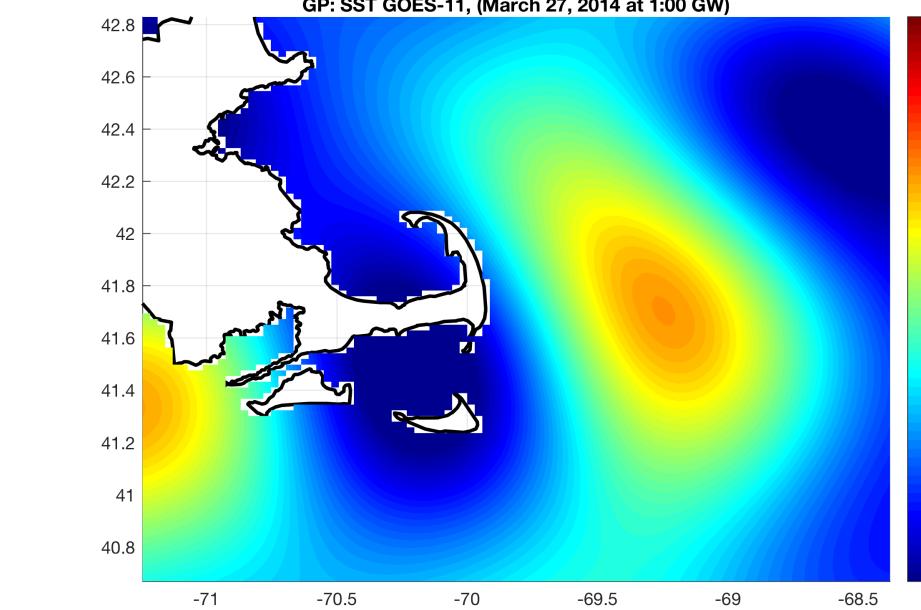
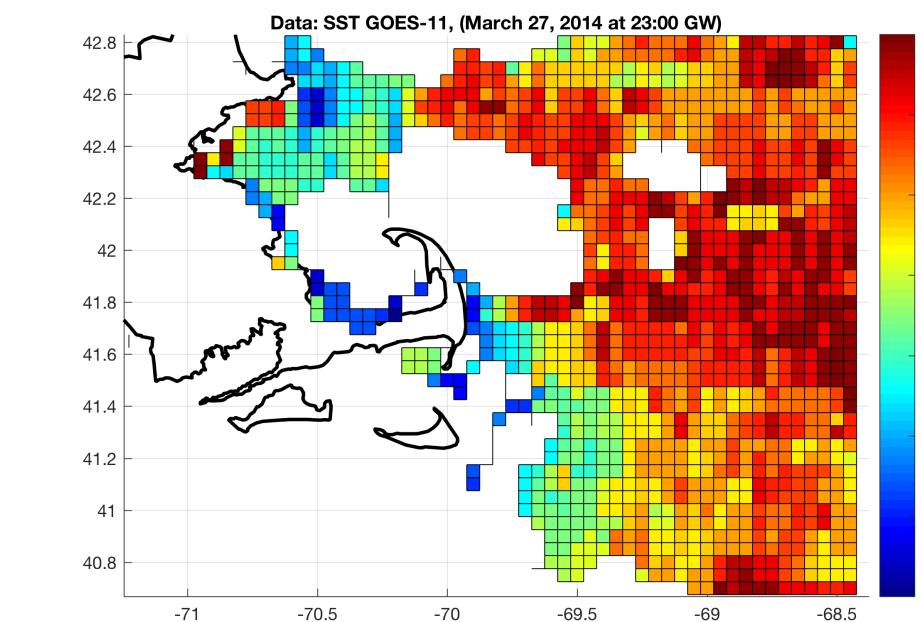
March 27, 2014 - 2:00 GW



March 27, 2014 - 13:00 GW

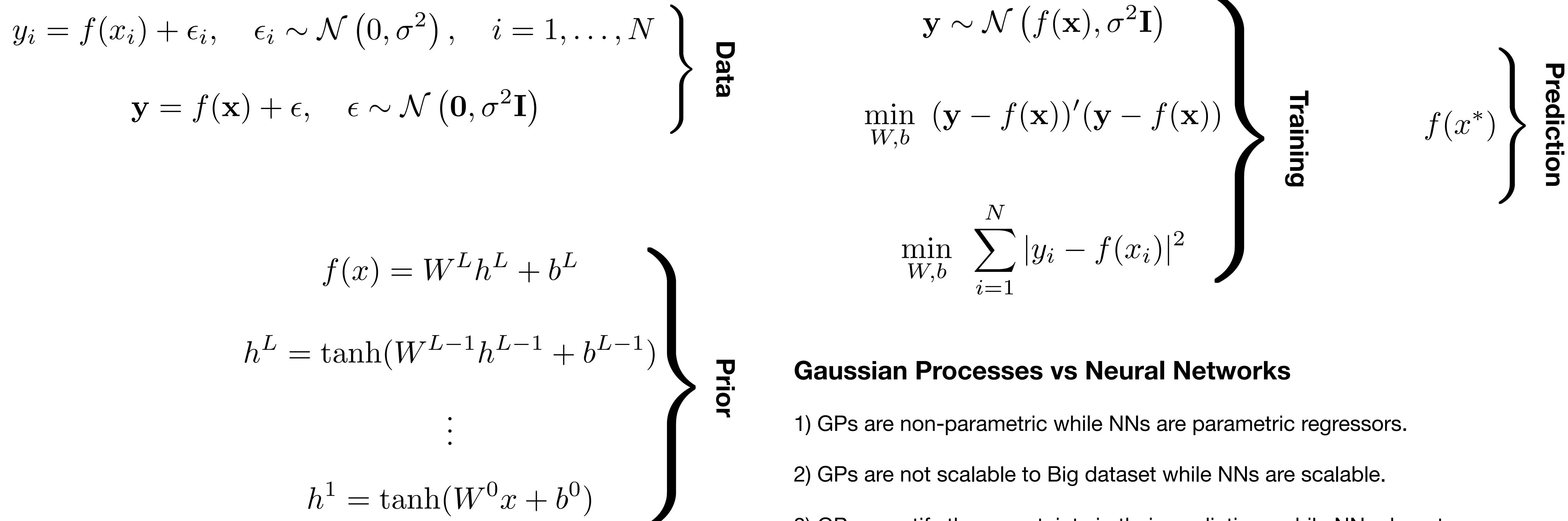


March 27, 2014 - 22:00 GW





Neural Networks Regression



Gaussian Processes vs Neural Networks

- 1) GPs are non-parametric while NNs are parametric regressors.
- 2) GPs are not scalable to Big dataset while NNs are scalable.
- 3) GPs quantify the uncertainty in their predictions while NNs do not.
- 4) GPs automatically balance the tradeoff between data fit and model complexity.



Physics Informed Neural Networks (PINNs)

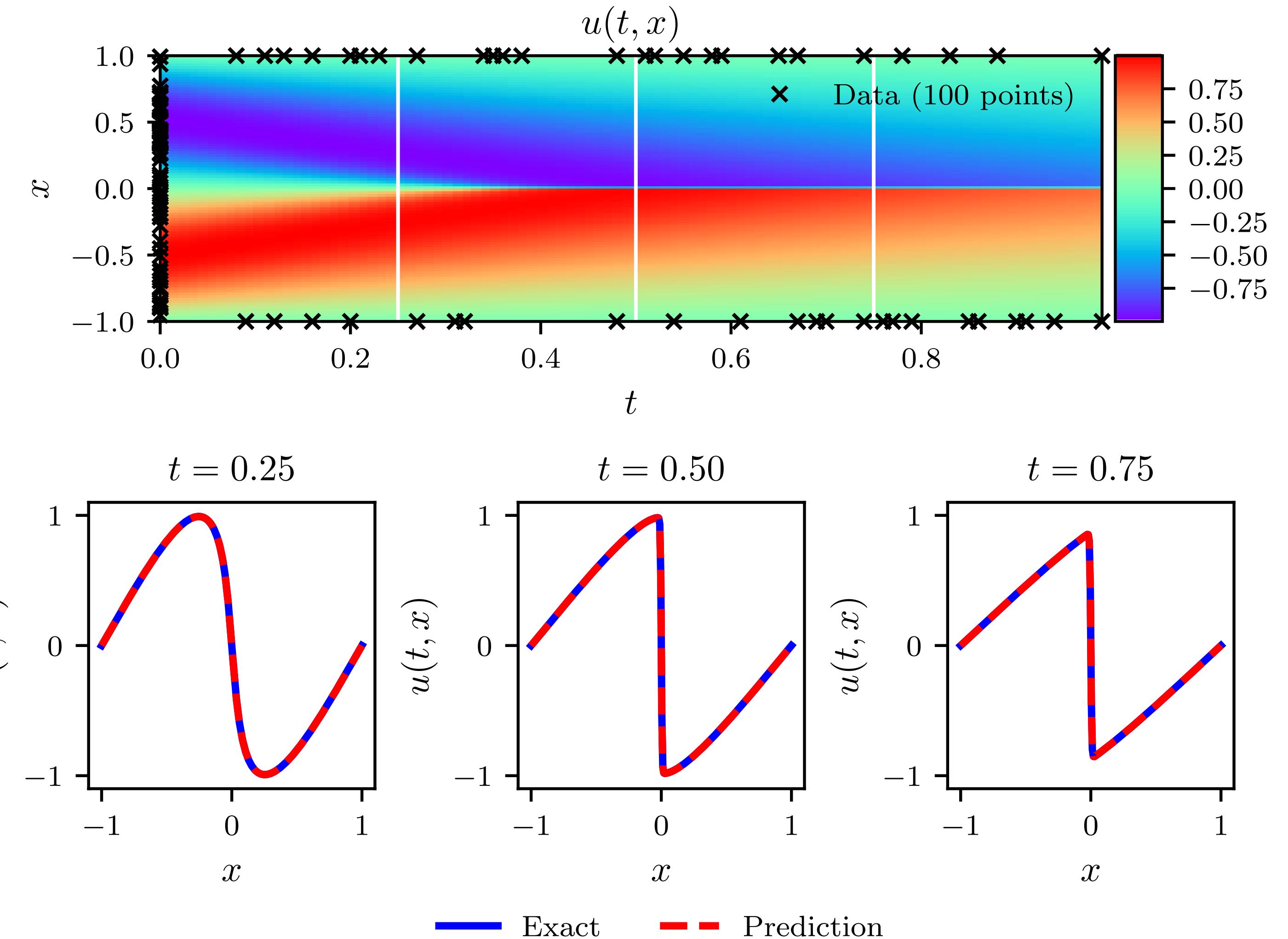


$$u_t + uu_x - (0.01/\pi)u_{xx} = 0$$

```
def u(t, x):
    u = neural_net(tf.concat([t,x],1), weights, biases)
    return u
```

```
def f(t, x):
    u = u(t, x)
    u_t = tf.gradients(u, t)[0]
    u_x = tf.gradients(u, x)[0]
    u_xx = tf.gradients(u_x, x)[0]
    f = u_t + u*u_x - (0.01/tf.pi)*u_xx
    return f
```

$$\sum_{i=1}^{N_u} |u(t_u^i, x_u^i) - u^i|^2 + \sum_{i=1}^{N_f} |f(t_f^i, x_f^i)|^2$$



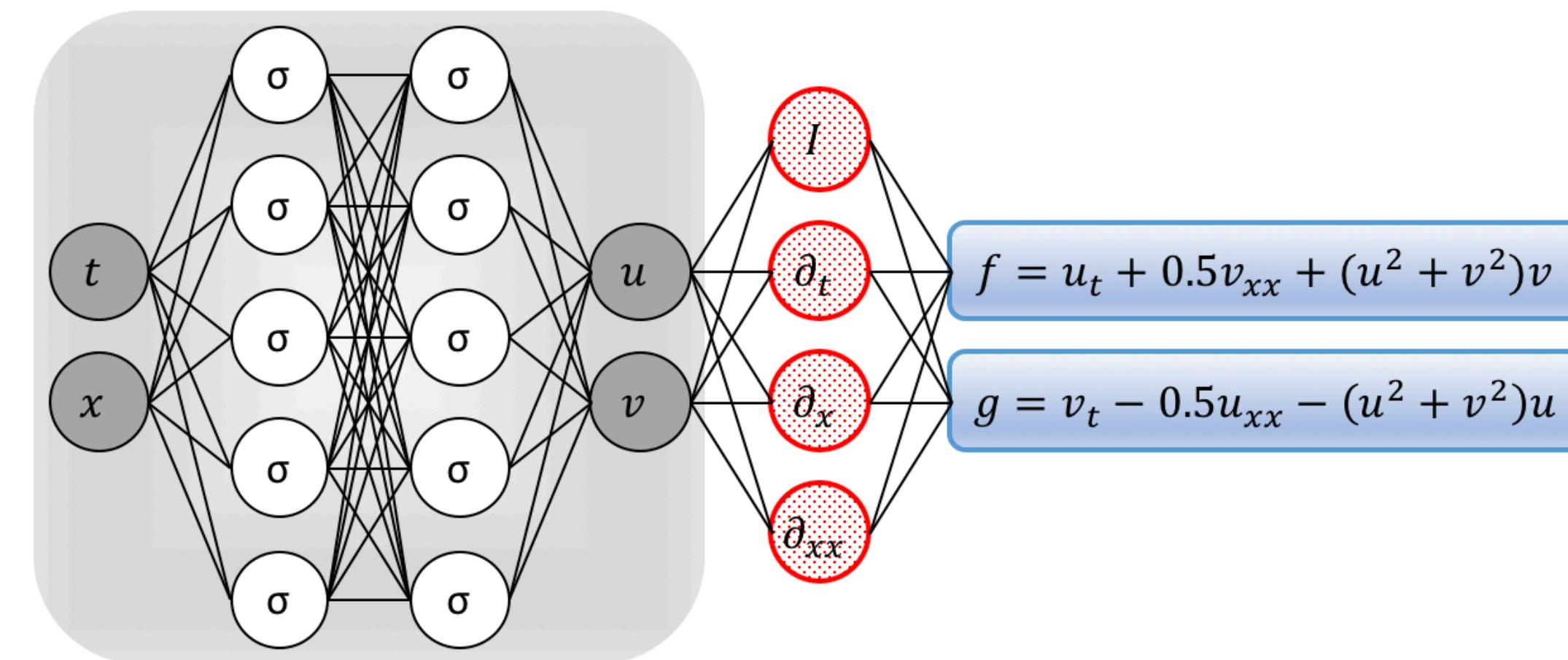


Physics Informed Neural Networks (PINNs)

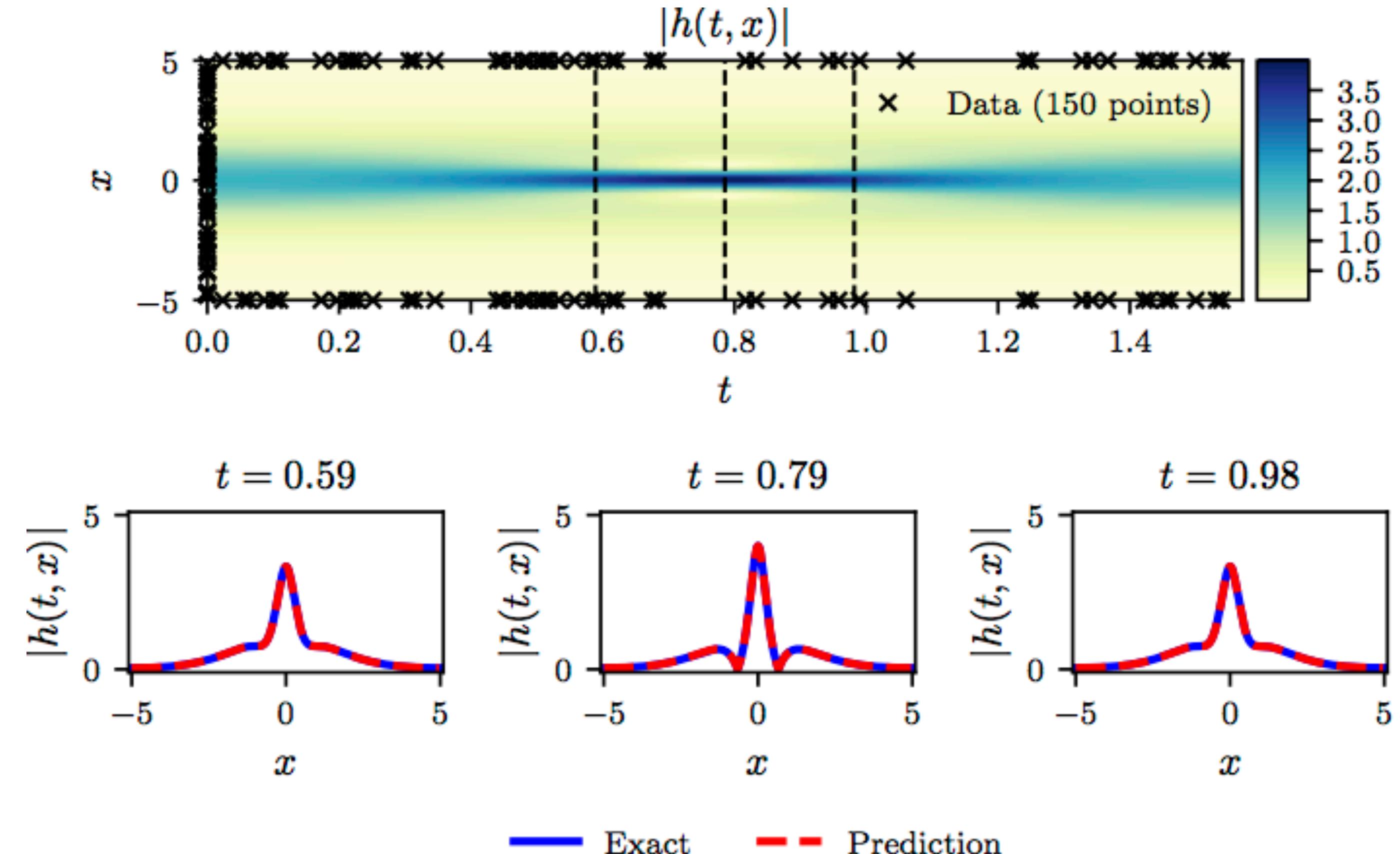


$$ih_t + 0.5h_{xx} + |h|^2 h = 0$$

$$u = \text{Real}(h), \quad v = \text{Imag}(h)$$



$$MSE = MSE_0 + MSE_b + MSE_f + MSE_g$$





Physics Informed Neural Networks (PINNs)



	FEM/FVM/FDM	PINNs	ROMs
Solution Space	Basis Functions	Neural Networks	Smart Basis Functions
Differential Operators	Discretization/Weak-form	Automatic Differentiation	Discretization/Weak-form
Solver	Linear/non-linear/Iterative	Gradient Descent (Training)	Linear/non-linear/Iterative
Evaluate	Interpolation	Inference	Interpolation



