

# Hidden Physics Models

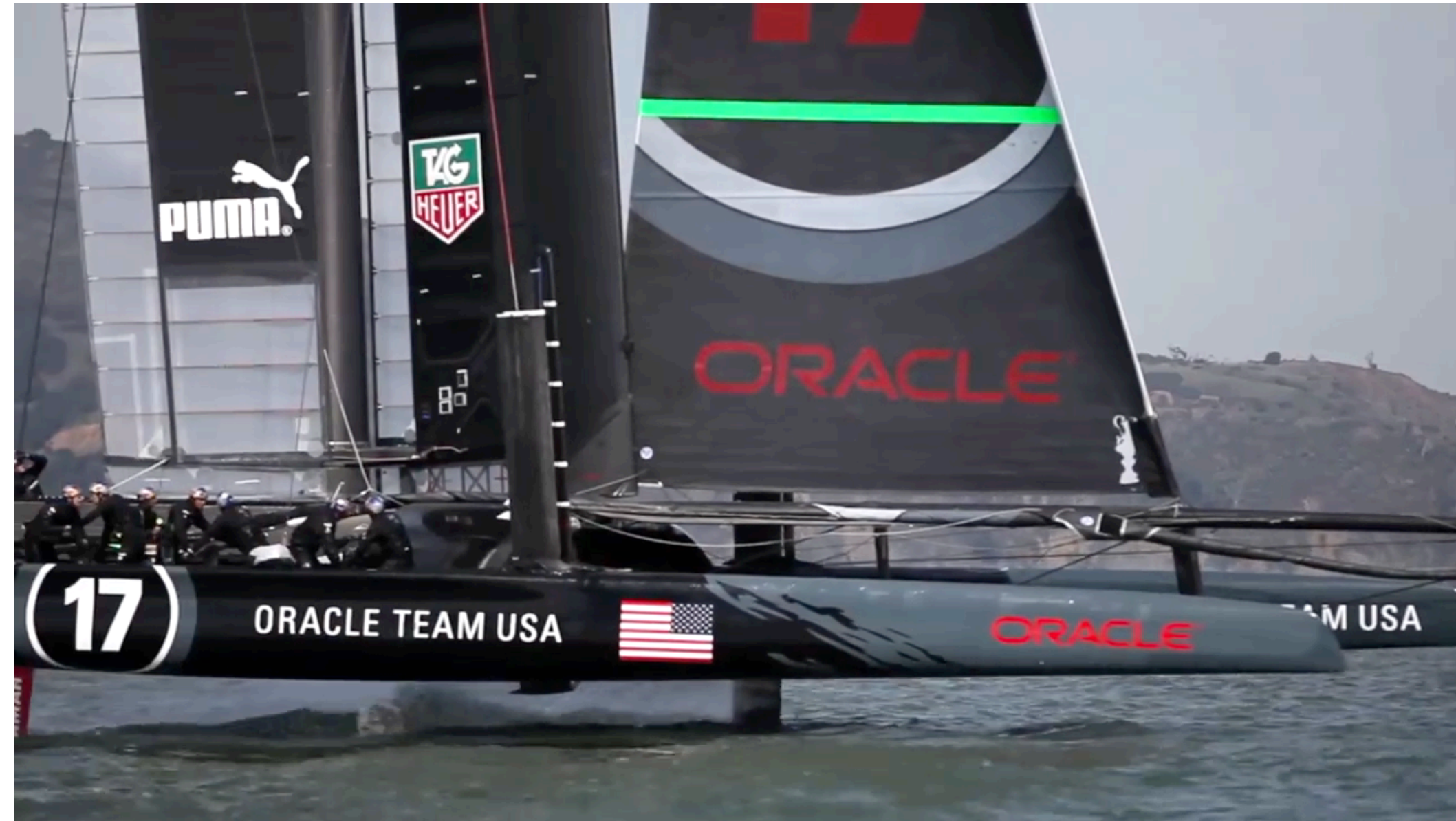
**Maziar Raissi**

**Assistant Professor**

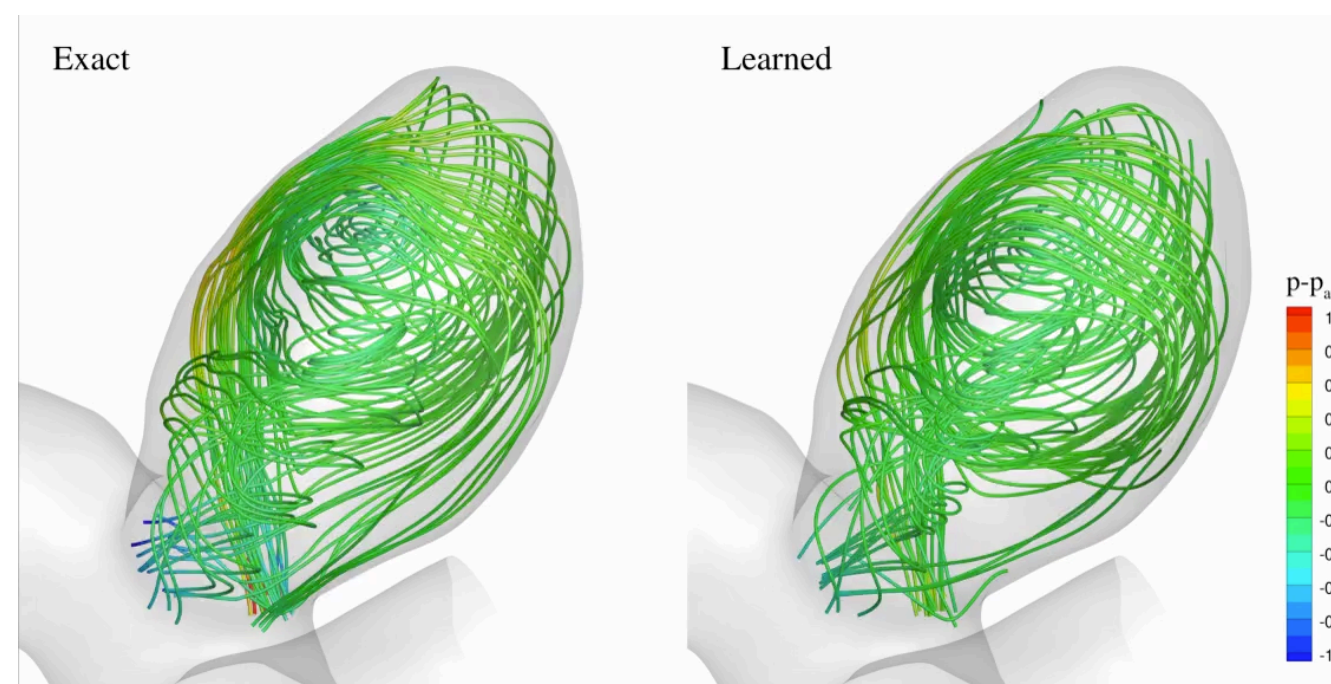
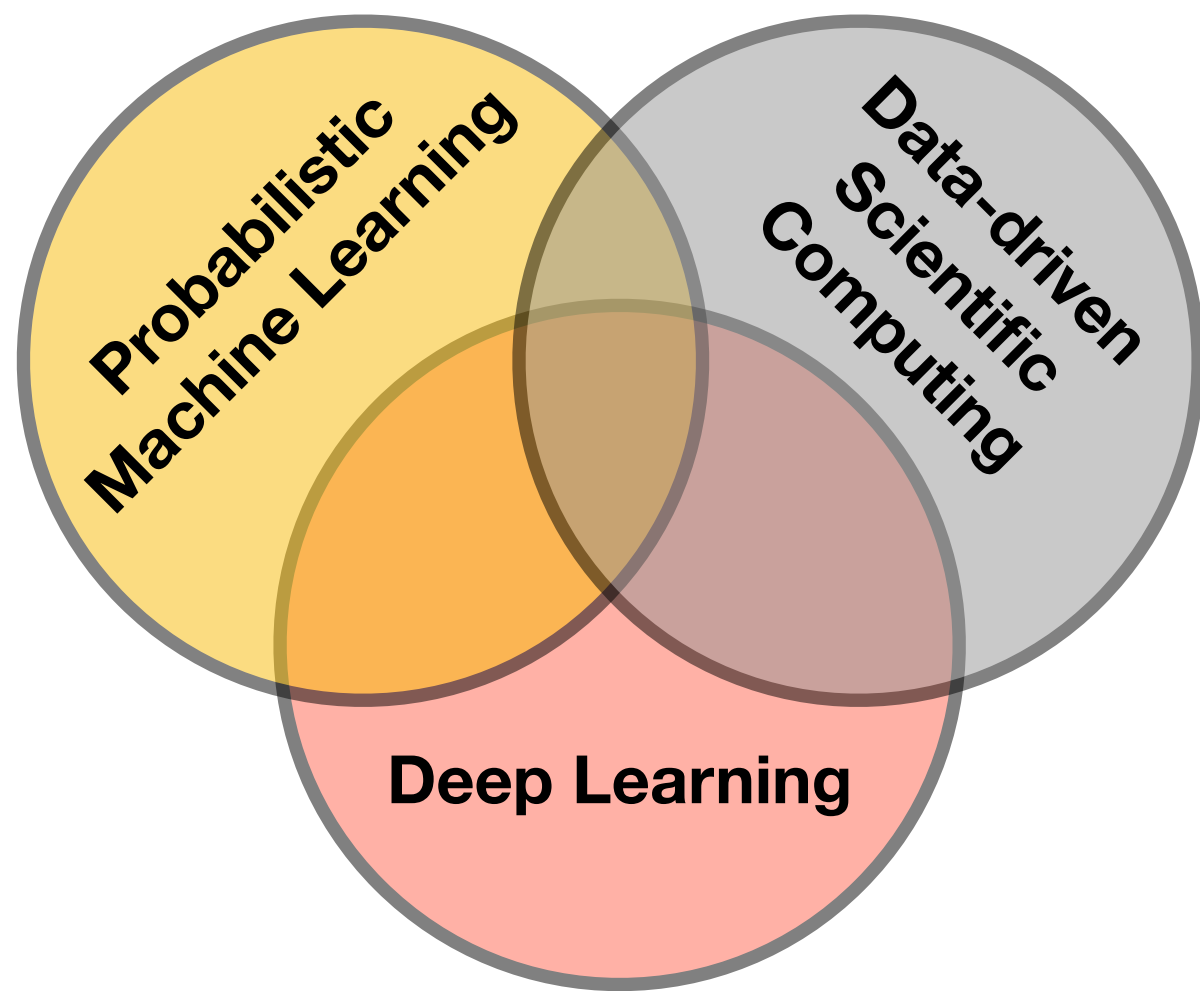
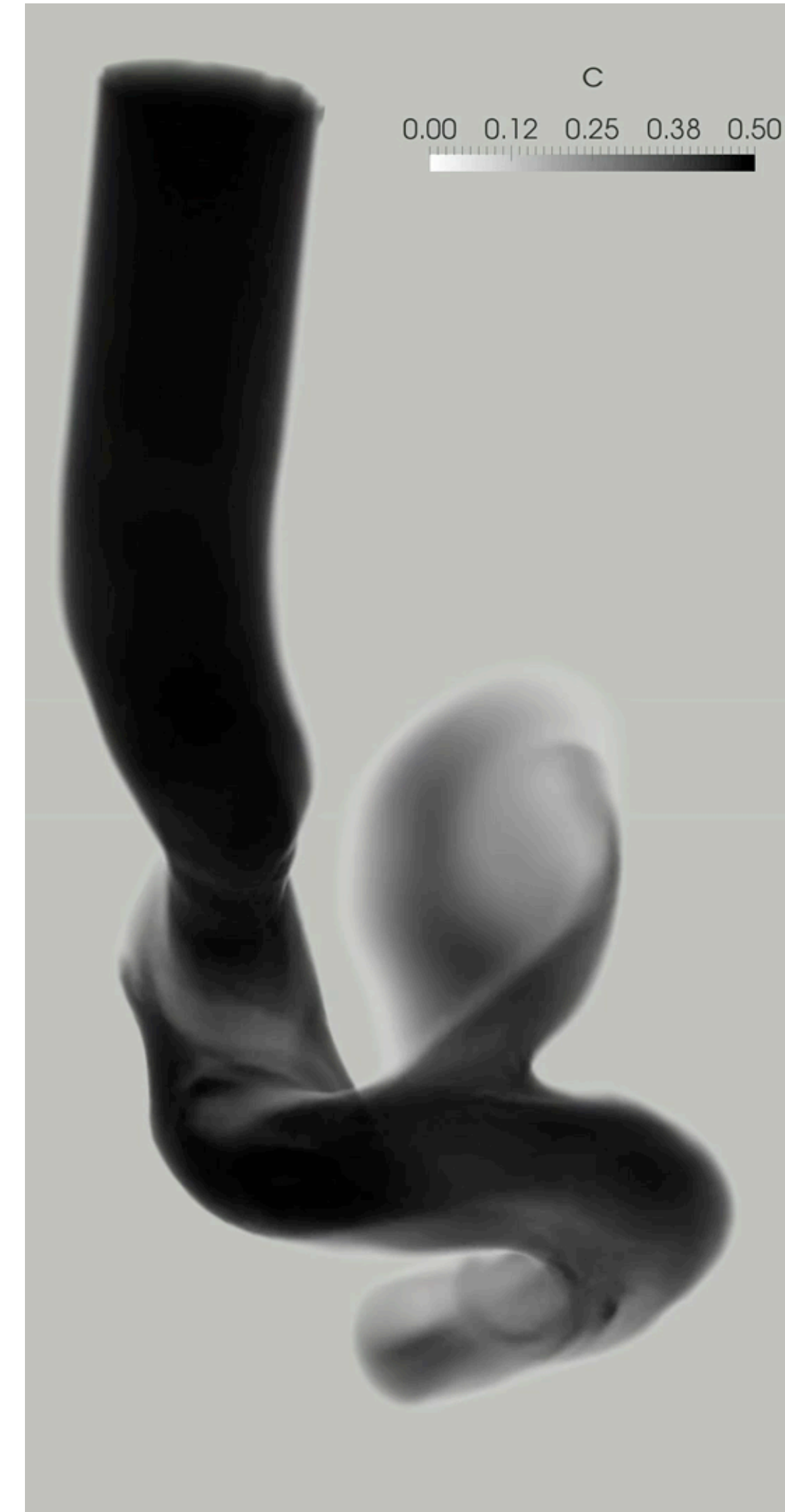
Department of Applied Mathematics

University of Colorado Boulder

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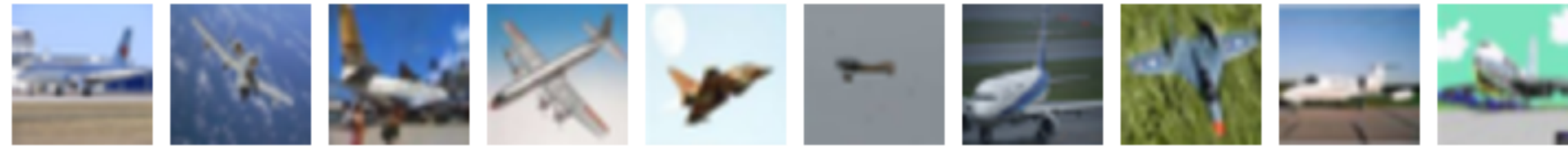


The ORACLE TEAM USA crew flying their AC72 "17" on foils.



# Machine/Deep Learning

airplane



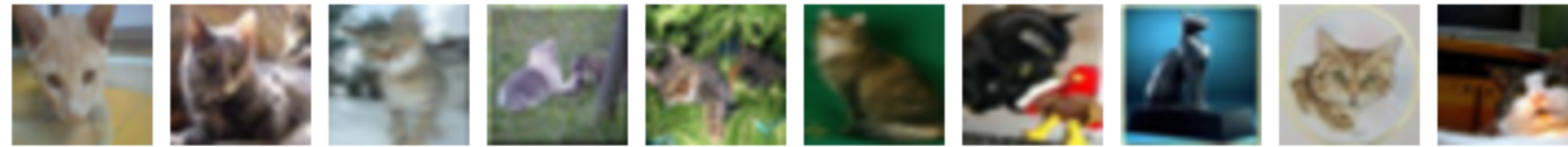
automobile



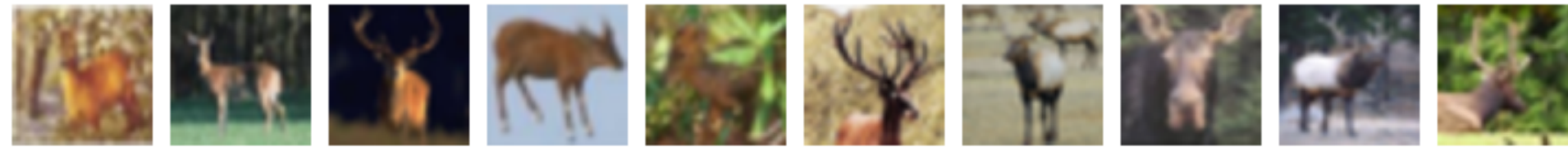
bird



cat



deer



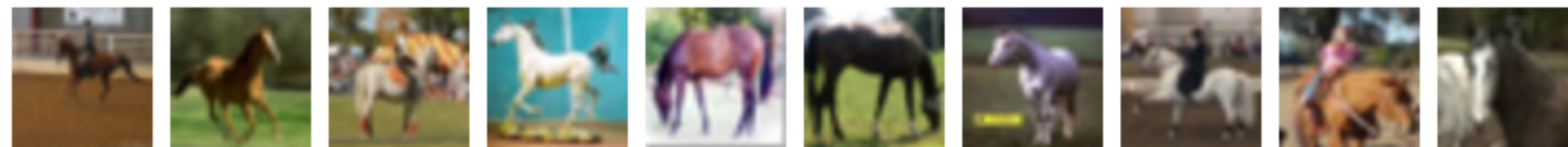
dog



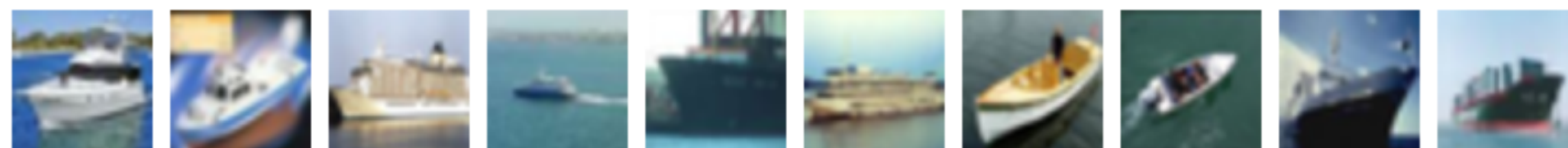
frog



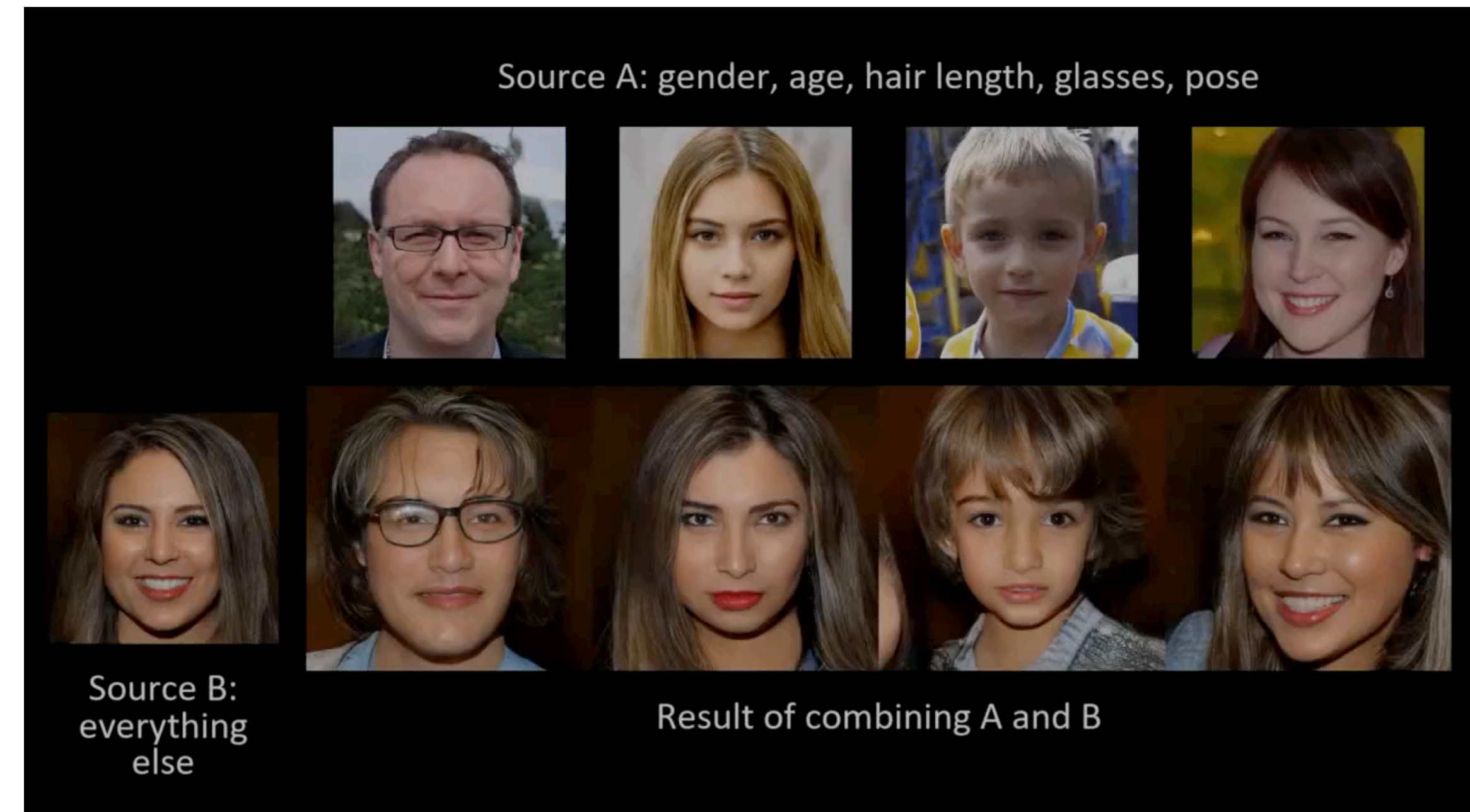
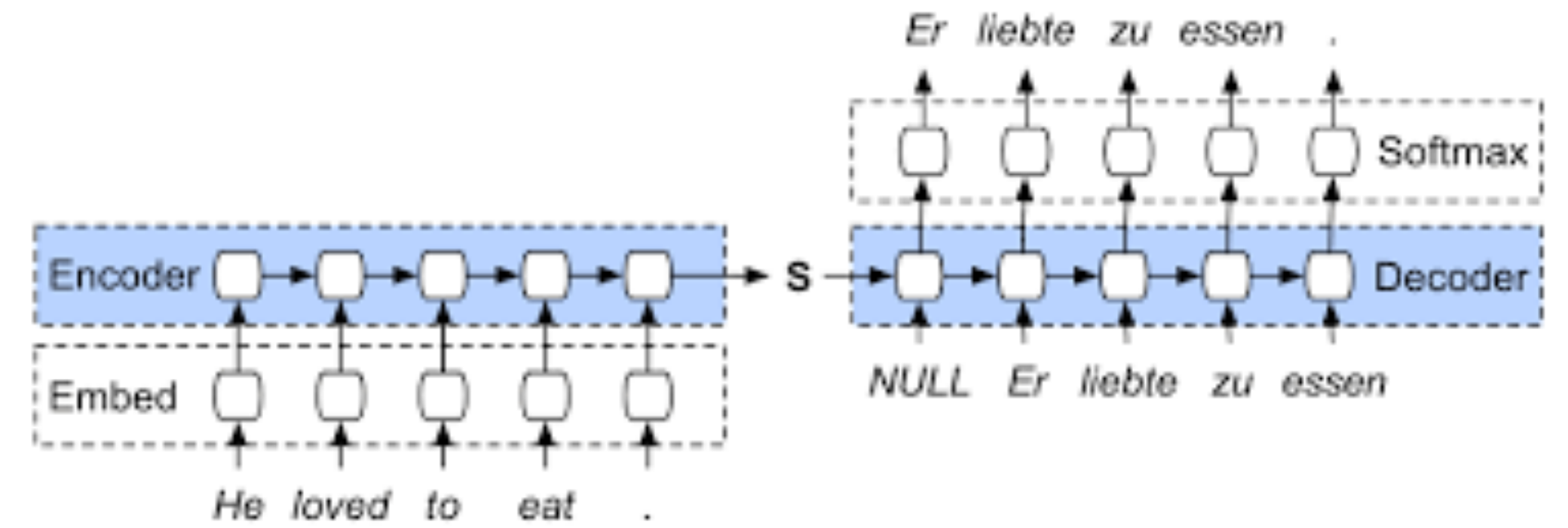
horse



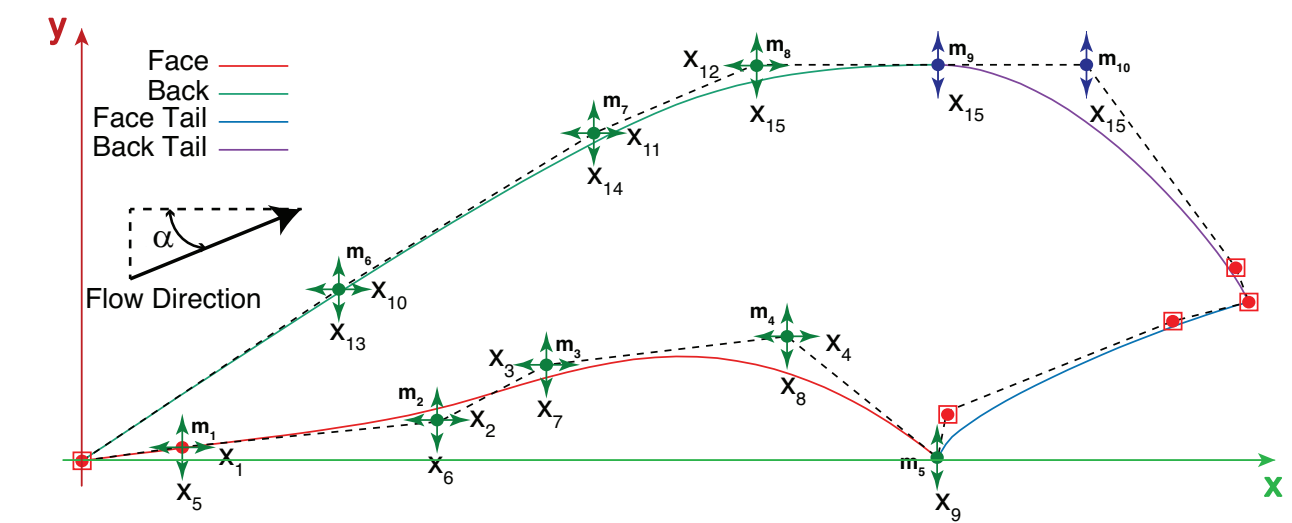
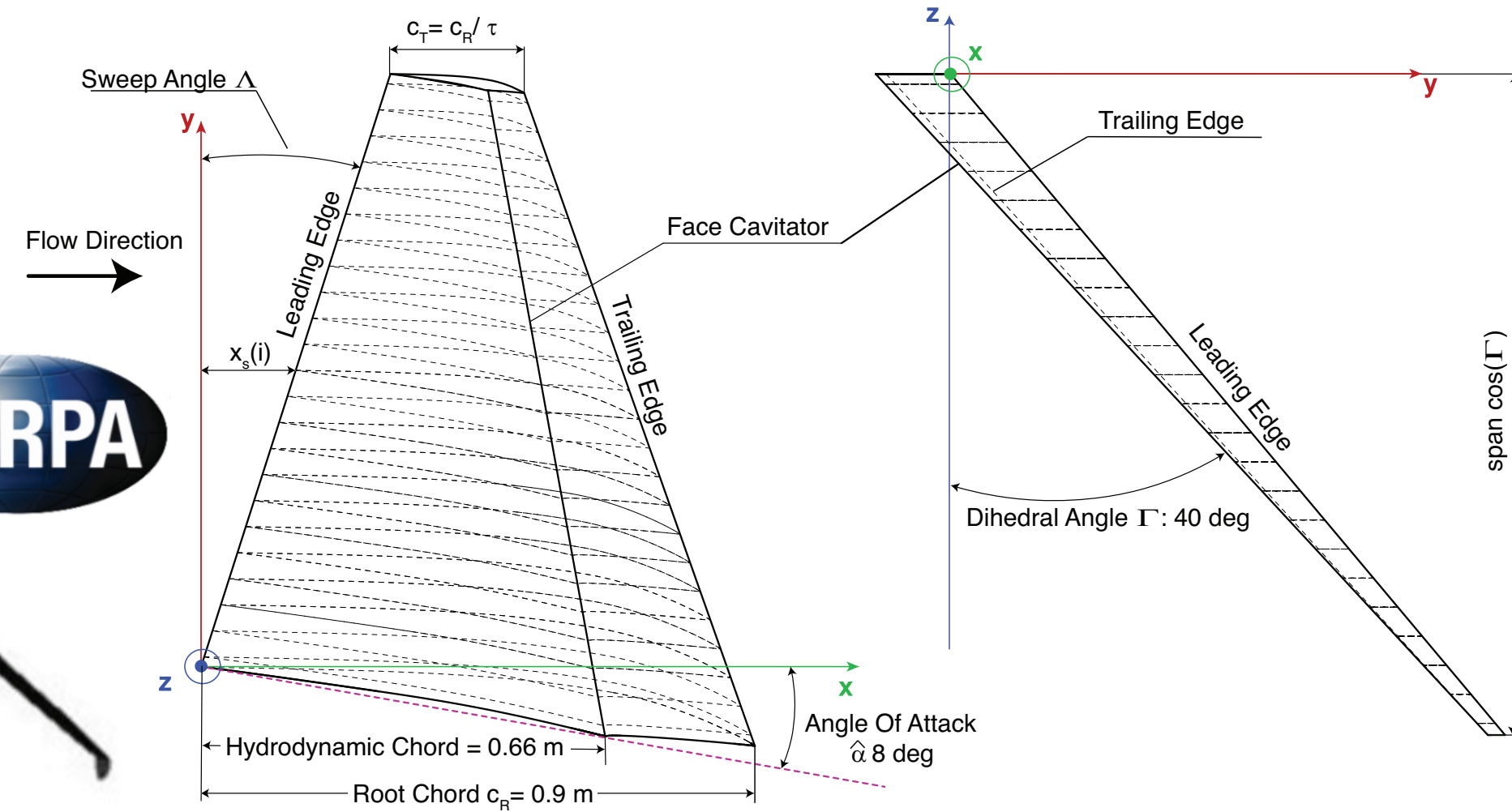
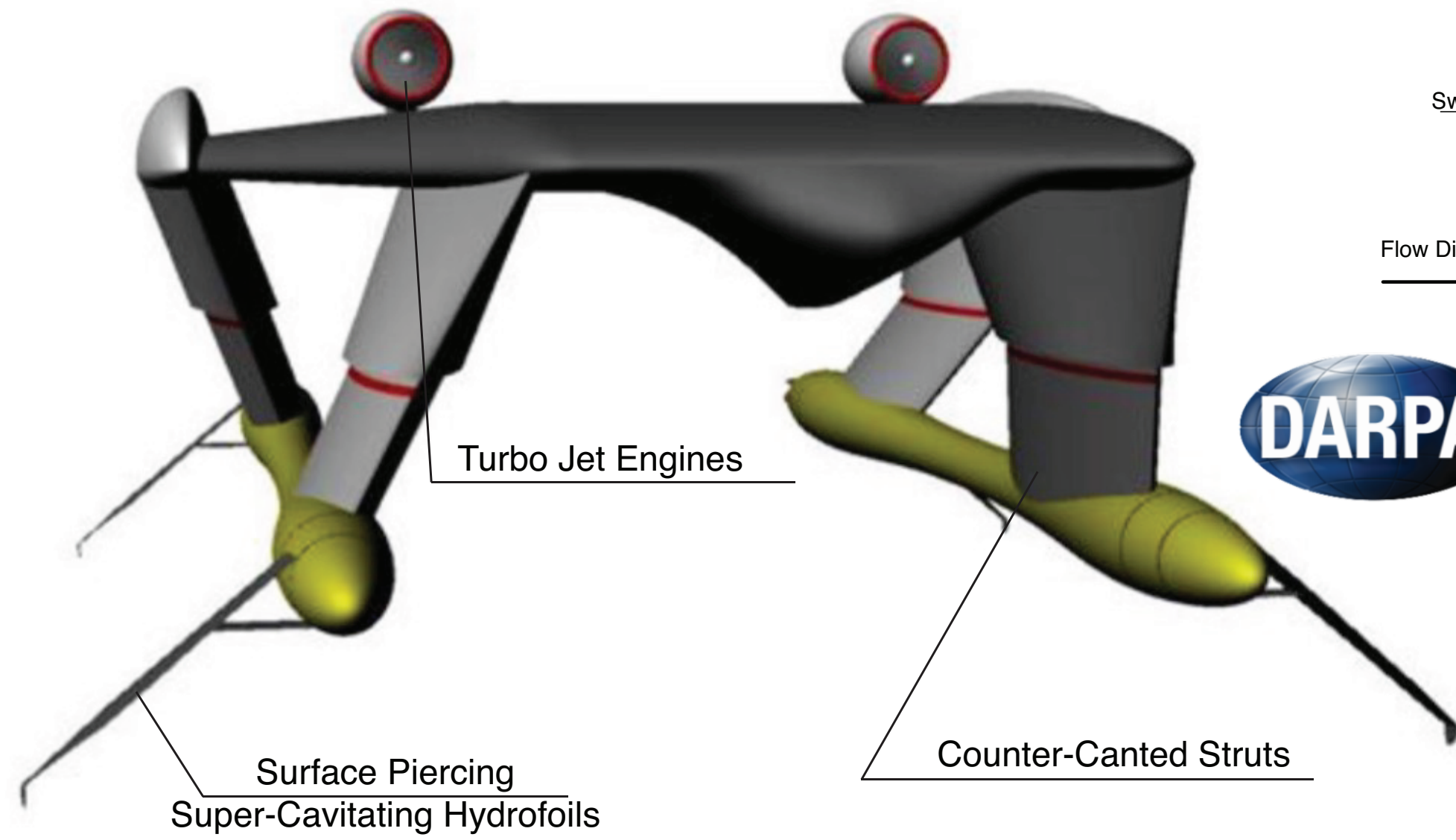
ship



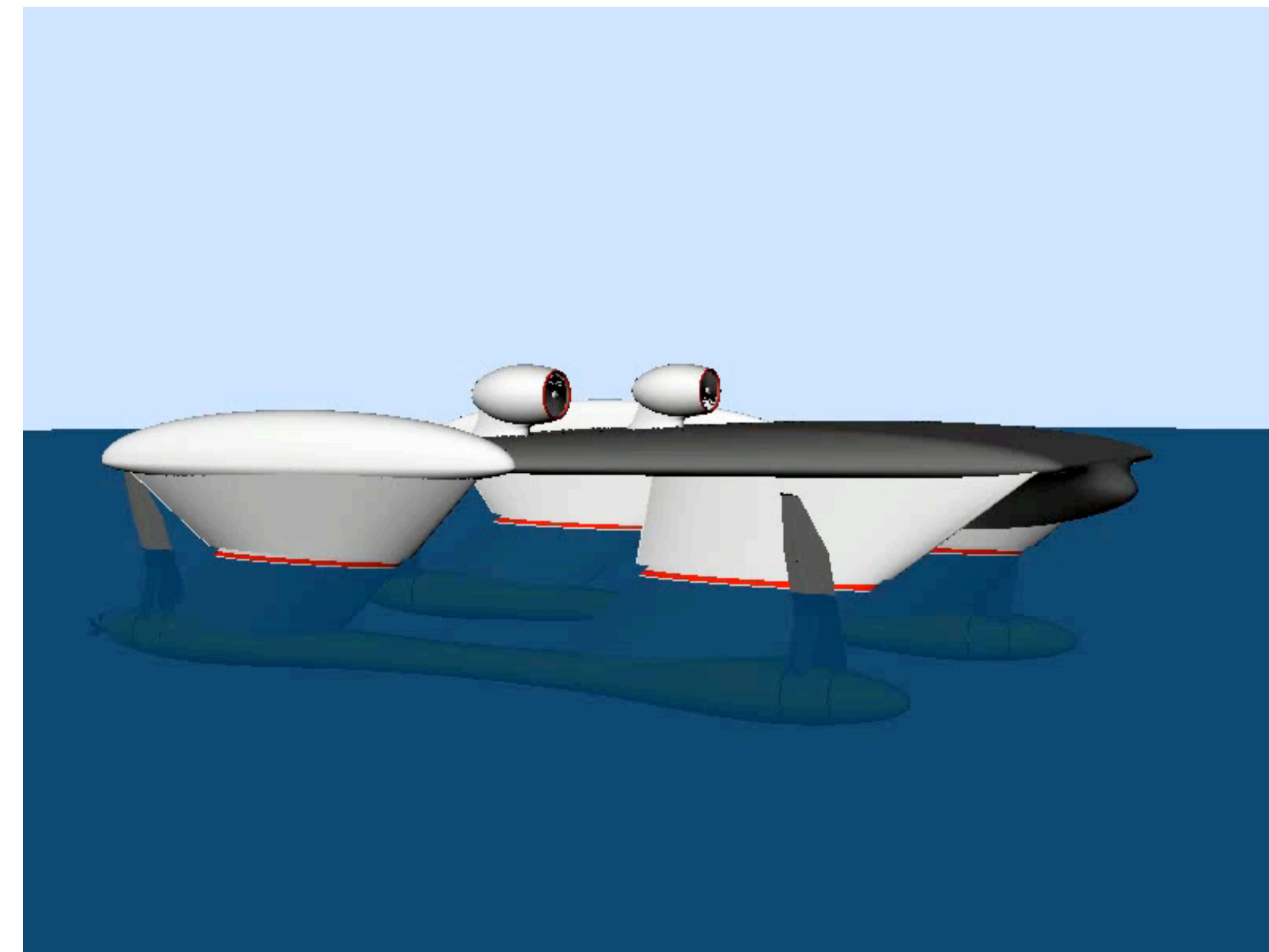
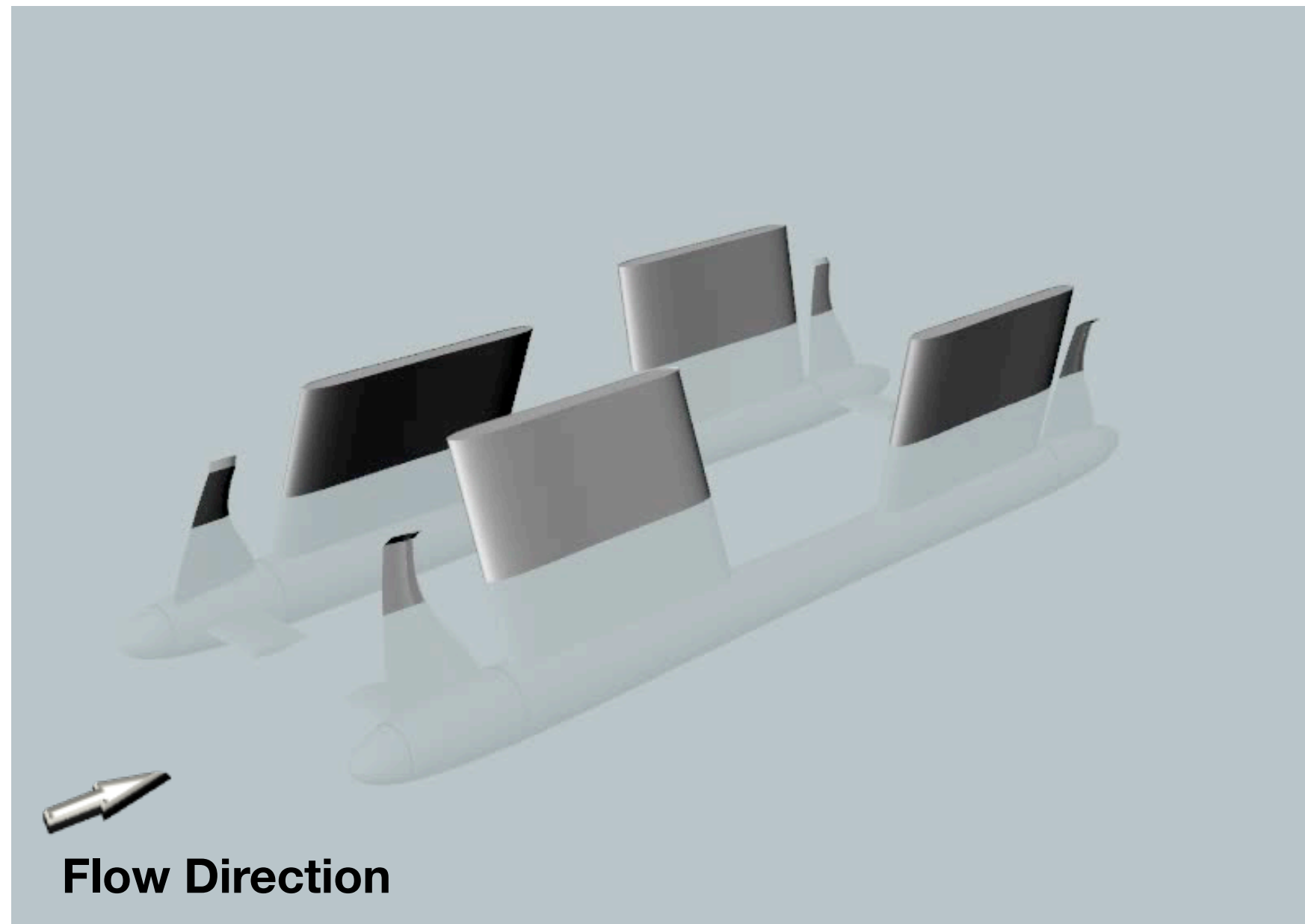
truck



# Design Optimization



lift/drag



# Gaussian Process Regression

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

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

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

$$\left[ \begin{array}{c} f(x) \\ f(x') \end{array} \right] \sim \mathcal{N} \left( \left[ \begin{array}{c} \mathbf{0} \\ 0 \end{array} \right], \left[ \begin{array}{cc} k(x, x; \theta) & k(x, x'; \theta) \\ k(x', x; \theta) & k(x', x'; \theta) \end{array} \right] \right) \left. \vphantom{\left[ \begin{array}{c} f(x) \\ f(x') \end{array} \right]} \right\} \text{Prior}$$

$$k(x, x'; \gamma, \omega) = \gamma^2 \exp(-0.5 \omega^2 (x - x')^2)$$

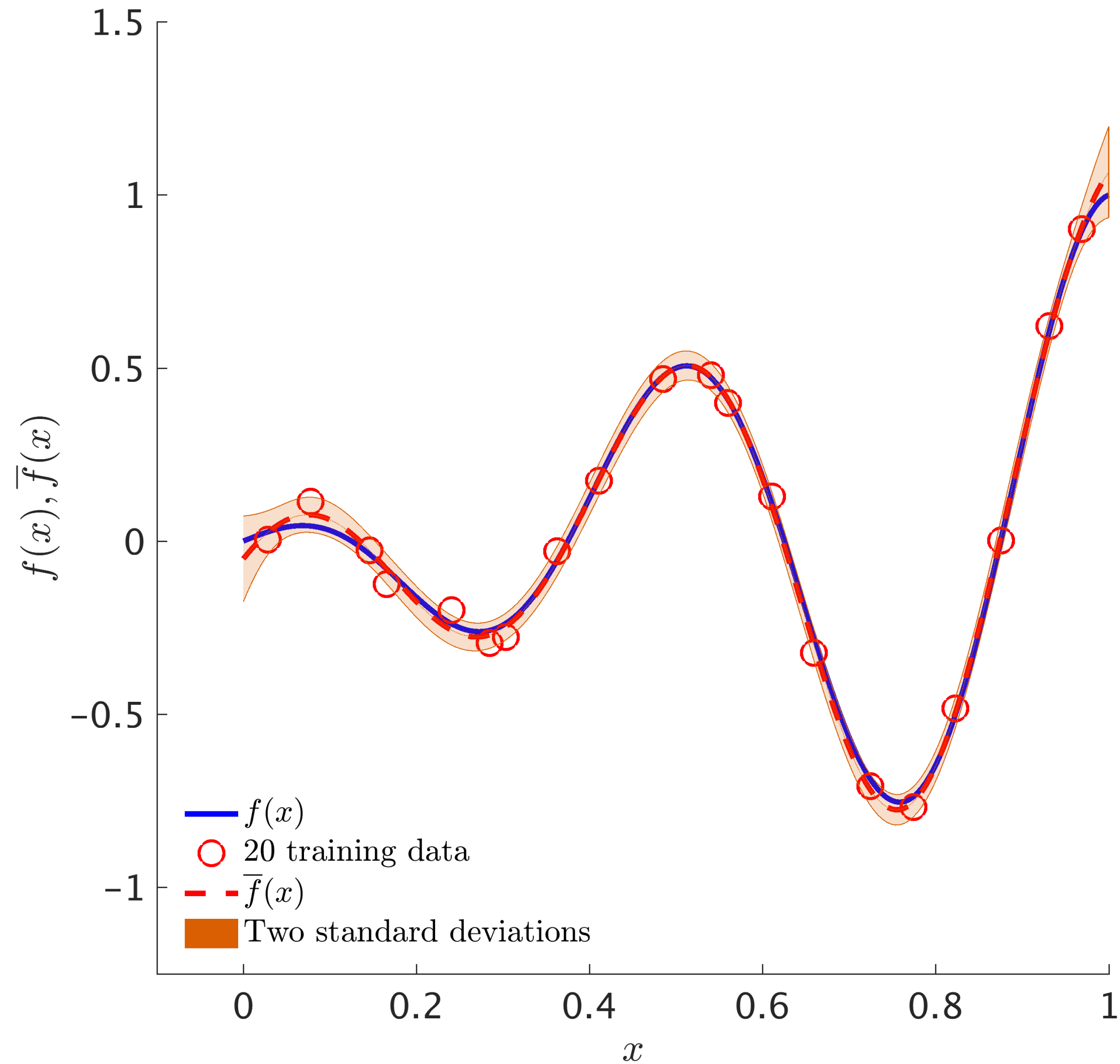
$$\left[ \begin{array}{c} f(x^*) \\ \mathbf{y} \end{array} \right] \sim \mathcal{N} \left( \left[ \begin{array}{c} 0 \\ \mathbf{0} \end{array} \right], \left[ \begin{array}{cc} k(x^*, x^*) & k(x^*, \mathbf{x}) \\ k(\mathbf{x}, x^*) & \mathbf{K} \end{array} \right] \right) \left. \vphantom{\left[ \begin{array}{c} f(x^*) \\ \mathbf{y} \end{array} \right]} \right\} \text{Prediction}$$

$$f(x^*) | \mathbf{x}, \mathbf{y} \sim \mathcal{N}(m(x^*), S(x^*, x^*))$$

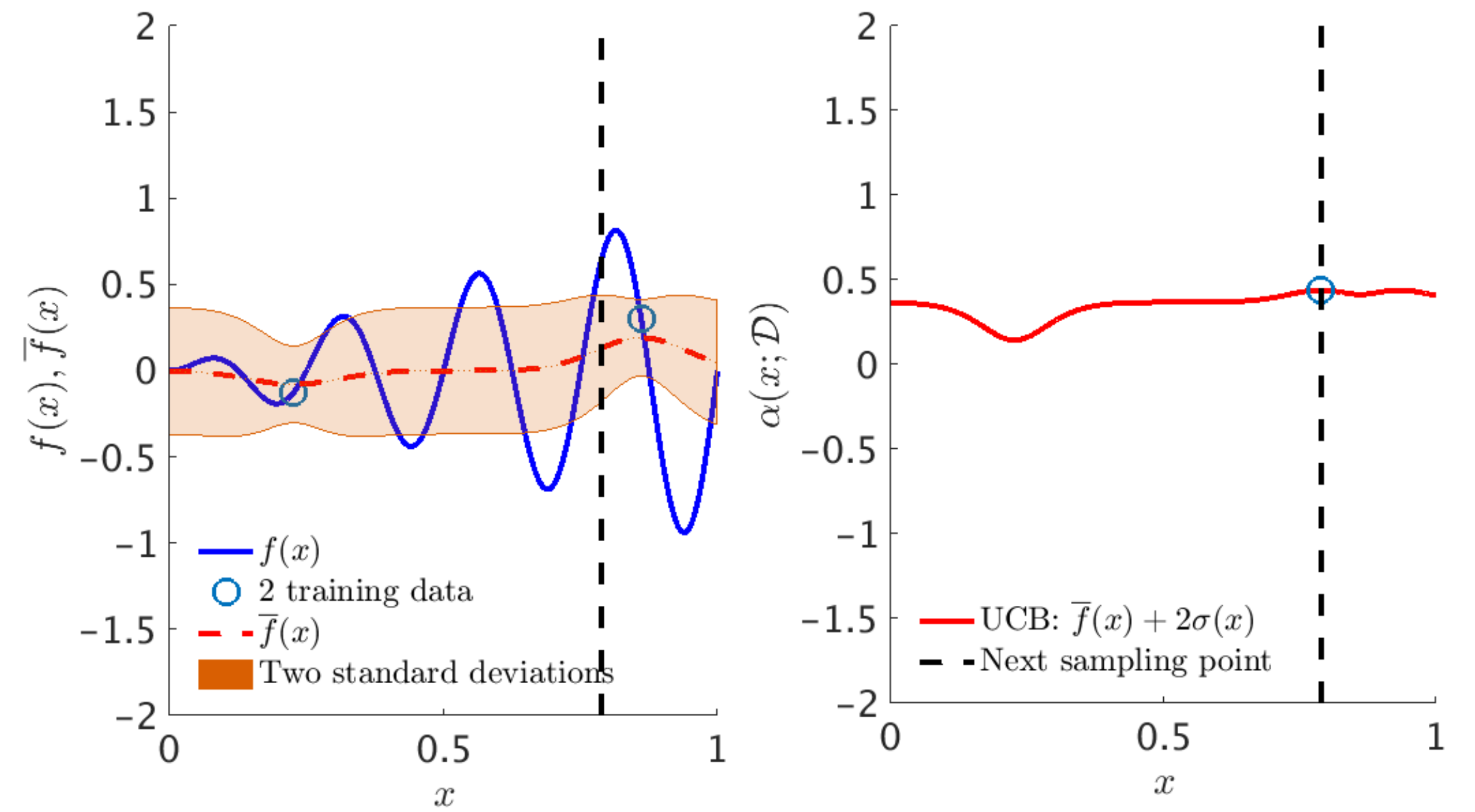
$$m(x^*) = k(x^*, \mathbf{x}) \mathbf{K}^{-1} \mathbf{y}$$

$$S(x^*, x^*) = k(x^*, x^*) - k(x^*, \mathbf{x}) \mathbf{K}^{-1} k(\mathbf{x}, x^*)$$

# Gaussian Process Regression

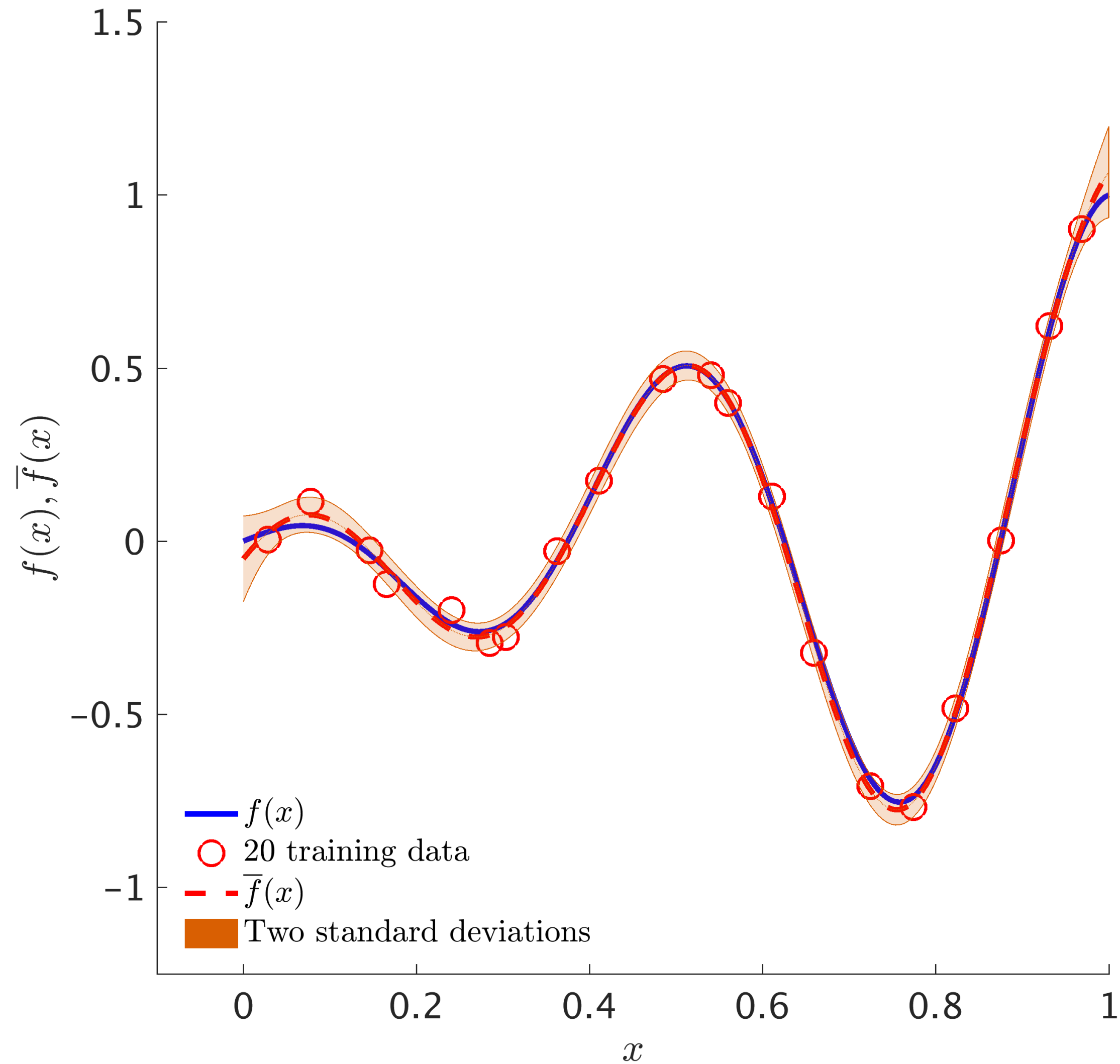


## Bayesian Optimization

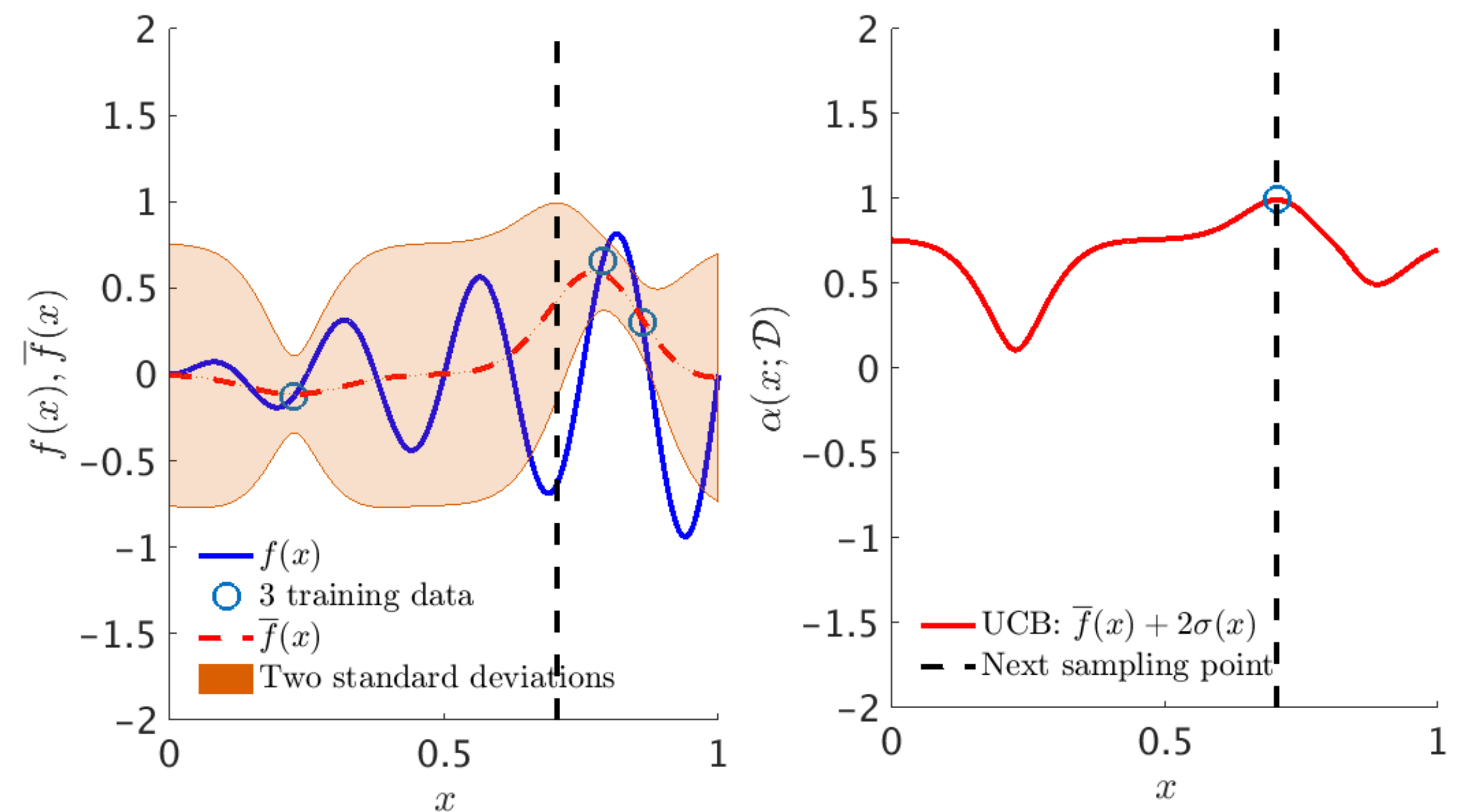


Shahriari, Bobak, et al. "Taking the human out of the loop: A review of bayesian optimization." *Proceedings of the IEEE* 104.1 (2016): 148-175.

# Gaussian Process Regression

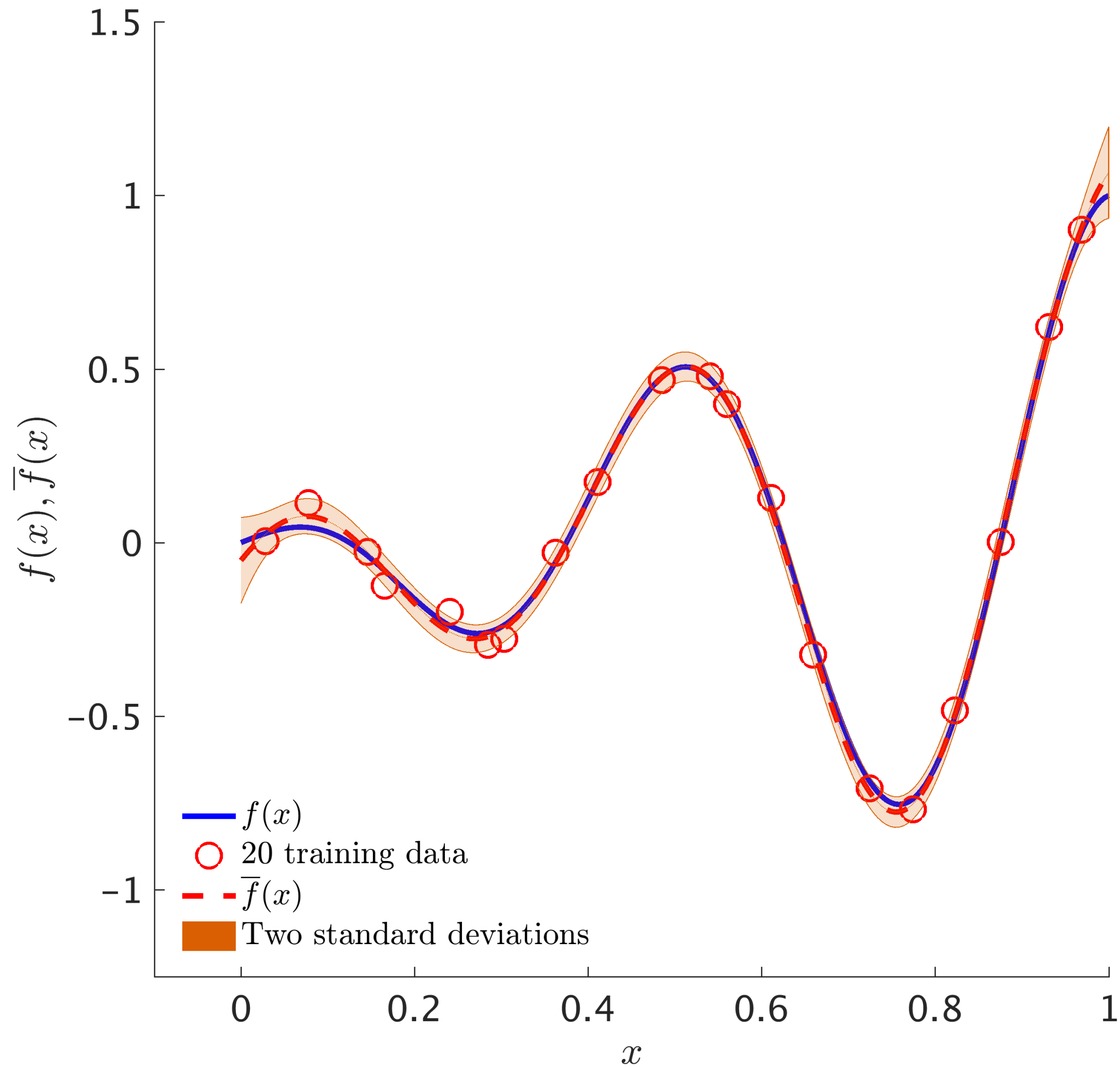


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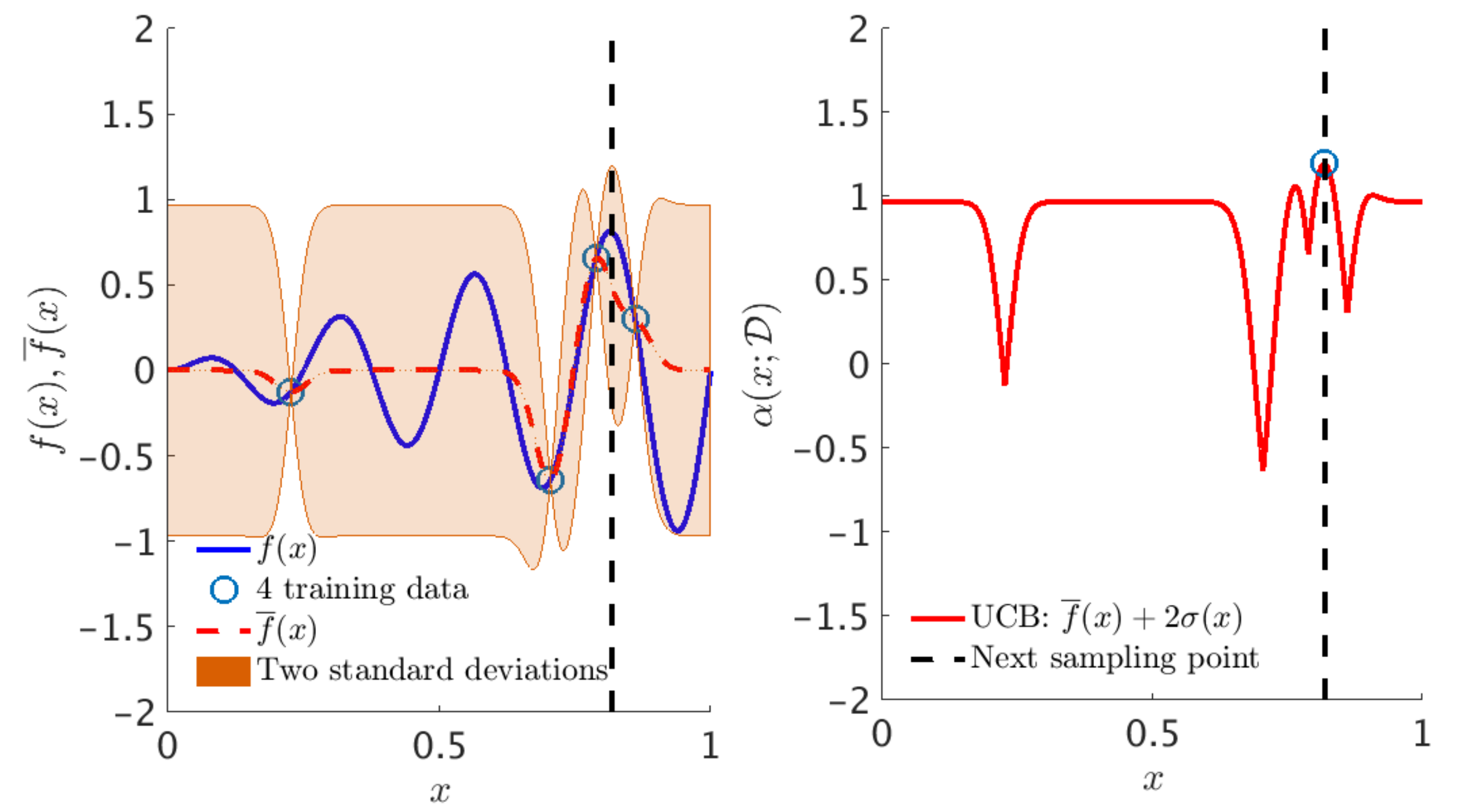


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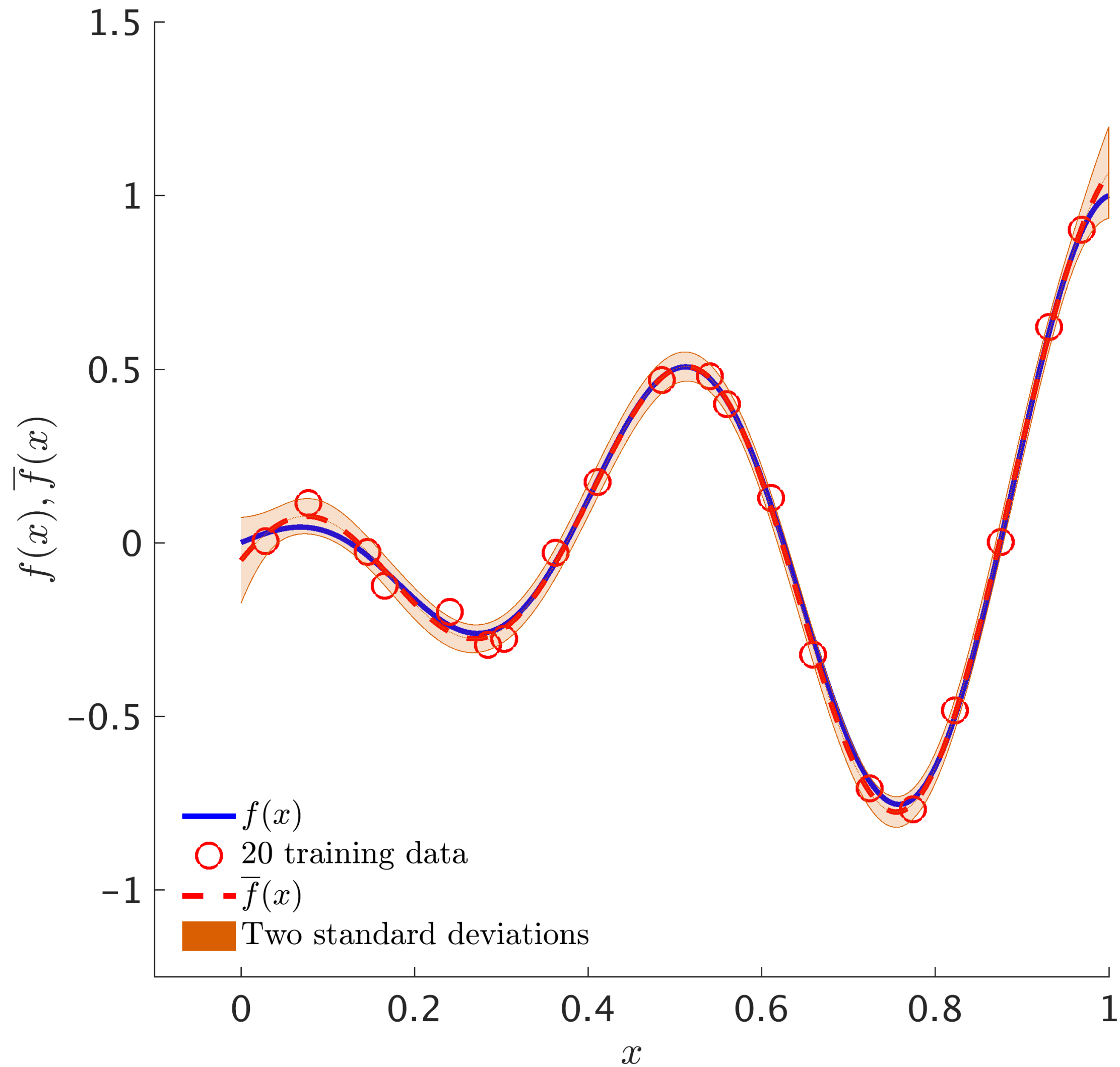