Forward-Backward Stochastic Neural Networks



Deep Learning of High-dimensional Partial Differential Equations

$$\begin{aligned} dX_t &= \mu(t, X_t, Y_t, Z_t)dt + \sigma(t, X_t, Y_t)dW_t \\ X_0 &= \xi \\ dY_t &= \varphi(t, X_t, Y_t, Z_t)dt + Z'_t\sigma(t, X_t, Y_t)dW_t \\ Y_T &= g(X_T) \end{aligned}$$

$$\begin{aligned} Y_t &= u(t, X_t) \\ Z_t &= Du(t, X_t) \end{aligned}$$

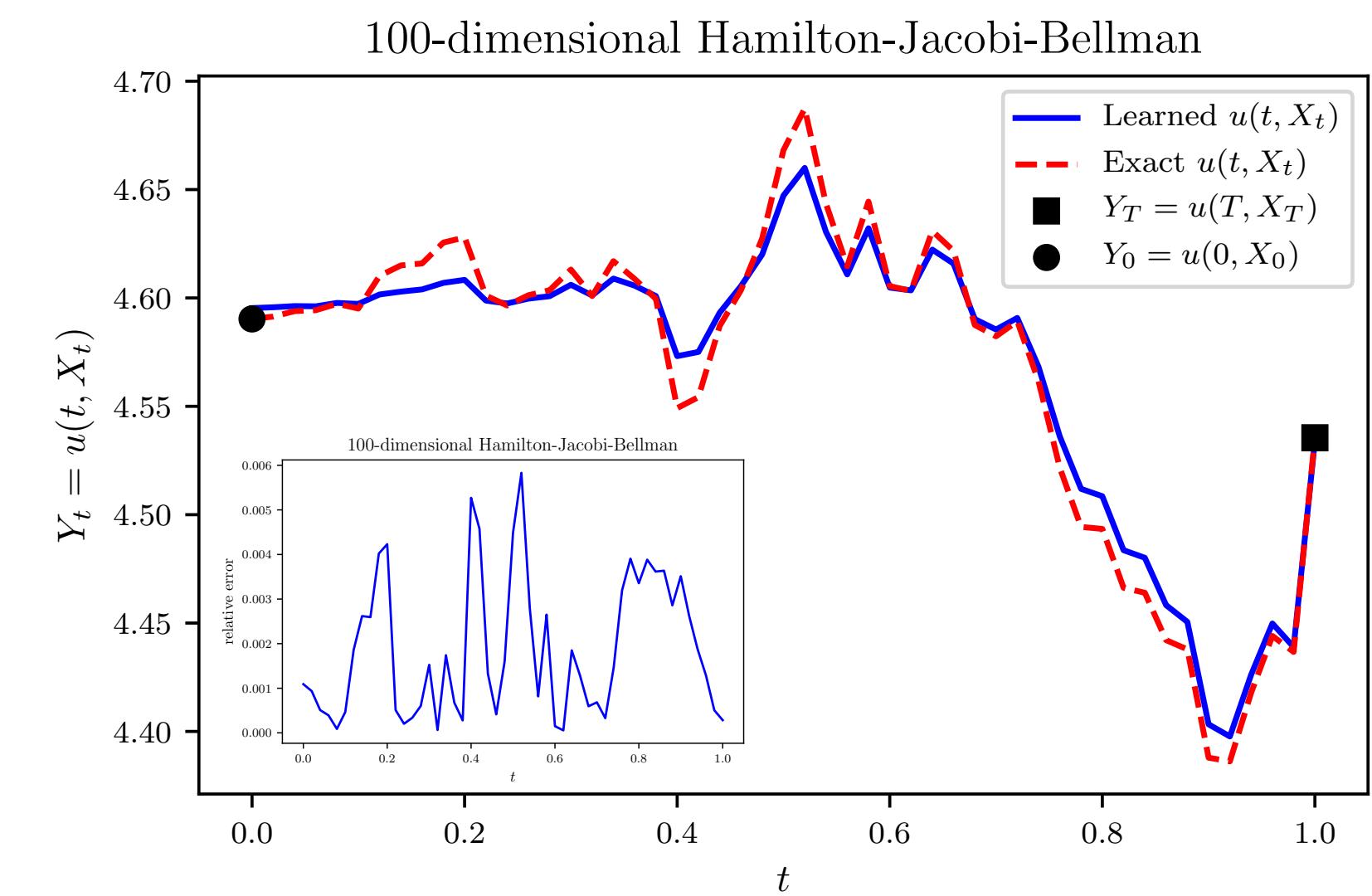
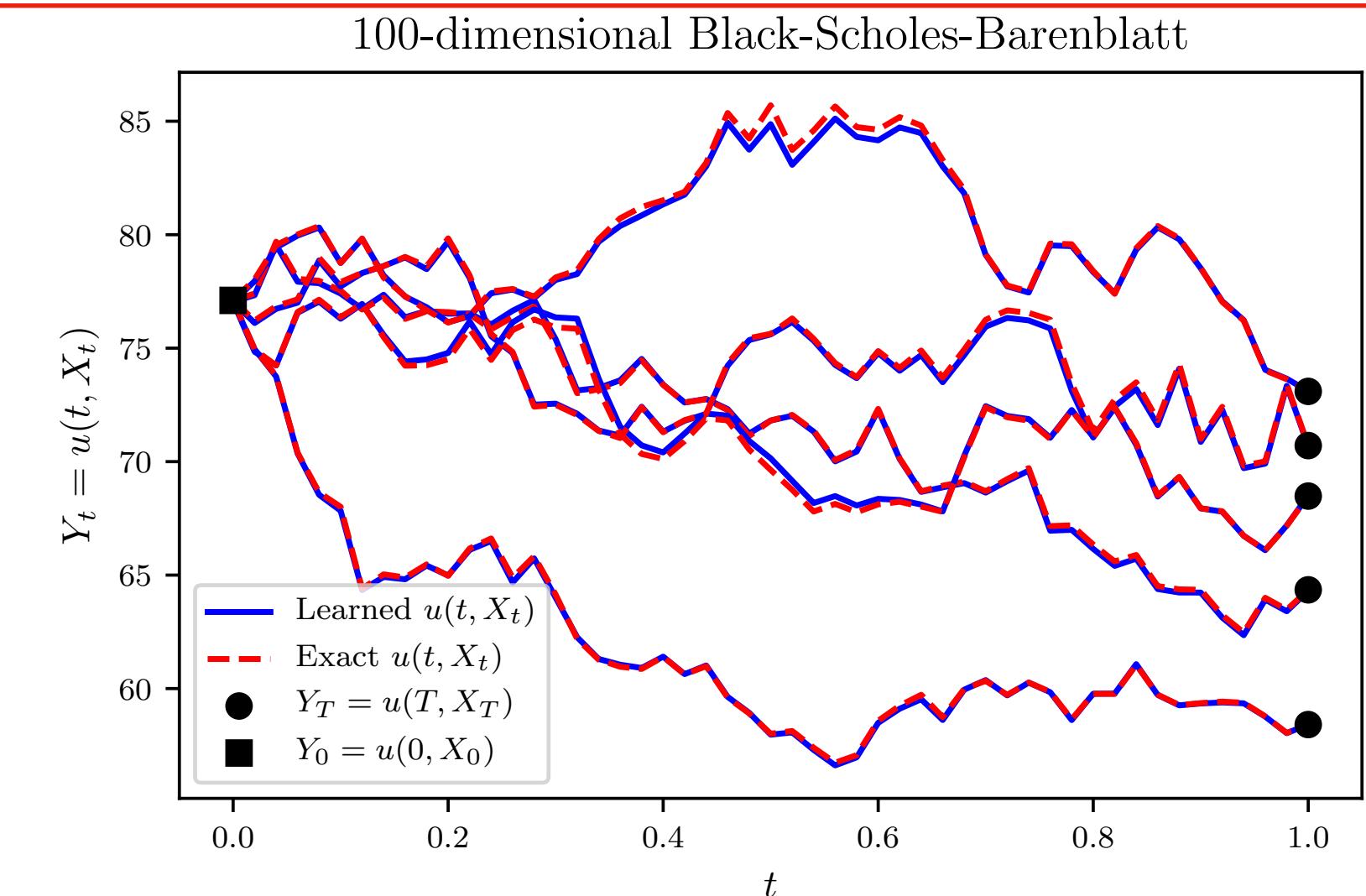


Forward-Backward Stochastic Differential Equation

$u(t, x) \rightarrow$ Deep Neural Network
 $Du(t, x) \rightarrow$ Automatic Differentiation

$$\begin{aligned} \frac{\partial u}{\partial t} &= \varphi(t, x, u, Du) - \mu(t, x, u, Du)'Du - \frac{1}{2}\text{Tr}[\sigma(t, x, u)\sigma(t, x, u)'D^2u] \\ u(T, x) &= g(x) \end{aligned}$$

 Quasi-Linear Partial Differential Equation

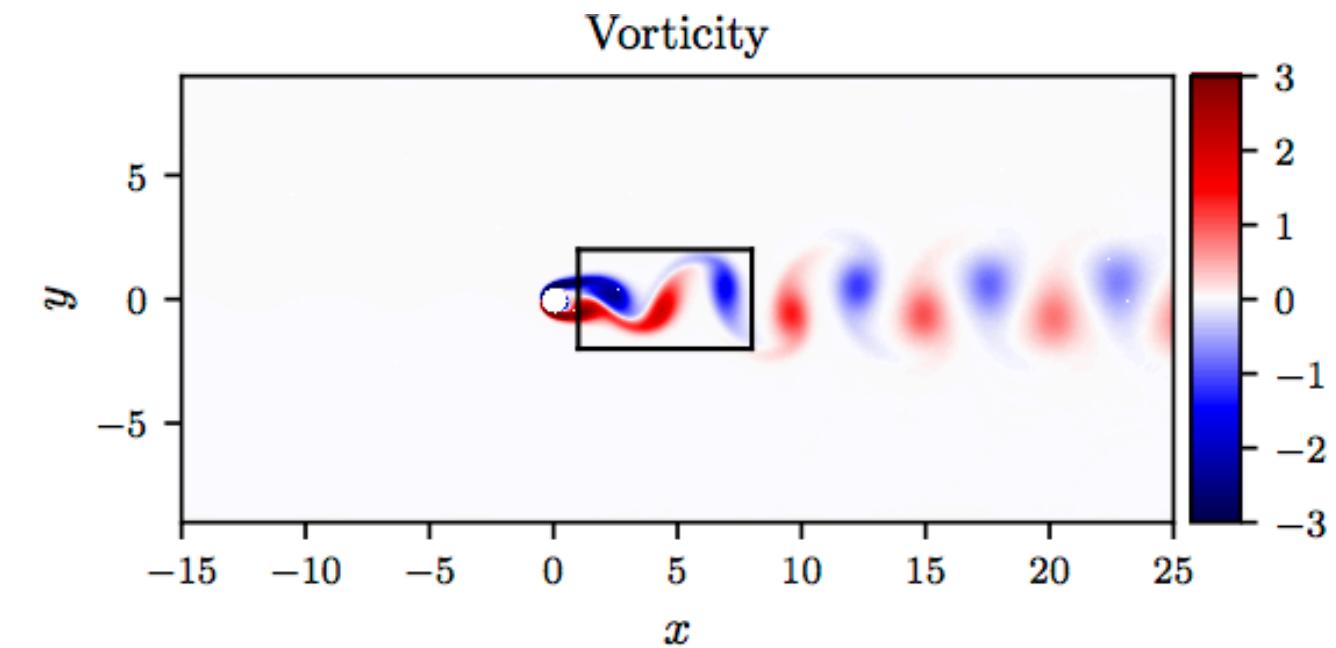




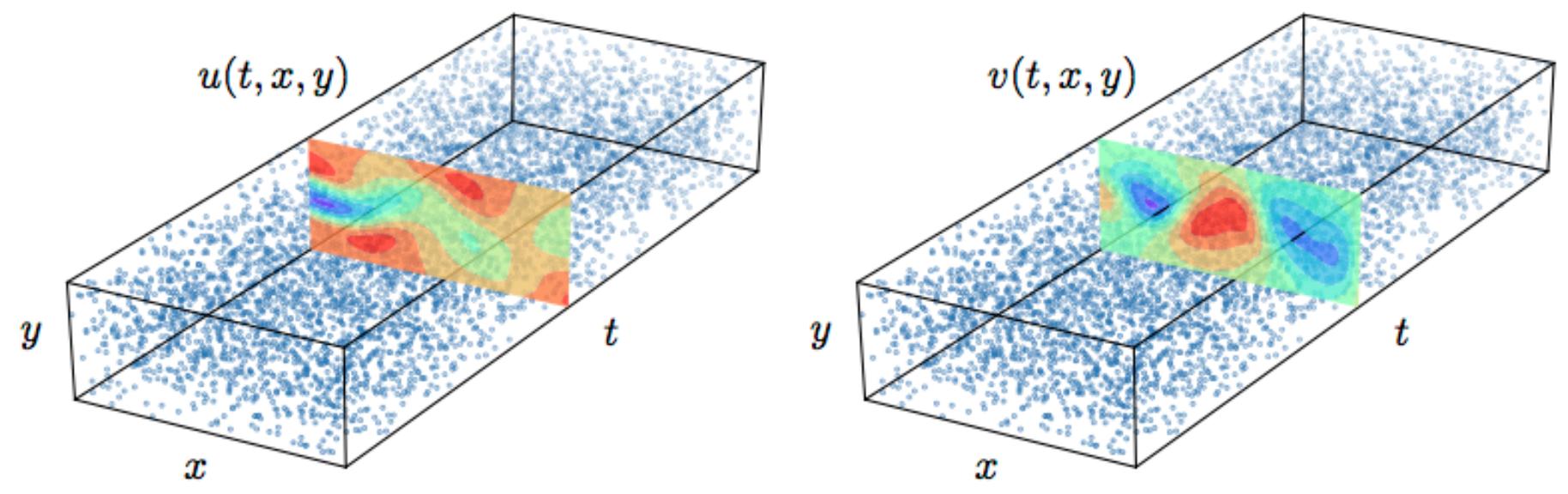
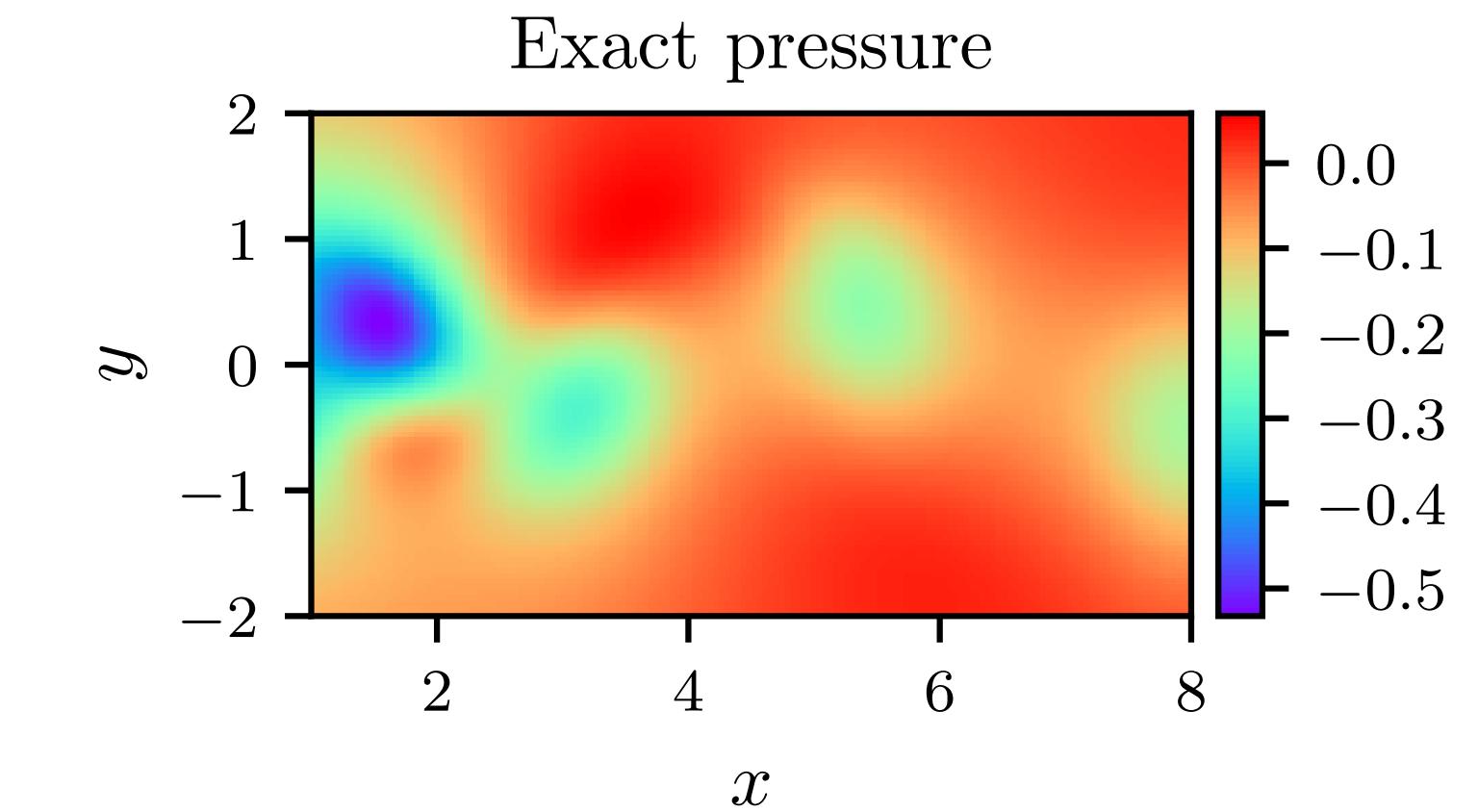
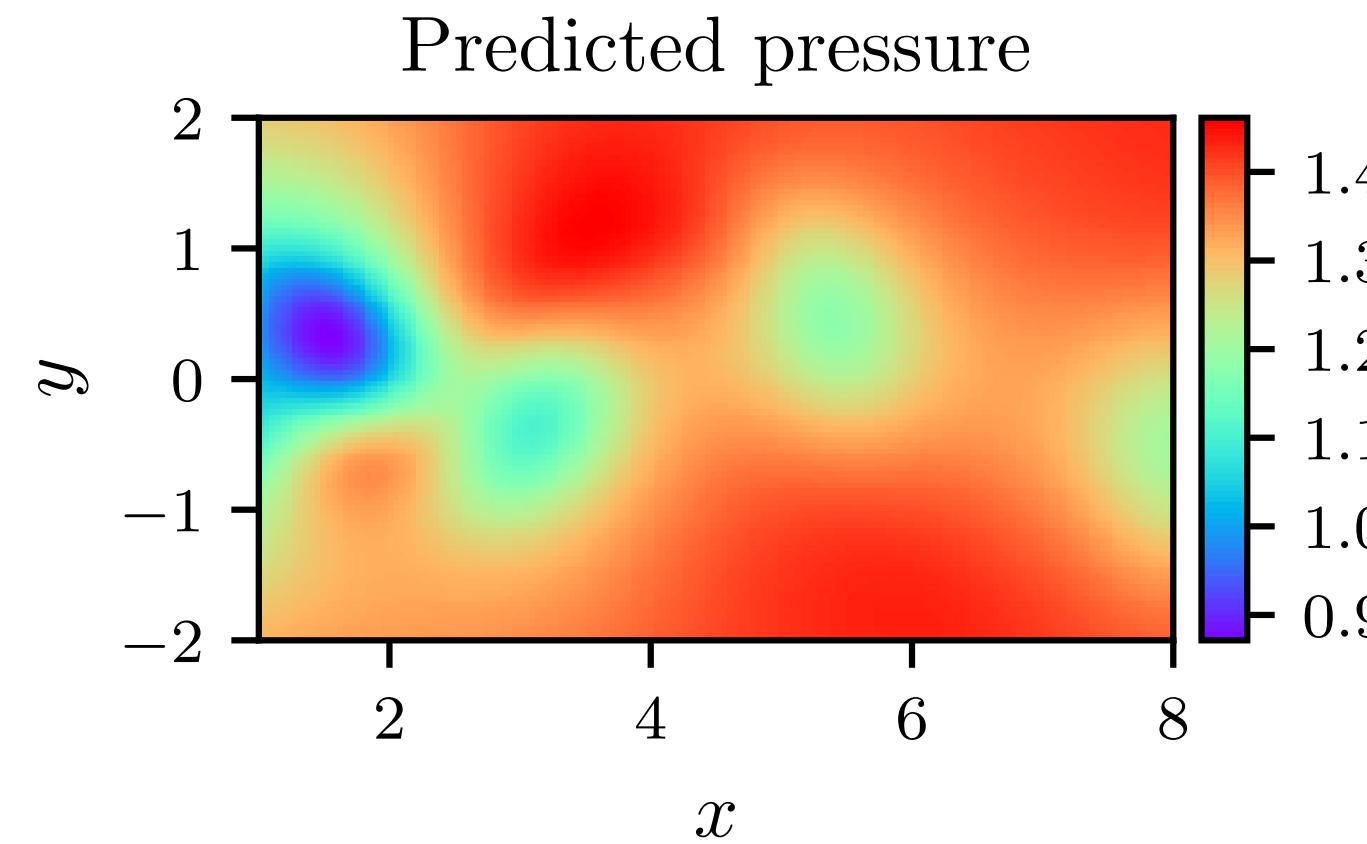
Physics Informed Neural Networks (PINNs)