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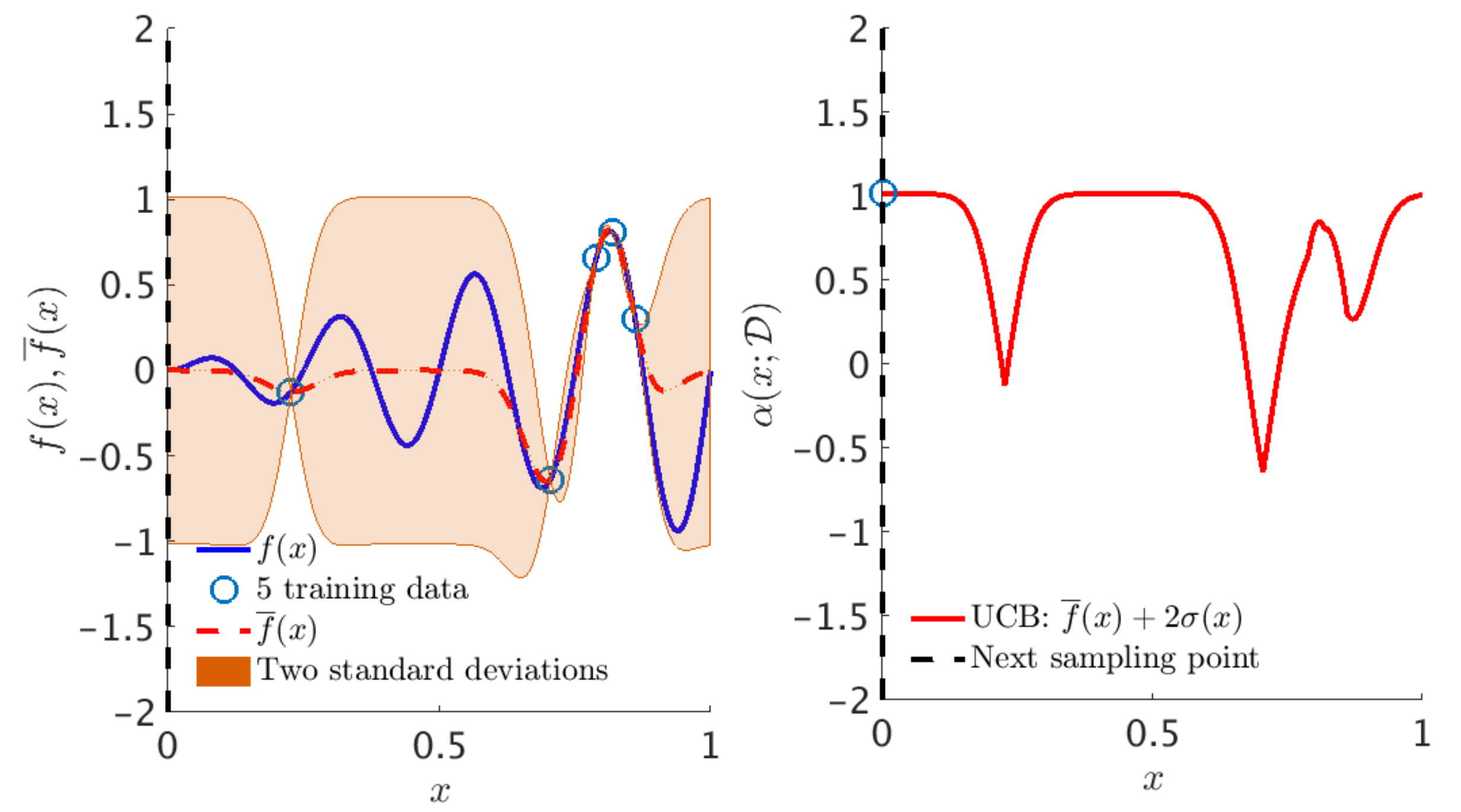


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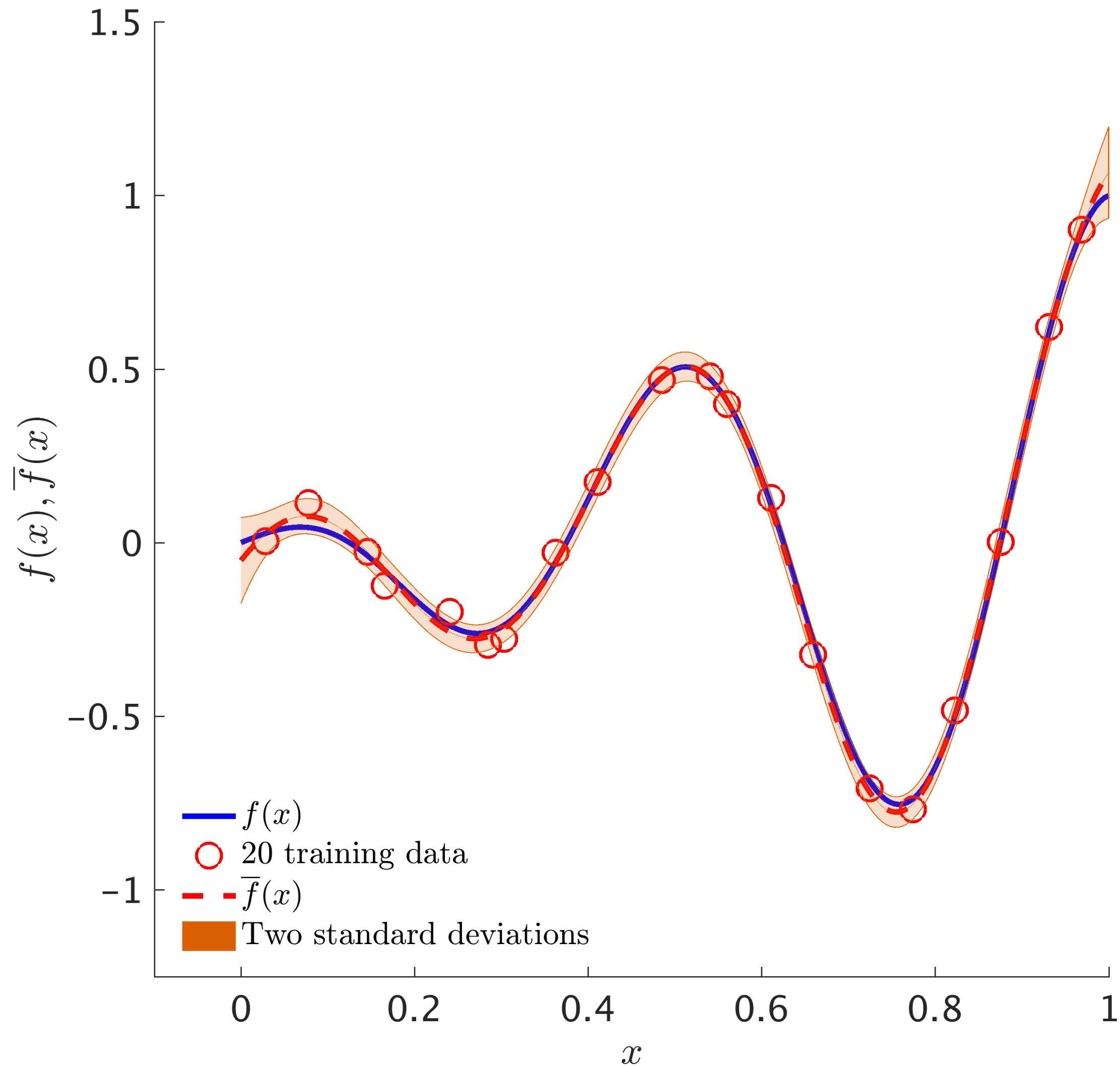
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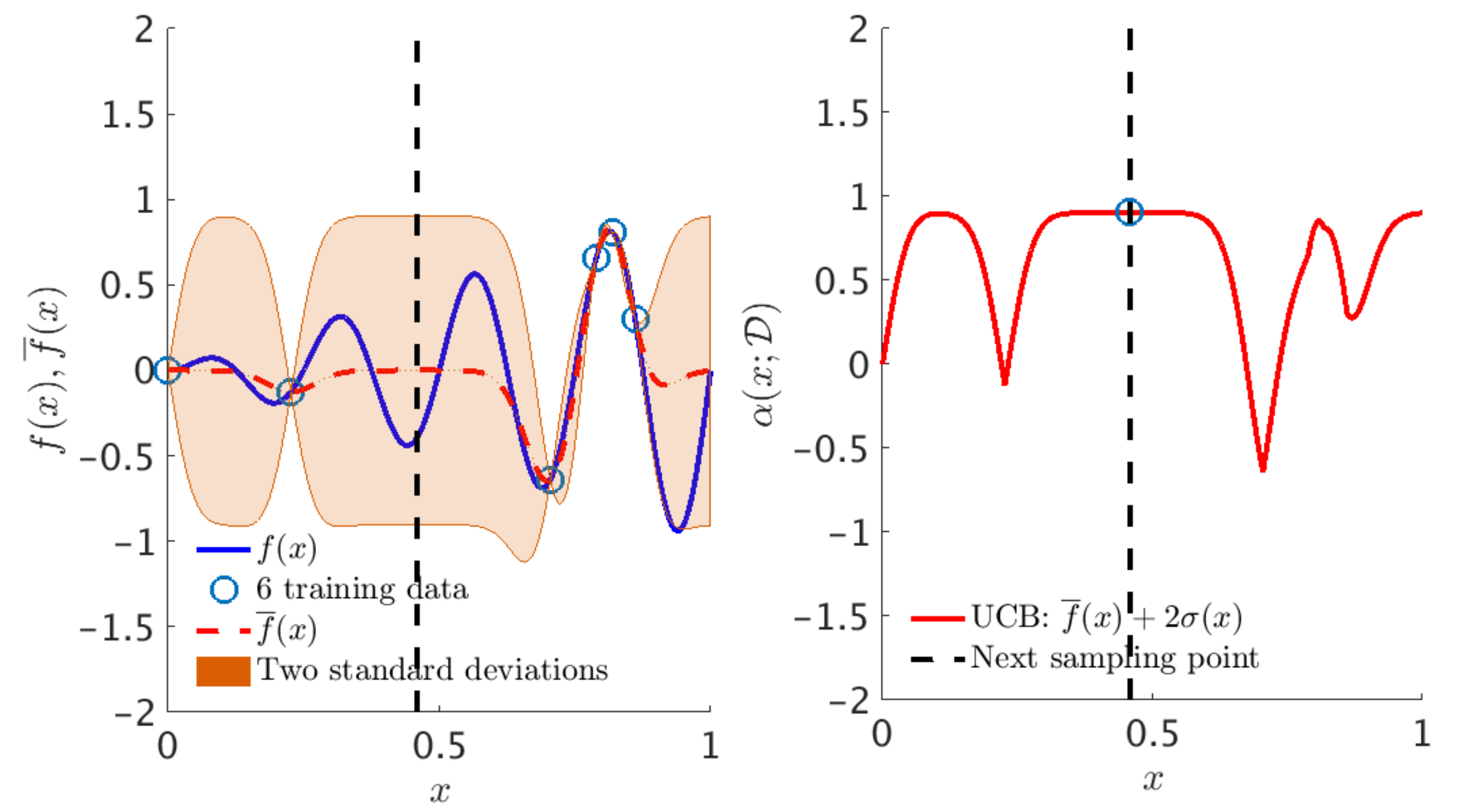
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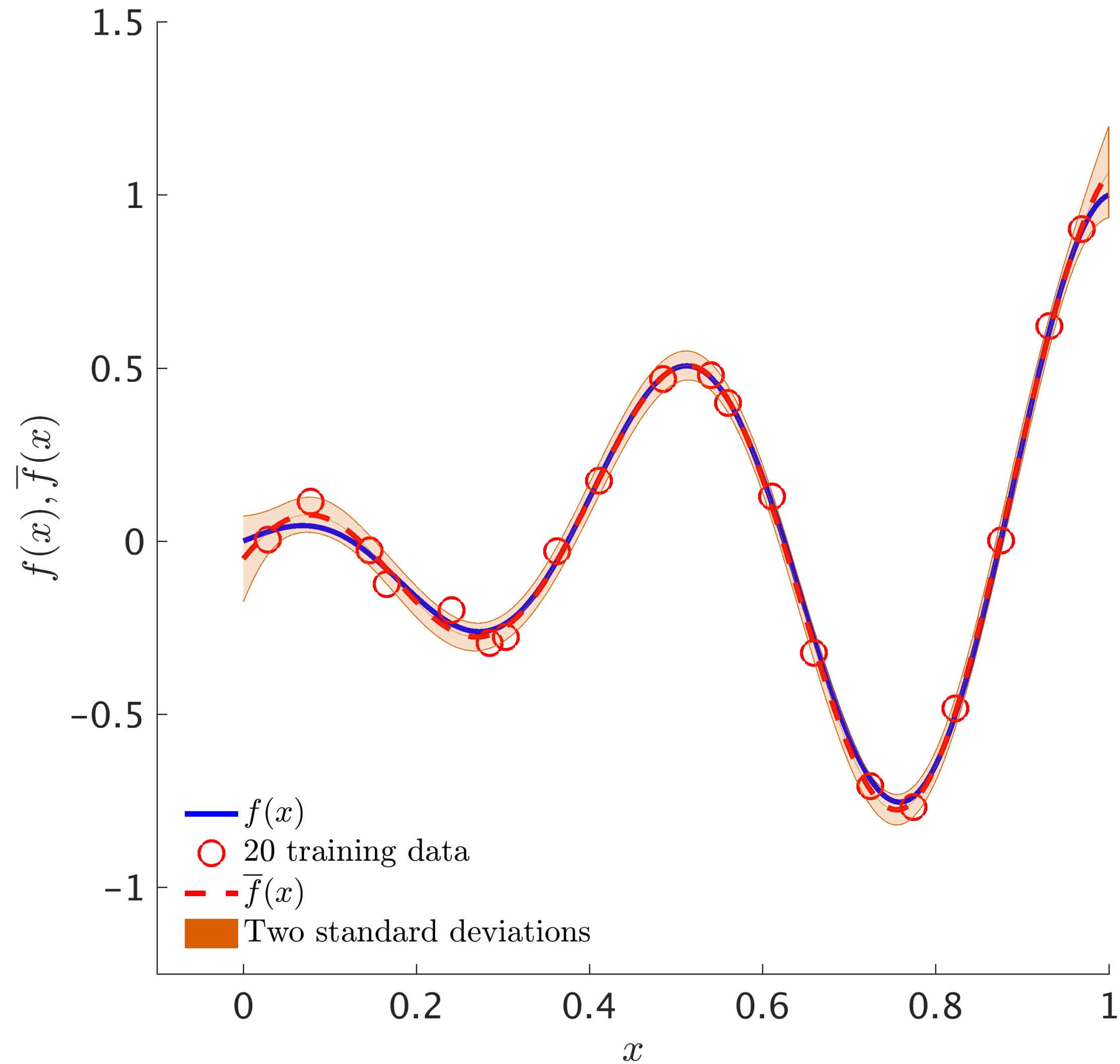


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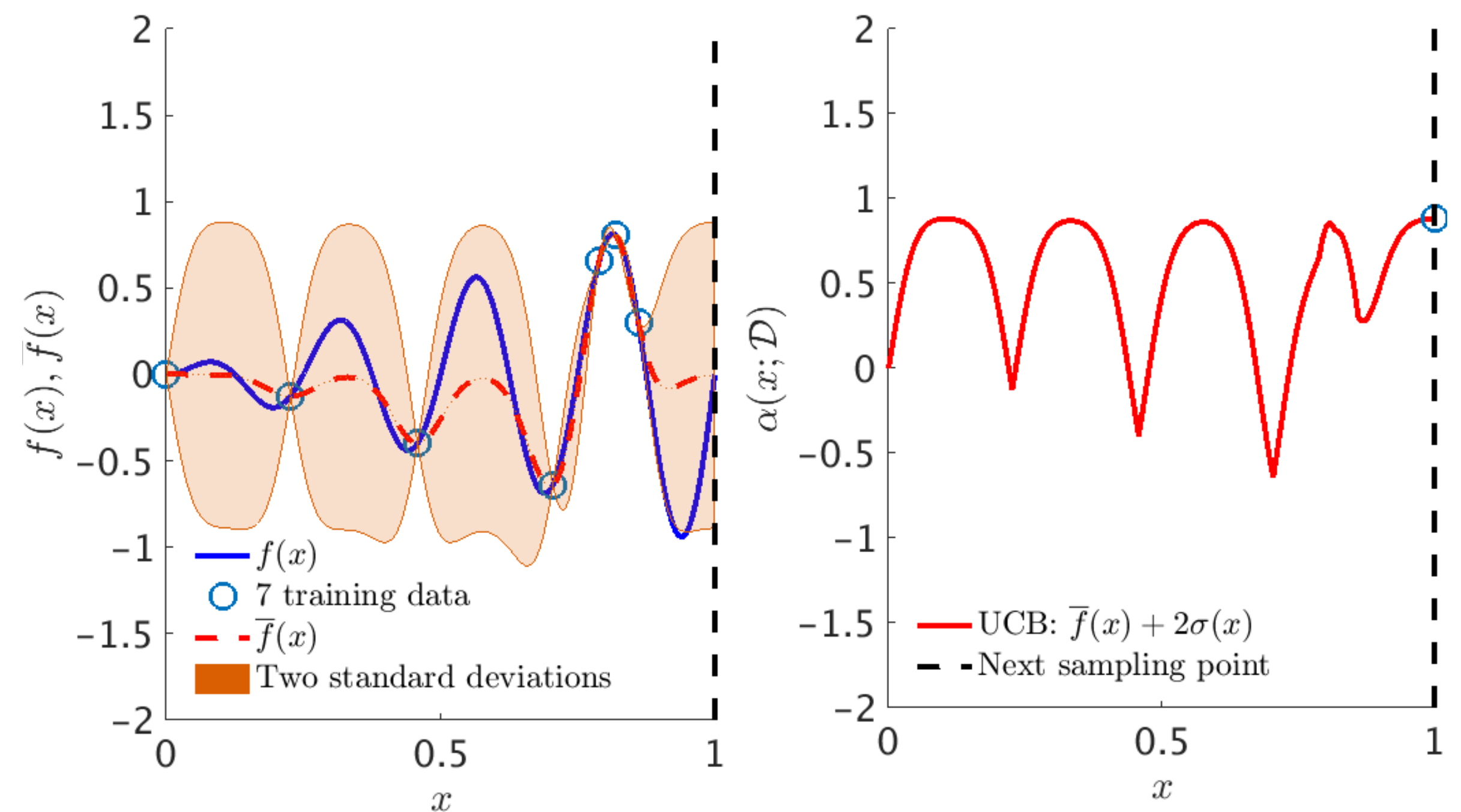


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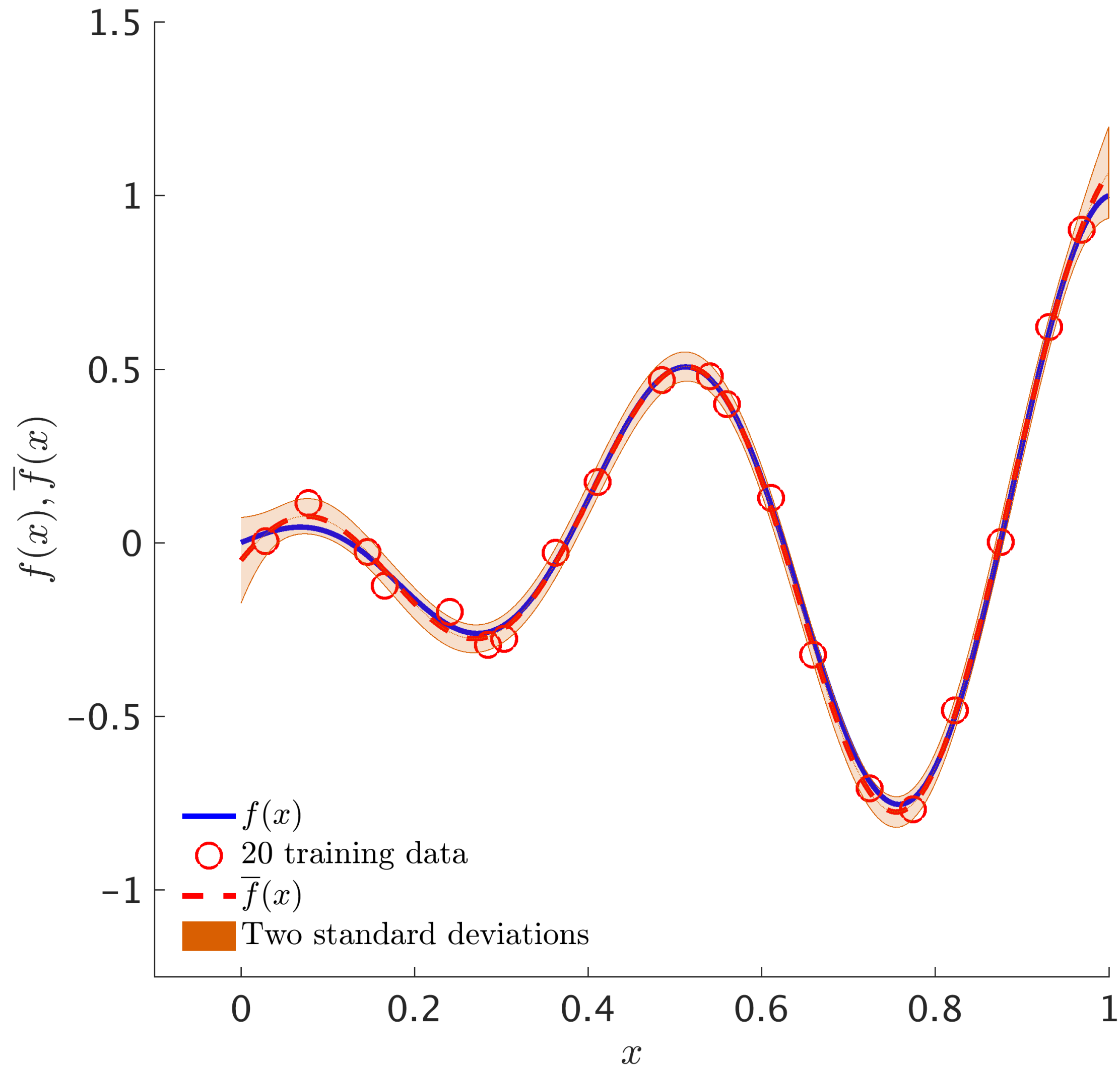


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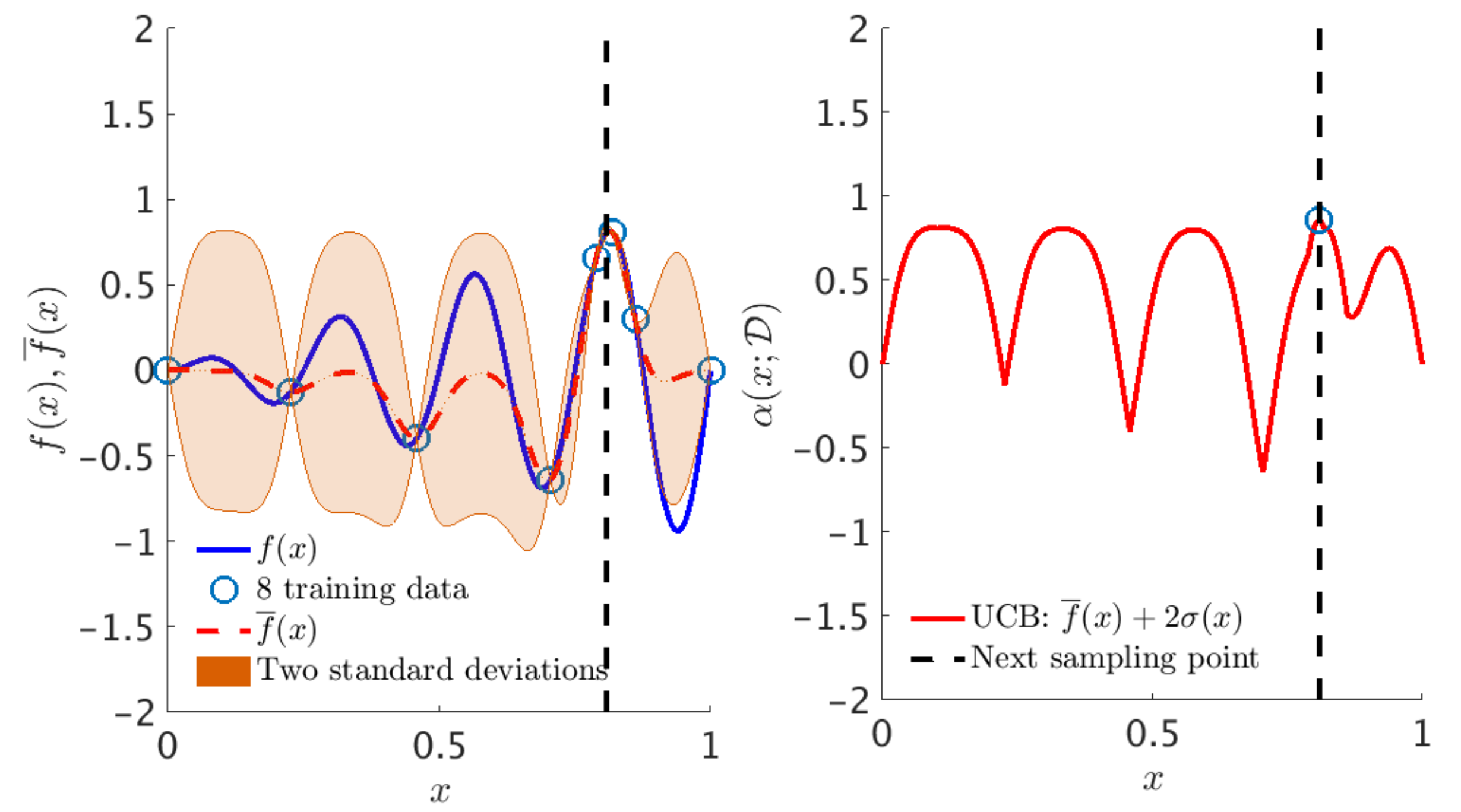


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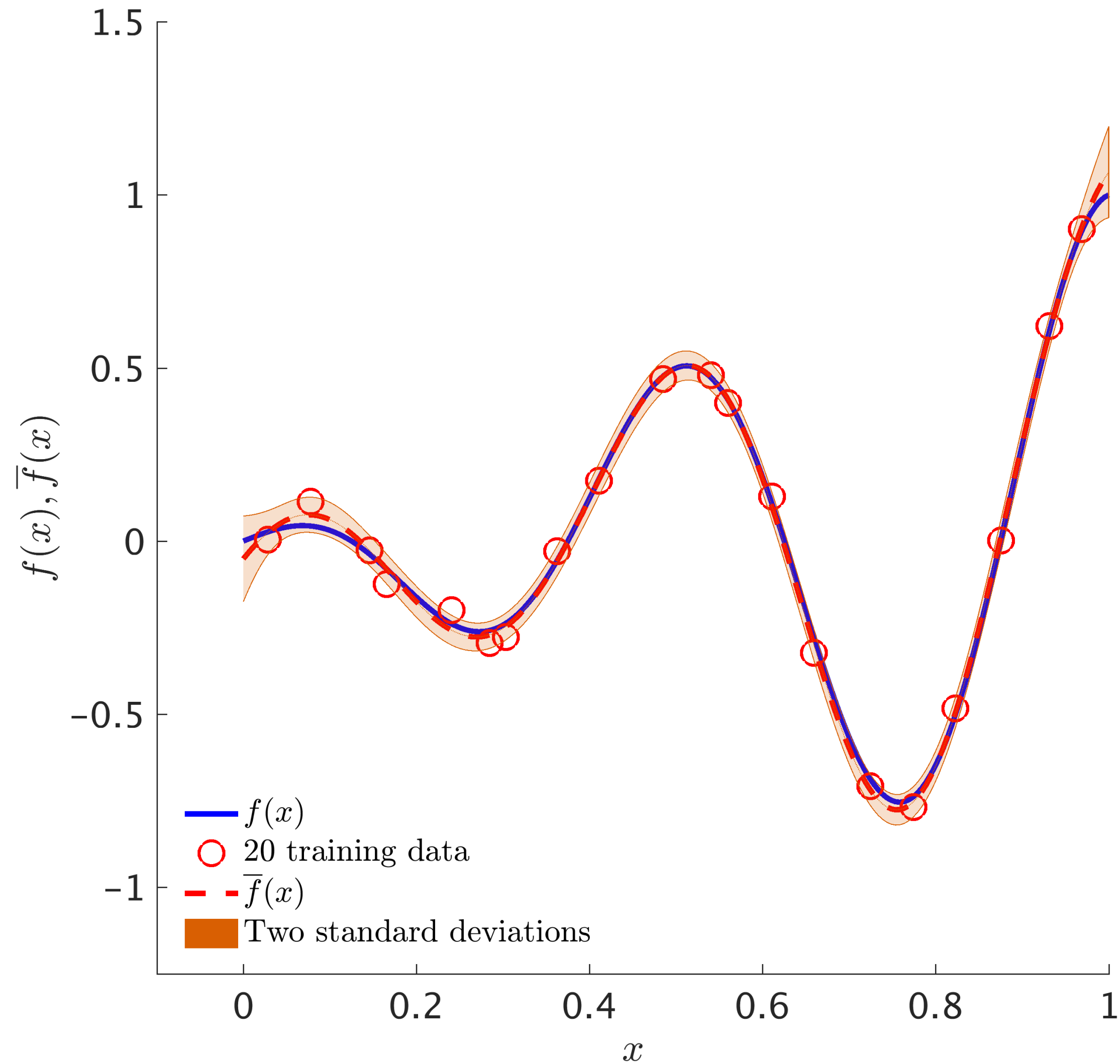


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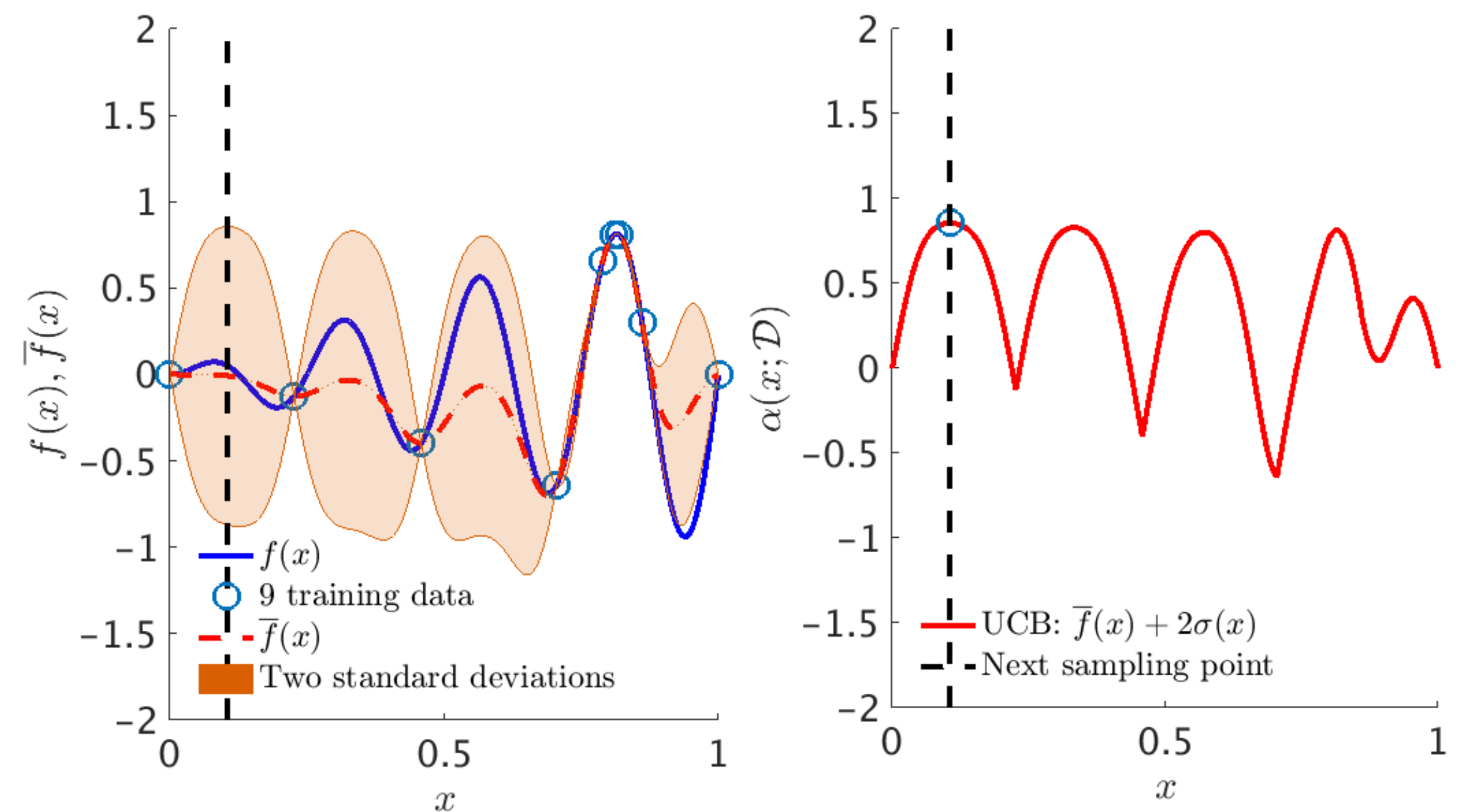


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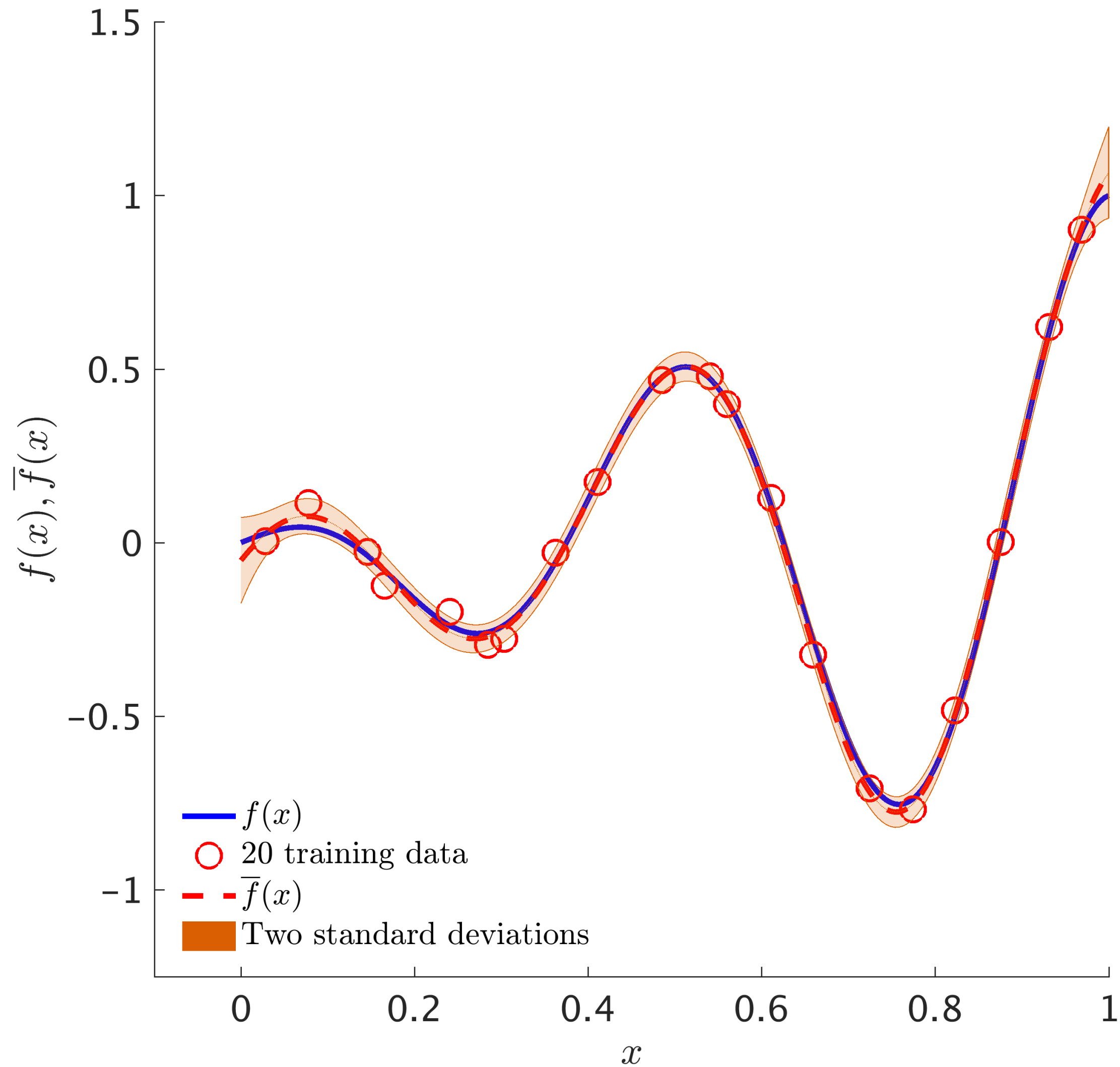