$$\begin{aligned} u_t + \lambda_1(uu_x + vu_y) &= -p_x + \lambda_2(u_{xx} + u_{yy}) \\ v_t + \lambda_1(uv_x + vv_y) &= -p_y + \lambda_2(v_{xx} + v_{yy}) \\ u_x + v_y &= 0 \end{aligned}$$



$$\begin{aligned} f &:= u_t + \lambda_1(uu_x + vu_y) + p_x - \lambda_2(u_{xx} + u_{yy}) \\ g &:= v_t + \lambda_1(uv_x + vv_y) + p_y - \lambda_2(v_{xx} + v_{yy}) \\ h &:= u_x + v_y \end{aligned}$$



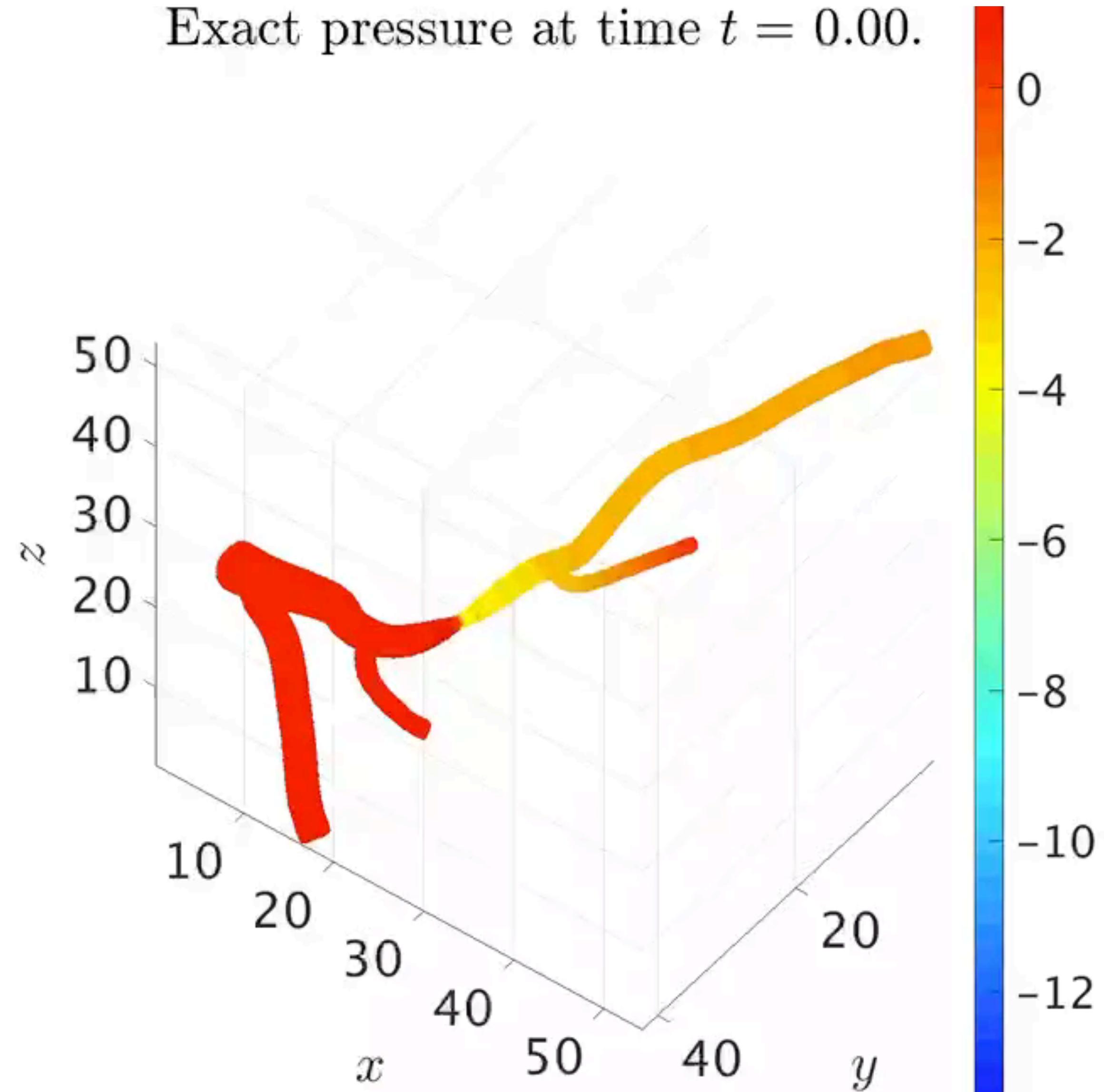
Correct PDE	$u_t + (uu_x + vu_y) = -p_x + 0.01(u_{xx} + u_{yy})$ $v_t + (uv_x + vv_y) = -p_y + 0.01(v_{xx} + v_{yy})$
Identified PDE (clean data)	$u_t + 0.999(uu_x + vu_y) = -p_x + 0.01047(u_{xx} + u_{yy})$ $v_t + 0.999(uv_x + vv_y) = -p_y + 0.01047(v_{xx} + v_{yy})$
Identified PDE (1% noise)	$u_t + 0.998(uu_x + vu_y) = -p_x + 0.01057(u_{xx} + u_{yy})$ $v_t + 0.998(uv_x + vv_y) = -p_y + 0.01057(v_{xx} + v_{yy})$



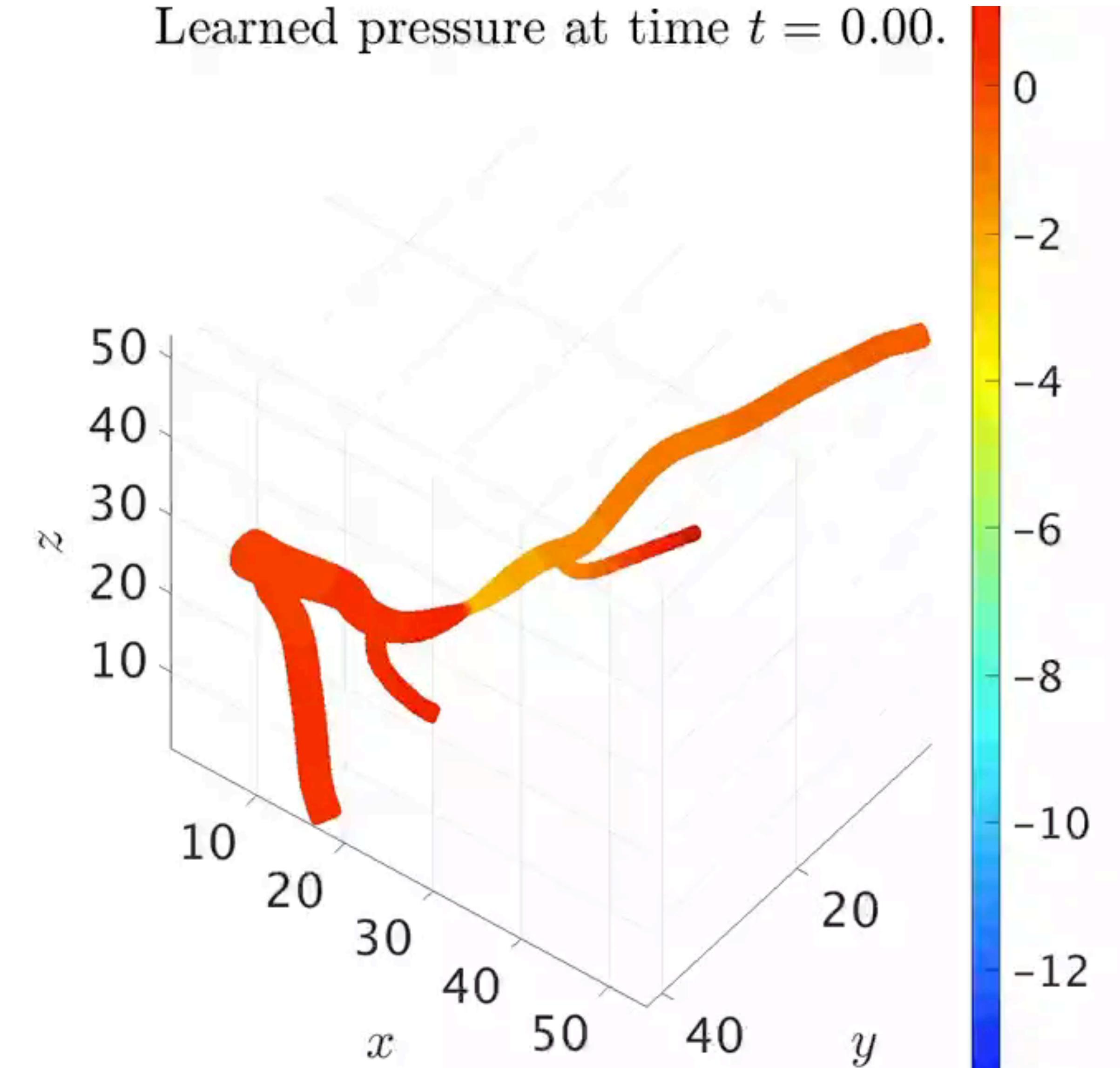
Physics Informed Neural Networks (PINNs)



Exact pressure at time $t = 0.00$.

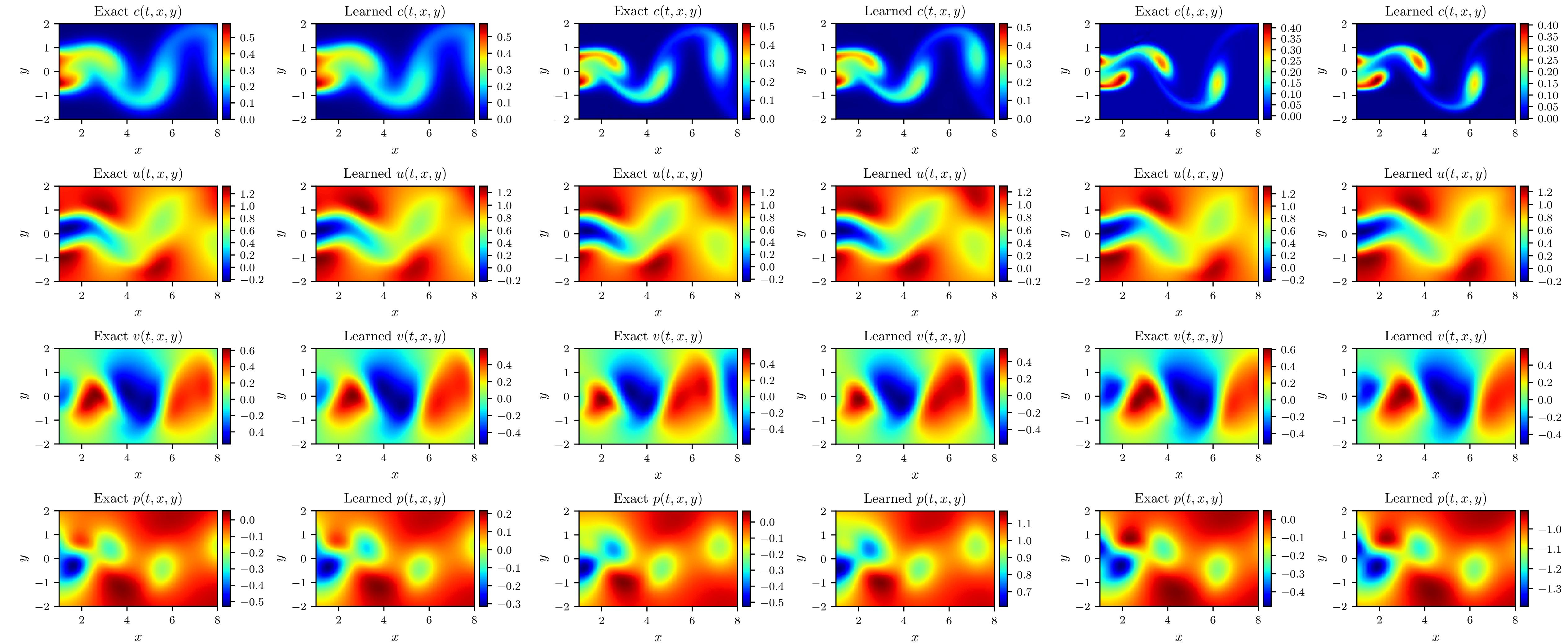


Learned pressure at time $t = 0.00$.





Hidden Fluid Mechanics



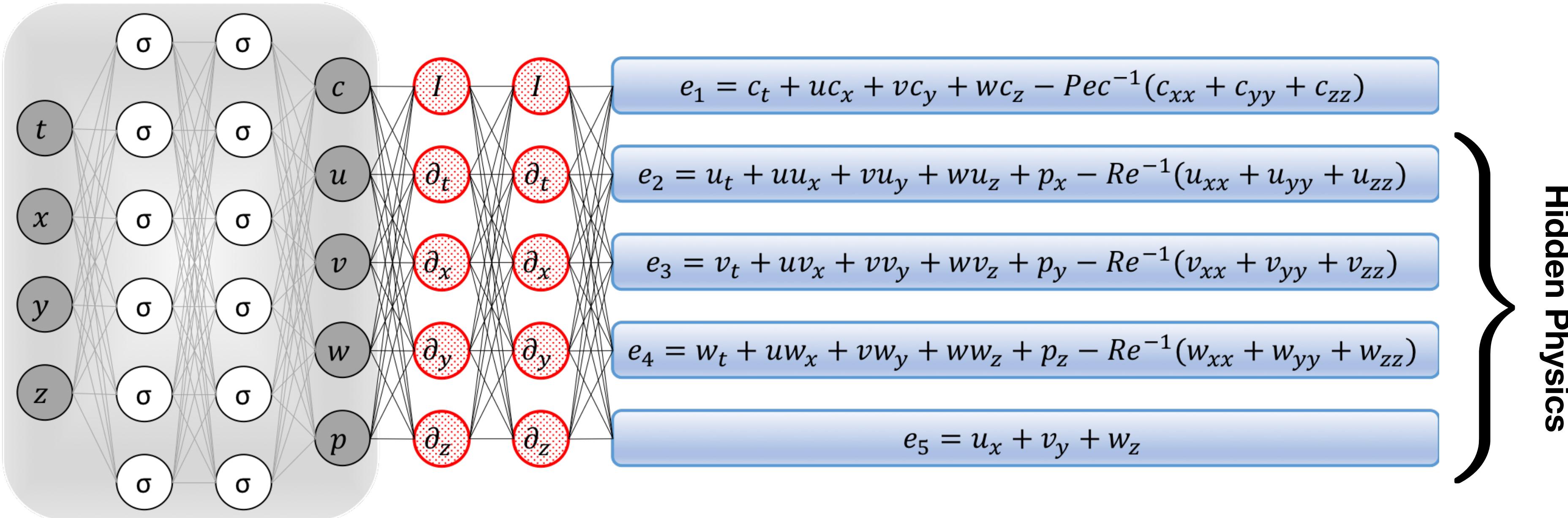
Pec = 40

Pec = 100

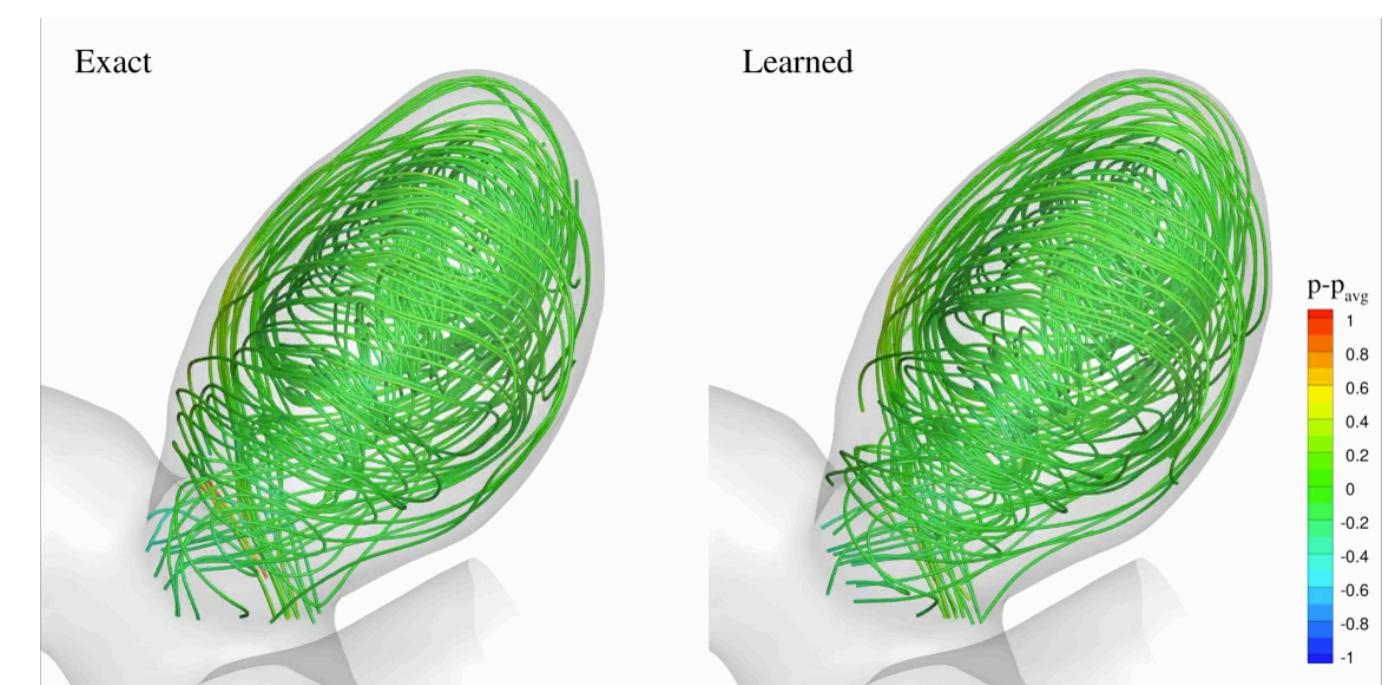
Pec = 250



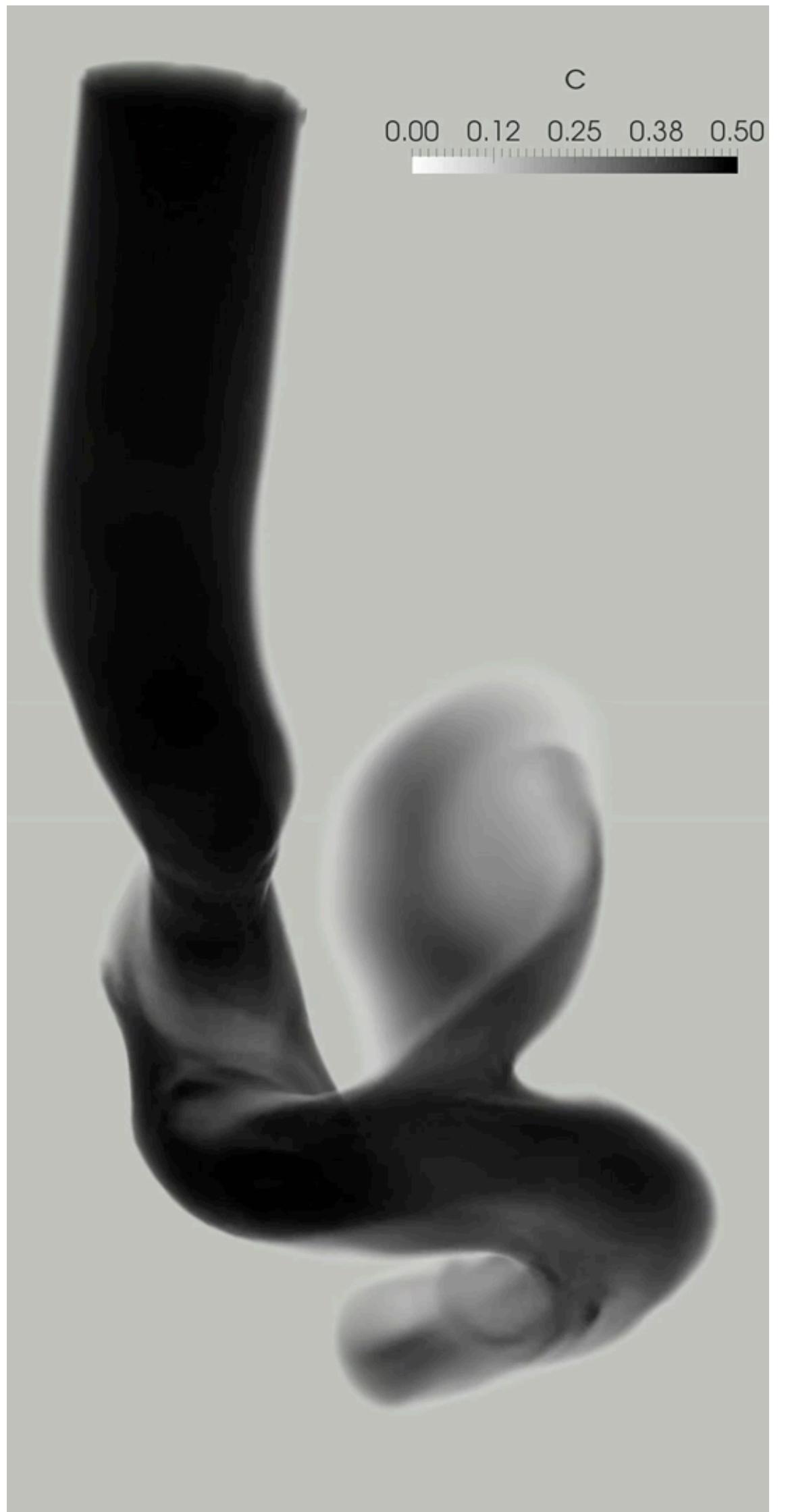
Hidden Fluid Mechanics



$$SSE = \sum_{n=1}^N |c(t^n, x^n, y^n, z^n) - c^n|^2 + \sum_{i=1}^5 \sum_{n=1}^N |e_i(t^n, x^n, y^n, z^n)|^2$$

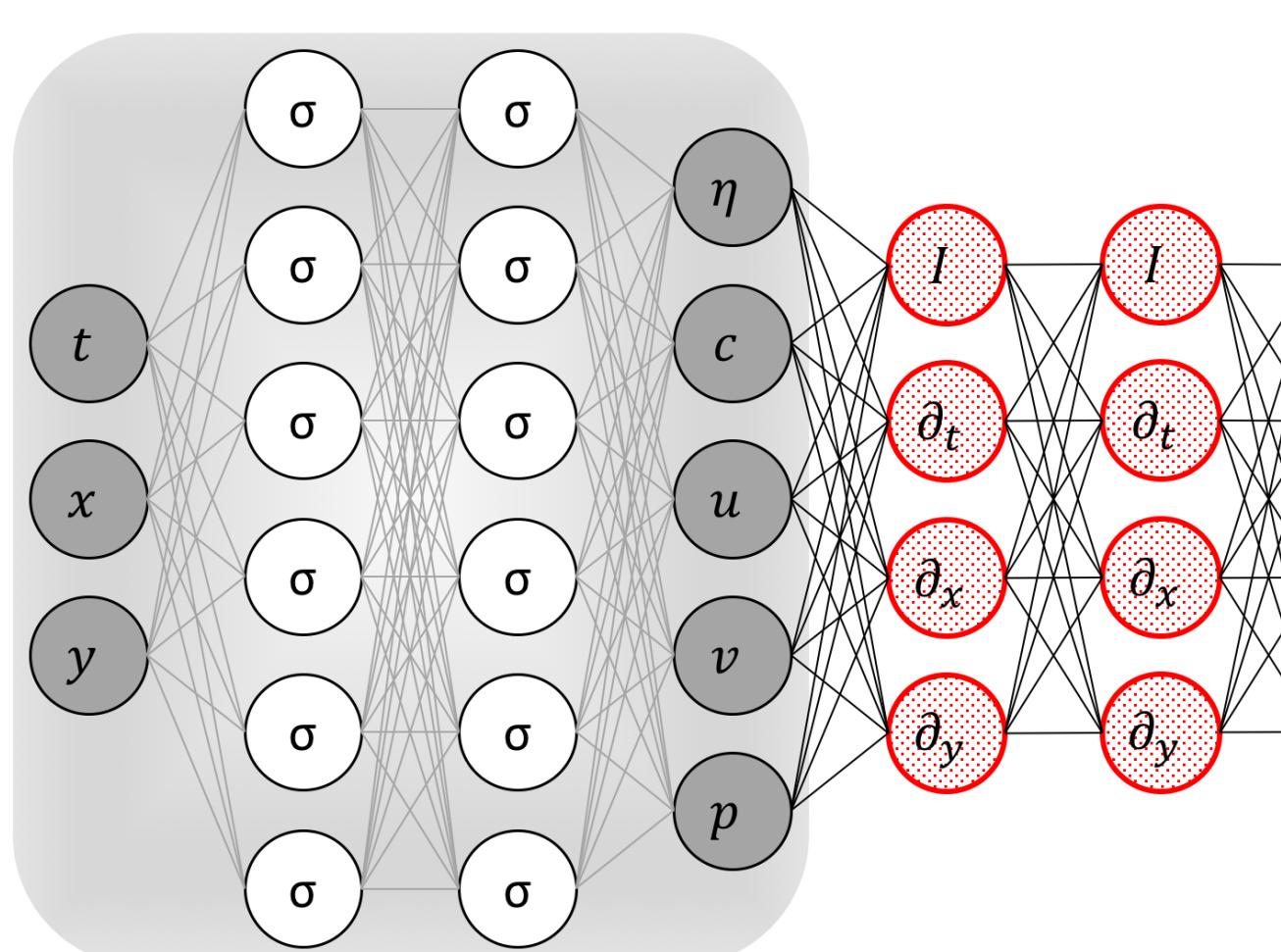


Raissi, Maziar, Alireza Yazdani, and George Em Karniadakis.
"Hidden Fluid Mechanics: A Navier-Stokes Informed Deep Learning Framework for Assimilating Flow Visualization Data."
arXiv preprint arXiv:1808.04327 (2018).



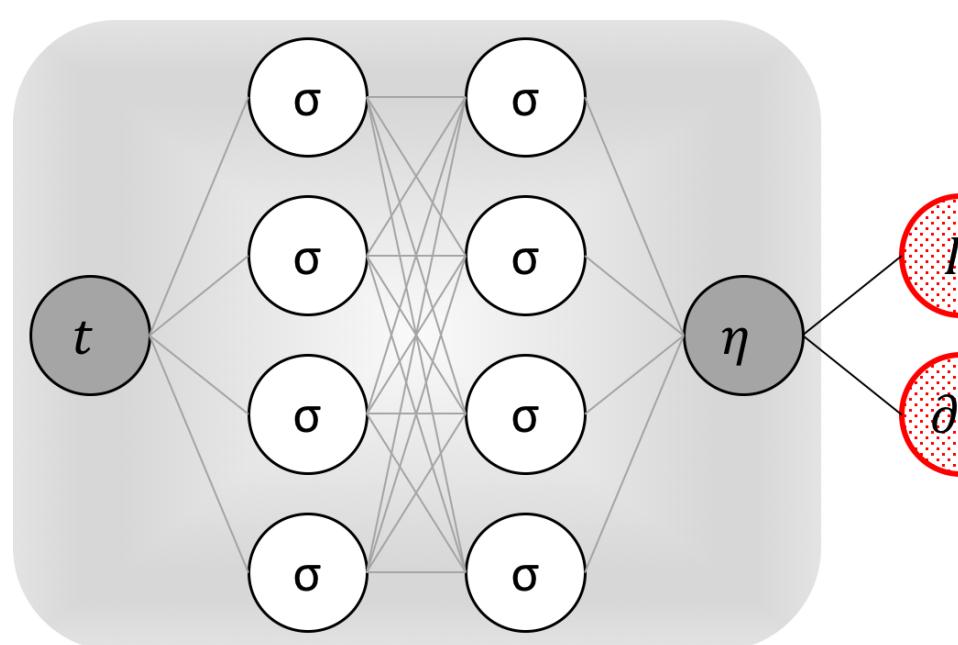


Deep Learning of Vortex Induced Vibrations



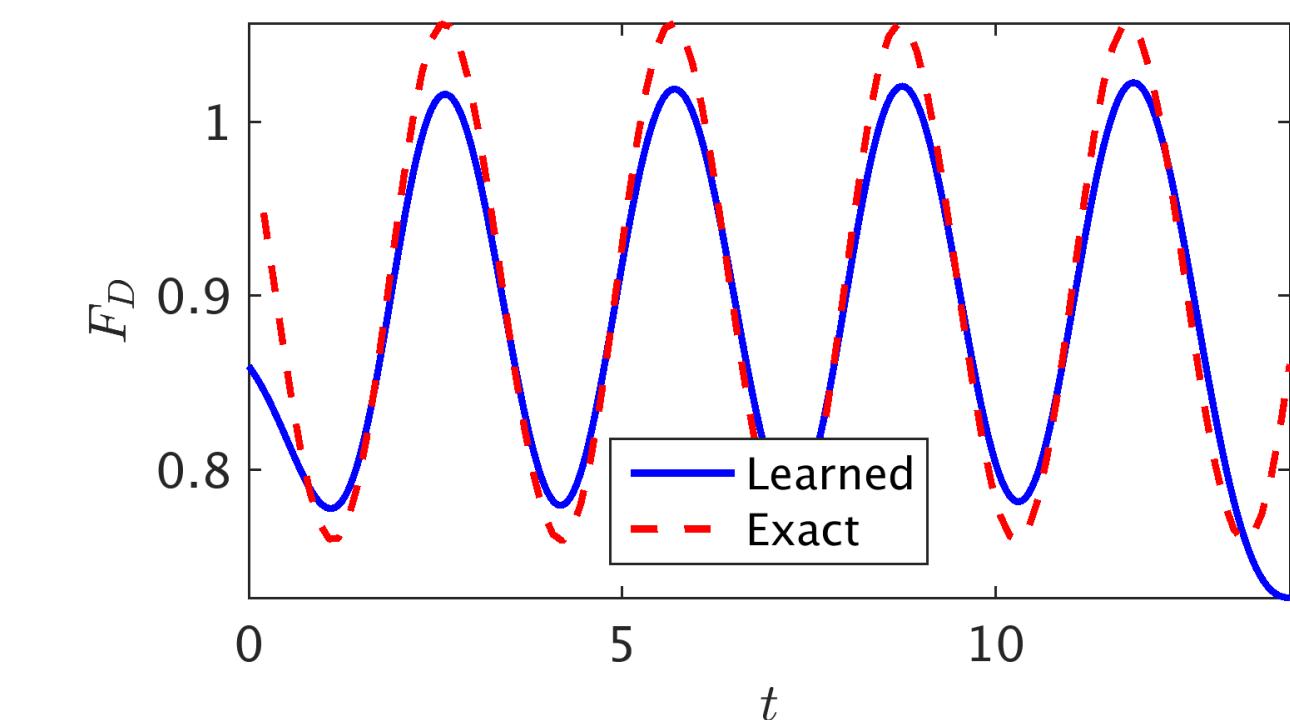
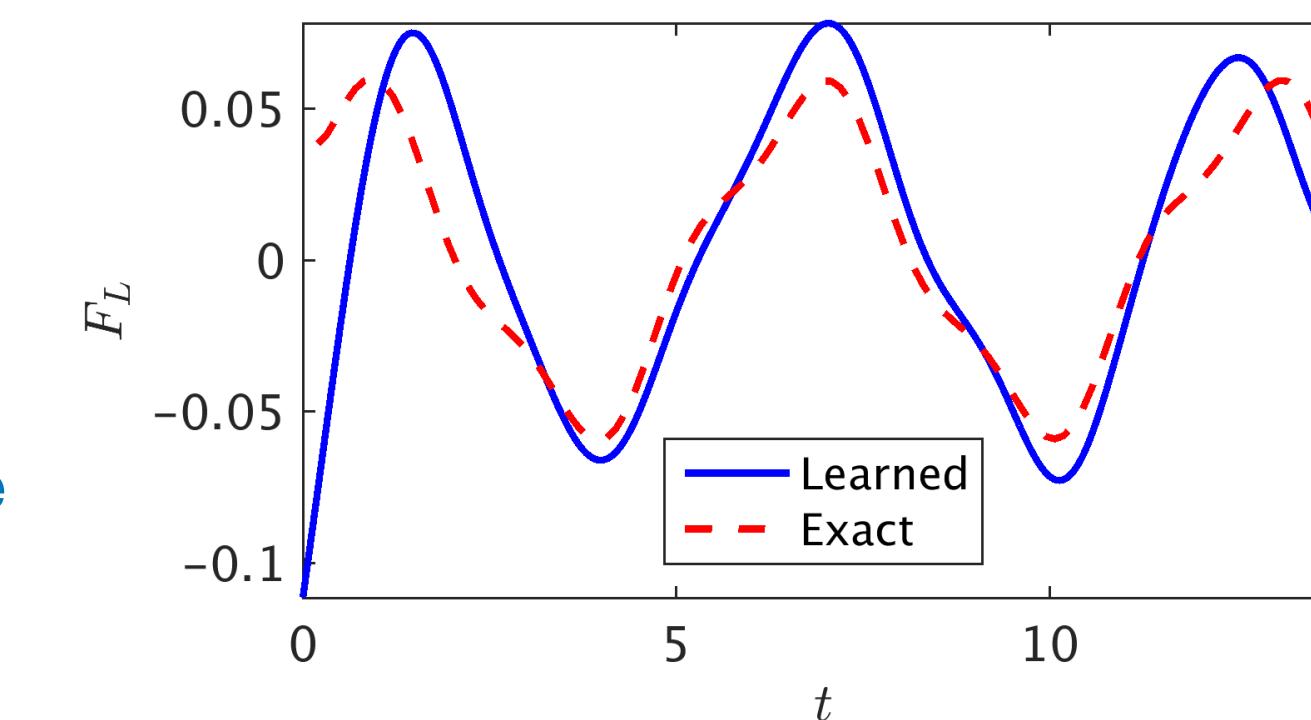
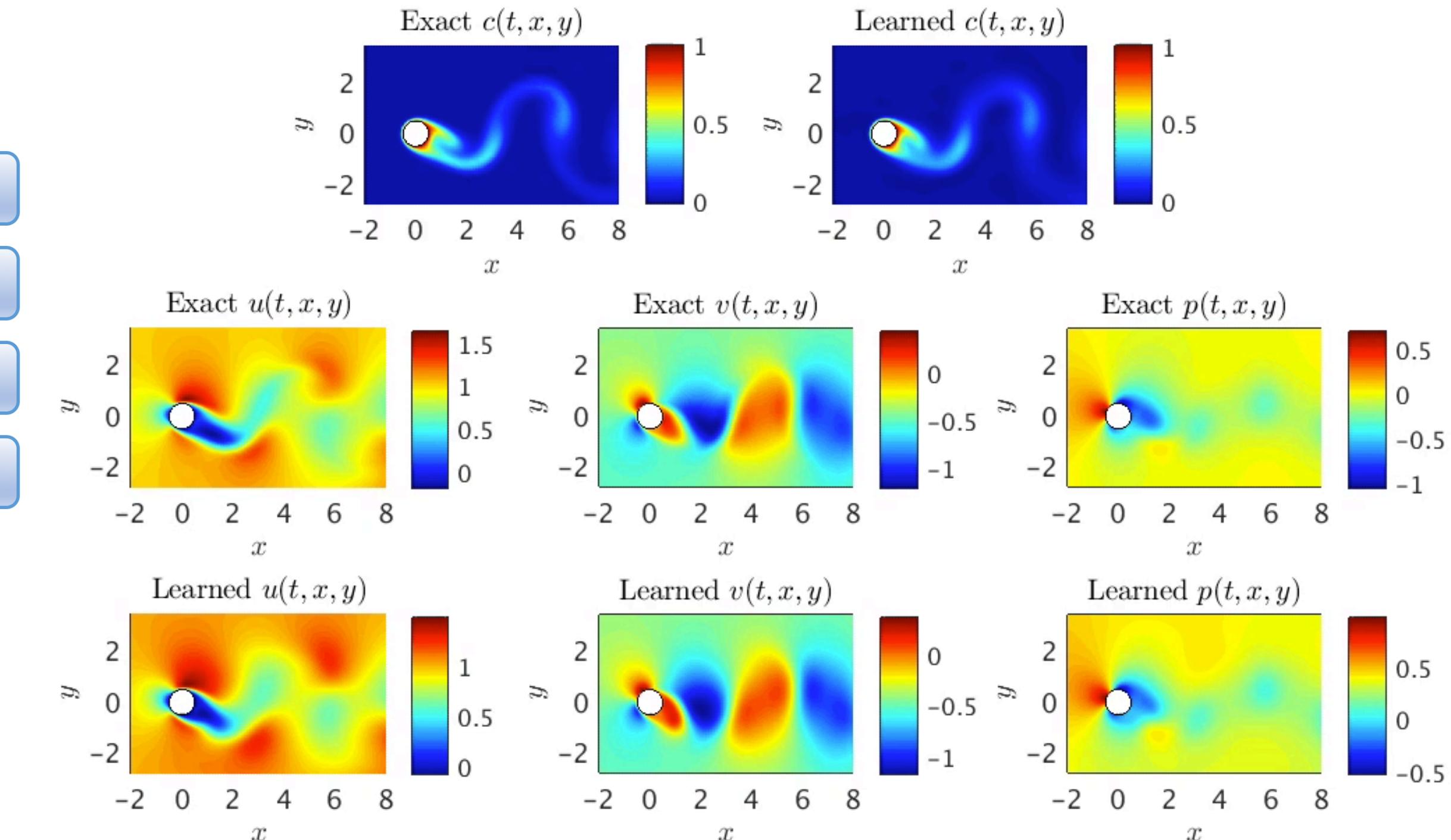
$$\begin{aligned} e_1 &= u_t + uu_x + vu_y + p_x - Re^{-1}(u_{xx} + u_{yy}) \\ e_2 &= v_t + uv_x + vv_y + p_y - Re^{-1}(v_{xx} + v_{yy}) + \eta_{tt} \\ e_3 &= u_x + v_y \\ e_4 &= c_t + uc_x + vc_y - Pe^{-1}(c_{xx} + c_{yy}) \end{aligned}$$