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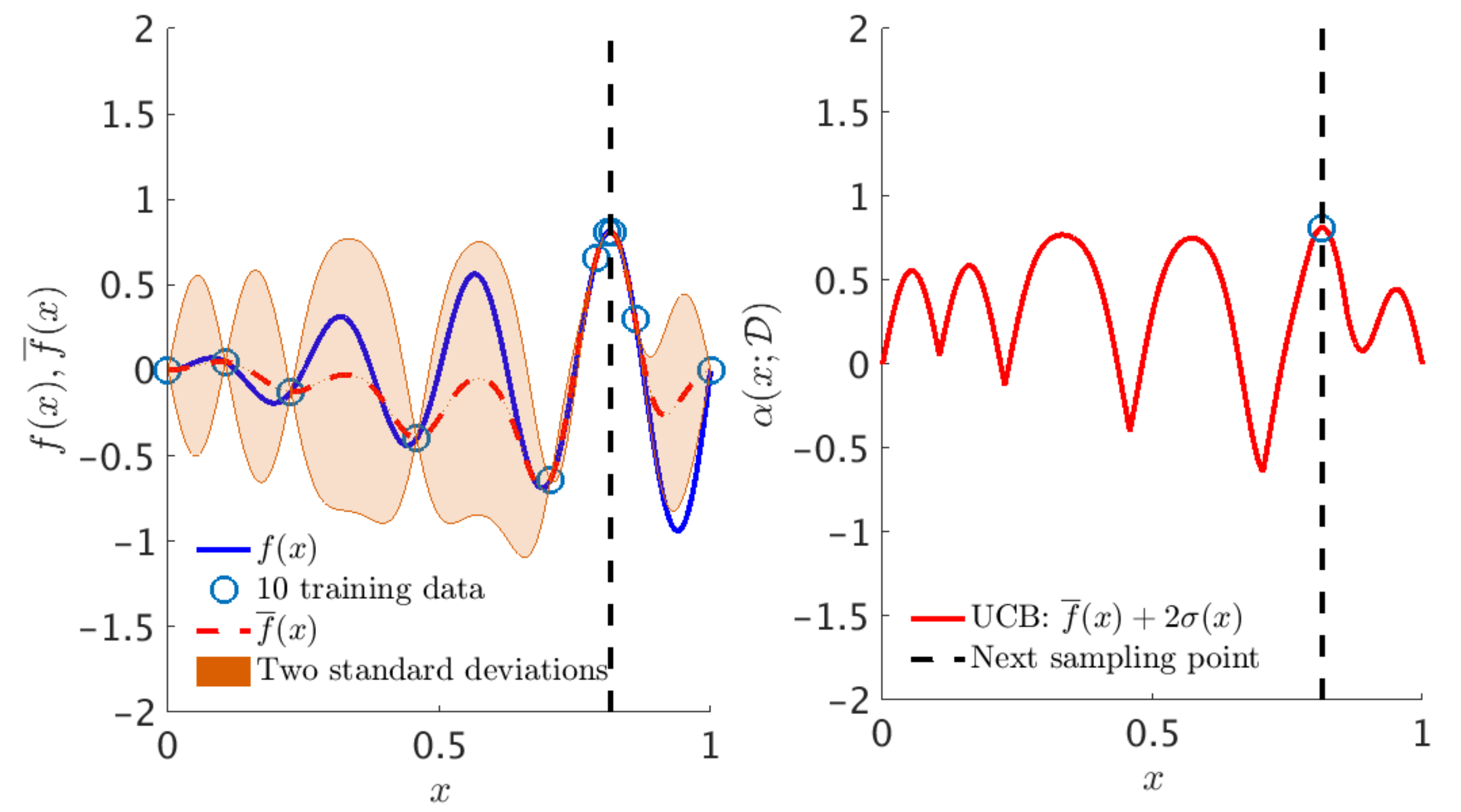


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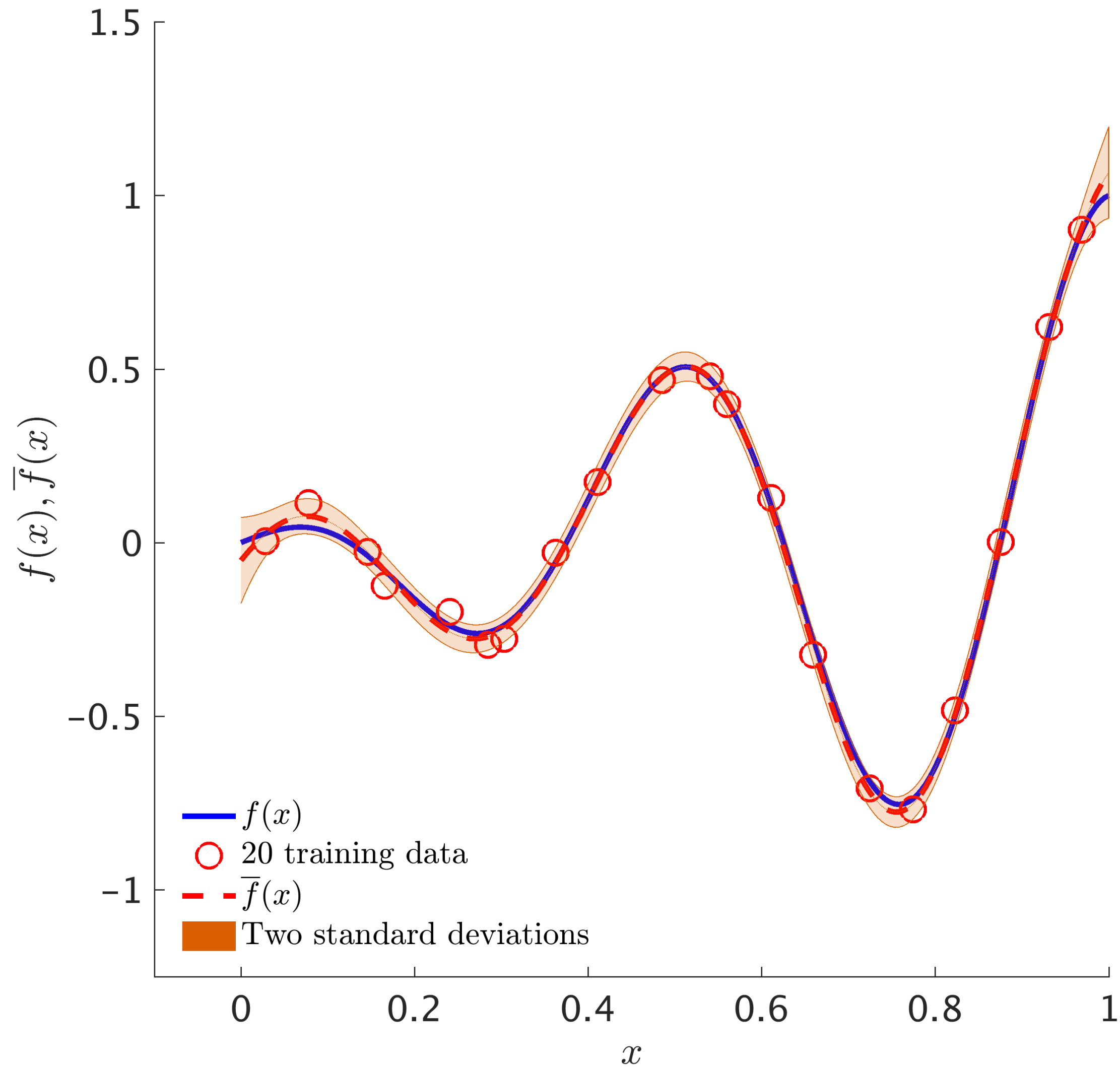


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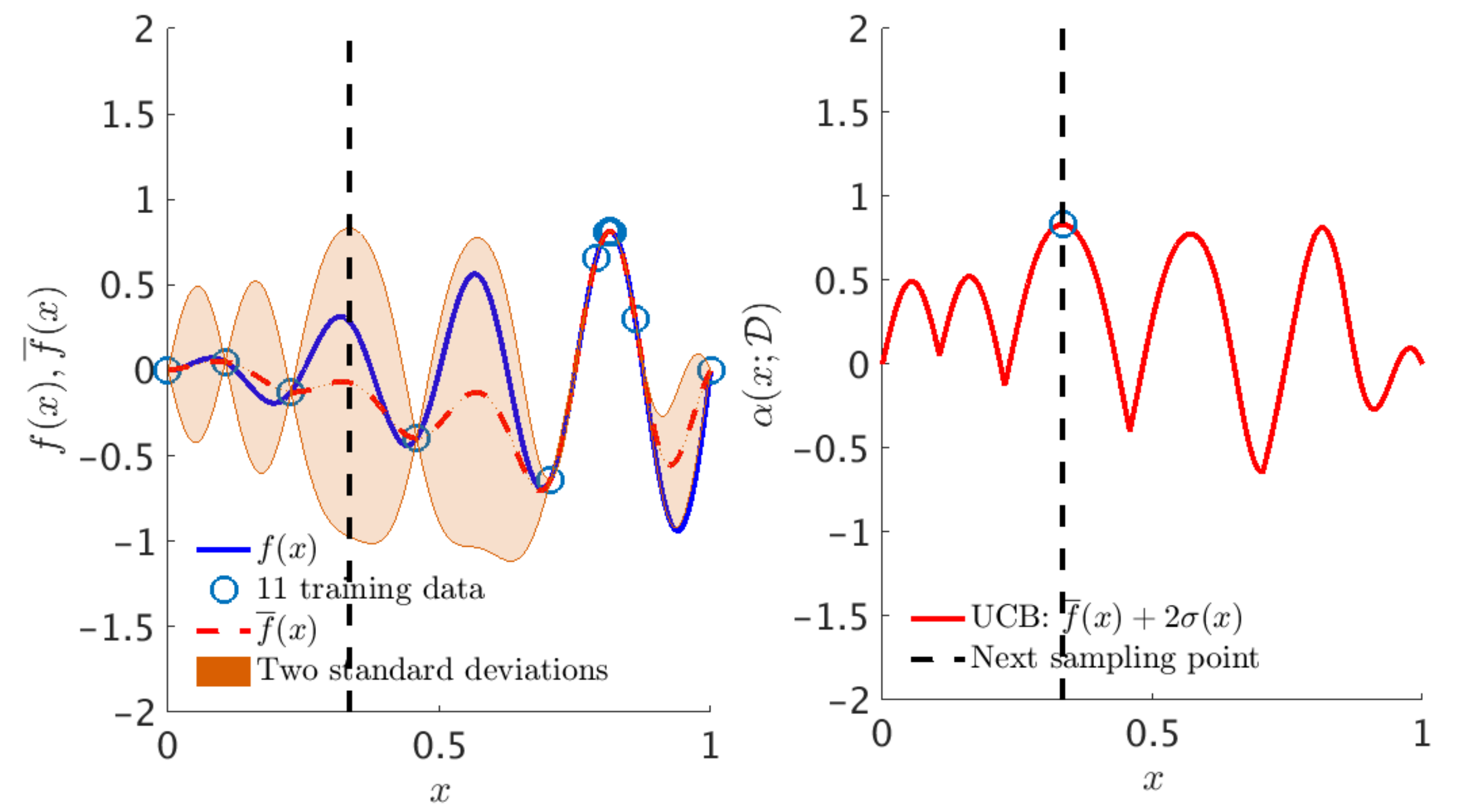


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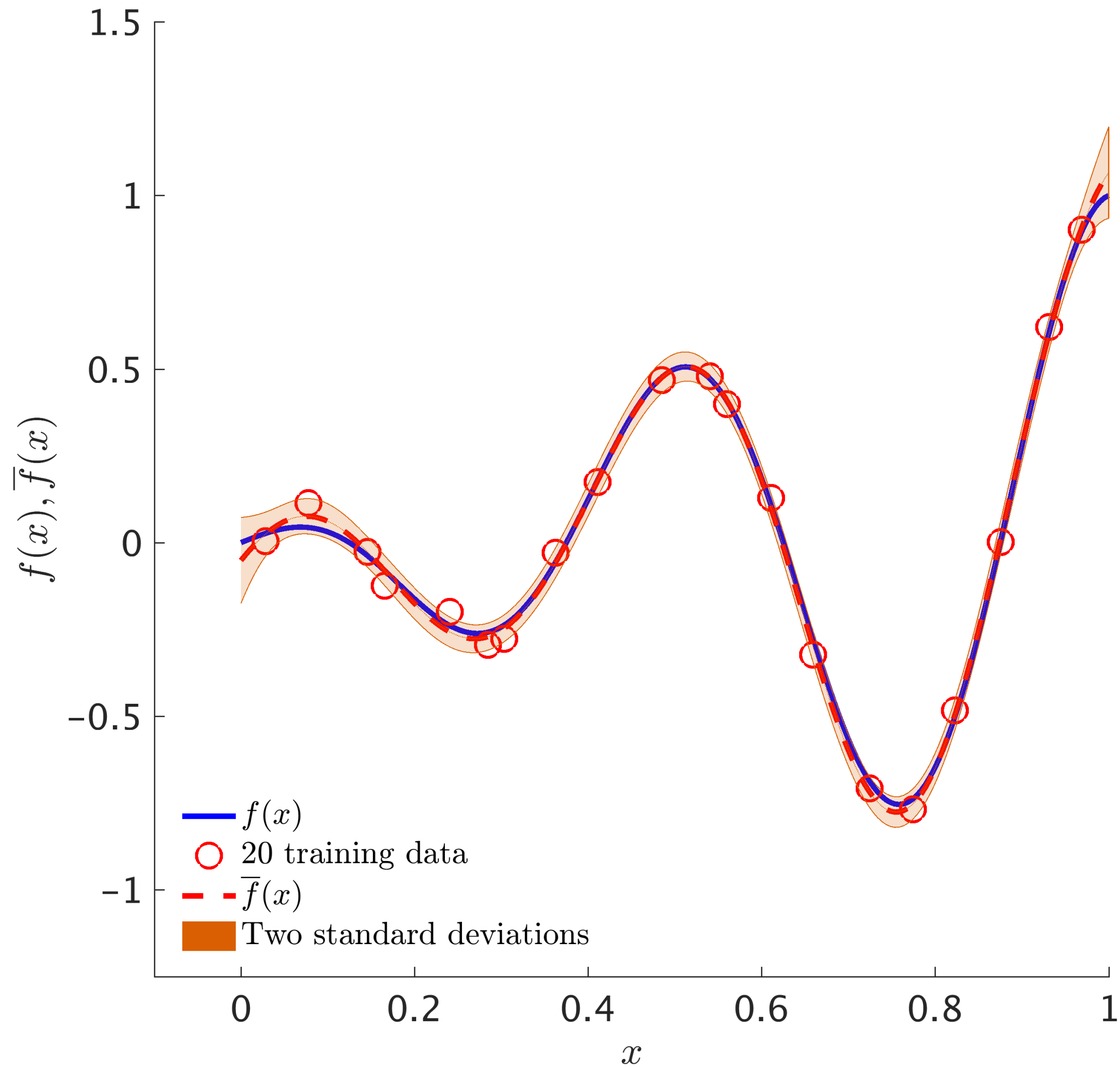


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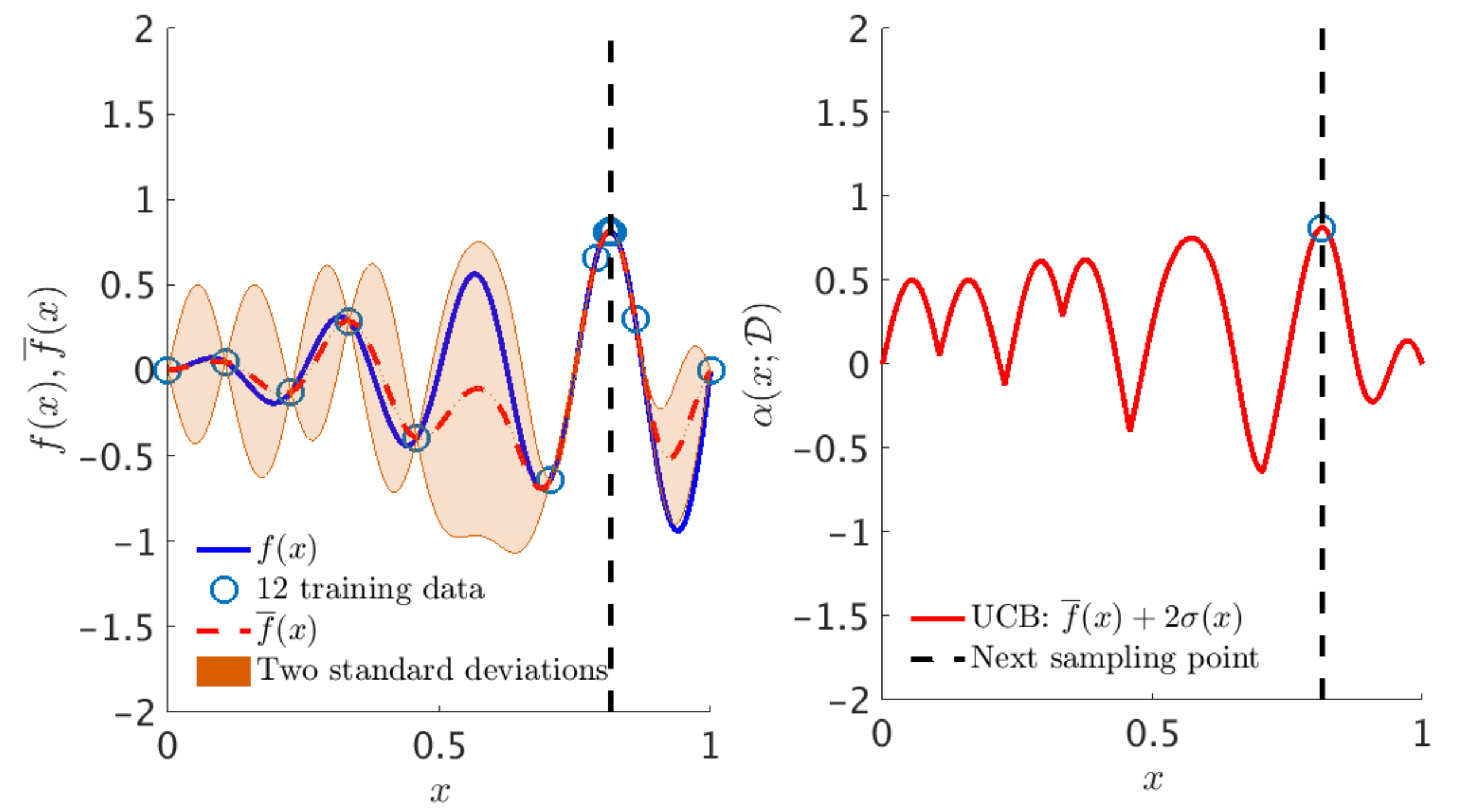


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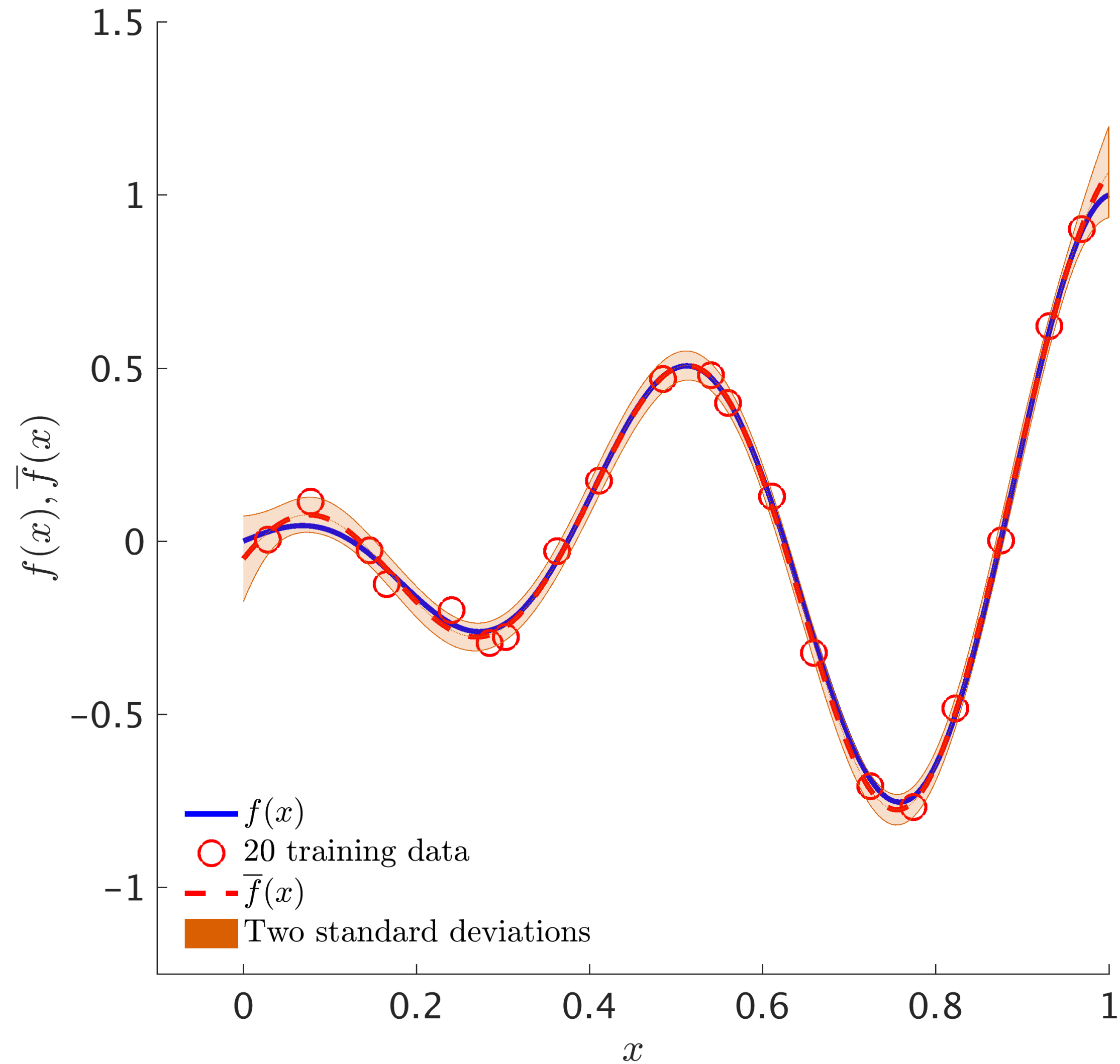


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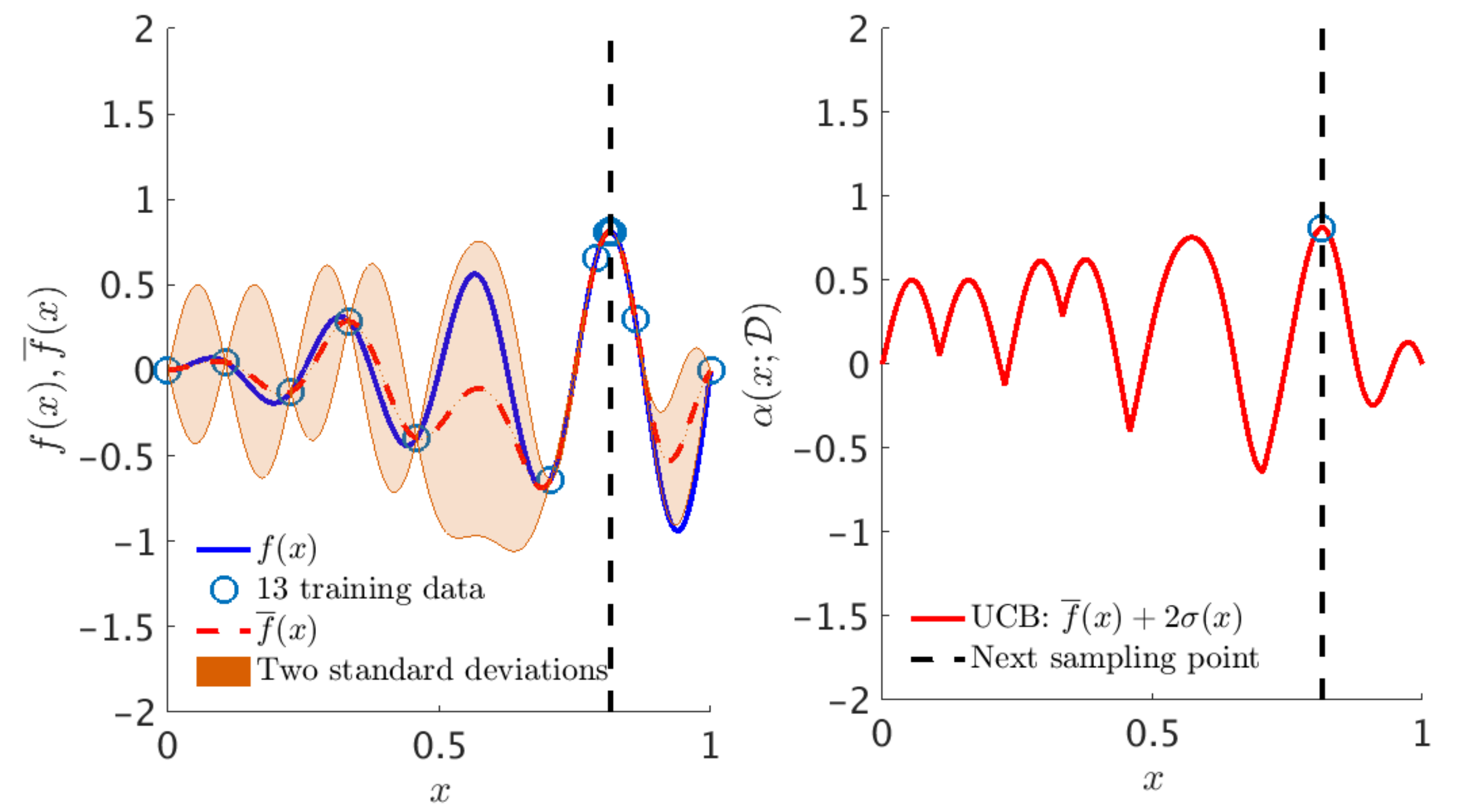


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# Gaussian Process Regression



## Bayesian Optimization



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# Multi-fidelity Modeling

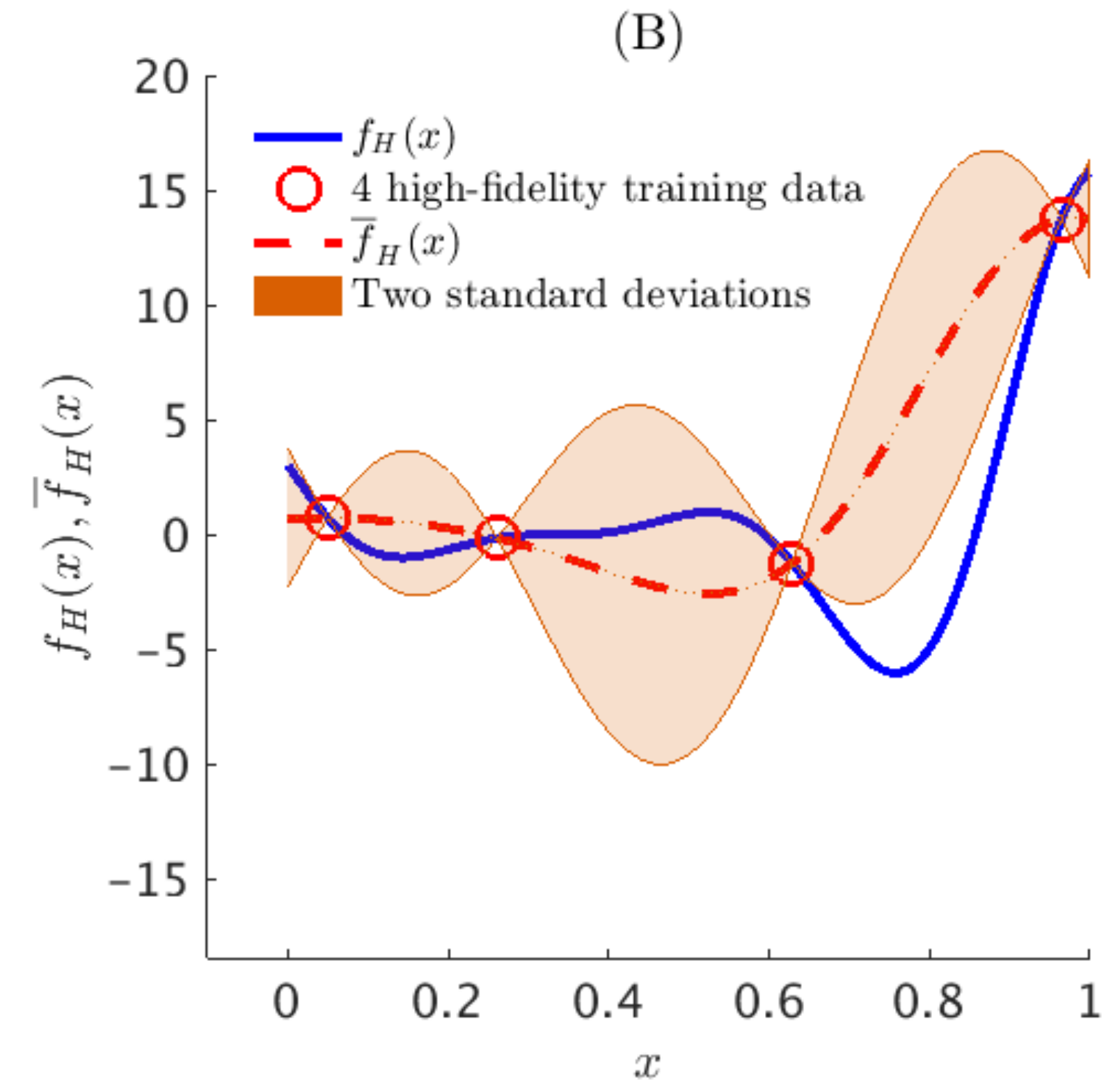
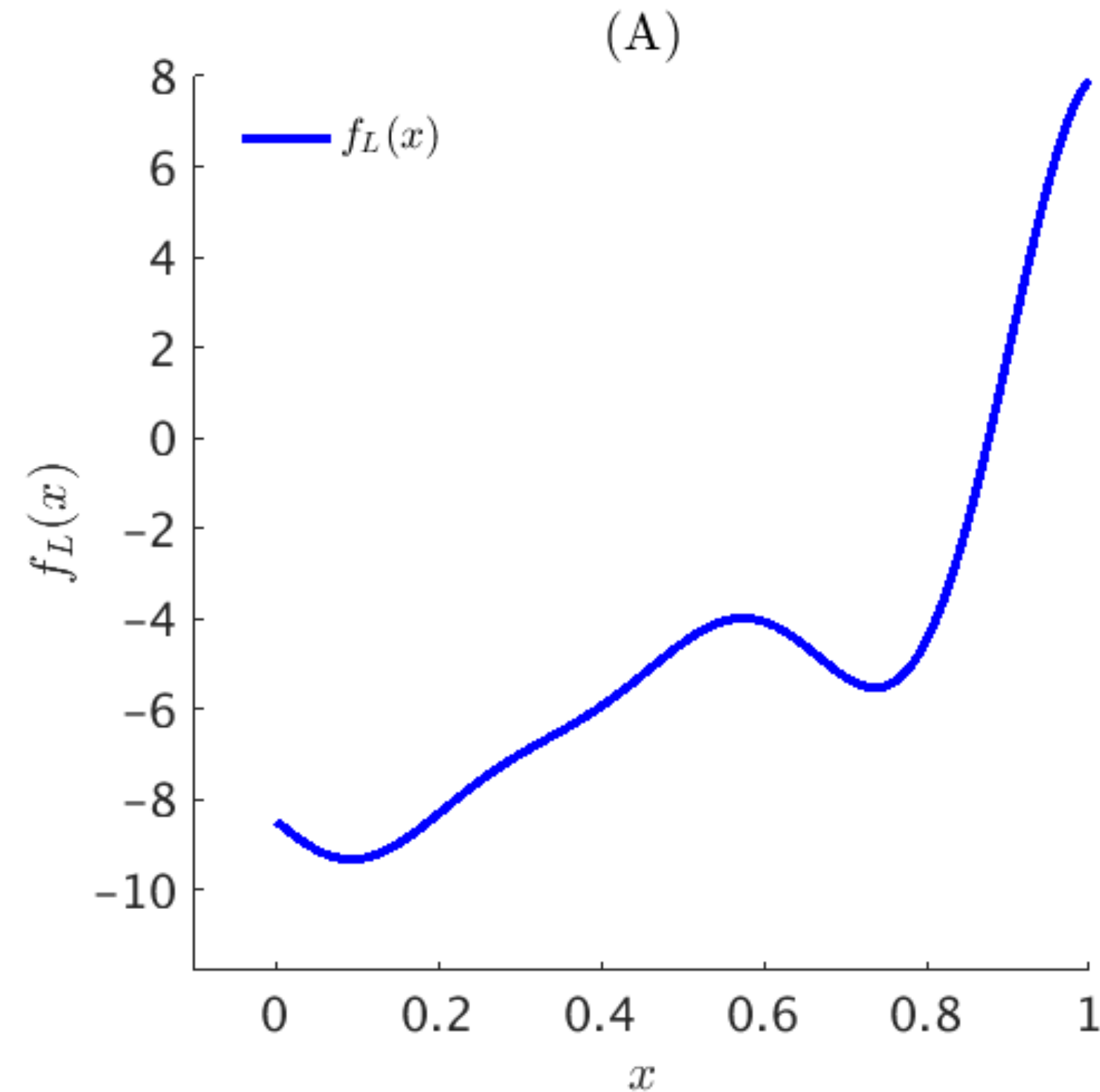
$$f_H(x) = \rho f_L(x) + \delta(x),$$