	Damping	Stiffness
Exact	$b = 0.084$	$k = 2.2020$
Learned	$b = 0.08600664$	$k = 2.2395933$
Error	2.39%	1.71%



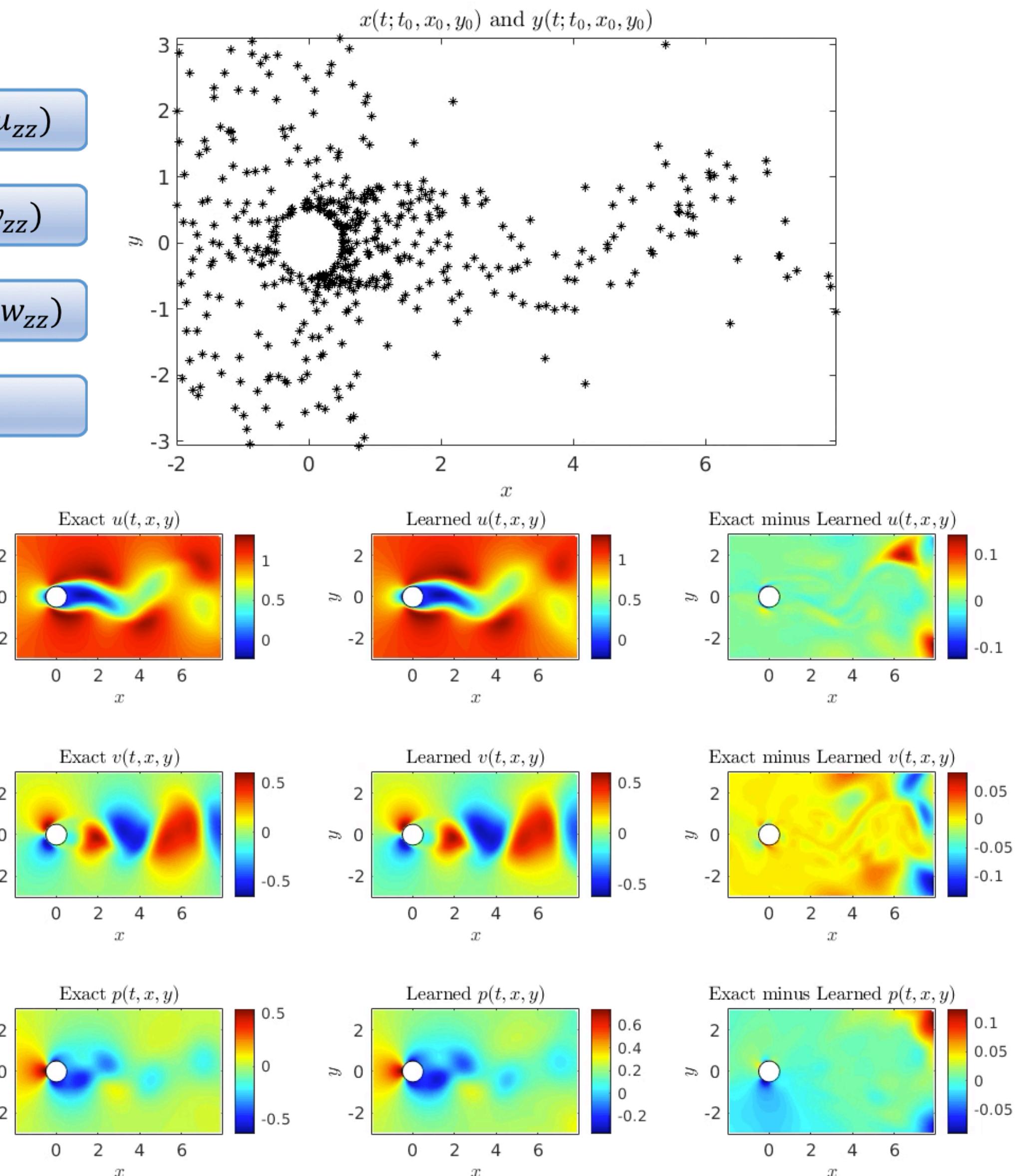
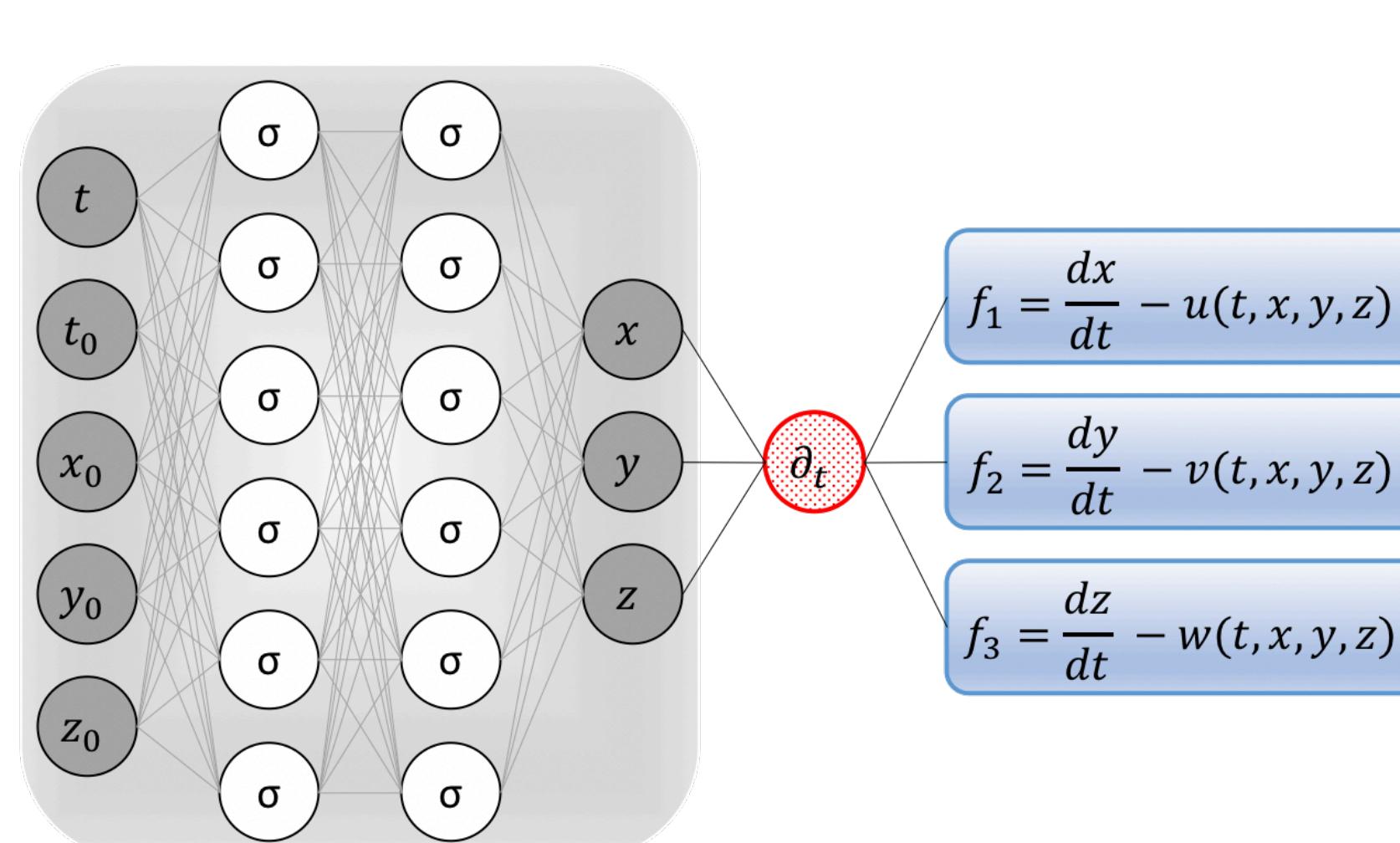
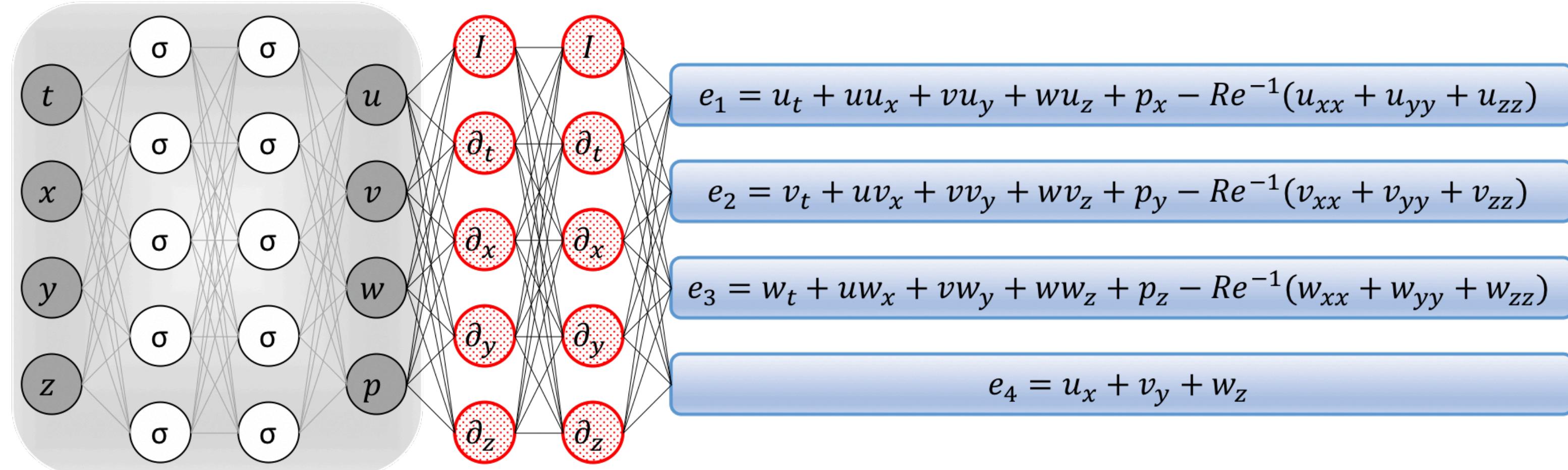
$$f_L = \rho\eta_{tt} + b\eta_t + k\eta$$

Raissi, Maziar, Zhicheng Wang, Michael S. Triantafyllou, and George Em Karniadakis. "Deep Learning of Vortex Induced Vibrations." *Journal of Fluid Mechanics* (2018).



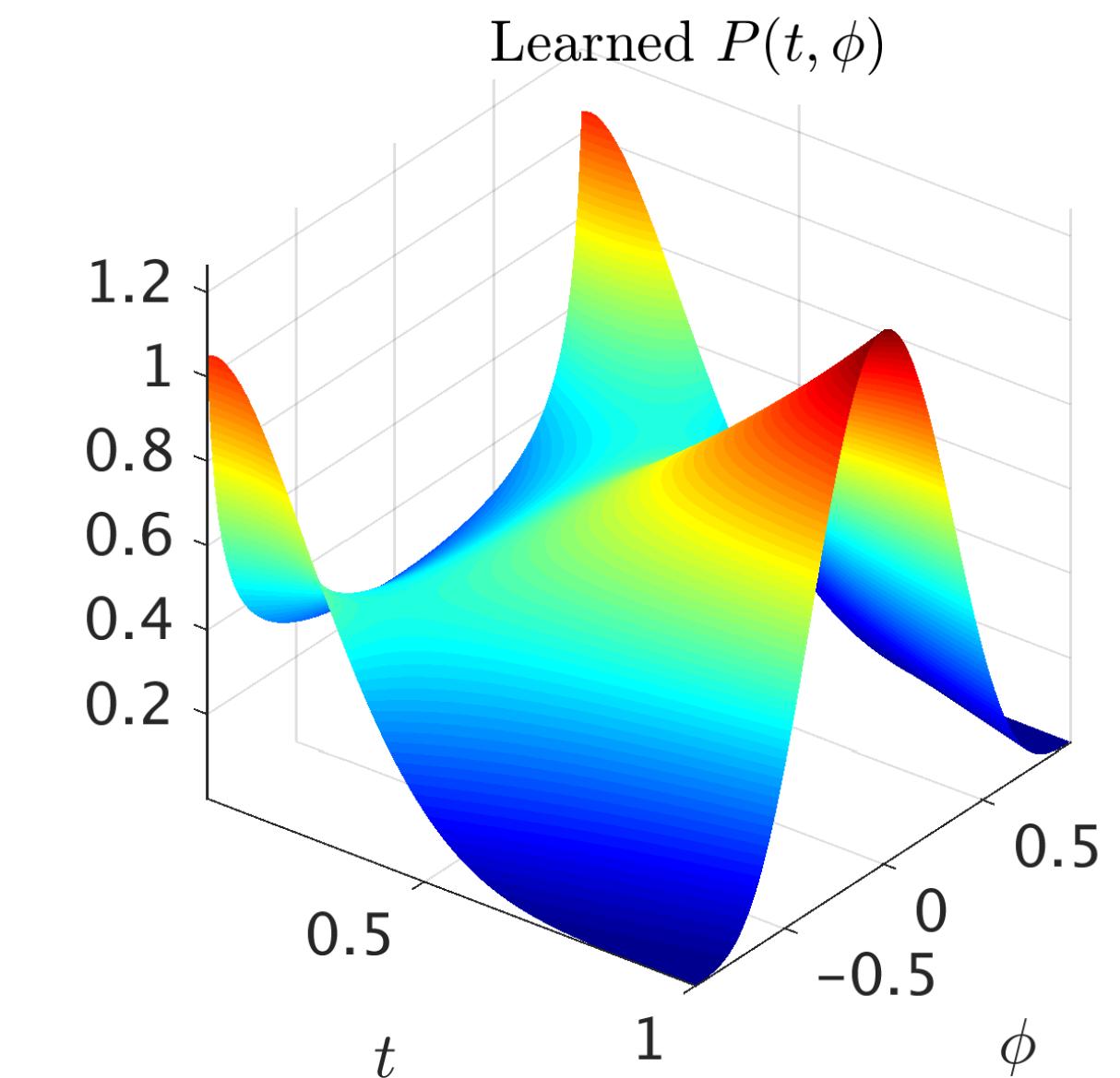
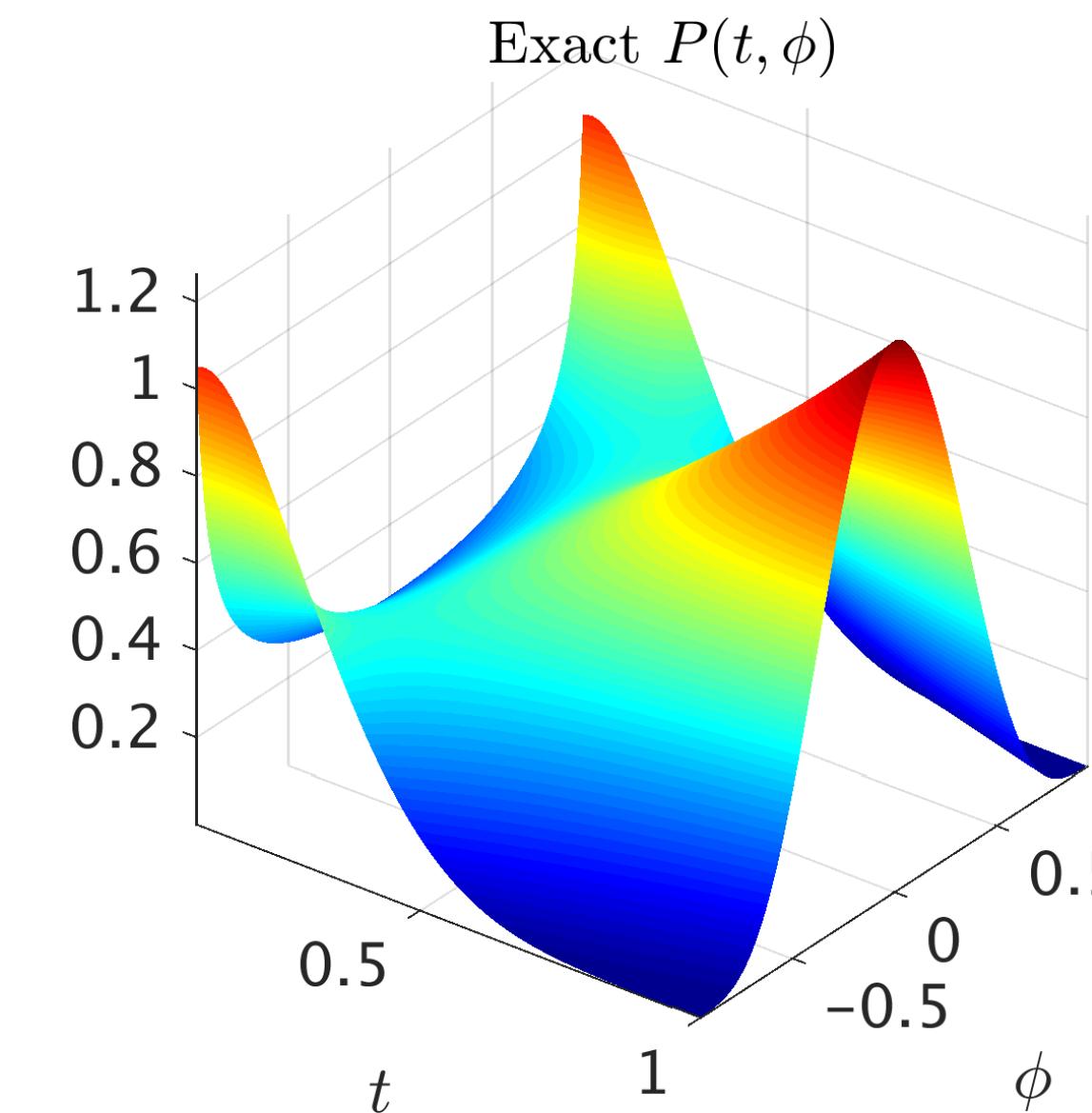
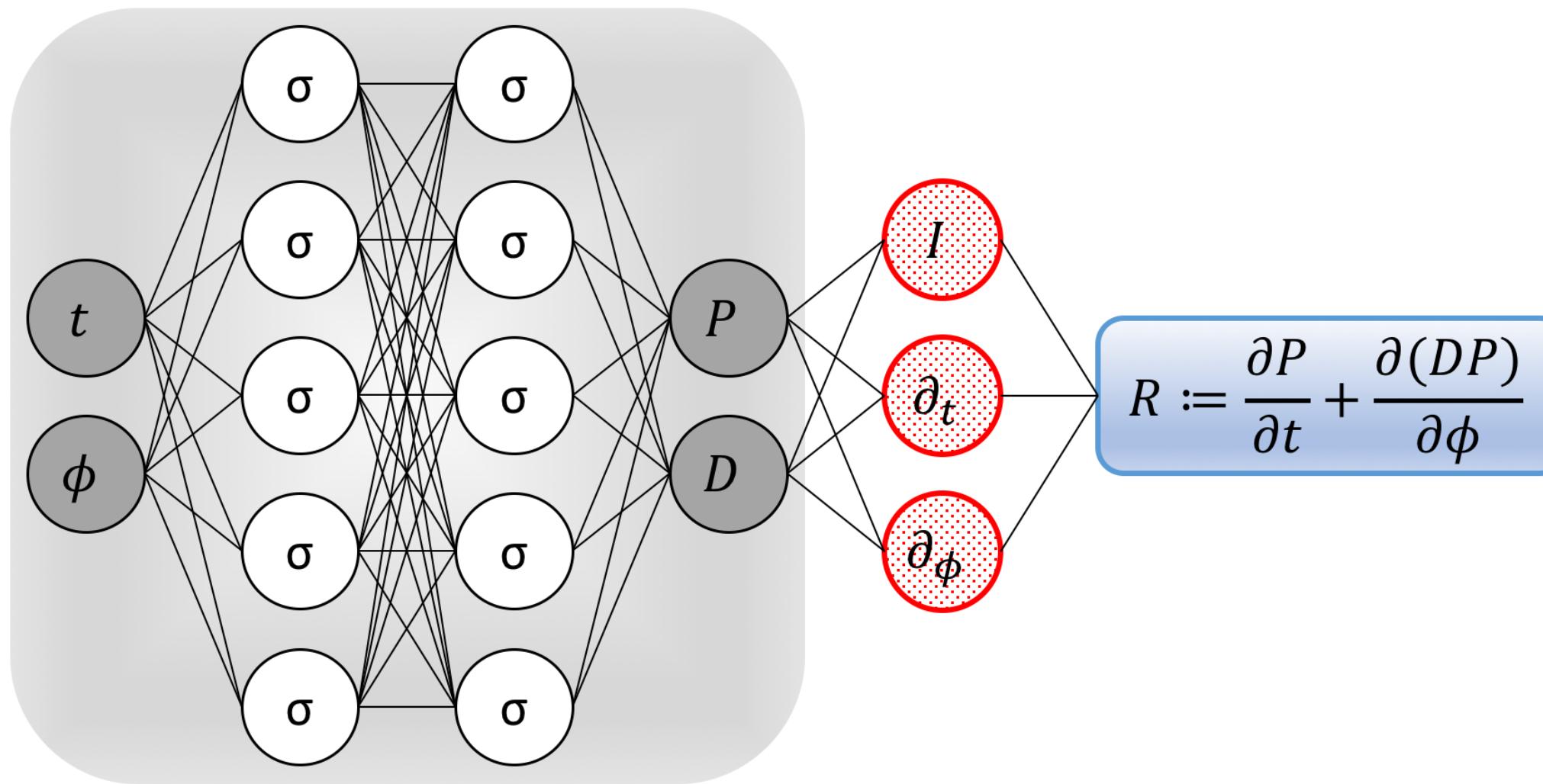