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

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

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

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



# Multi-fidelity Modeling

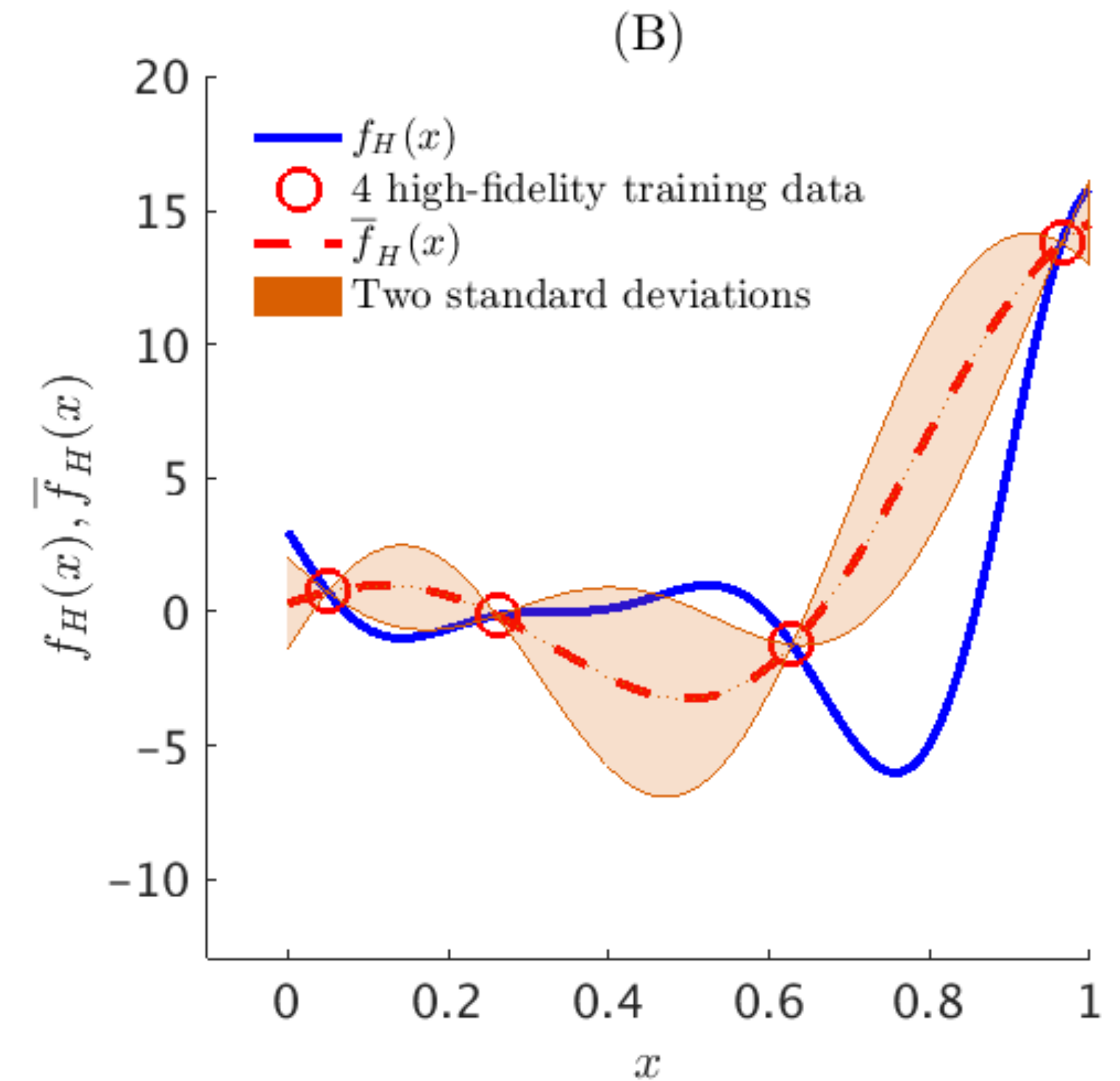
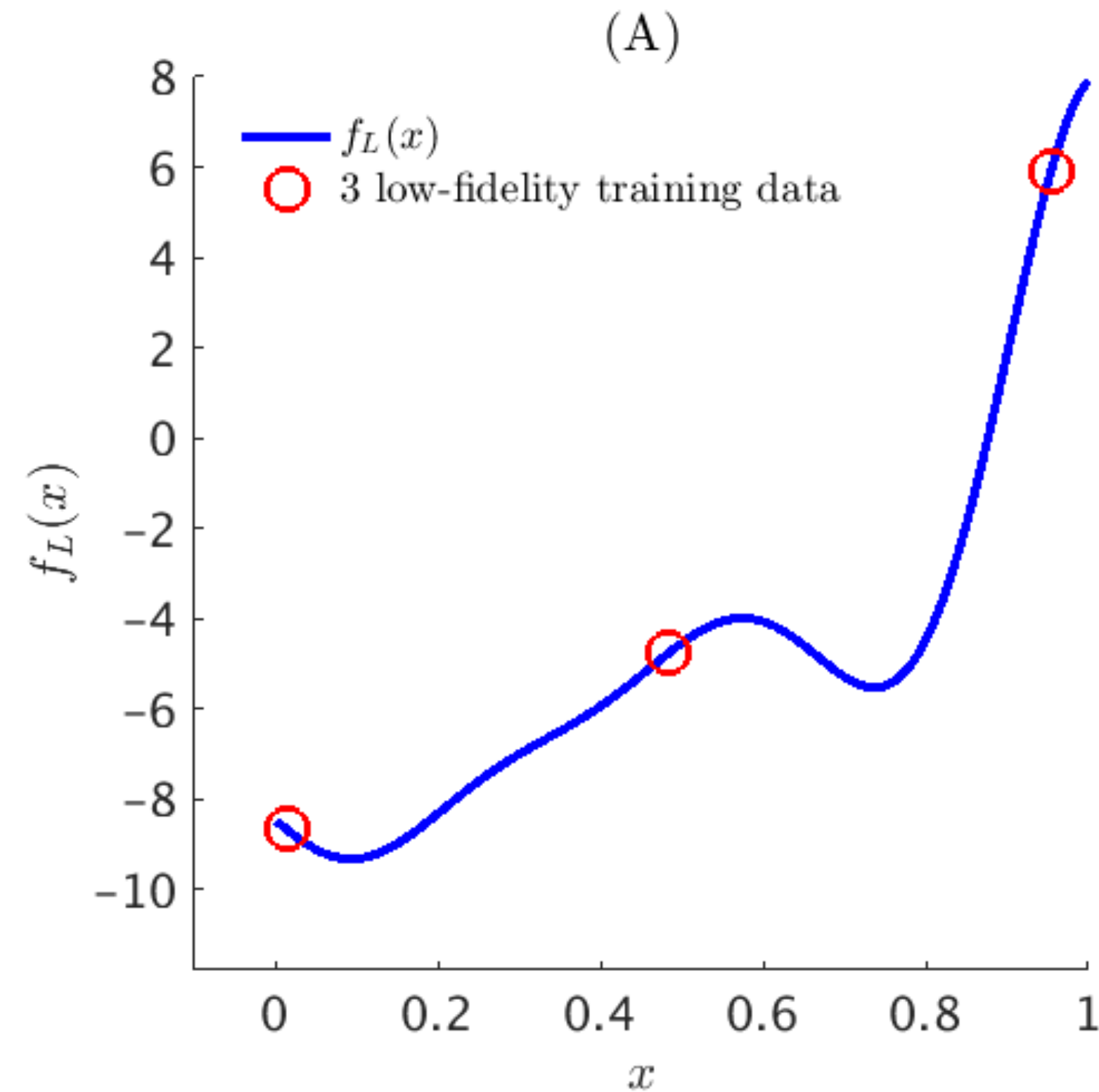
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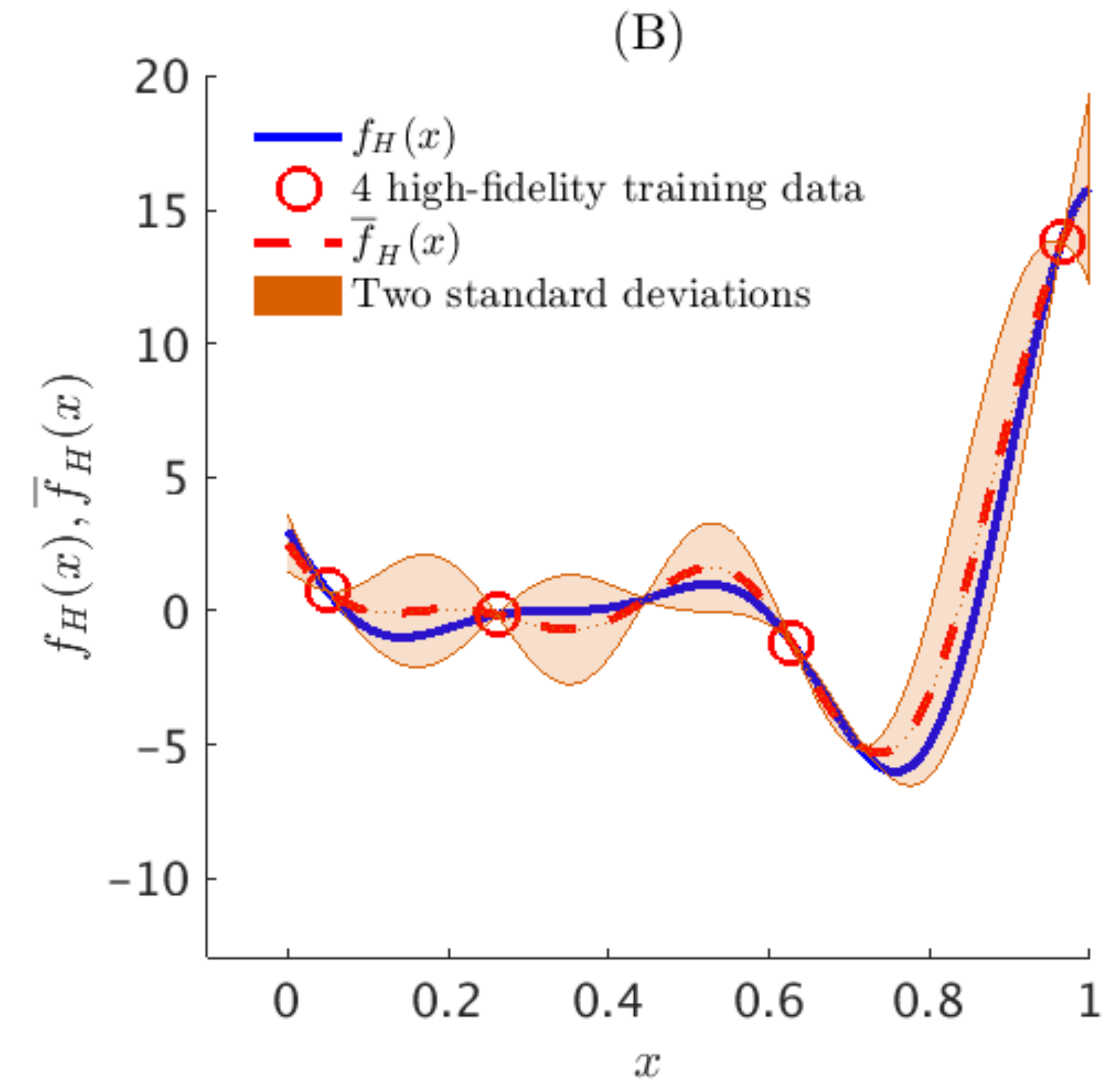
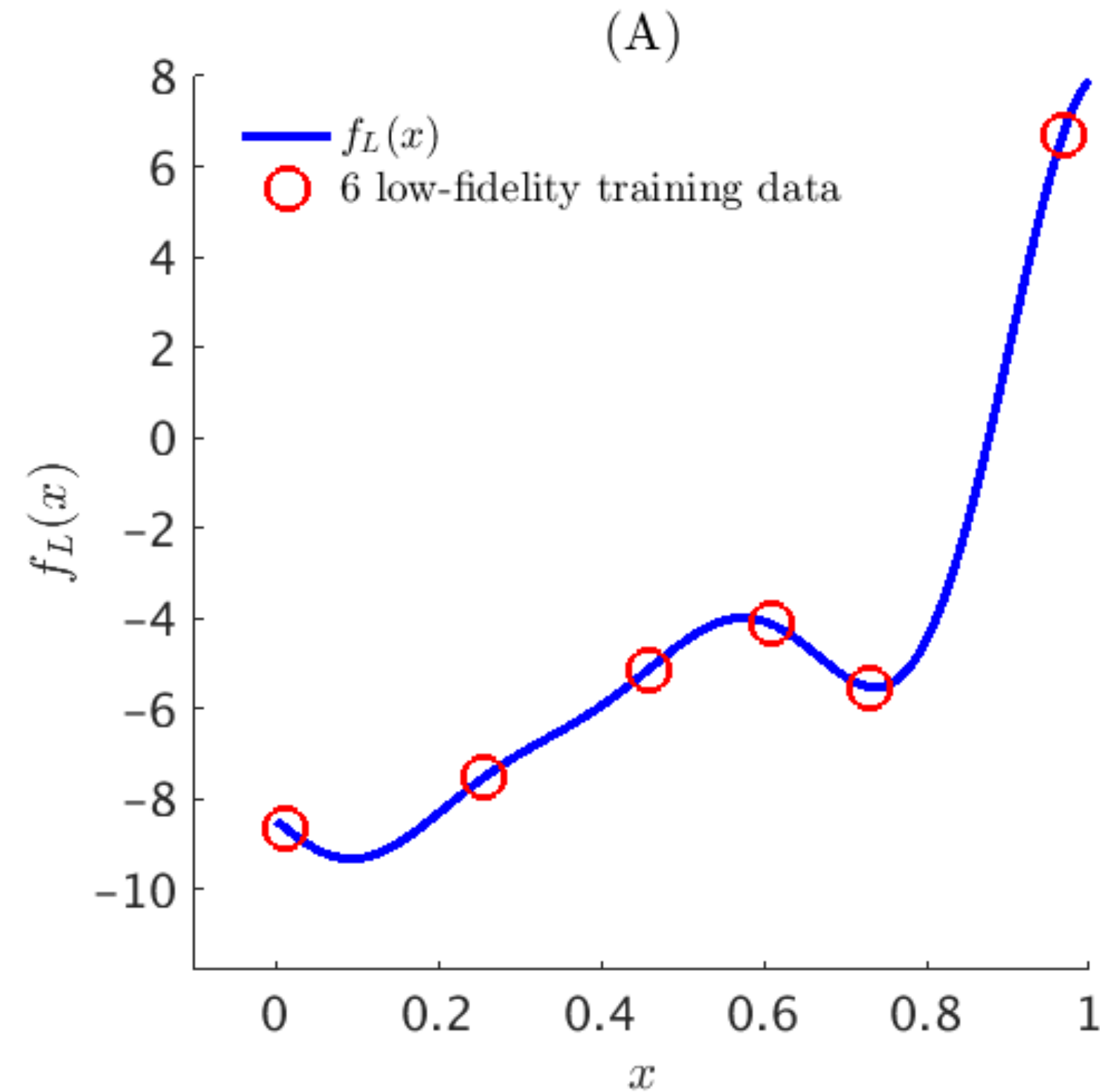
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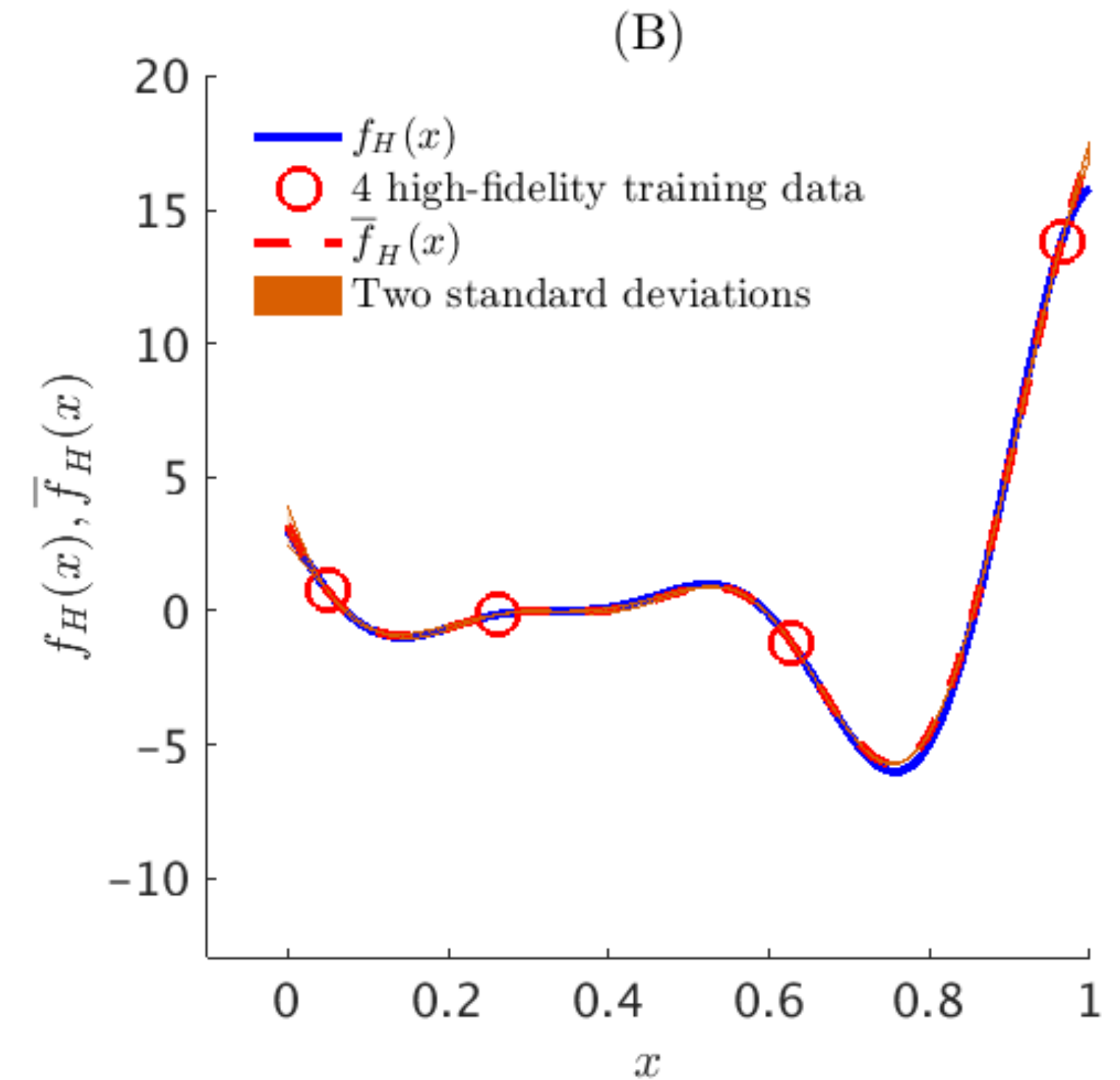
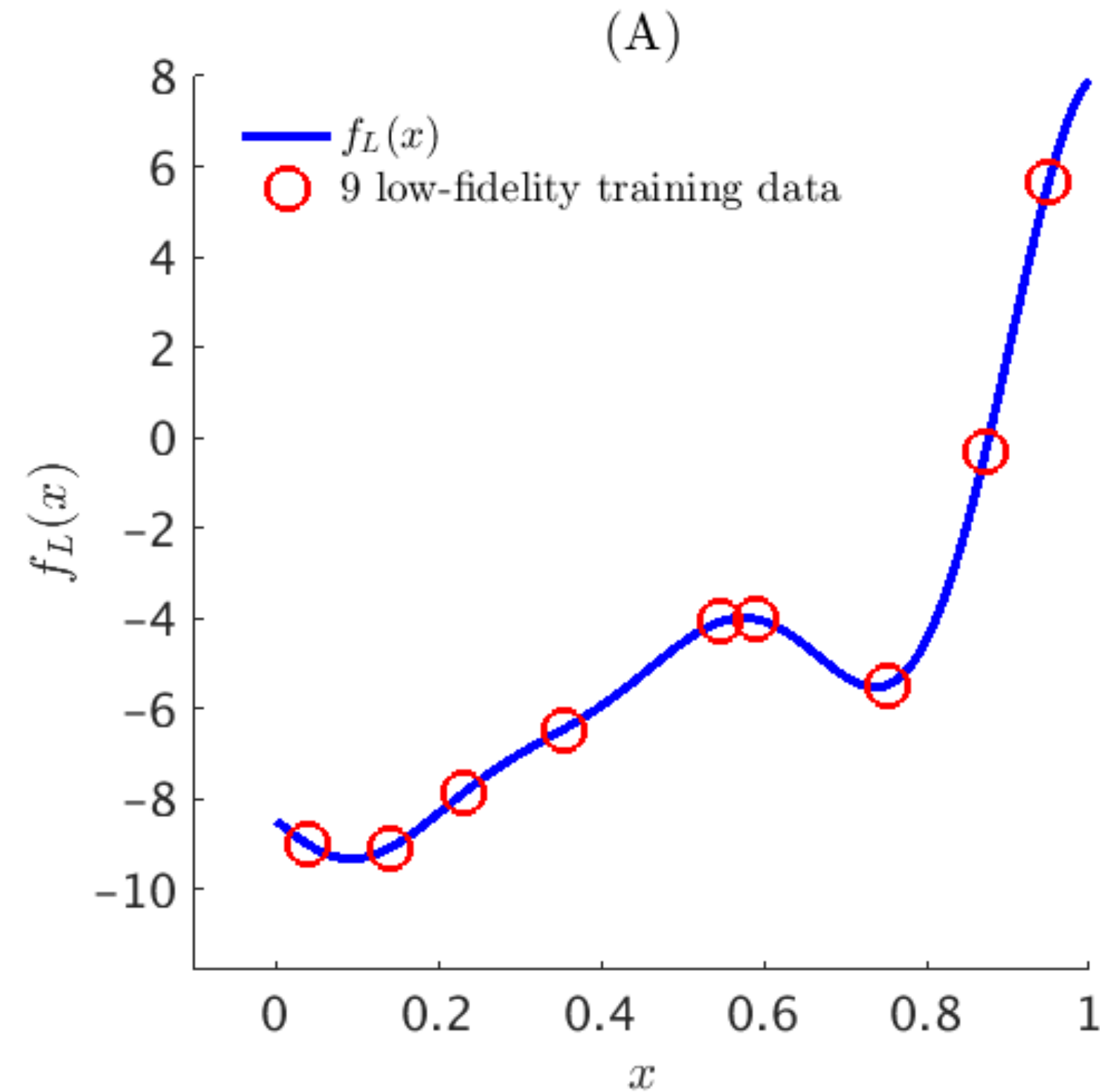
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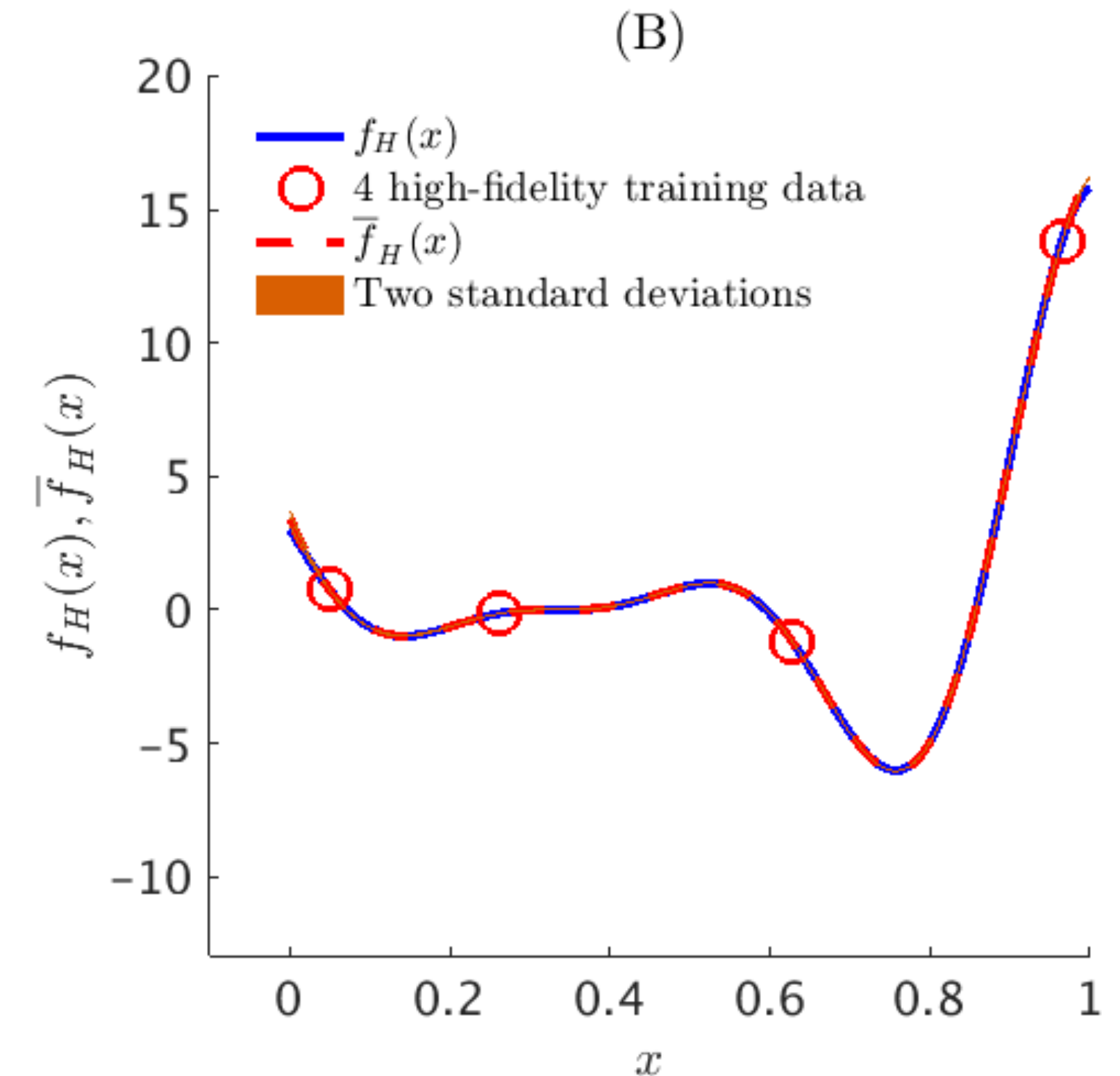
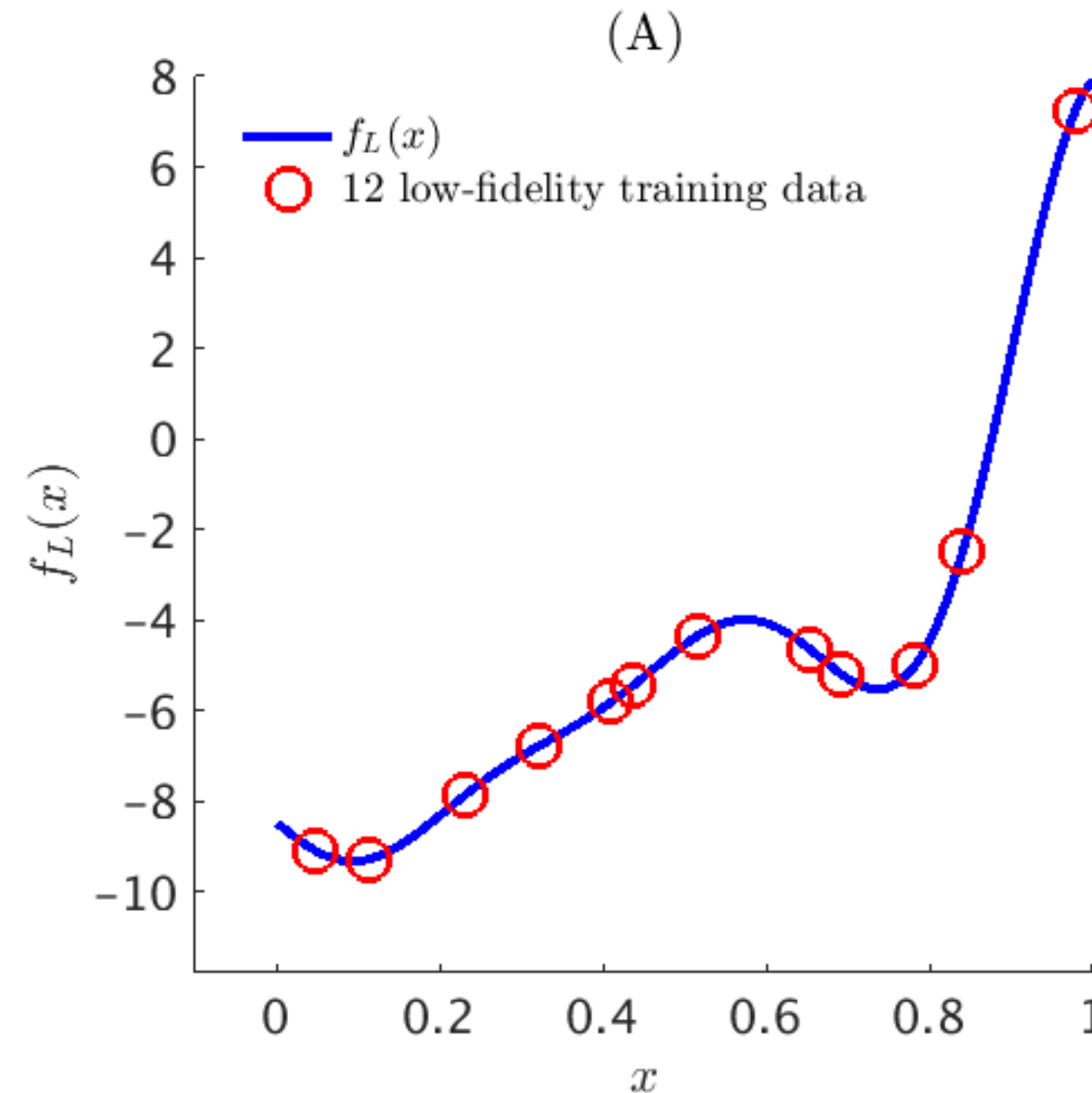
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# Multi-fidelity Modeling

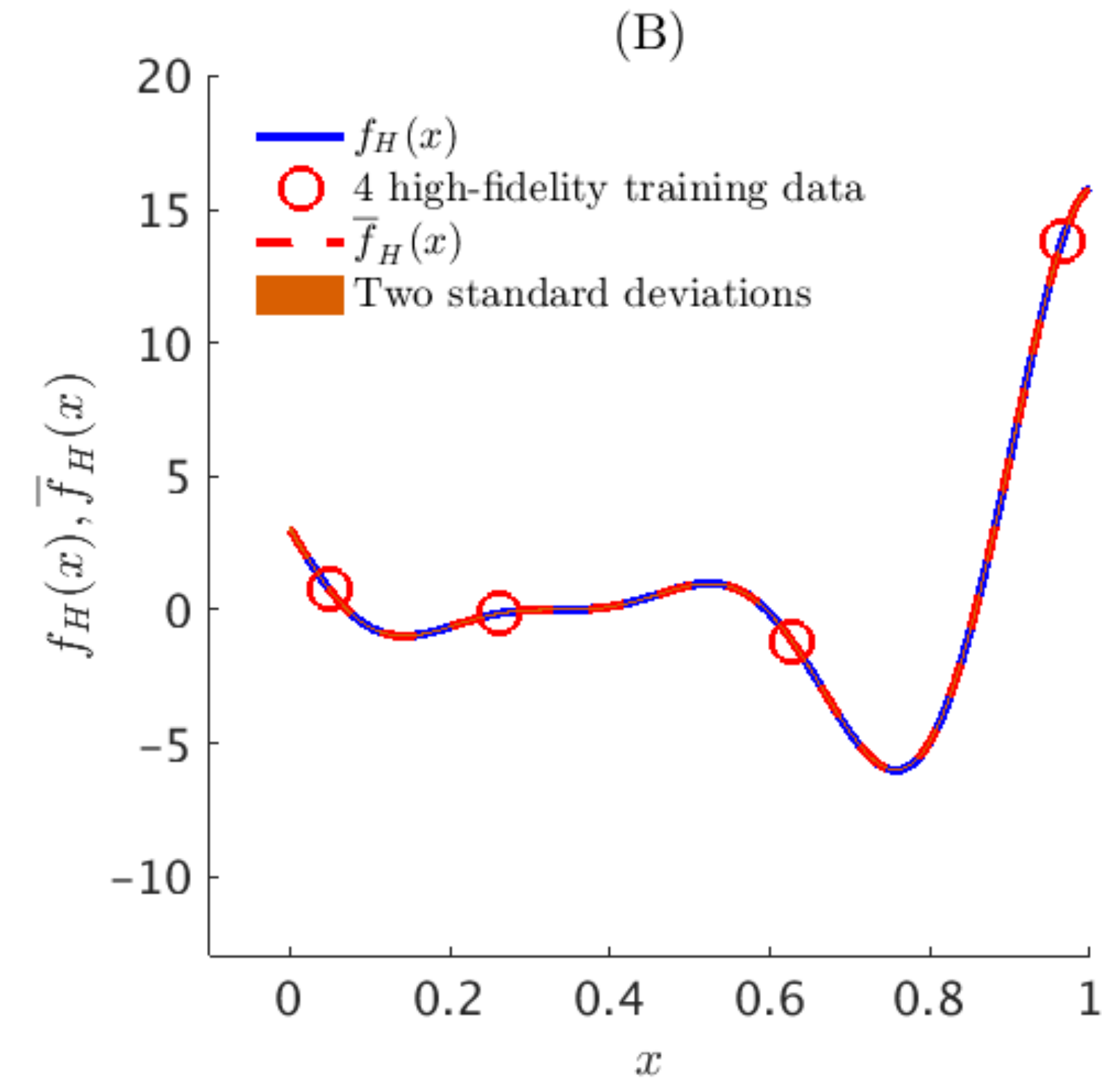
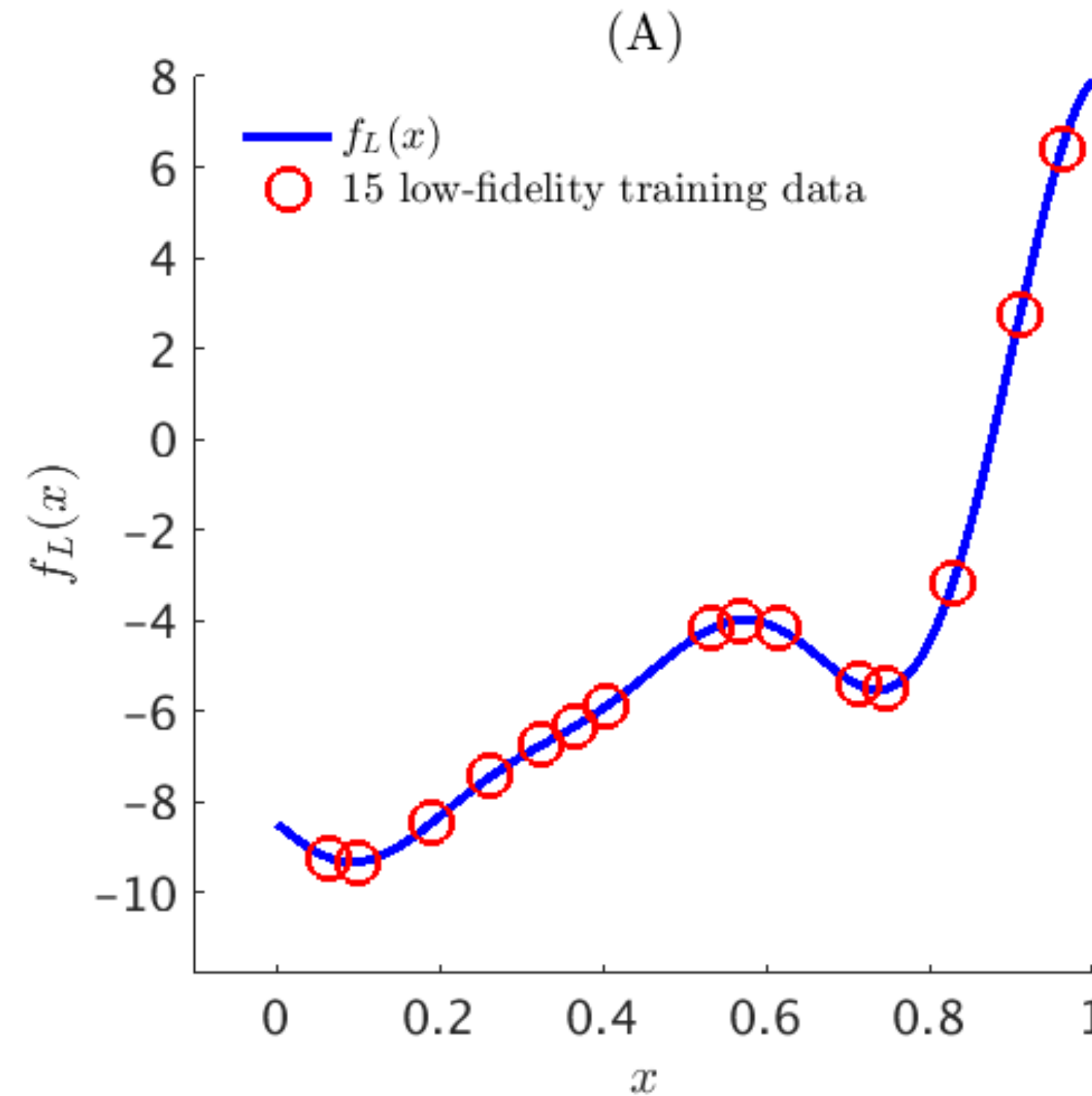
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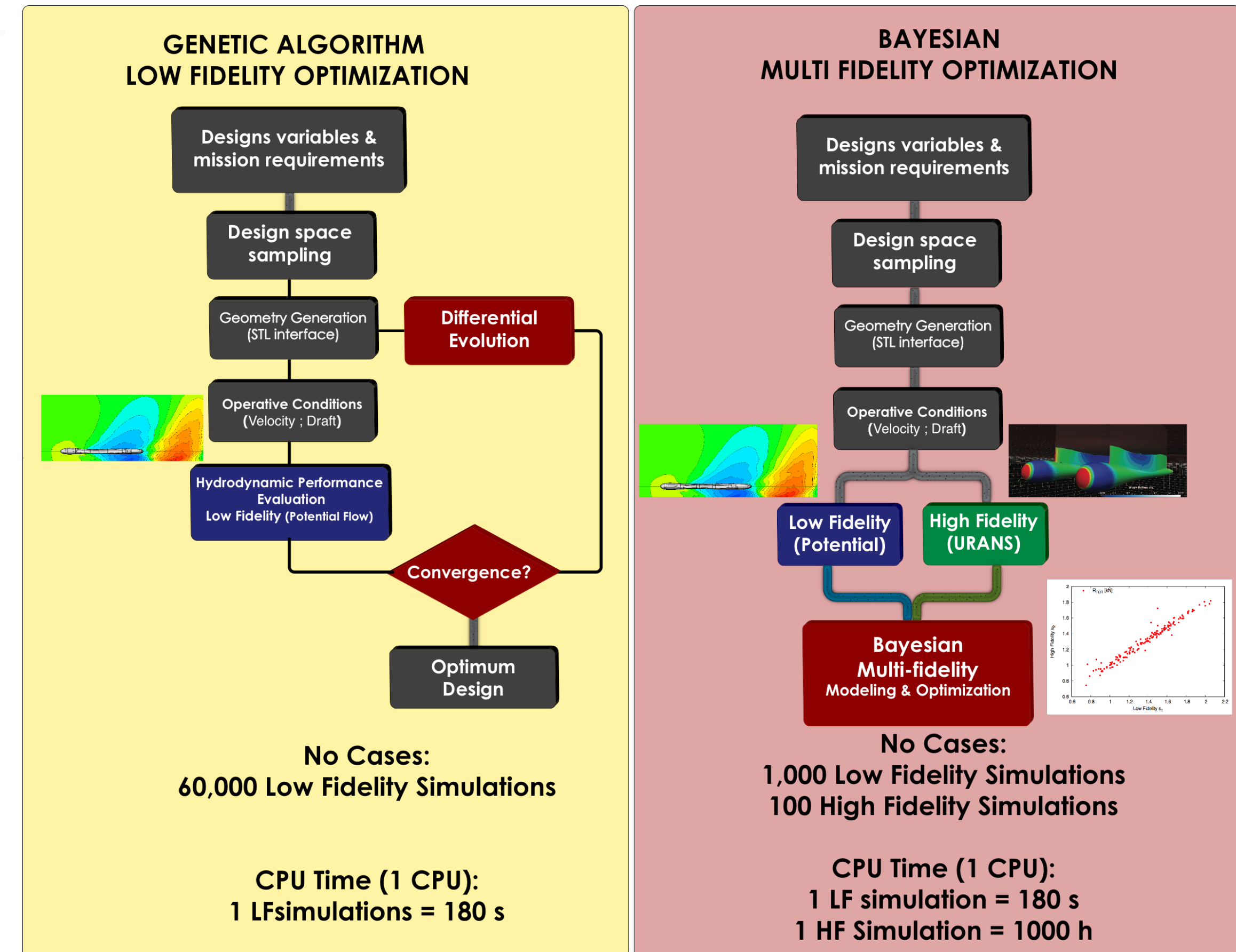
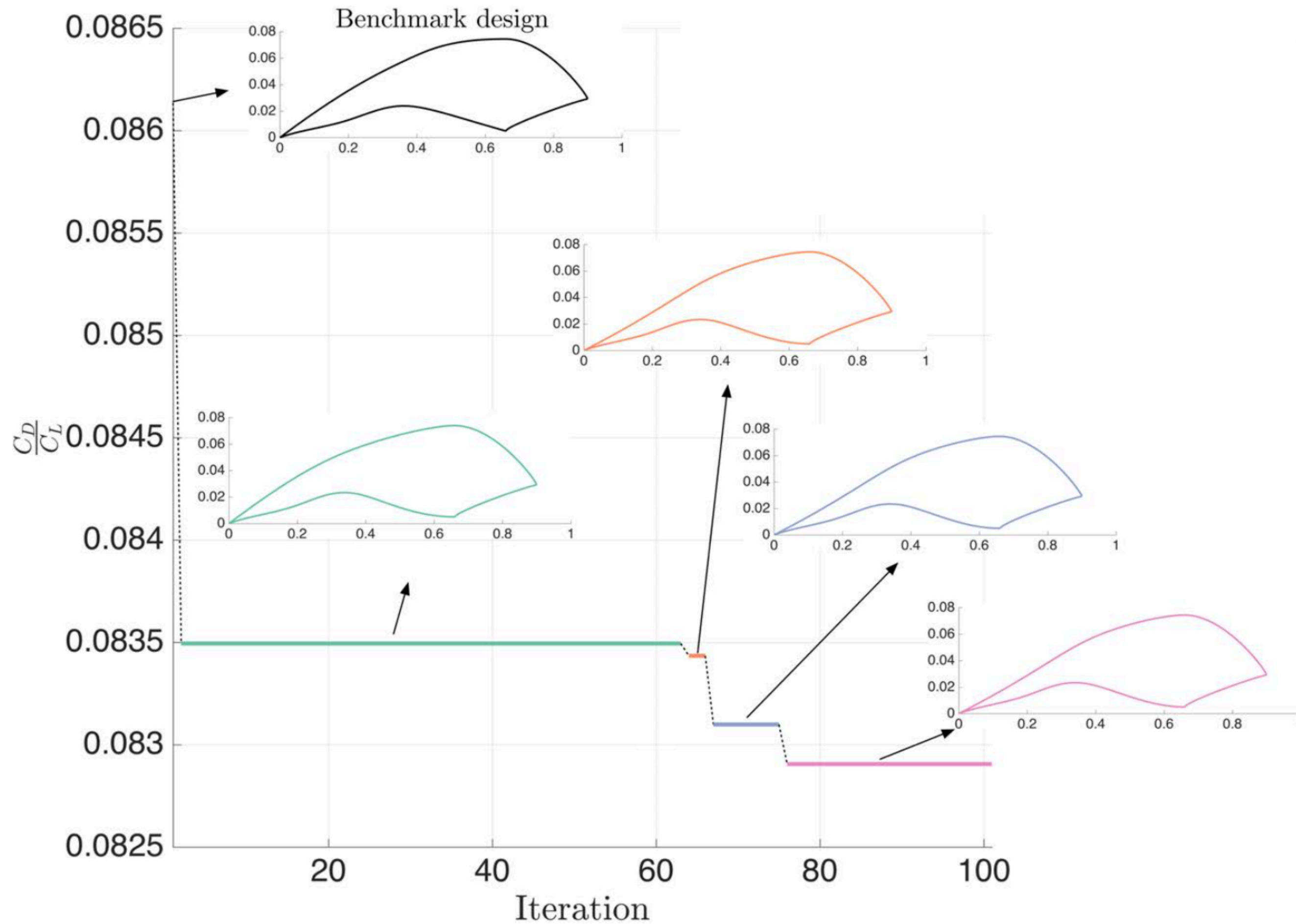
$$\begin{bmatrix} f_H \\ f_L \end{bmatrix} \sim \mathcal{GP} \left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} k_{HH} & k_{HL} \\ k_{LH} & k_{LL} \end{bmatrix} \right),$$