Eulerian-Lagrangian Neural Networks

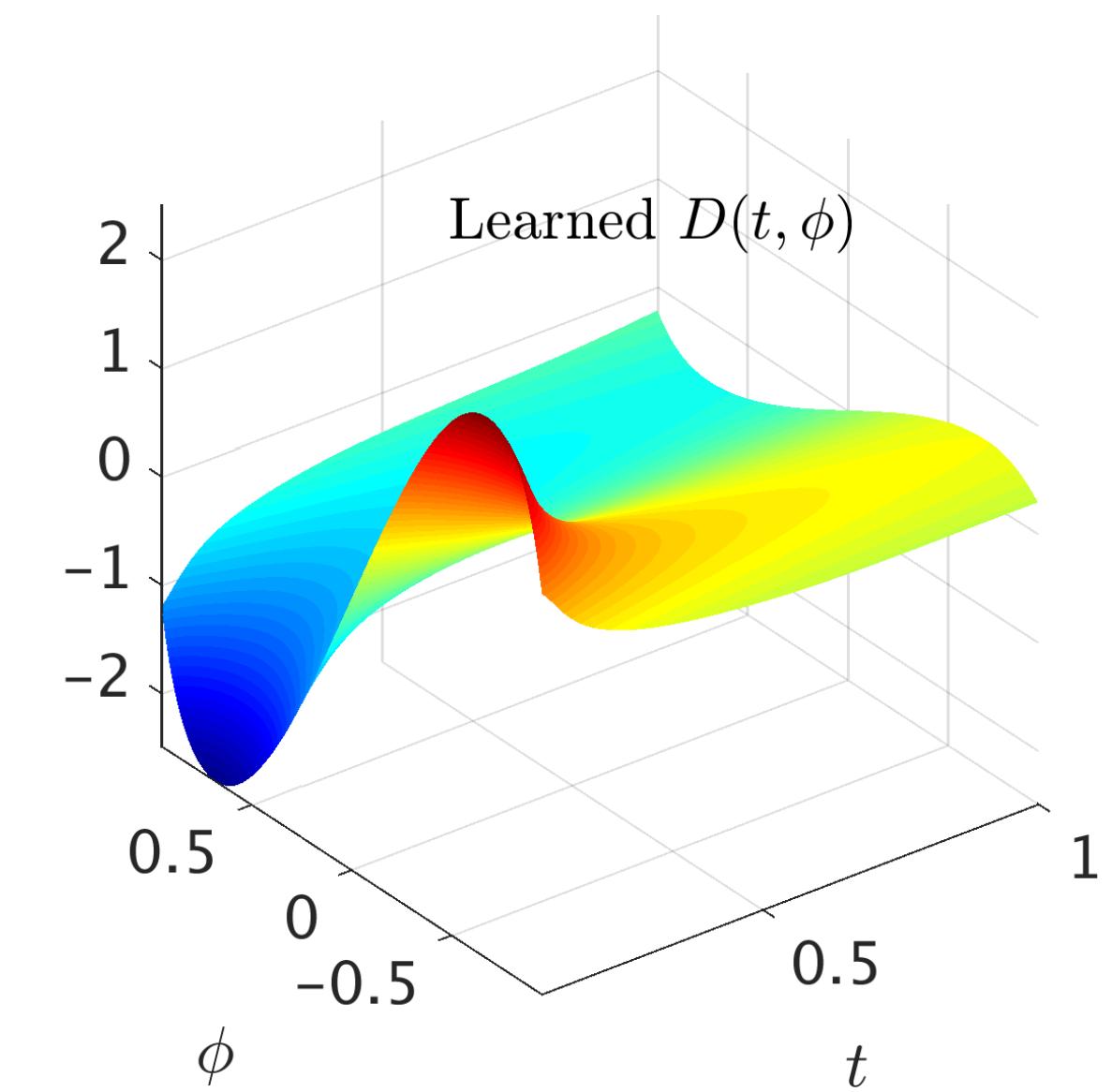
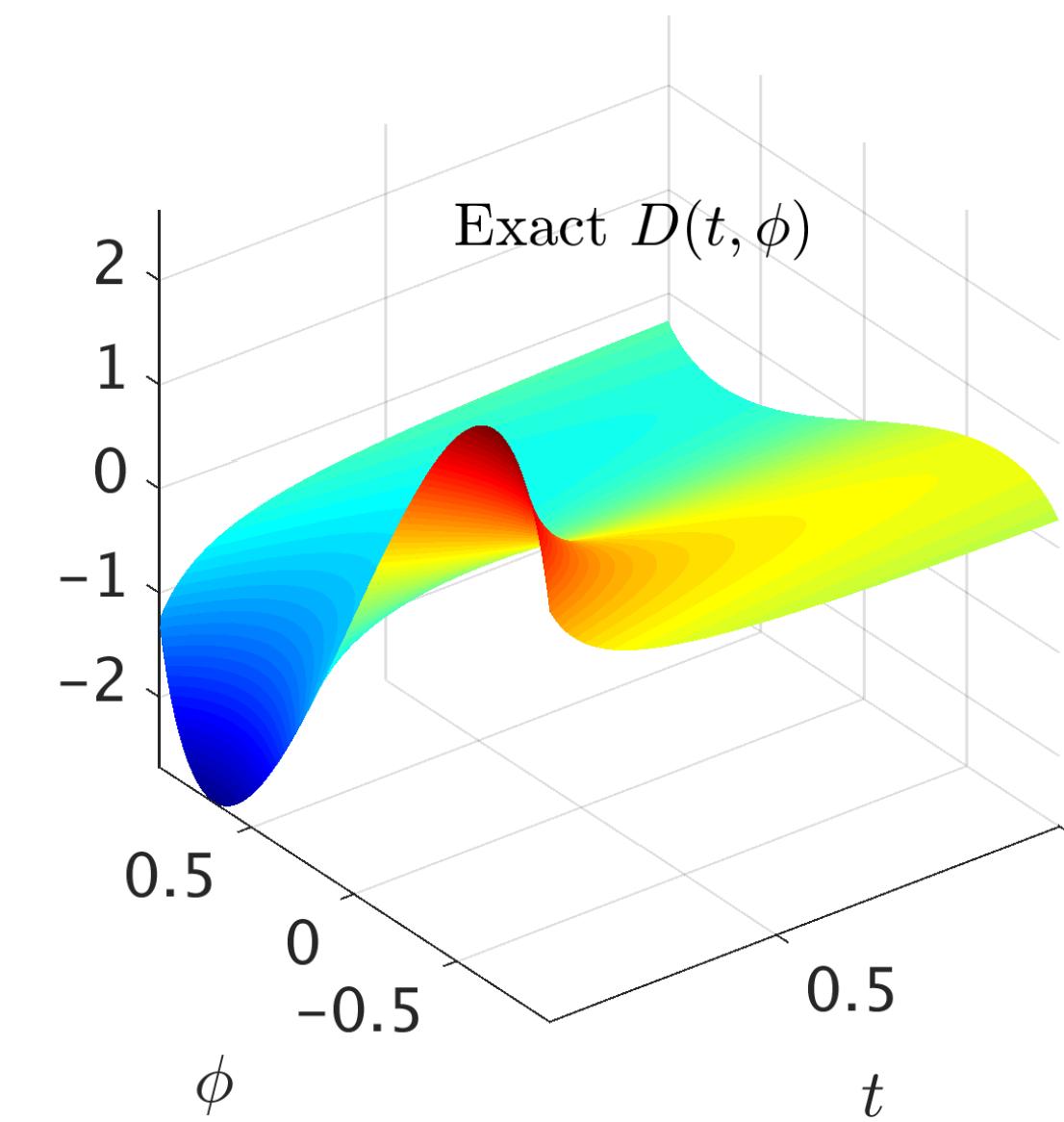




Deep Learning of Turbulent Scalar Mixing



$$SSE = \sum_{n=1}^N |P(t^n, \phi^n) - P^n|^2 + \sum_{n=1}^N |R(t^n, \phi^n)|^2$$



Raissi, Maziar, Hessam Babaee, and Peyman Givi. "Deep Learning of Turbulent Scalar Mixing." *Physical Review Fluids* (to appear).



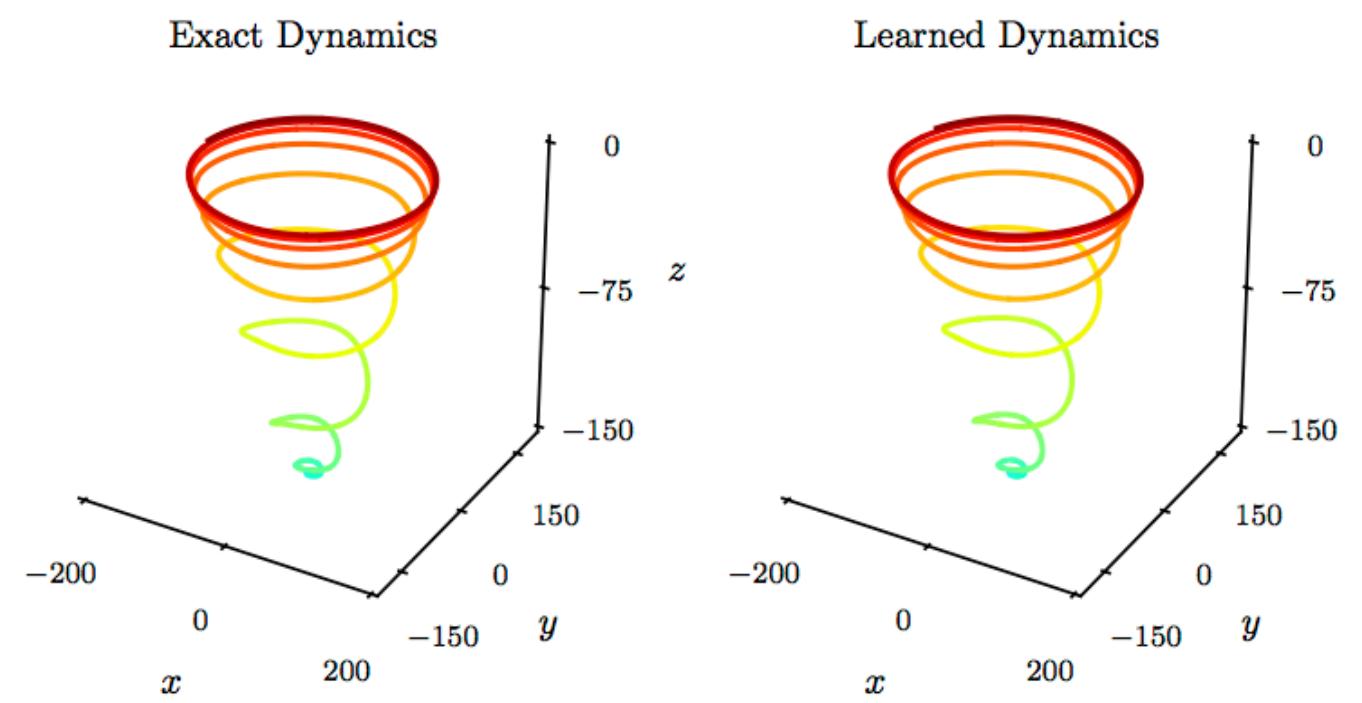
Multi-step Neural Networks



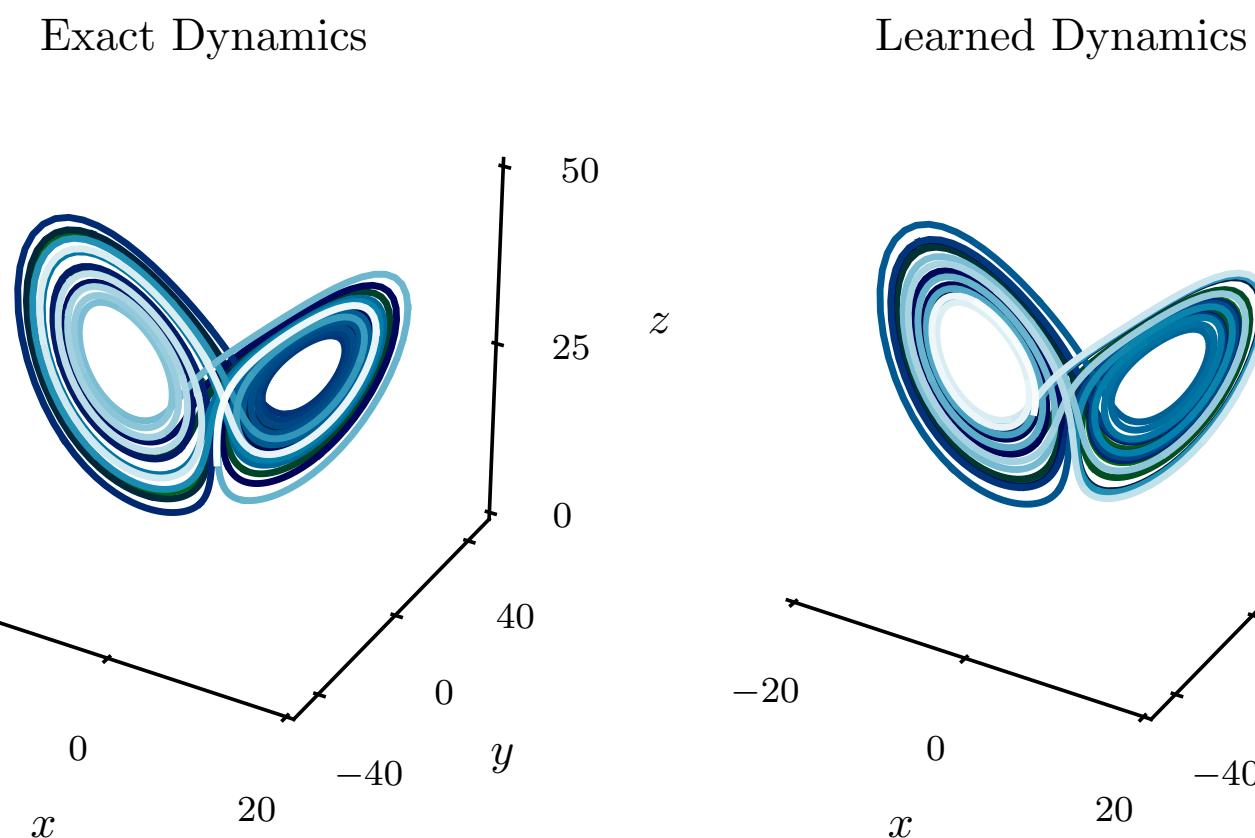
$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$$

$$\mathbf{x}^{n+1} = \mathbf{x}^n + \frac{\Delta t}{2} (\mathbf{f}(\mathbf{x}^n) + \mathbf{f}(\mathbf{x}^{n+1}))$$