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



# Multi-fidelity Bayesian Optimization

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



# Numerical Gaussian Processes

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

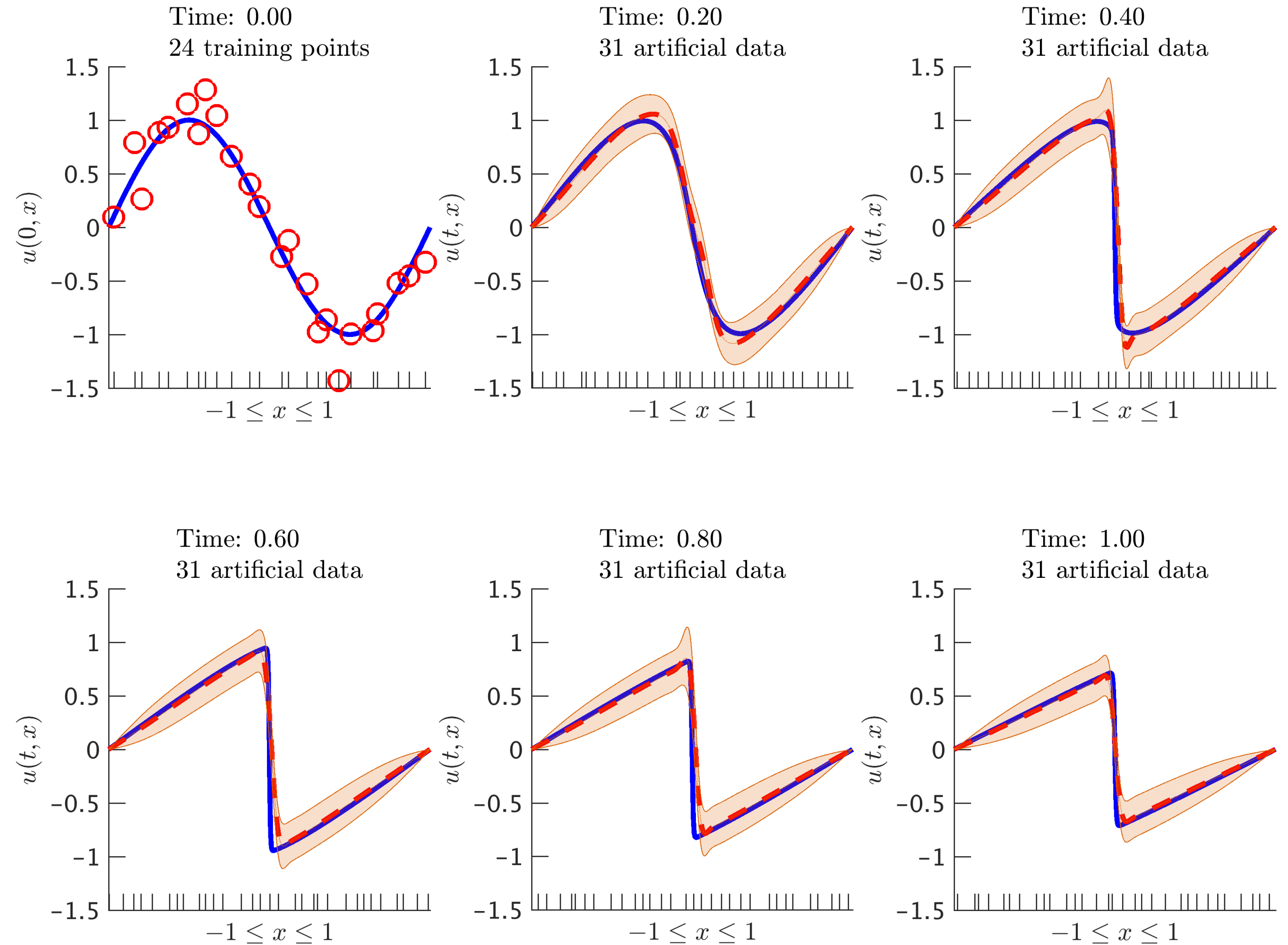
$$u^n + \Delta t (u^{n-1}u_x^n - (0.01/\pi)u_{xx}^n) = u^{n-1}$$

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

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

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

Physics Informed Prior





# Numerical Gaussian Processes

$$\begin{aligned} \begin{bmatrix} \mathbf{u}^n \\ \mathbf{u}^{n-1} \end{bmatrix} &\sim \mathcal{N}(0, \mathbf{K}) \\ \mathbf{K} &= \begin{bmatrix} k^{n,n}(\mathbf{x}^n, \mathbf{x}^n; \theta) + \sigma_n^2 \mathbf{I} & k^{n,n-1}(\mathbf{x}^n, \mathbf{x}^{n-1}; \theta) \\ k^{n-1,n}(\mathbf{x}^{n-1}, \mathbf{x}^n; \theta) & k^{n-1,n-1}(\mathbf{x}^{n-1}, \mathbf{x}^{n-1}; \theta) + \sigma_{n-1}^2 \mathbf{I} \end{bmatrix} \end{aligned} \quad \left. \vphantom{\begin{bmatrix} \mathbf{u}^n \\ \mathbf{u}^{n-1} \end{bmatrix}} \right\} \text{Training}$$

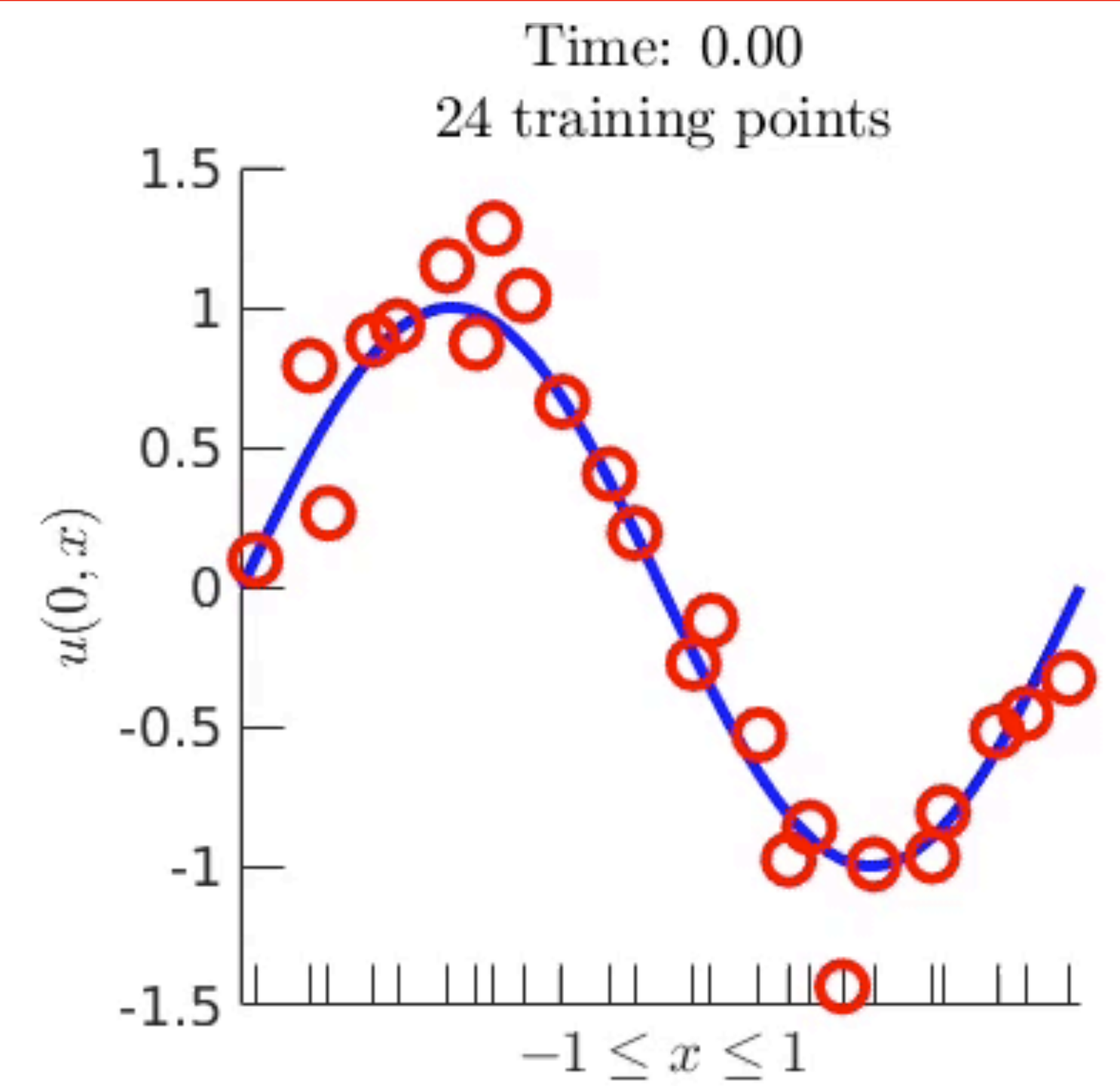
$$\min_{\theta, \sigma_n, \sigma_{n-1}} \begin{bmatrix} \mathbf{u}^n \\ \mathbf{u}^{n-1} \end{bmatrix}^T \mathbf{K}^{-1} \begin{bmatrix} \mathbf{u}^n \\ \mathbf{u}^{n-1} \end{bmatrix} + \log |\mathbf{K}|$$

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

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

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

Prediction



$$\left. \begin{aligned} \mathbf{u}^n &\sim \mathcal{N}(\mathbf{m}^n, \mathbf{S}^{n,n}) \\ \mathbf{m}^n &= m^n(\mathbf{x}^n) \\ \mathbf{S}^{n,n} &= S^{n,n}(\mathbf{x}^n, \mathbf{x}^n) \end{aligned} \right\} \text{Artificial Data}$$

# Hidden Physics Models

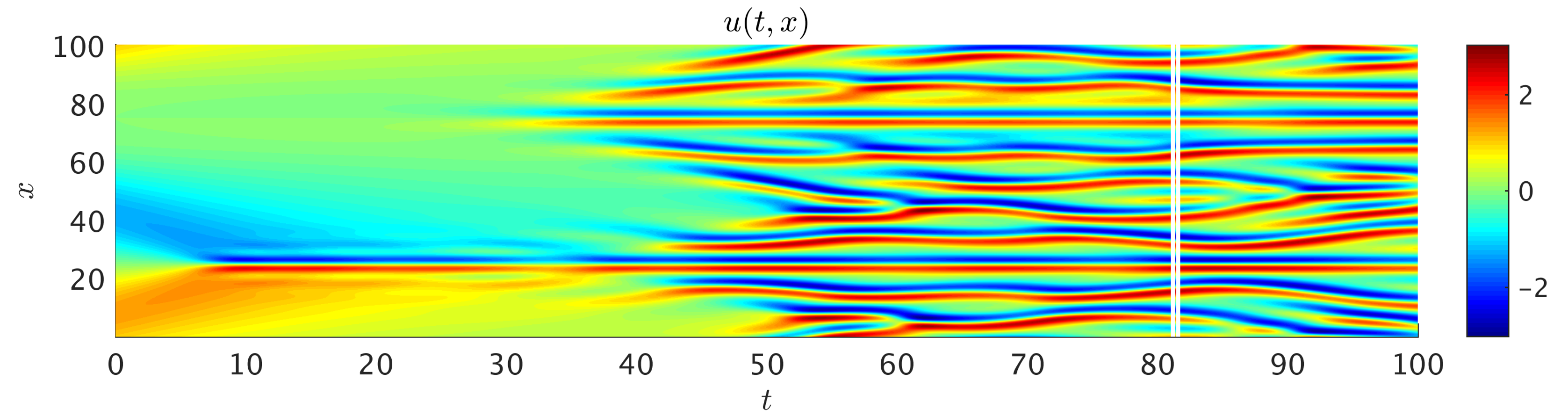
$$u_t + \lambda_1 u u_x + \lambda_2 u_{xx} + \lambda_3 u_{xxxx} = 0$$

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

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

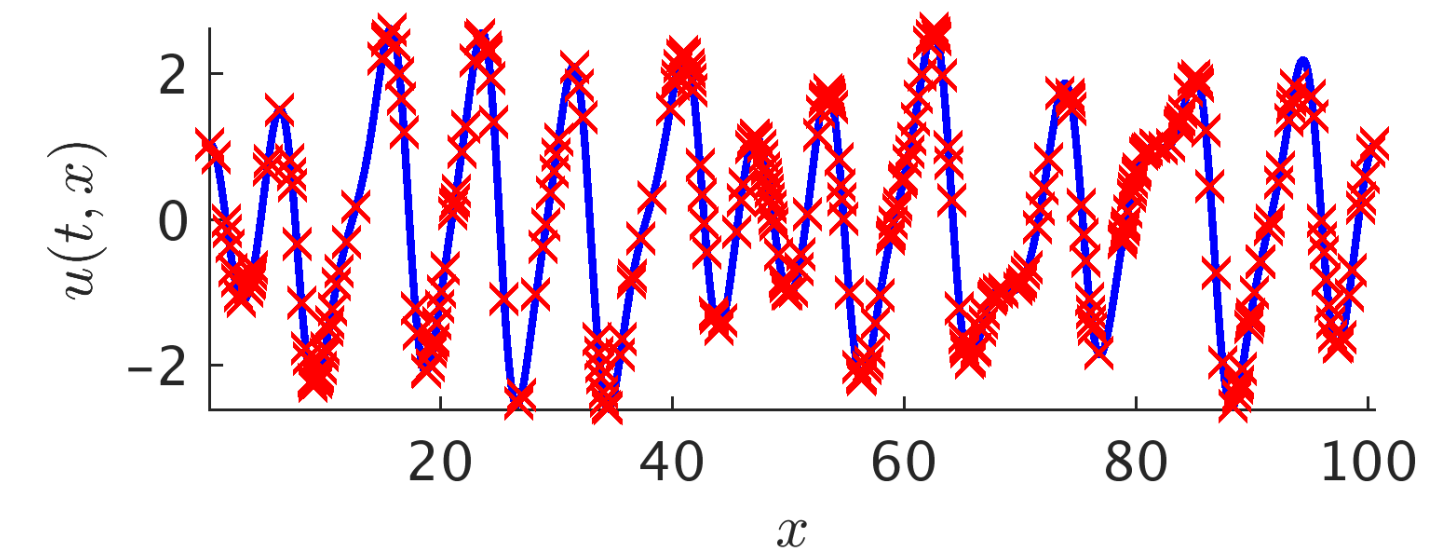
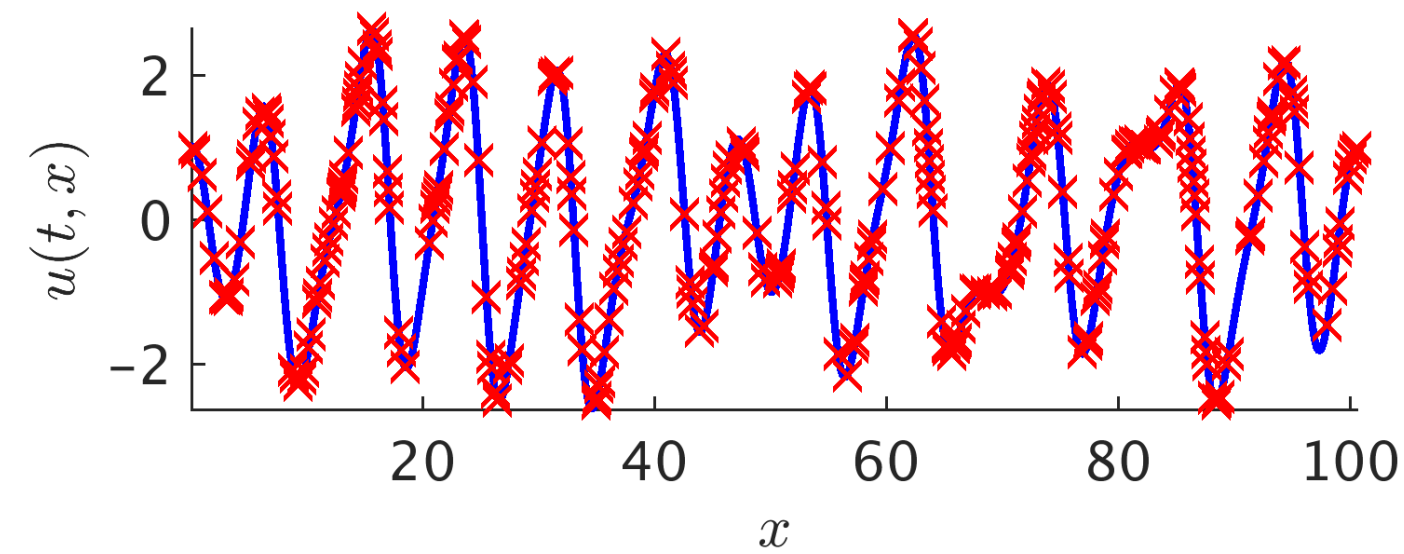
$$\begin{bmatrix} u^n \\ u^{n-1} \end{bmatrix} \sim \mathcal{GP} \left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} k^{n,n} & k^{n,n-1} \\ k^{n-1,n} & k^{n-1,n-1} \end{bmatrix} \right)$$

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



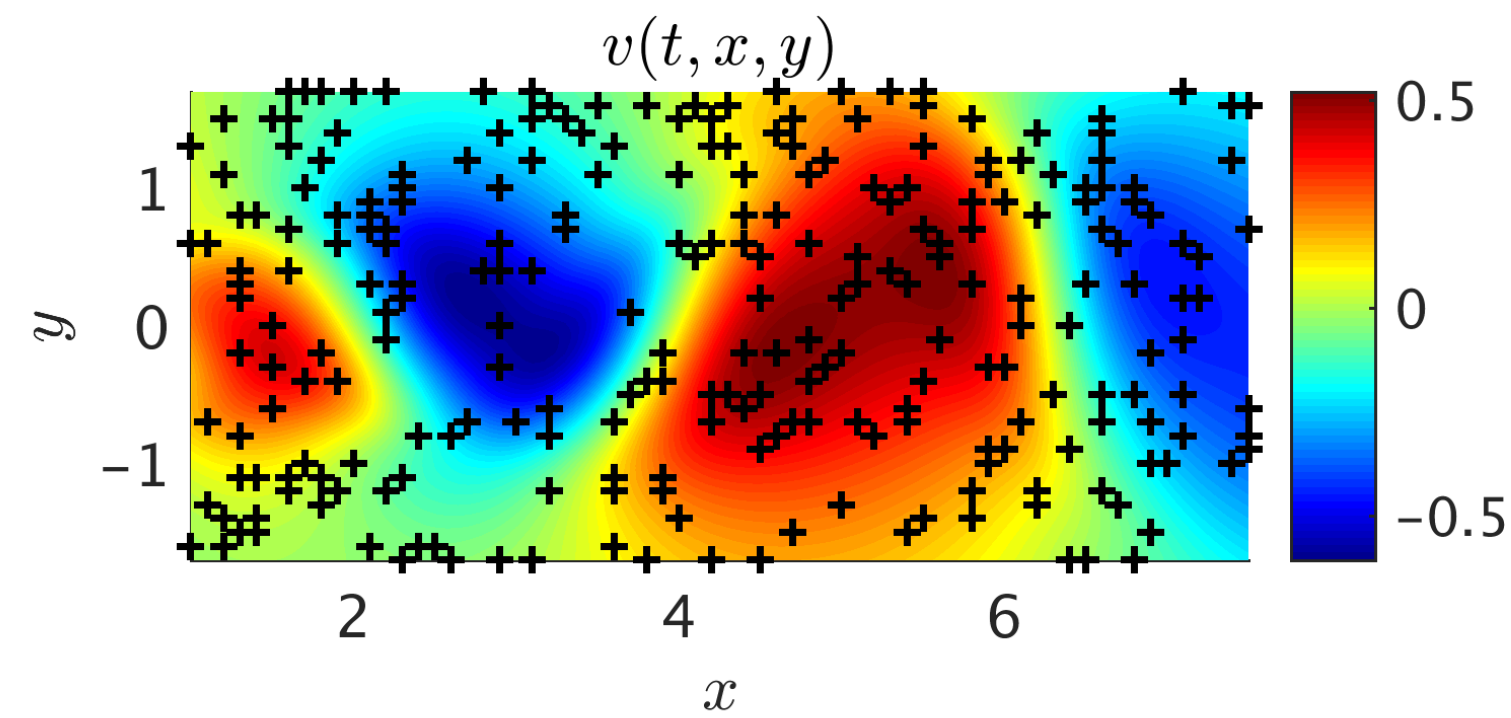
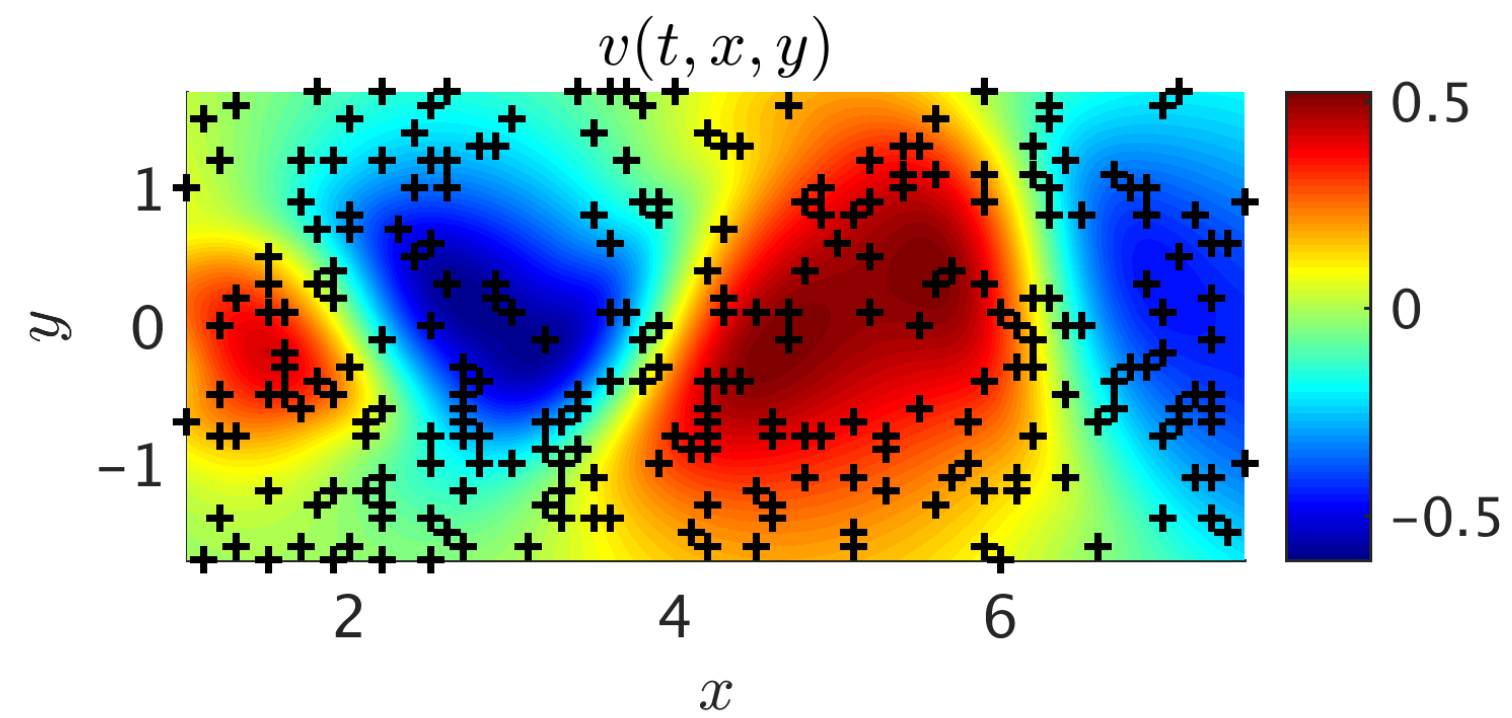
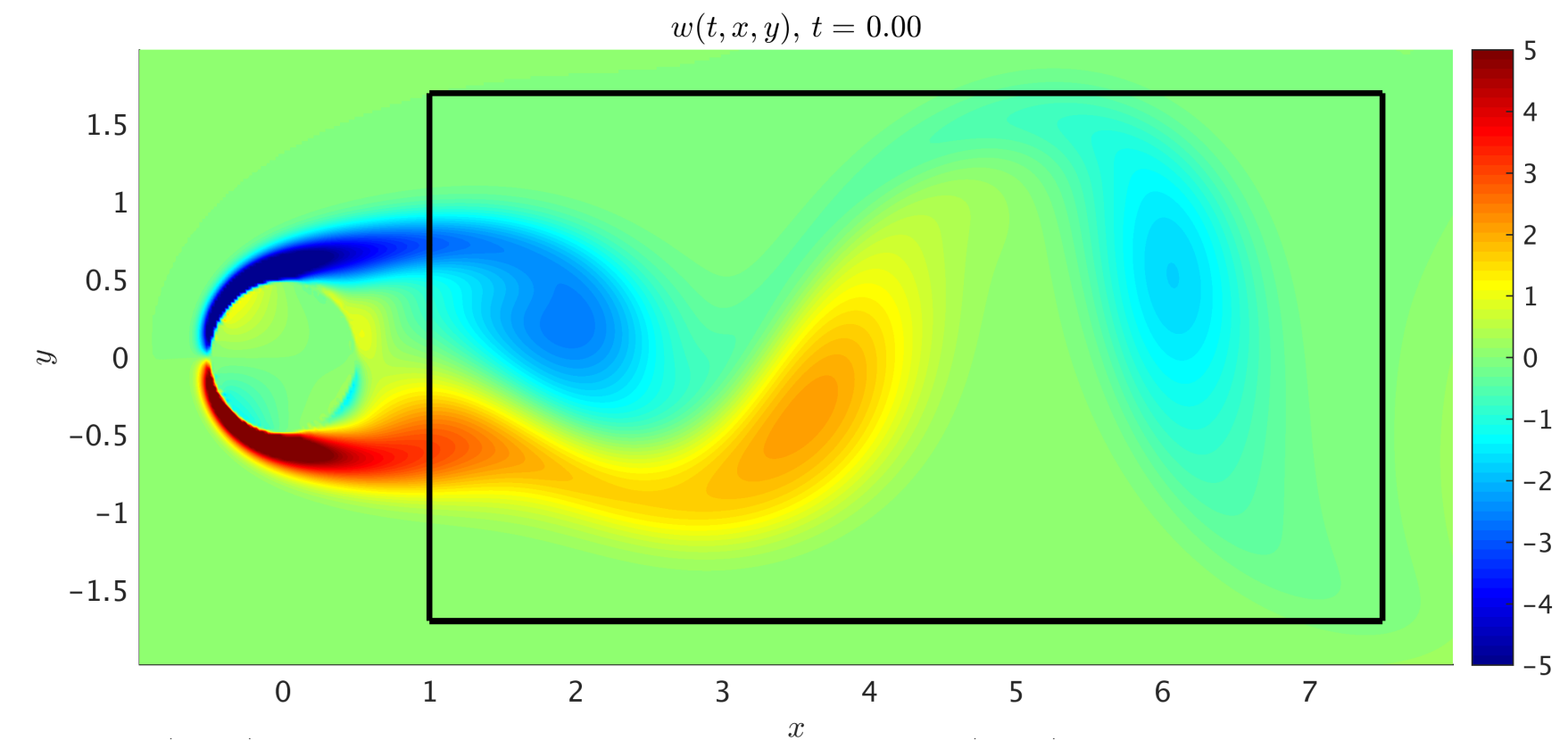
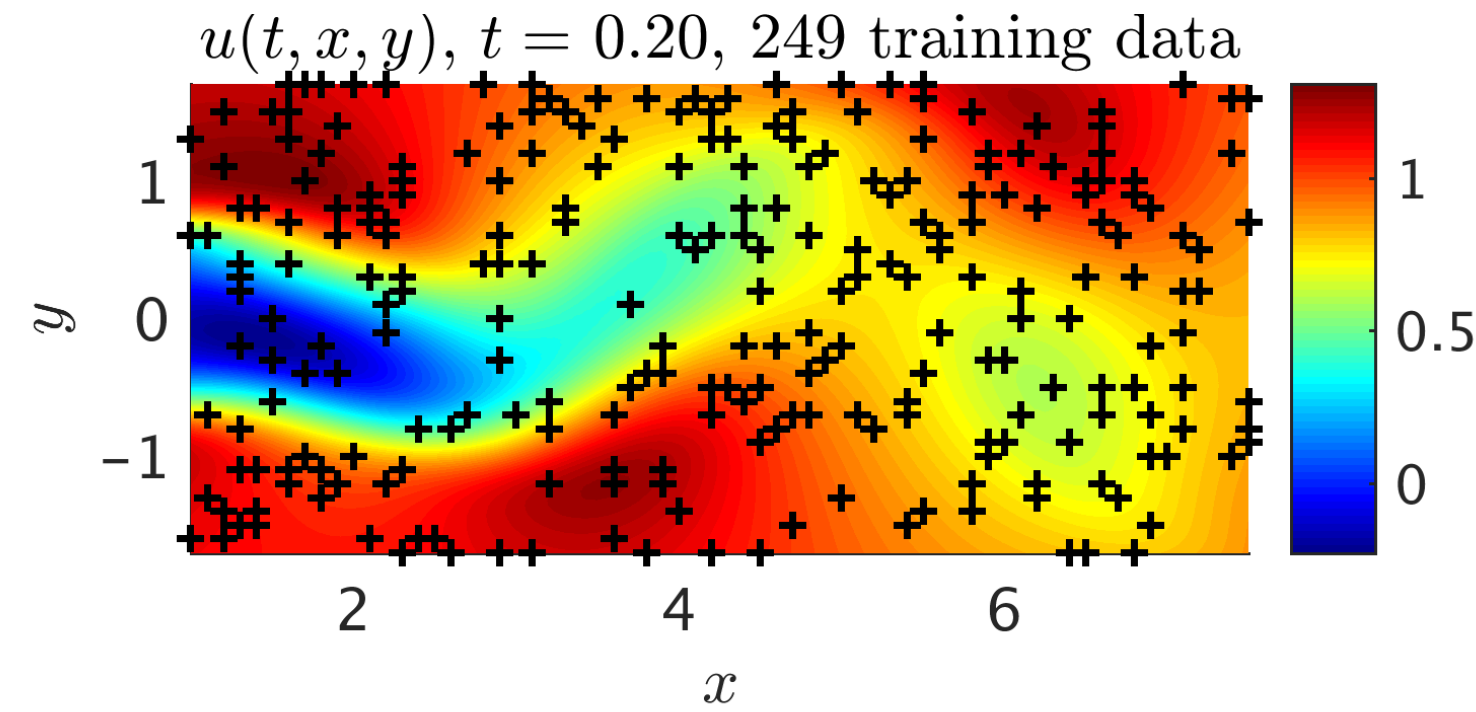
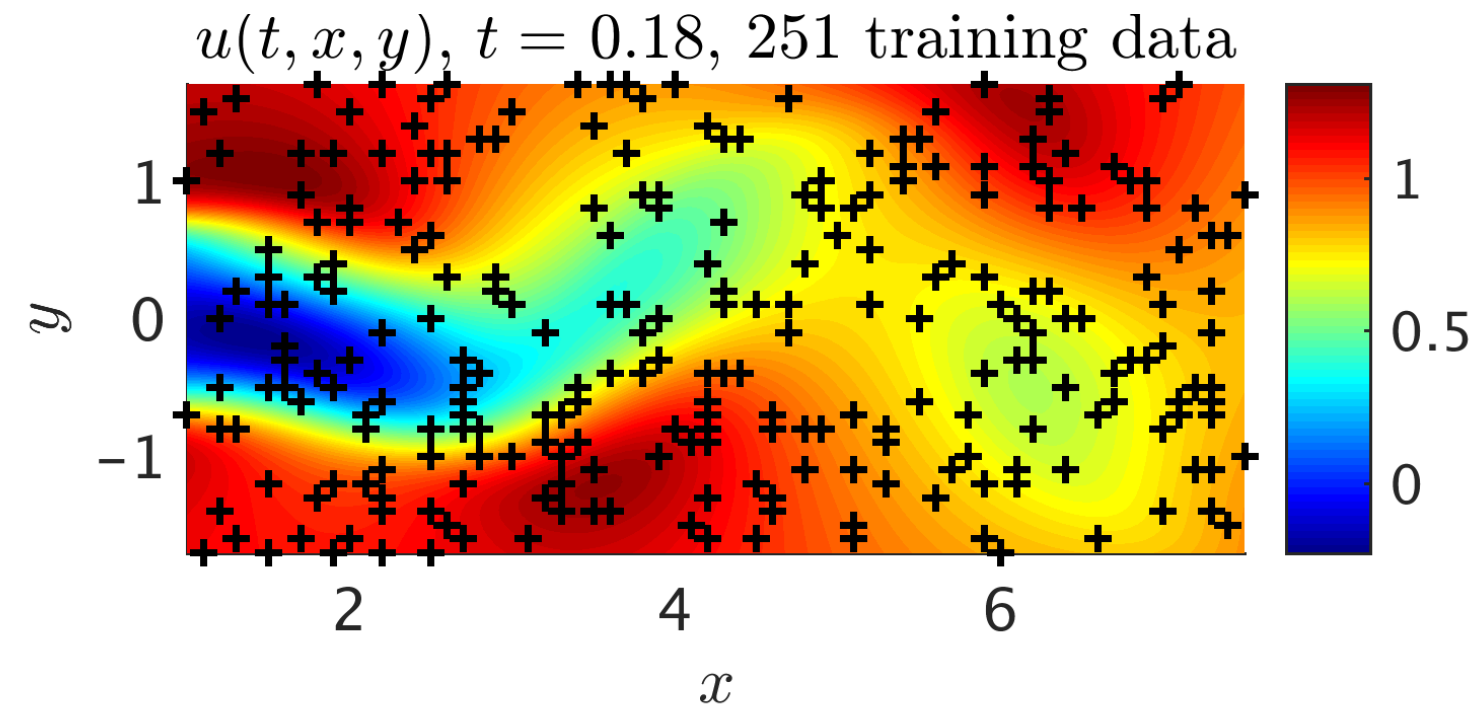
$t = 81.20$   
301 training data