Navier-Stokes Equations

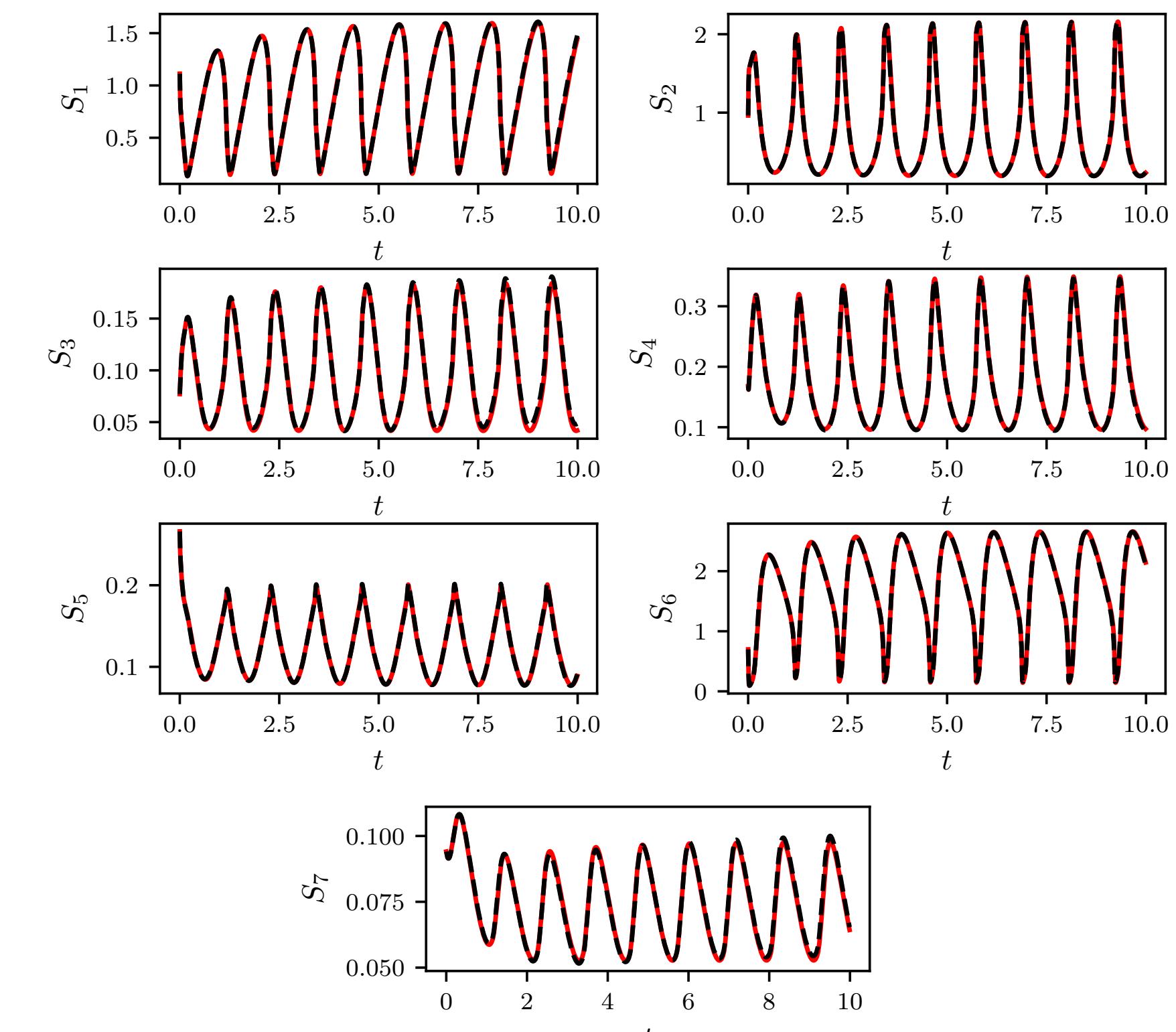


Lorenz System



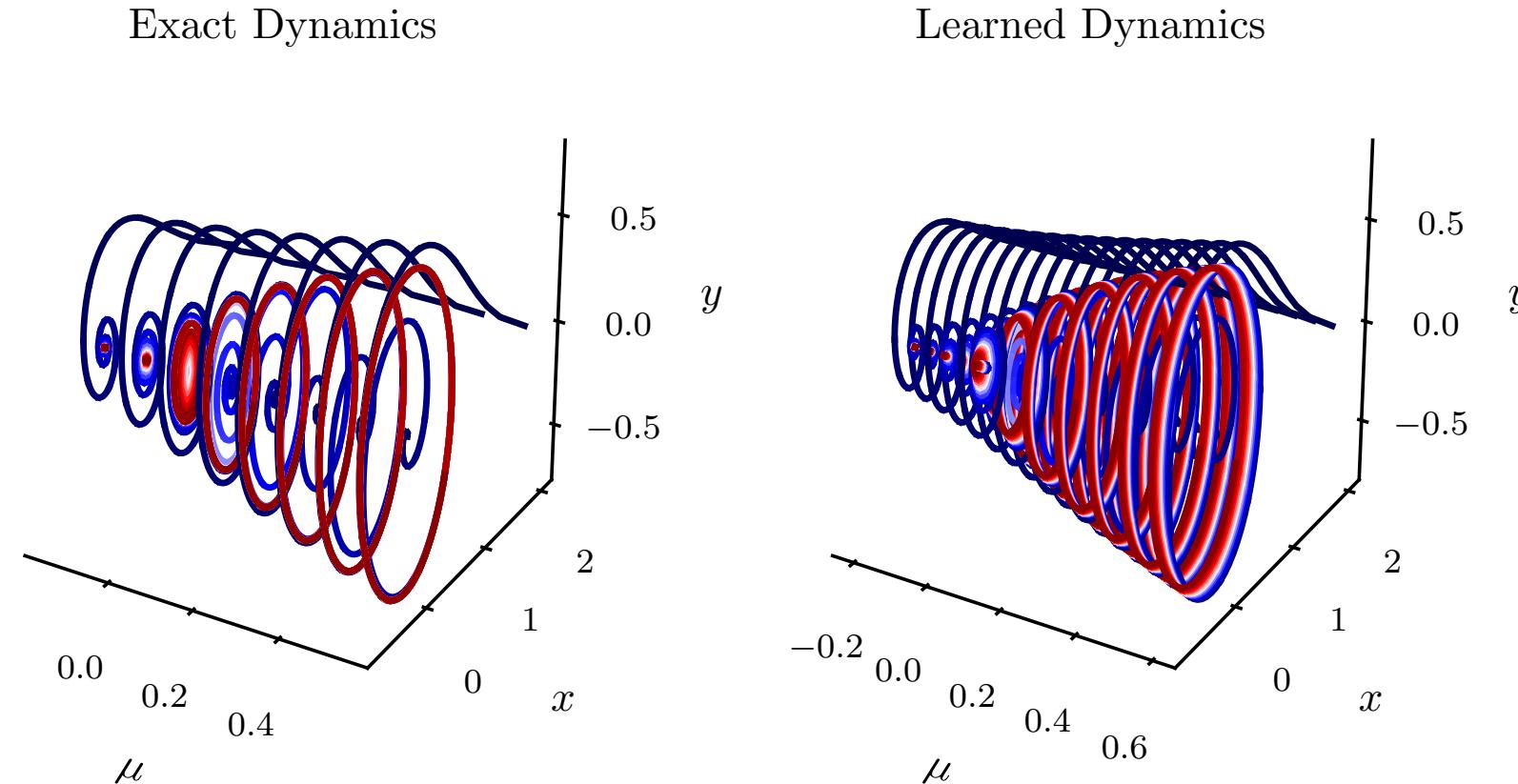
Learned Dynamics

Glycolytic Oscillator



— Exact Dynamics - - Learned Dynamics

Hopf Bifurcation





Deep Hidden Physics Models

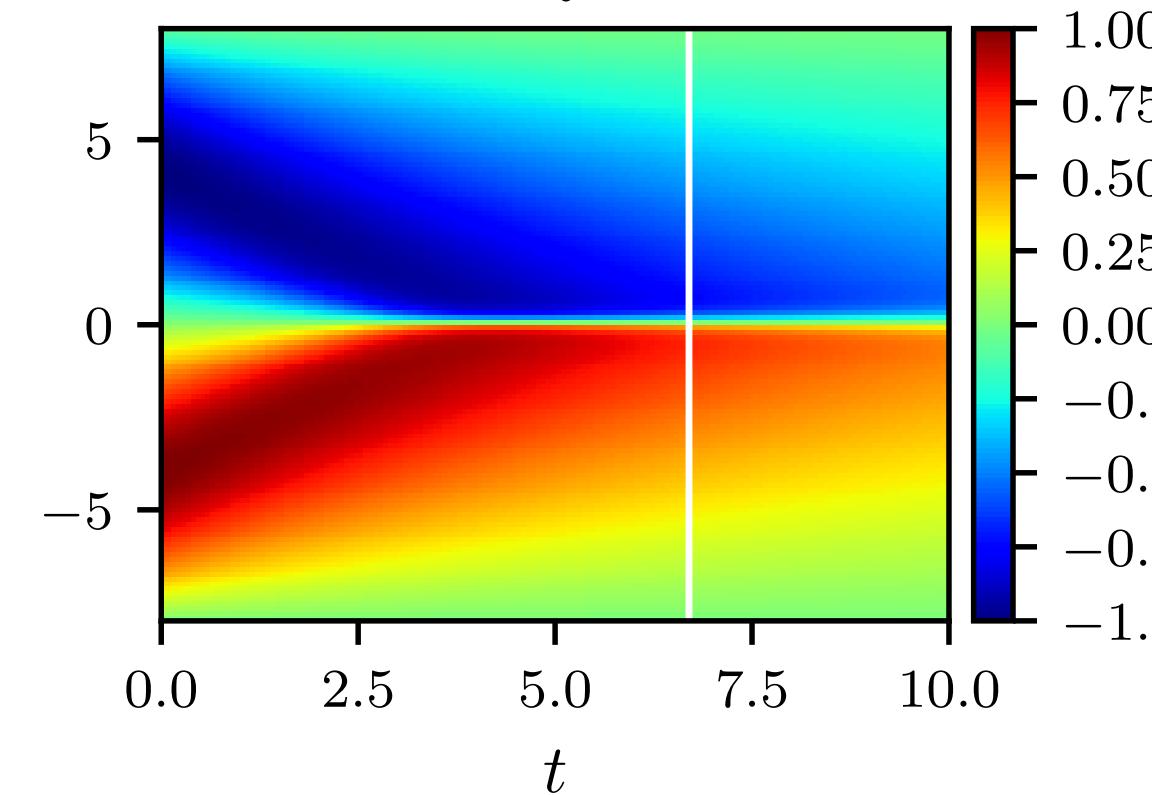


$$u_t = \mathcal{N}(t, x, u, u_x, u_{xx}, \dots)$$

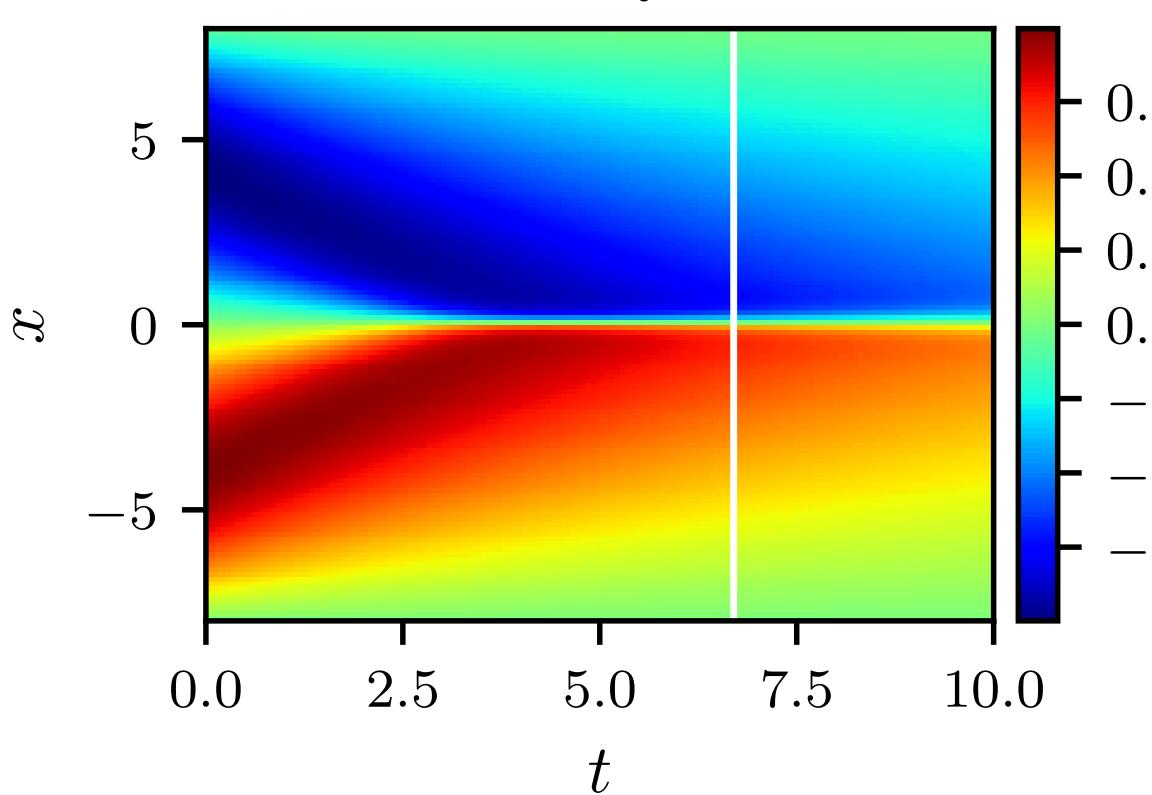
$$f = u_t - \mathcal{N}(t, x, u, u_x, u_{xx}, \dots)$$

$$\sum_{i=1}^N |u(t_i, x_i) - u_i|^2 + |f(t_i, x_i)|^2$$

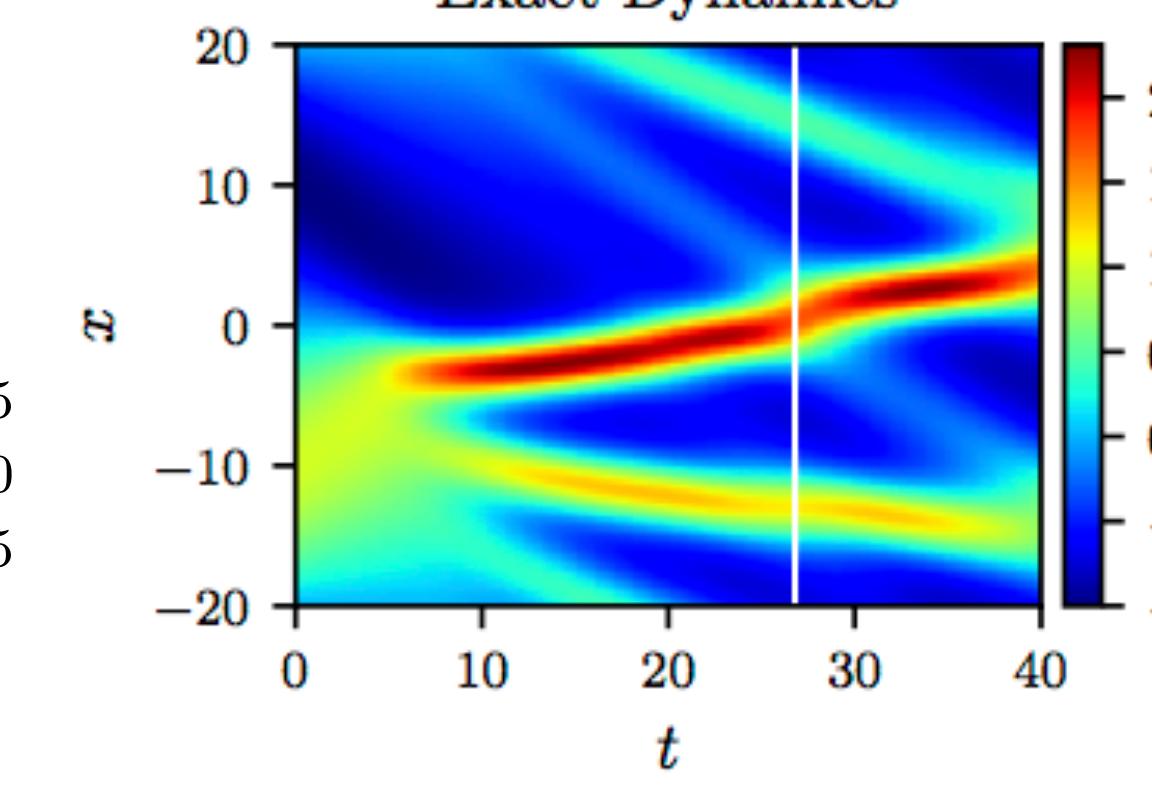
Exact Dynamics



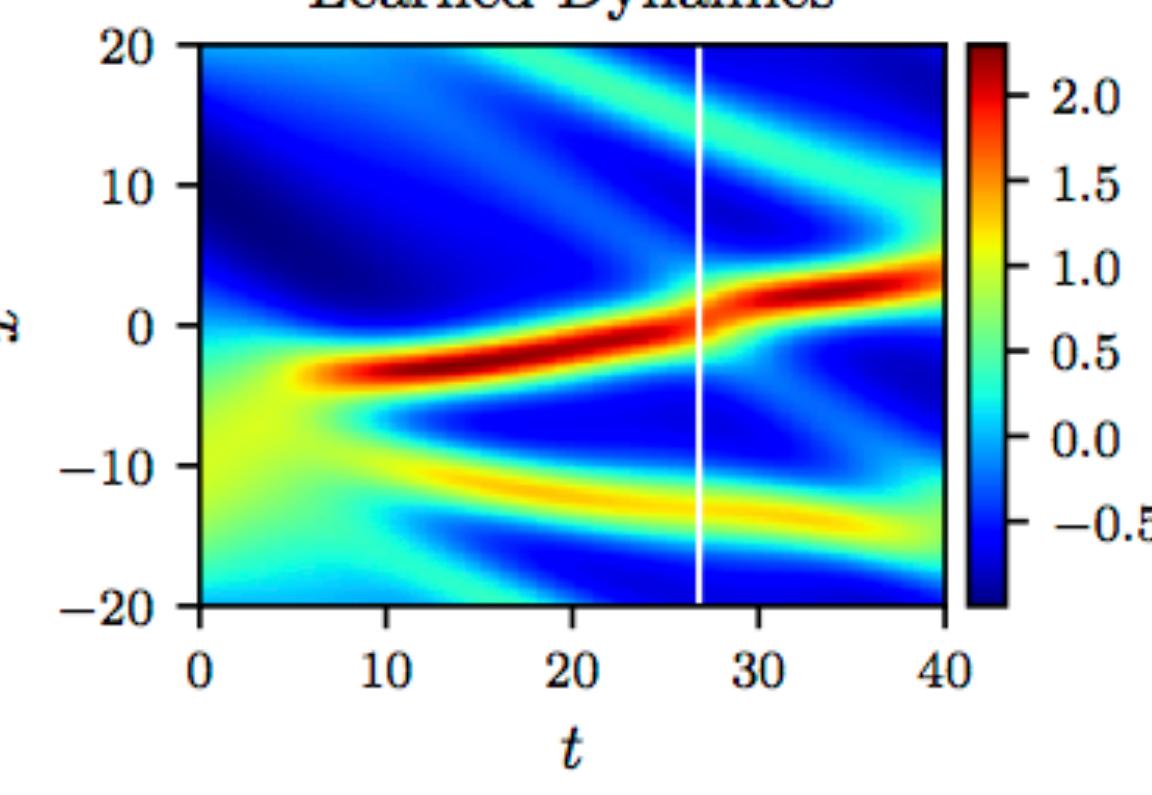
Learned Dynamics



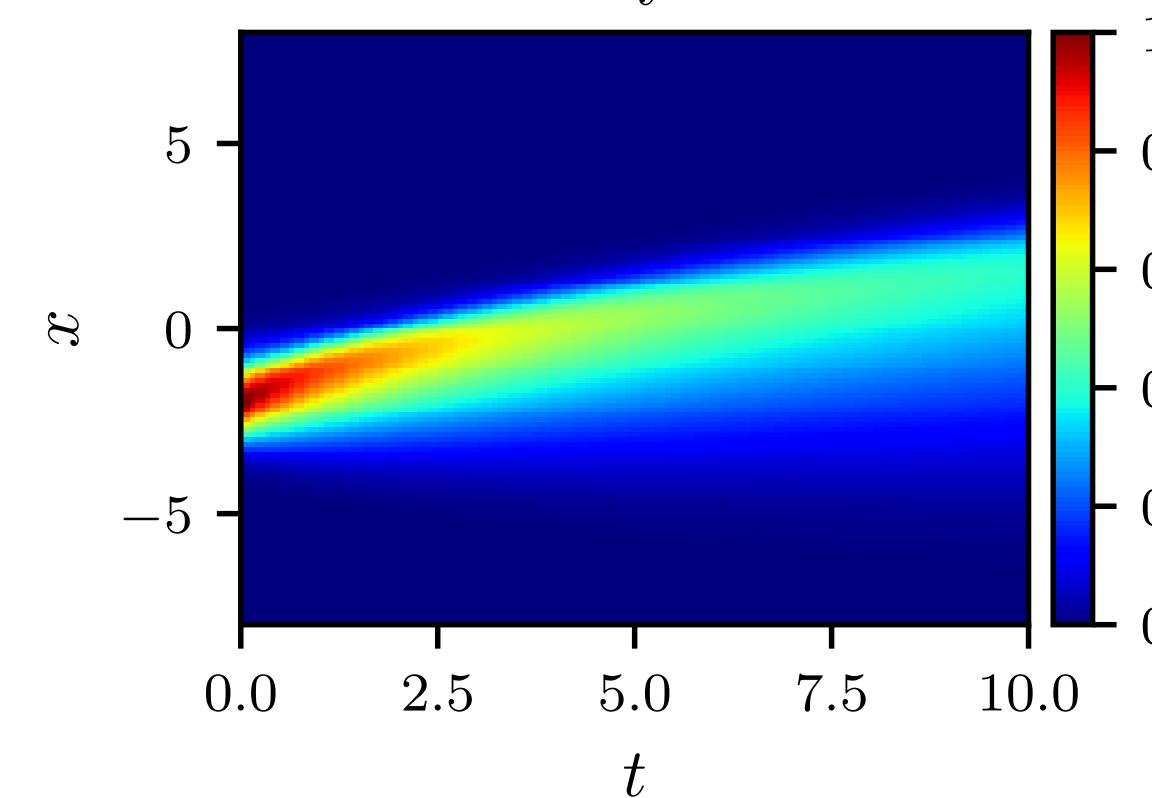
Exact Dynamics



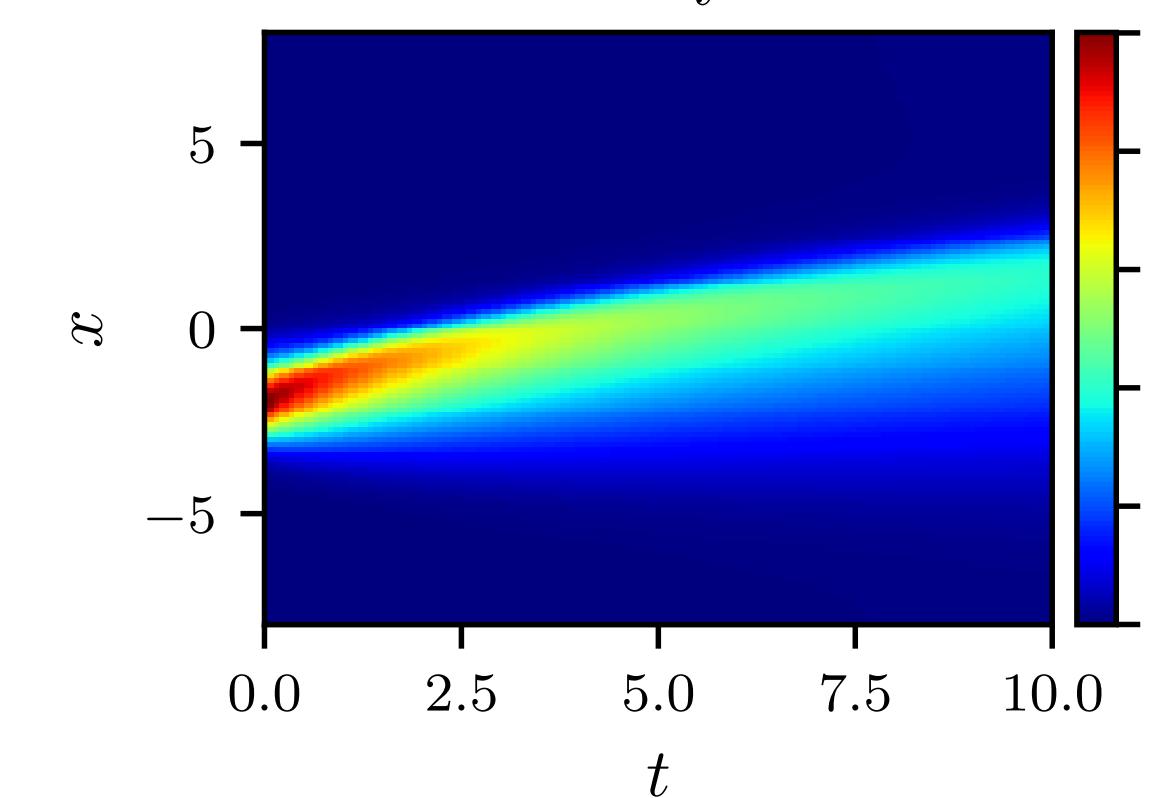
Learned Dynamics



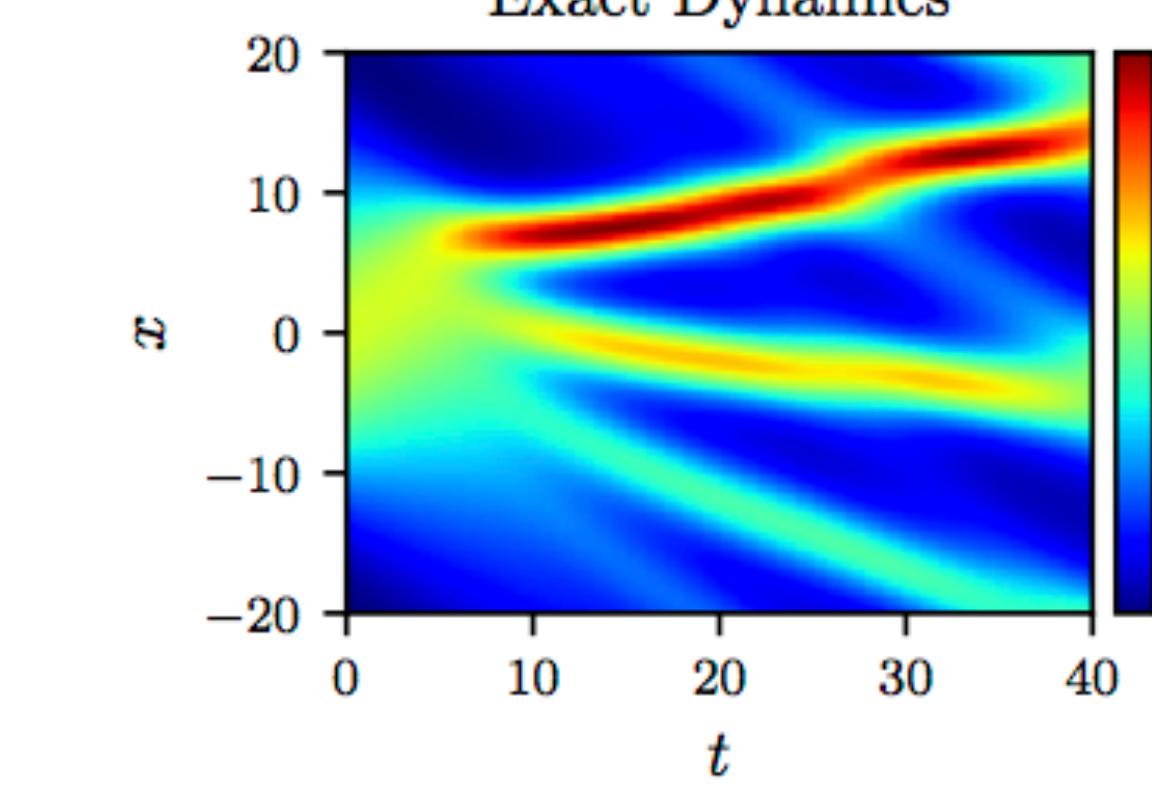
Exact Dynamics



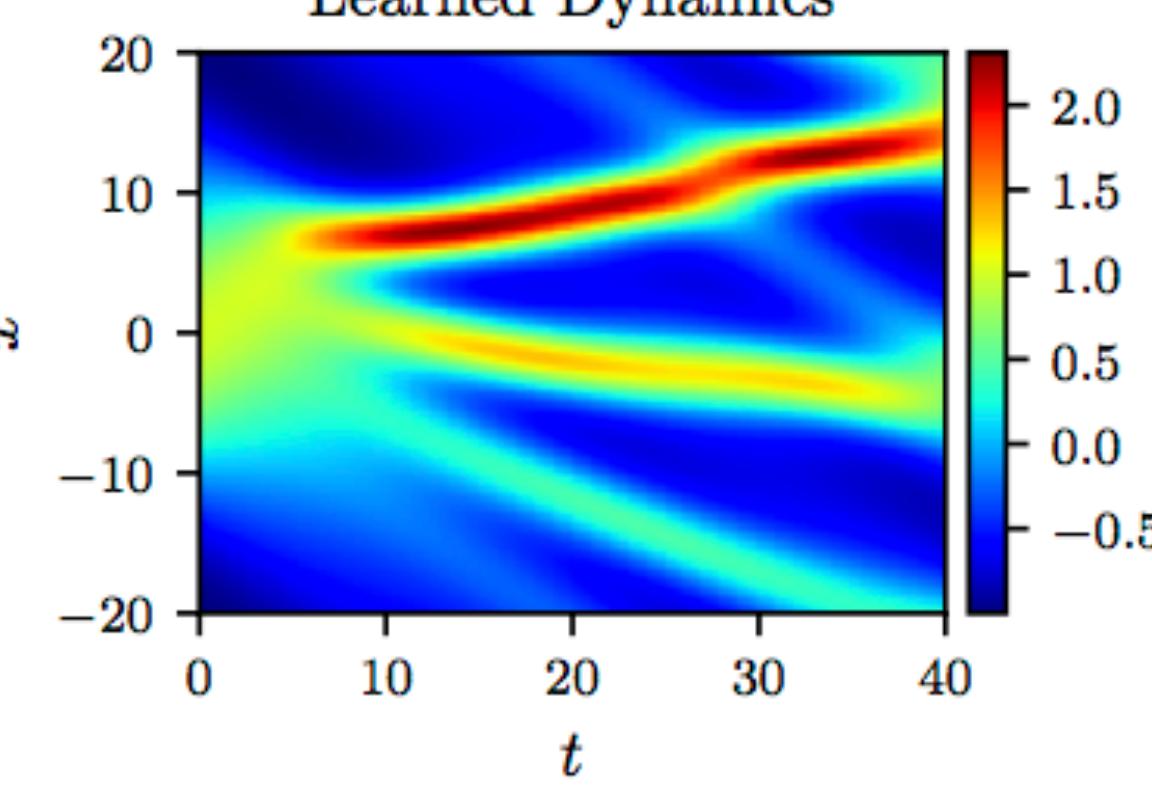
Learned Dynamics



Exact Dynamics



Learned Dynamics





Hidden Physics Models



Thank you!

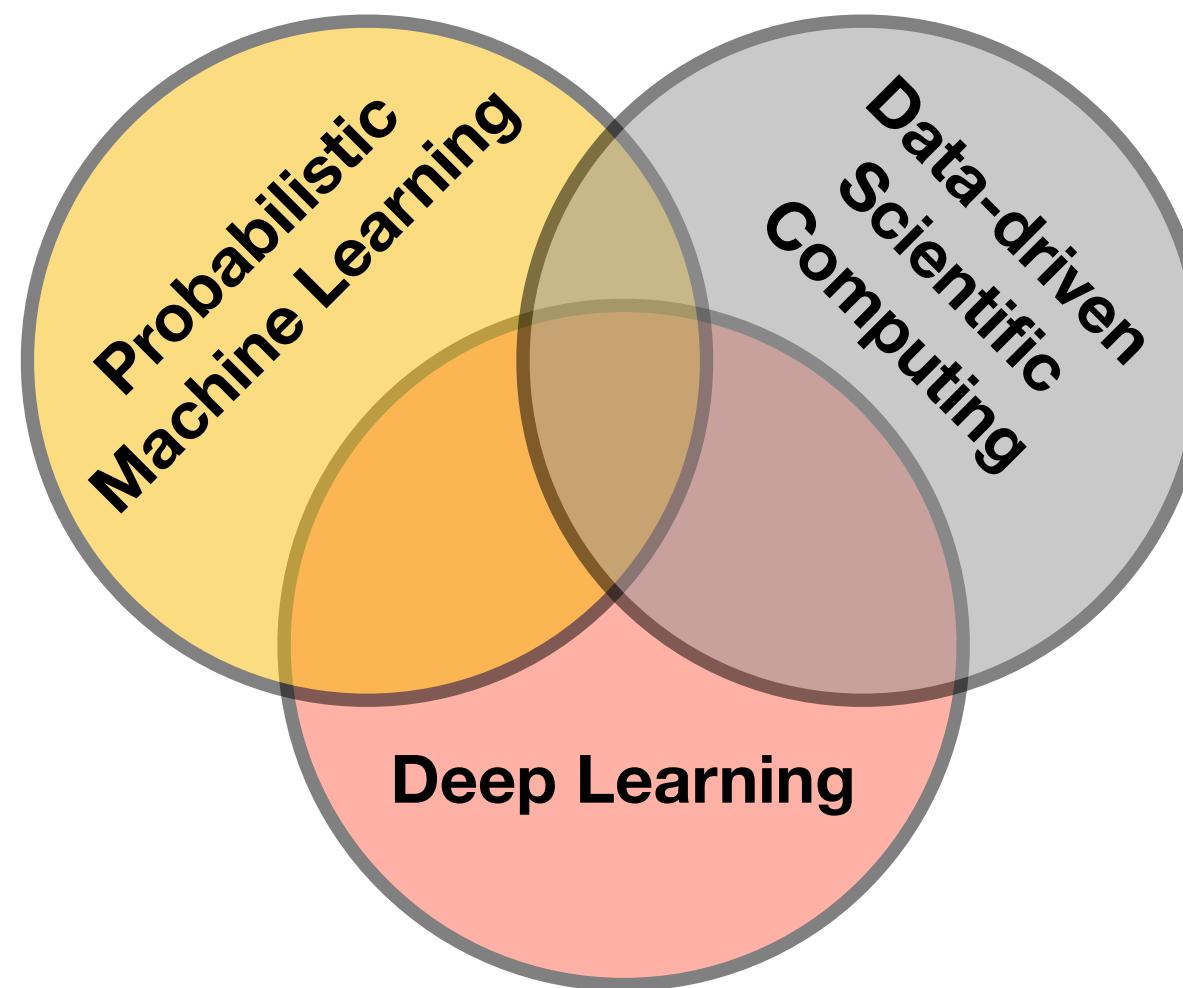
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MURI/ARO W911NF-15-1-0562

AFOSR FA9550-17-1-001

NIH U01HL116323

NSF DMS-1736088



Overview

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<https://github.com/maziarraissi>

NumericalGP

Numerical Gaussian Processes for Time-dependent and Non-linear Partial Differential Equations

● MATLAB ★ 18 ⚡ 18

HPM

Hidden physics models: Machine learning of nonlinear partial differential equations

● MATLAB ★ 36 ⚡ 30

ParametricGP

Parametric Gaussian Process Regression for Big Data

● Python ★ 18 ⚡ 9

DeepHPMs

Deep Hidden Physics Models: Deep Learning of Nonlinear Partial Differential Equations

● Python ★ 84 ⚡ 64

PINNs

Physics Informed Deep Learning: Data-driven Solutions and Discovery of Nonlinear Partial Differential Equations

● Python ★ 163 ⚡ 110

FBSNNs

Forward-Backward Stochastic Neural Networks: Deep Learning of High-dimensional Partial Differential Equations

● Python ★ 37 ⚡ 25