$t = 81.60$   
299 training data

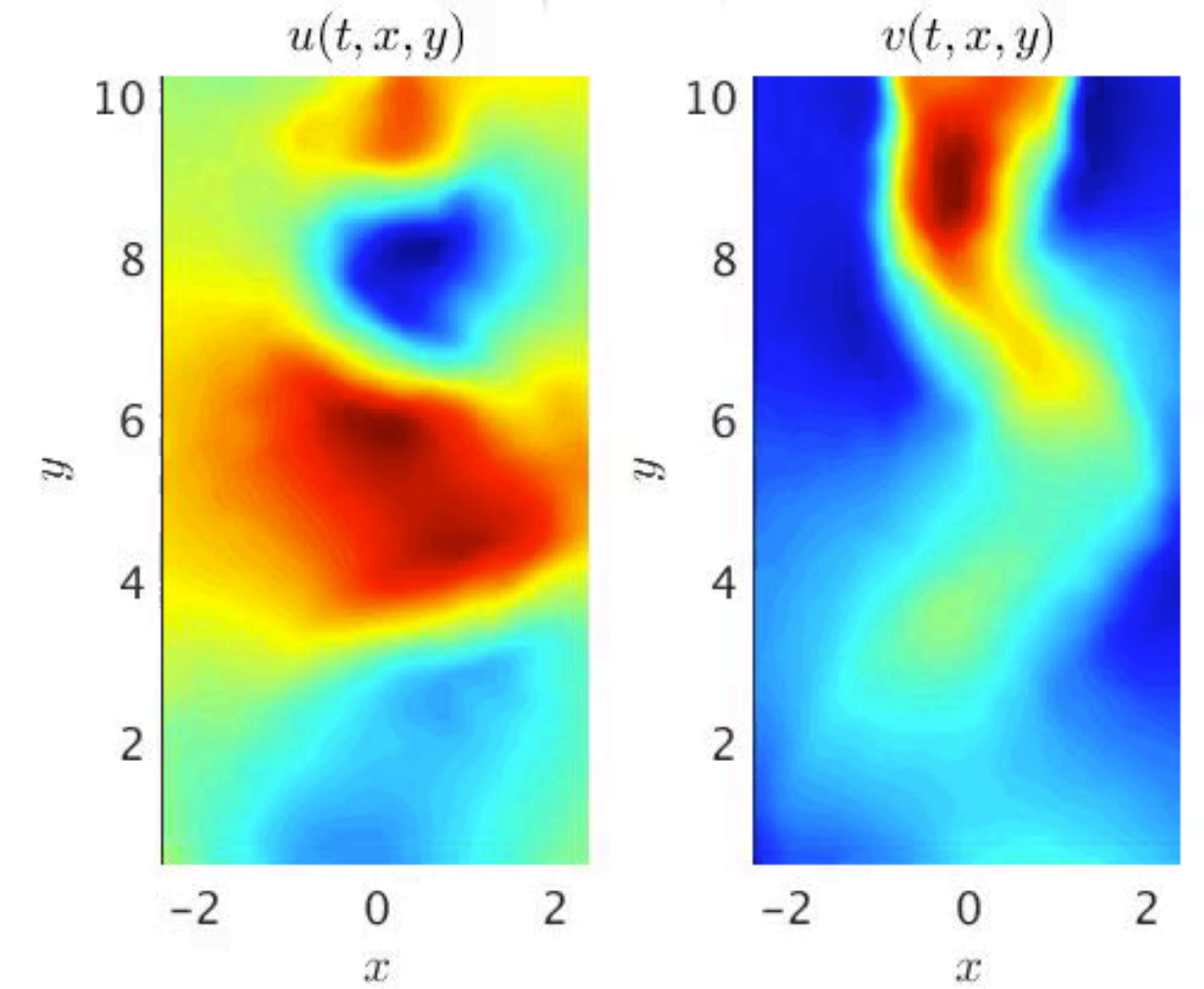


Correct PDE	$u_t + u u_x + u_{xx} + u_{xxxx} = 0$
Identified PDE (clean data)	$u_t + 0.952 u u_x + 1.005 u_{xx} + 0.980 u_{xxxx} = 0$
Identified PDE (1% noise)	$u_t + 0.908 u u_x + 0.951 u_{xx} + 0.927 u_{xxxx} = 0$

# Hidden Physics Models

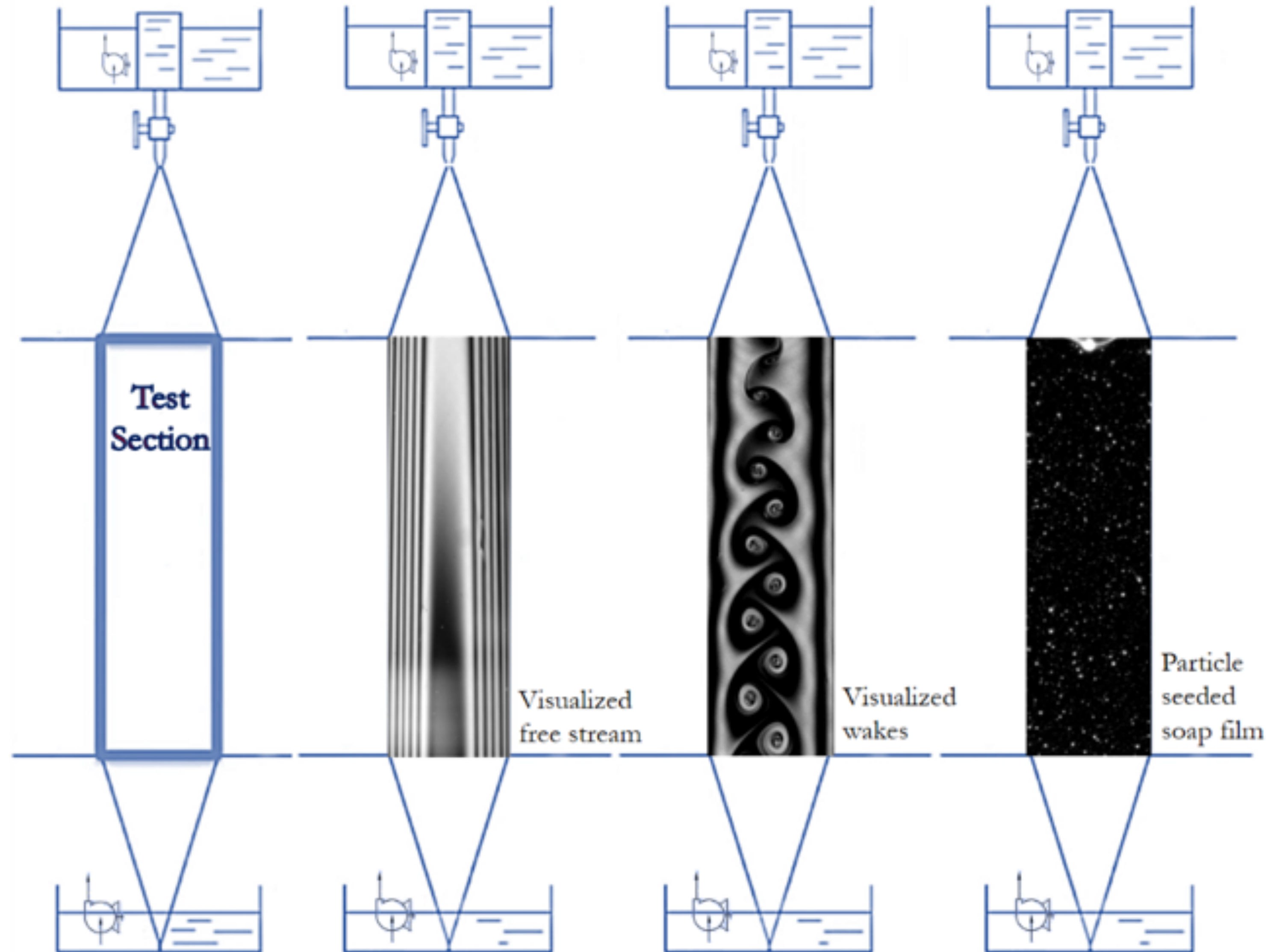
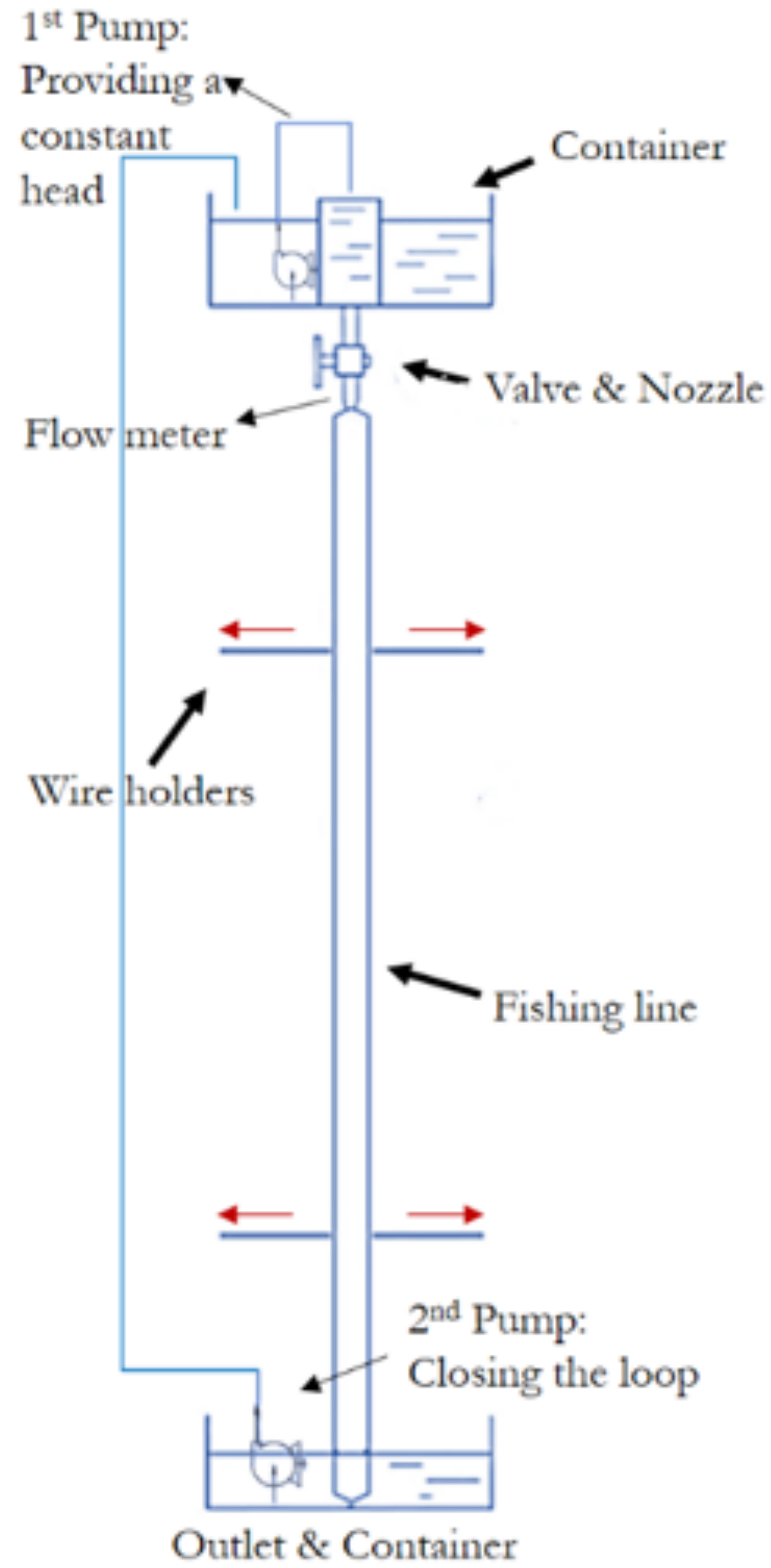


PIV Data



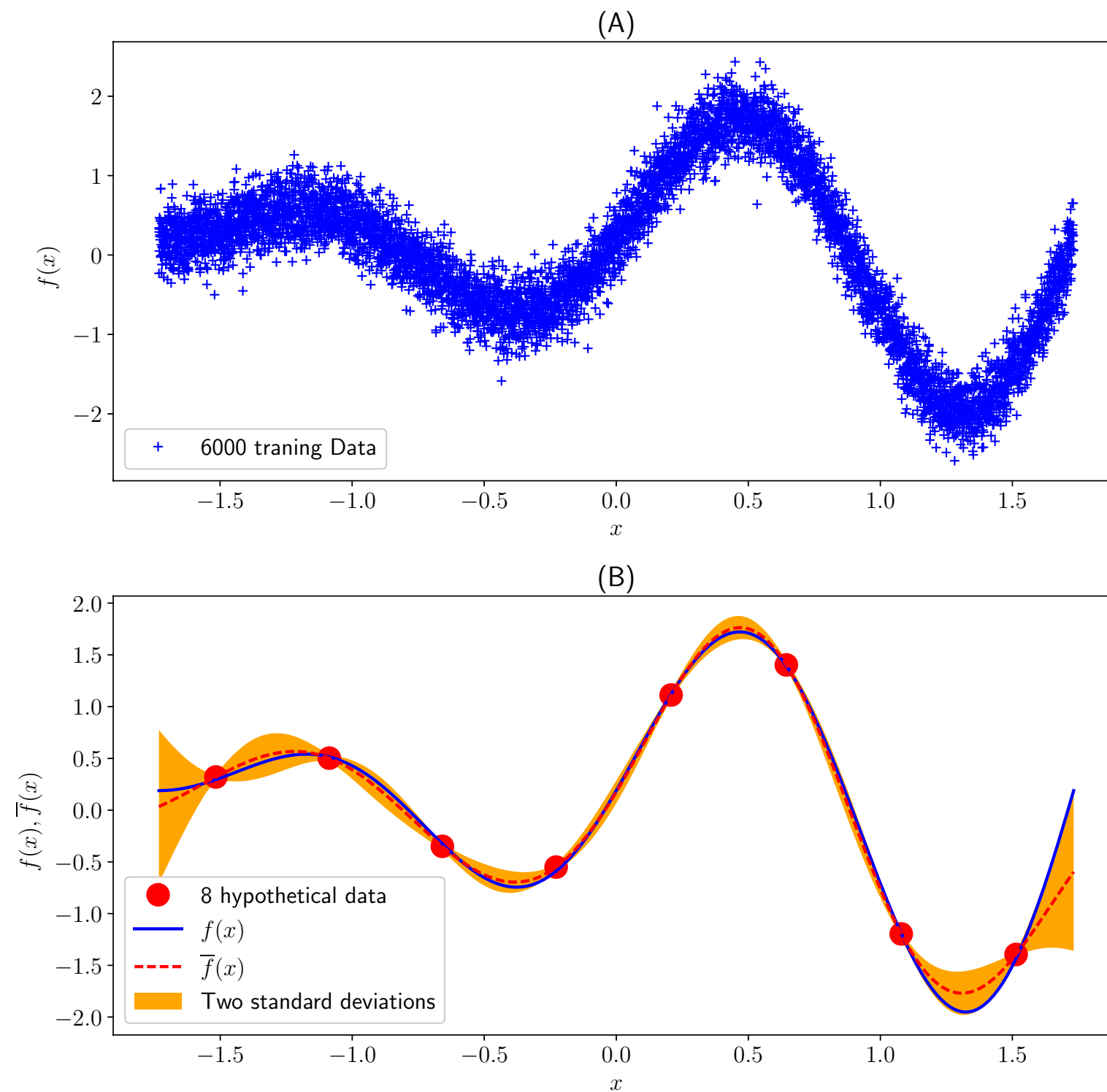
Correct PDE	$u_t + (uu_x + vv_y) = -p_x + 0.01(u_{xx} + u_{yy})$ $v_t + (uv_x + vv_y) = -p_y + 0.01(v_{xx} + v_{yy})$
Identified PDE (clean data)	$u_t + 0.983(uu_x + vv_y) = -p_x + 0.00826(u_{xx} + u_{yy})$ $v_t + 0.983(uv_x + vv_y) = -p_y + 0.00826(v_{xx} + v_{yy})$
Identified PDE (1% noise)	$u_t + 0.849(uu_x + vv_y) = -p_x + 0.01399(u_{xx} + u_{yy})$ $v_t + 0.849(uv_x + vv_y) = -p_y + 0.01399(v_{xx} + v_{yy})$

# Hidden Physics Models



# Parametric Gaussian Processes for Big Data

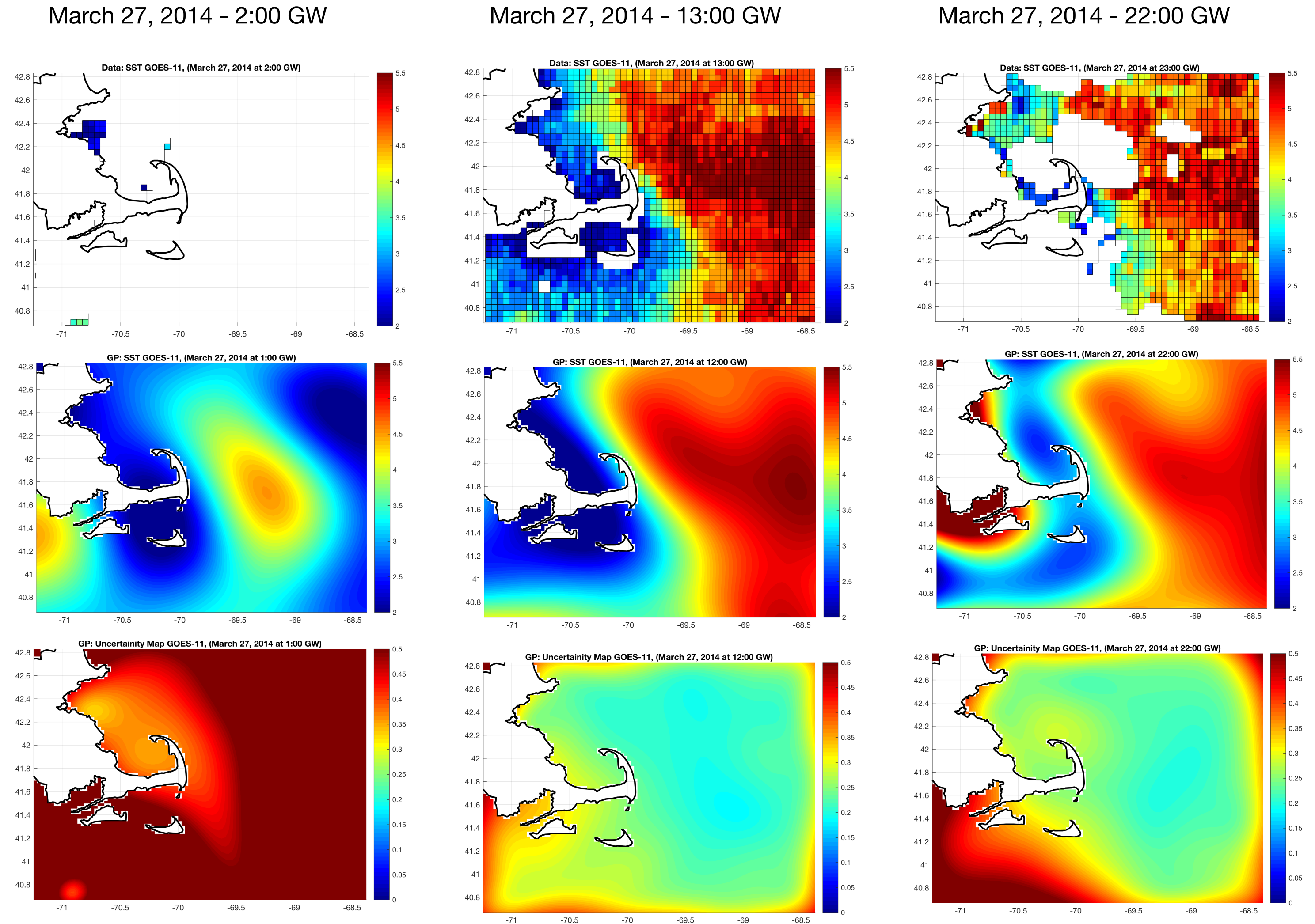
- 1) Parametric Gaussian process  
(producer of the hypothetical data)
- 2) Classical Gaussian process  
(consumer of the hypothetical data)



GOES\_11  
Satellite

Prediction

Uncertainty  
Map



# Neural Networks Regression

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

$$\left. \begin{aligned}
 f(x) &= W^L h^L + b^L \\
 h^L &= \tanh(W^{L-1} h^{L-1} + b^{L-1}) \\
 &\vdots \\
 h^1 &= \tanh(W^0 x + b^0)
 \end{aligned} \right\} \text{Prior}$$

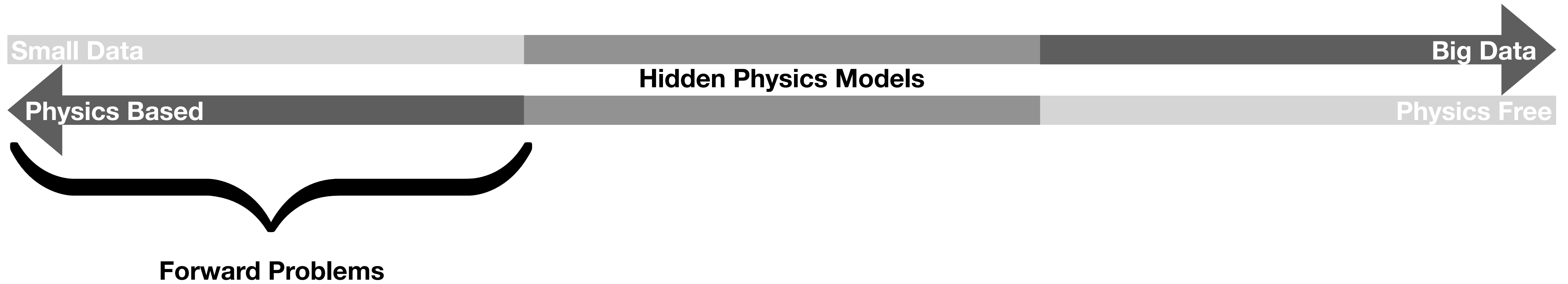
$$\left. \begin{aligned}
 \mathbf{y} &\sim \mathcal{N}(f(\mathbf{x}), \sigma^2 \mathbf{I}) \\
 \min_{W,b} & (\mathbf{y} - f(\mathbf{x}))' (\mathbf{y} - f(\mathbf{x})) \\
 \min_{W,b} & \sum_{i=1}^N |y_i - f(x_i)|^2
 \end{aligned} \right\} \text{Training}$$

$$\left. f(x^*) \right\} \text{Prediction}$$

## 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.

# Forward Problems



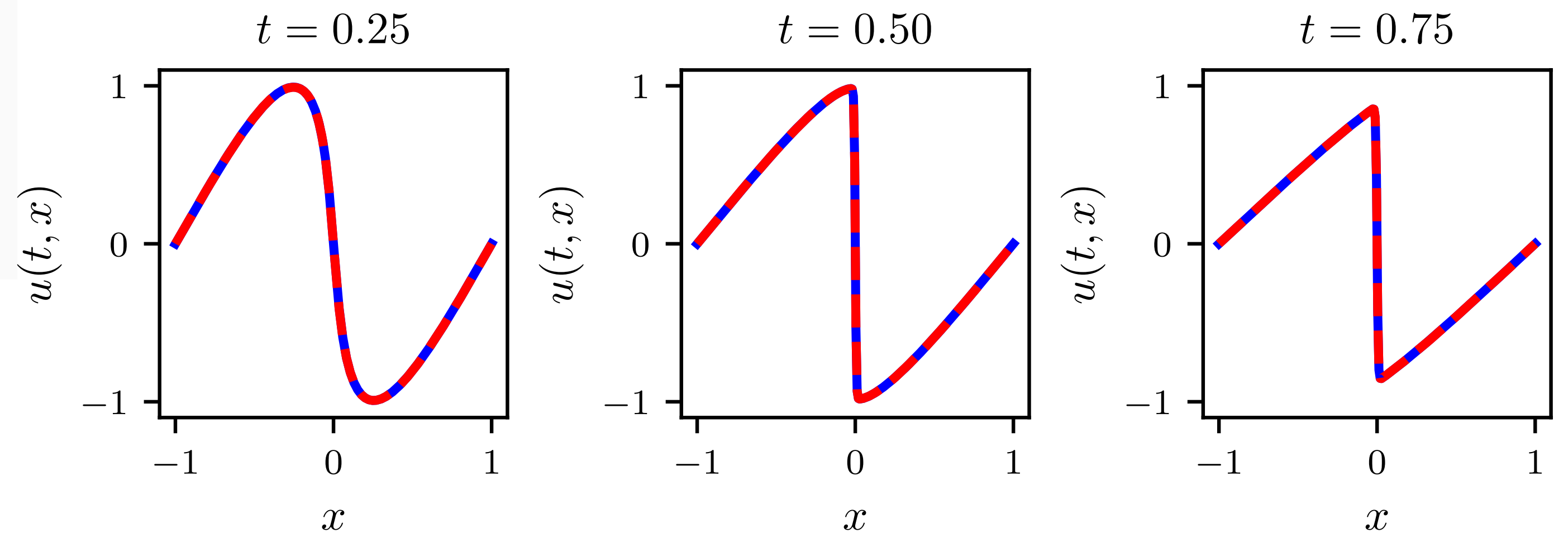
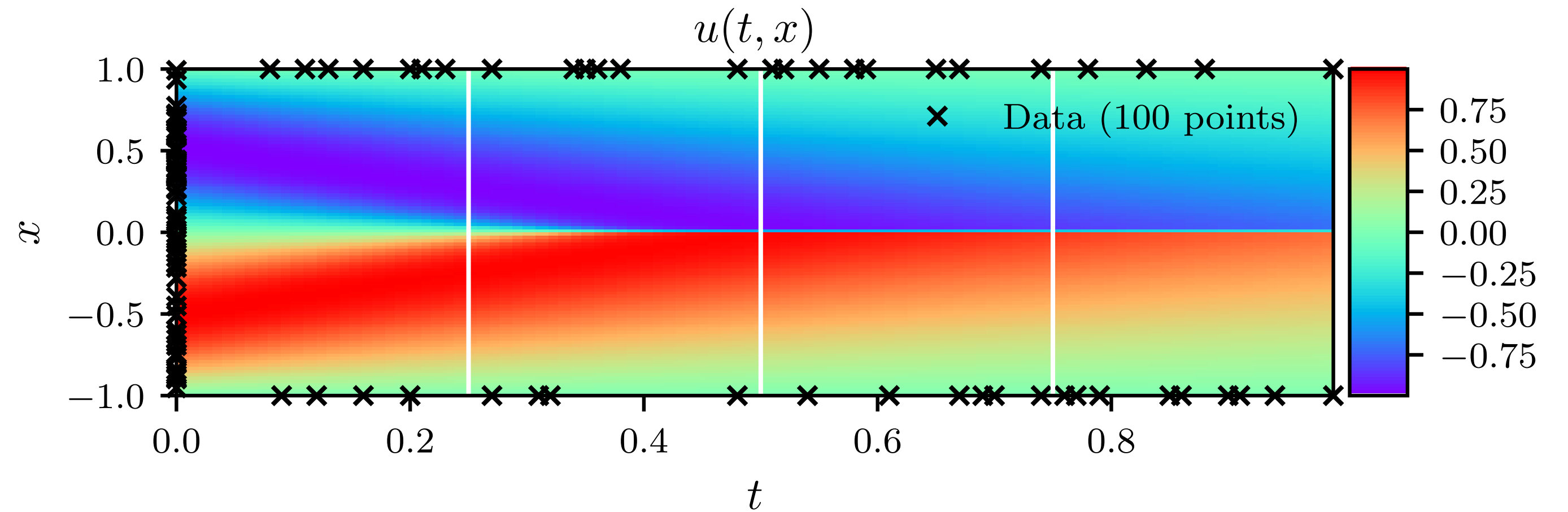
# Physics Informed Neural Networks (PINNs)

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

```
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
```

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



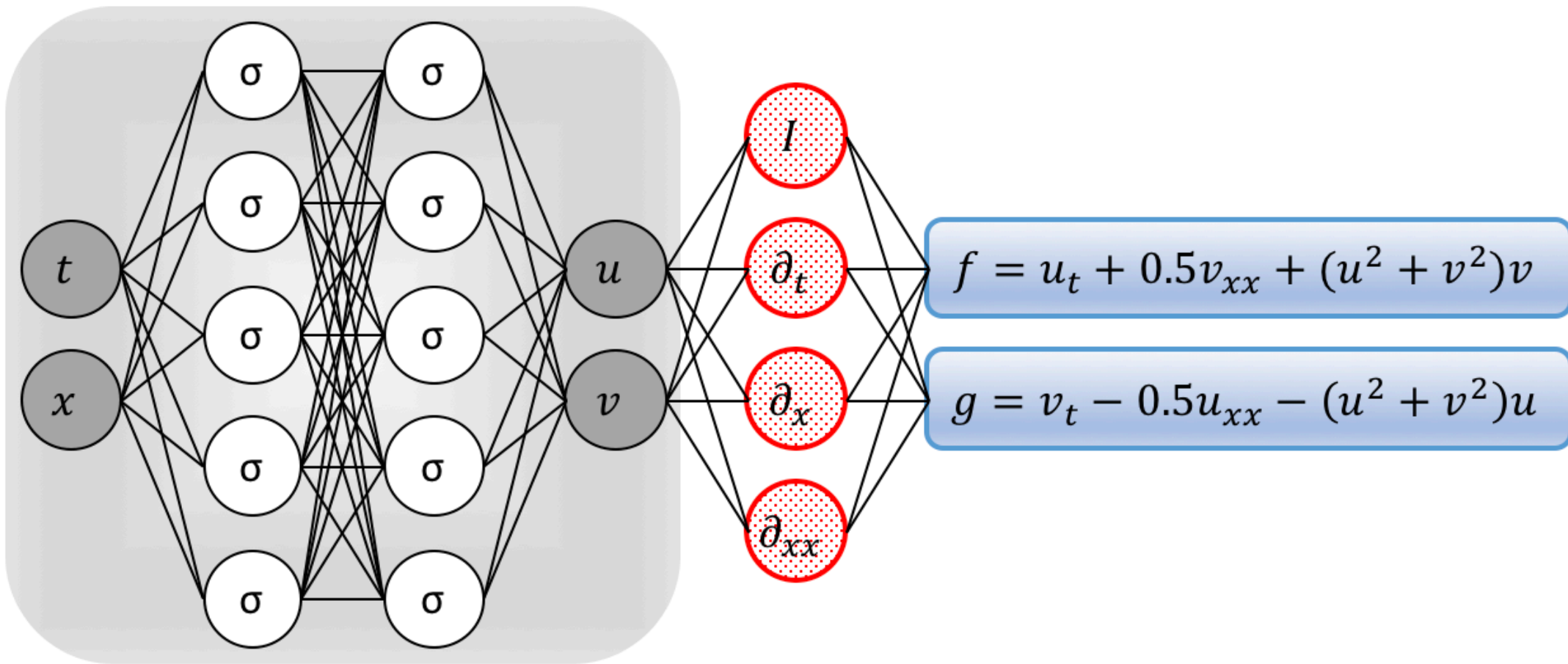
— Exact    - - - Prediction



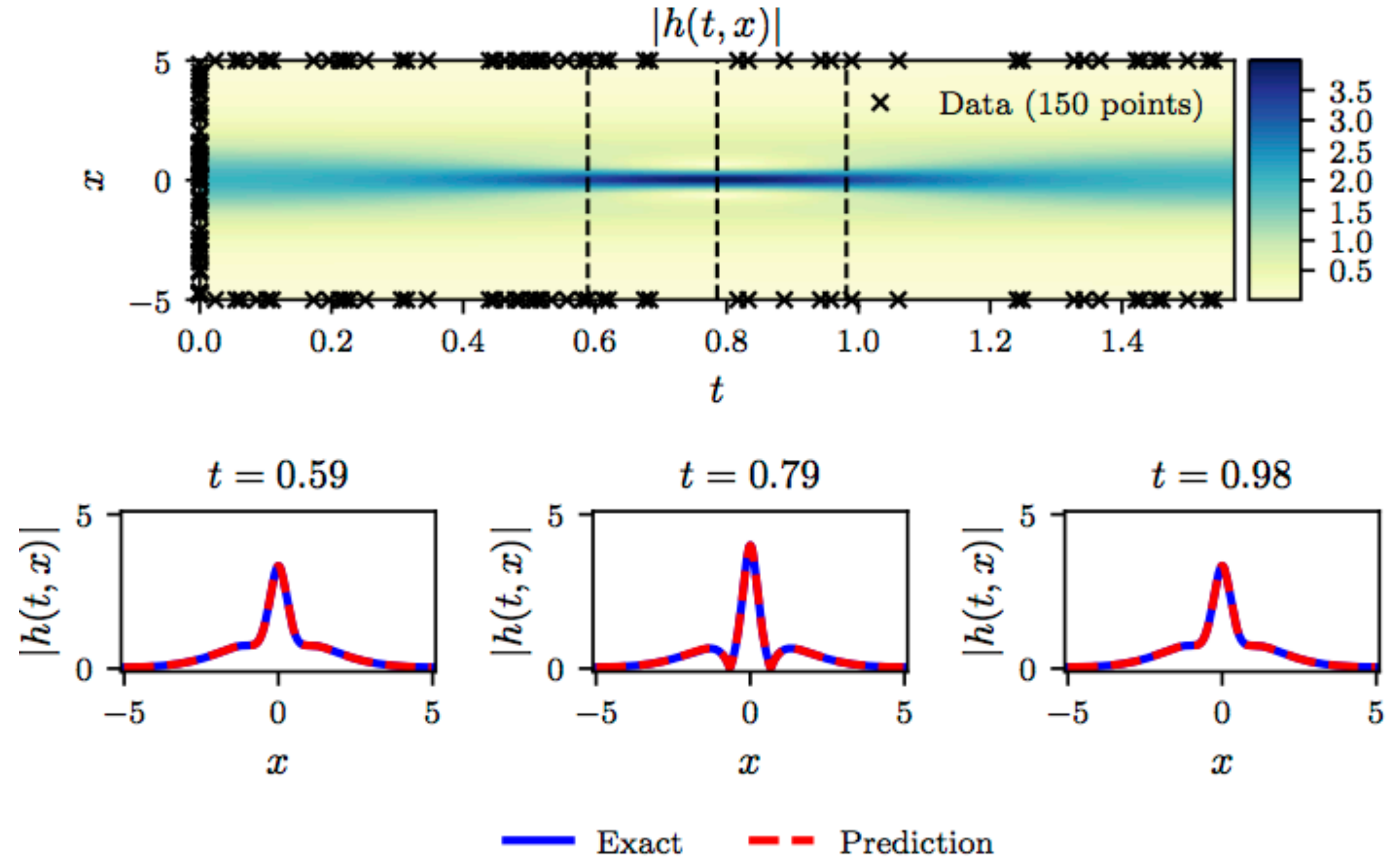
# Physics Informed Neural Networks (PINNs)

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

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



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





# 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

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

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



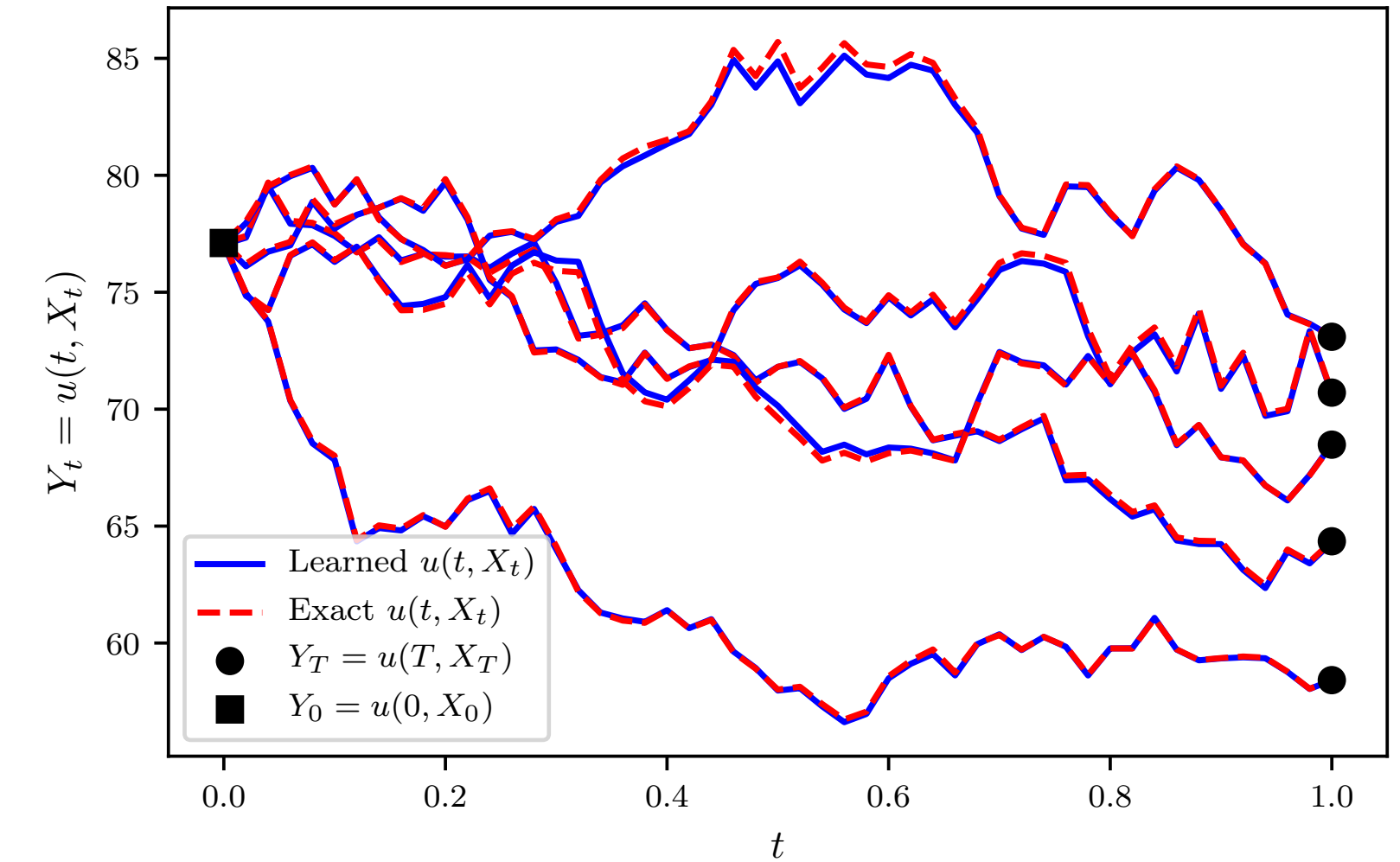
Forward-Backward Stochastic  
Differential Equation

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

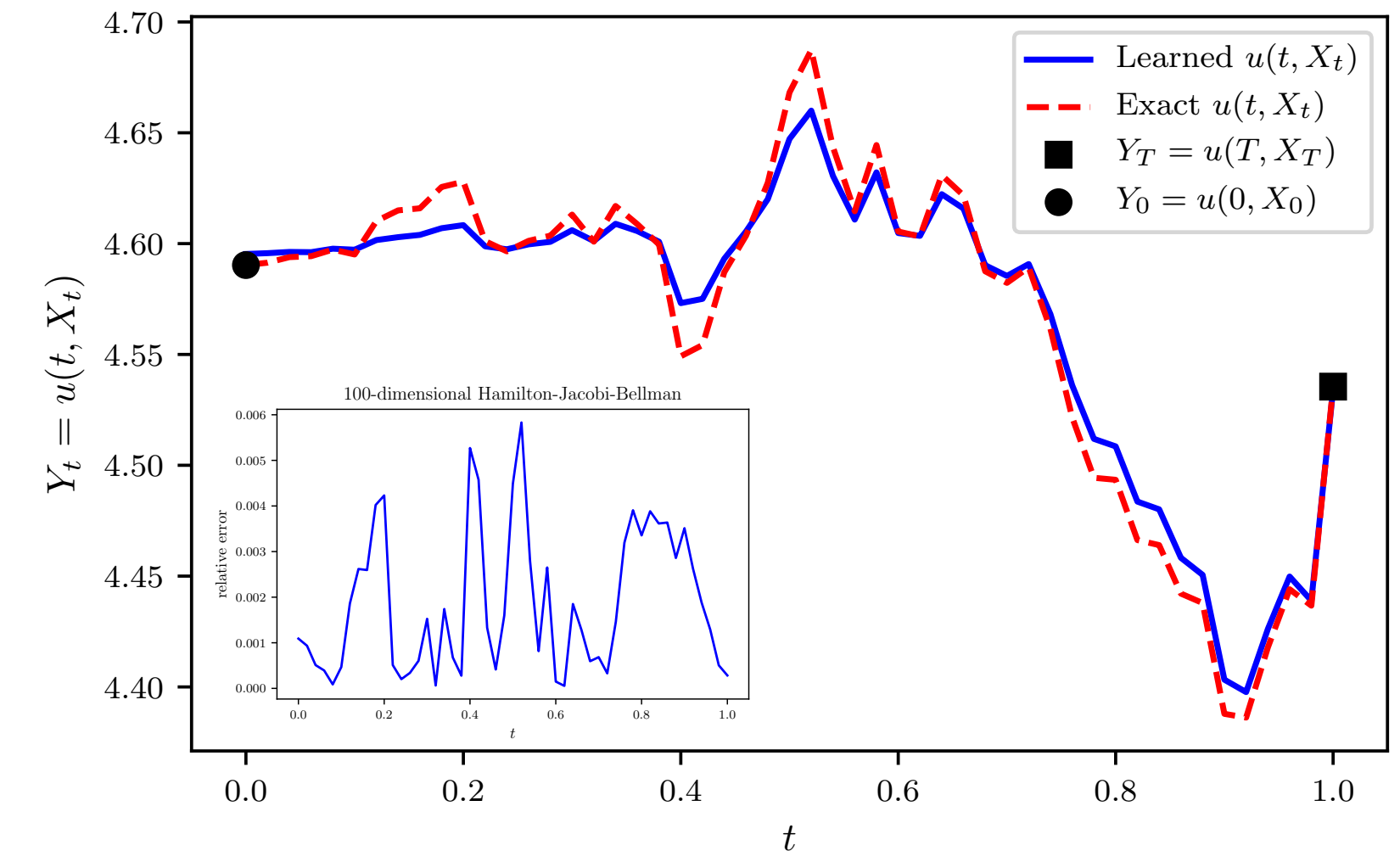
$$\begin{aligned}
 \frac{\partial u}{\partial t} &= \varphi(t, x, u, Du) - \mu(t, x, u, Du)' Du - \frac{1}{2} \text{Tr}[\sigma(t, x, u)\sigma(t, x, u)' D^2 u] \\
 u(T, x) &= g(x)
 \end{aligned}$$

Quasi-Linear Partial Differential Equation

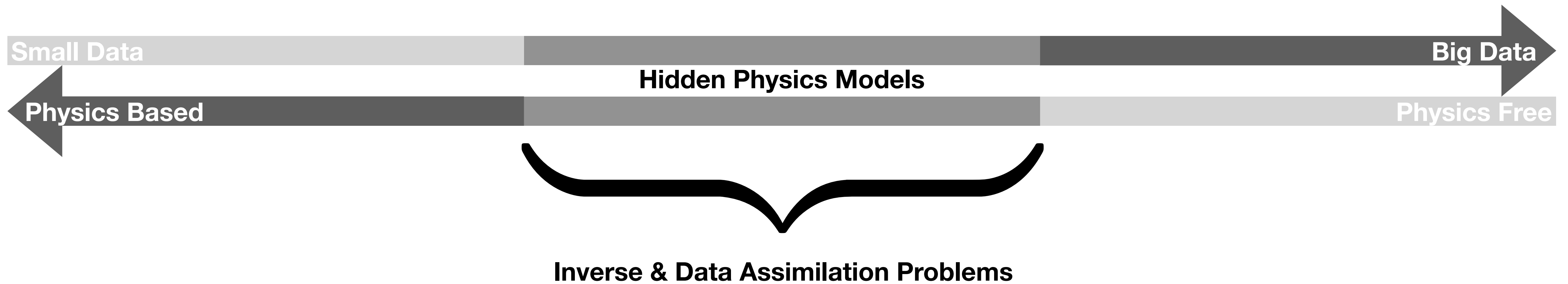
100-dimensional Black-Scholes-Barenblatt



100-dimensional Hamilton-Jacobi-Bellman



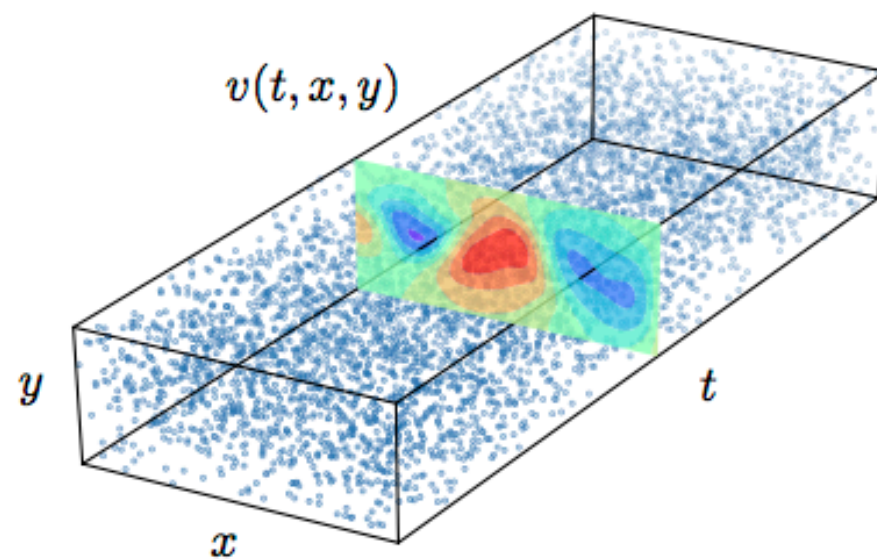
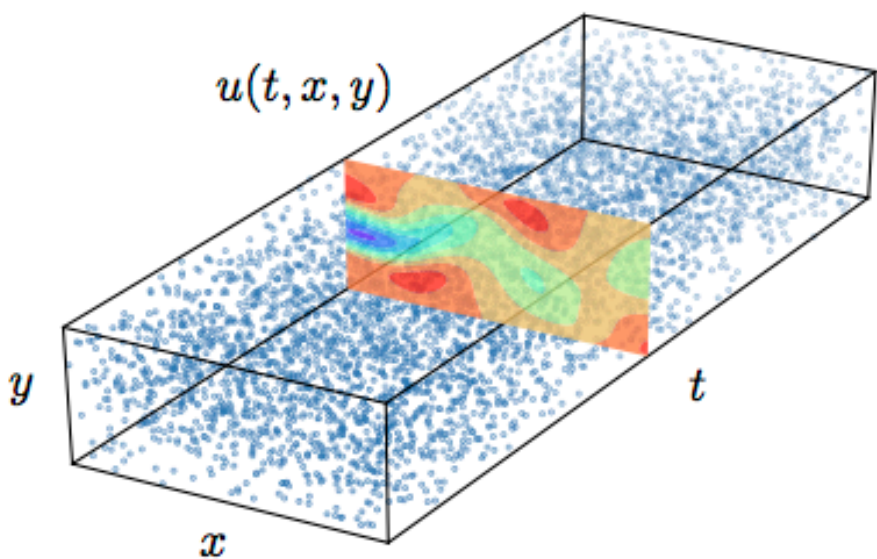
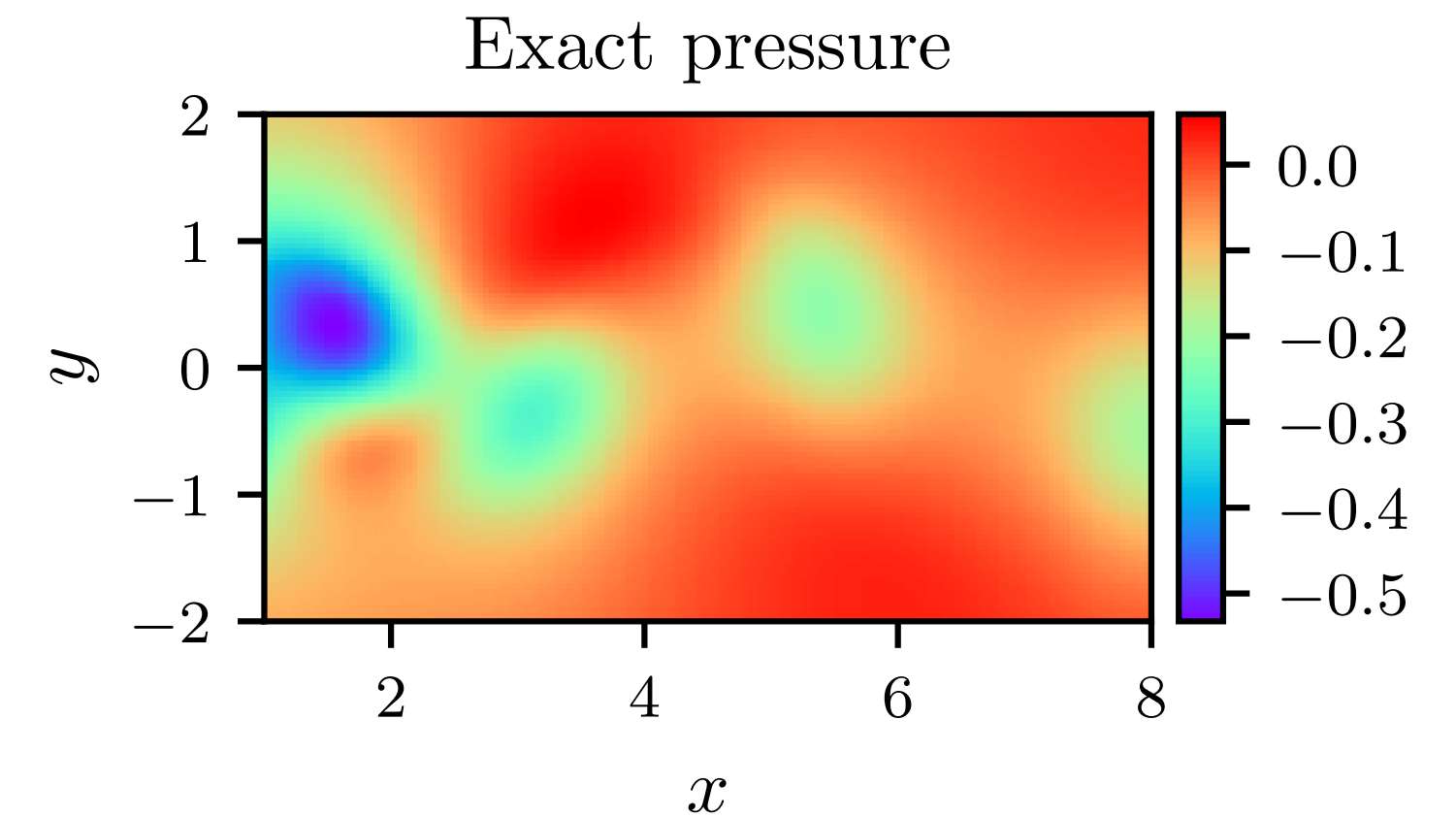
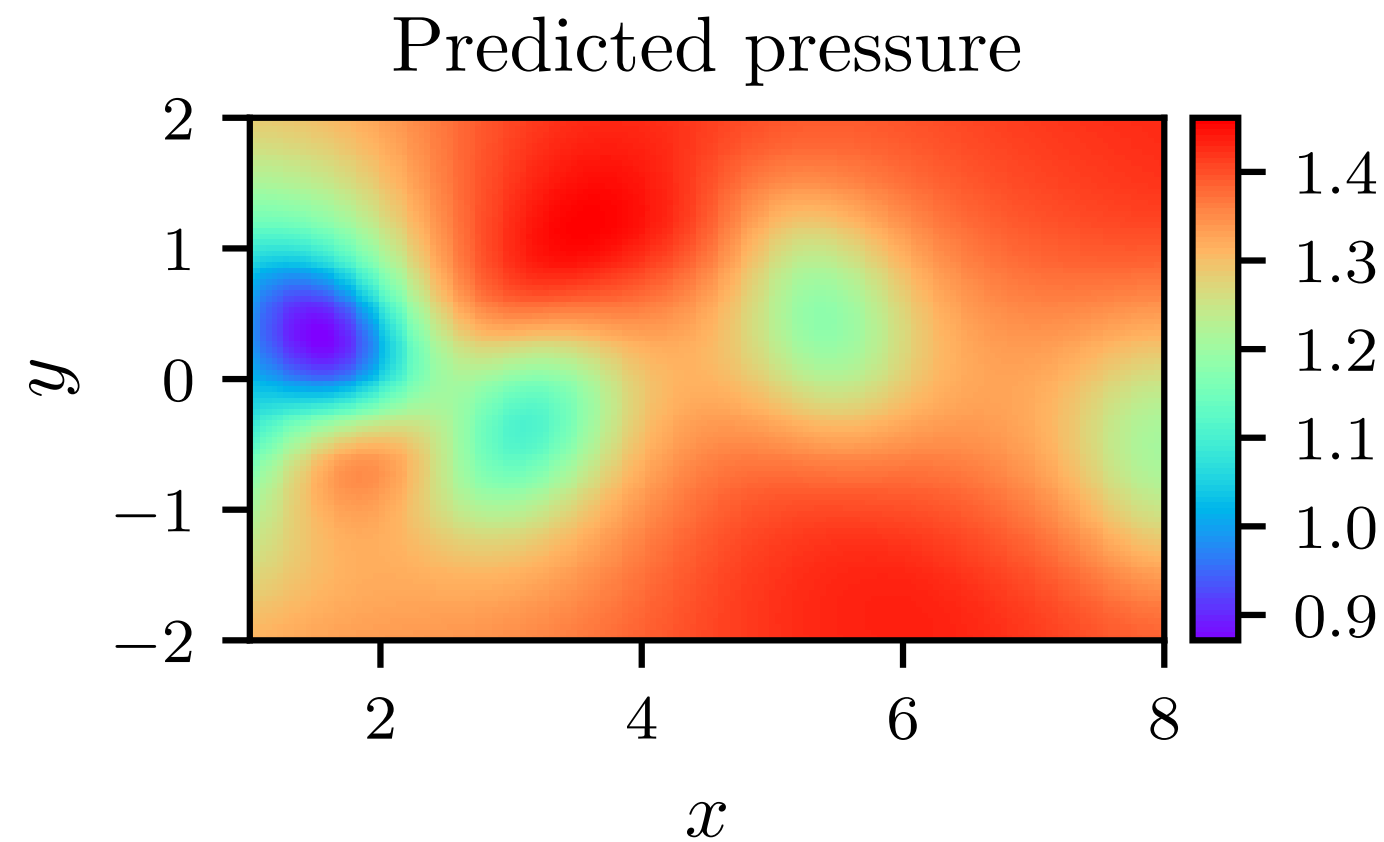
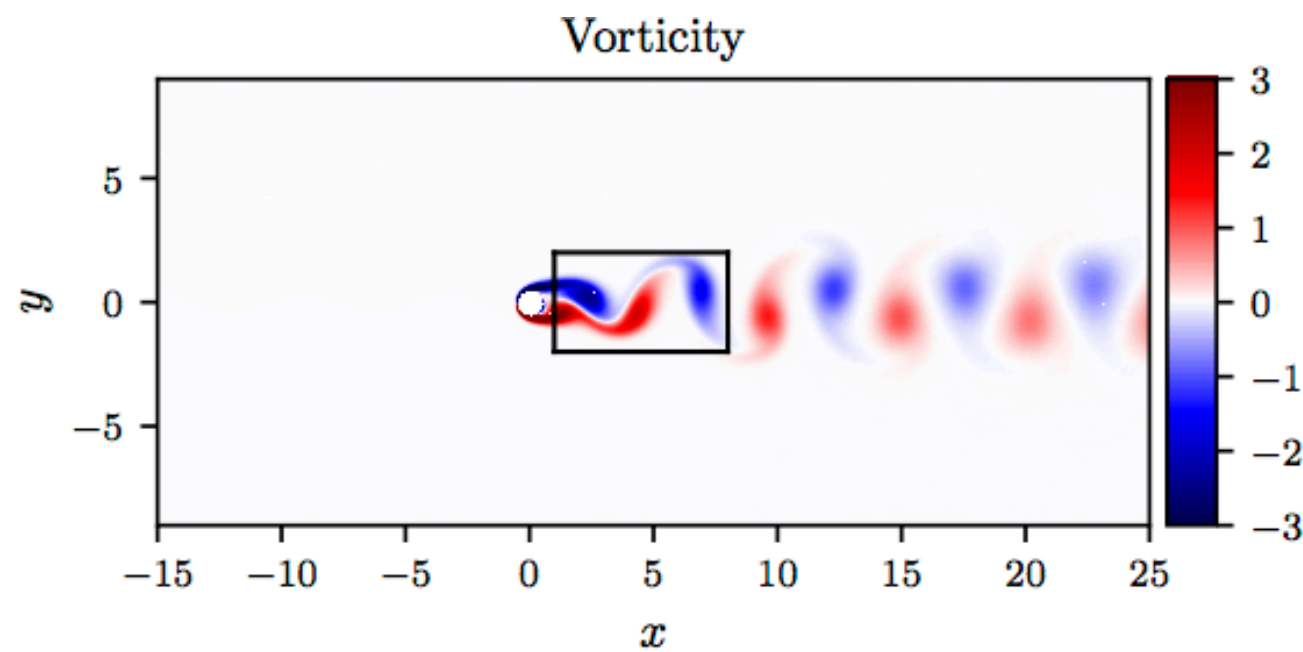
# Inverse & Data Assimilation Problems



# Physics Informed Neural Networks (PINNs)

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

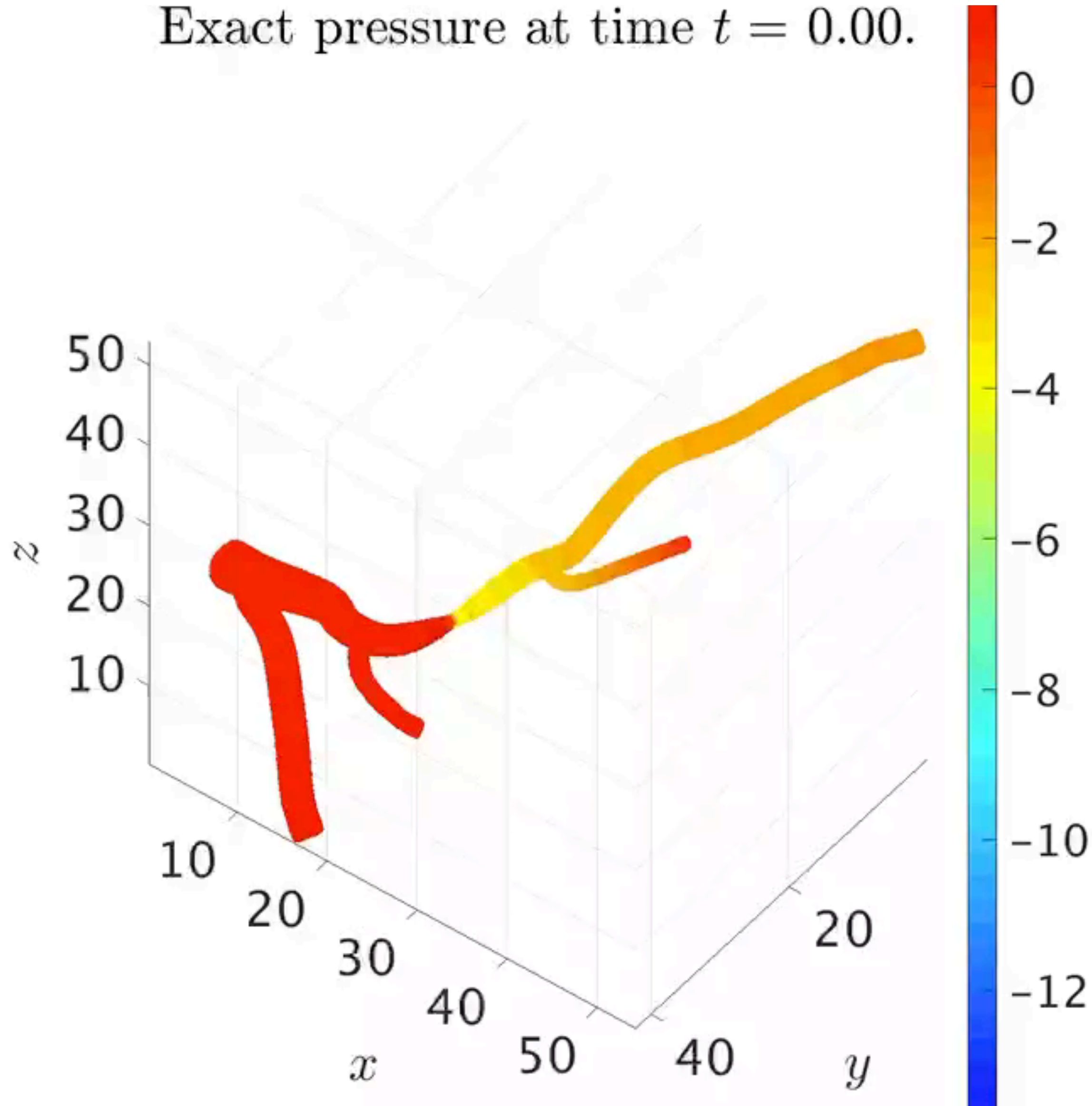
$$\begin{aligned}
 f &:= u_t + \lambda_1(uu_x + vu_y) + p_x - \lambda_2(u_{xx} + u_{yy}) \\
 g &:= v_t + \lambda_1(uv_x + vv_y) + p_y - \lambda_2(v_{xx} + v_{yy}) \\
 h &:= u_x + v_y
 \end{aligned}$$



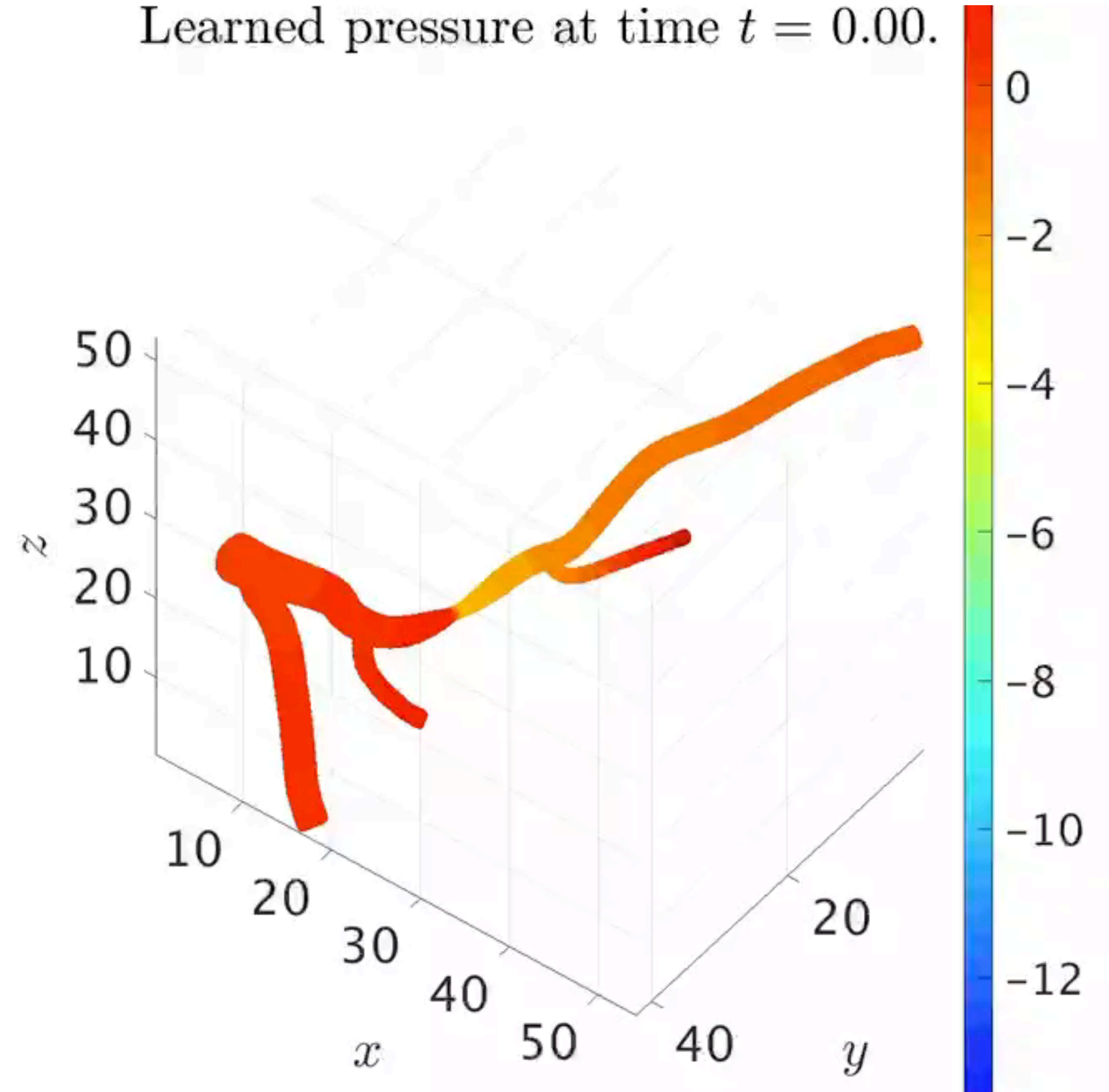
Correct PDE	$  \begin{aligned}  u_t + (uu_x + vu_y) &= -p_x + 0.01(u_{xx} + u_{yy}) \\  v_t + (uv_x + vv_y) &= -p_y + 0.01(v_{xx} + v_{yy})  \end{aligned}  $
Identified PDE (clean data)	$  \begin{aligned}  u_t + 0.999(uu_x + vu_y) &= -p_x + 0.01047(u_{xx} + u_{yy}) \\  v_t + 0.999(uv_x + vv_y) &= -p_y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

# Physics Informed Neural Networks (PINNs)

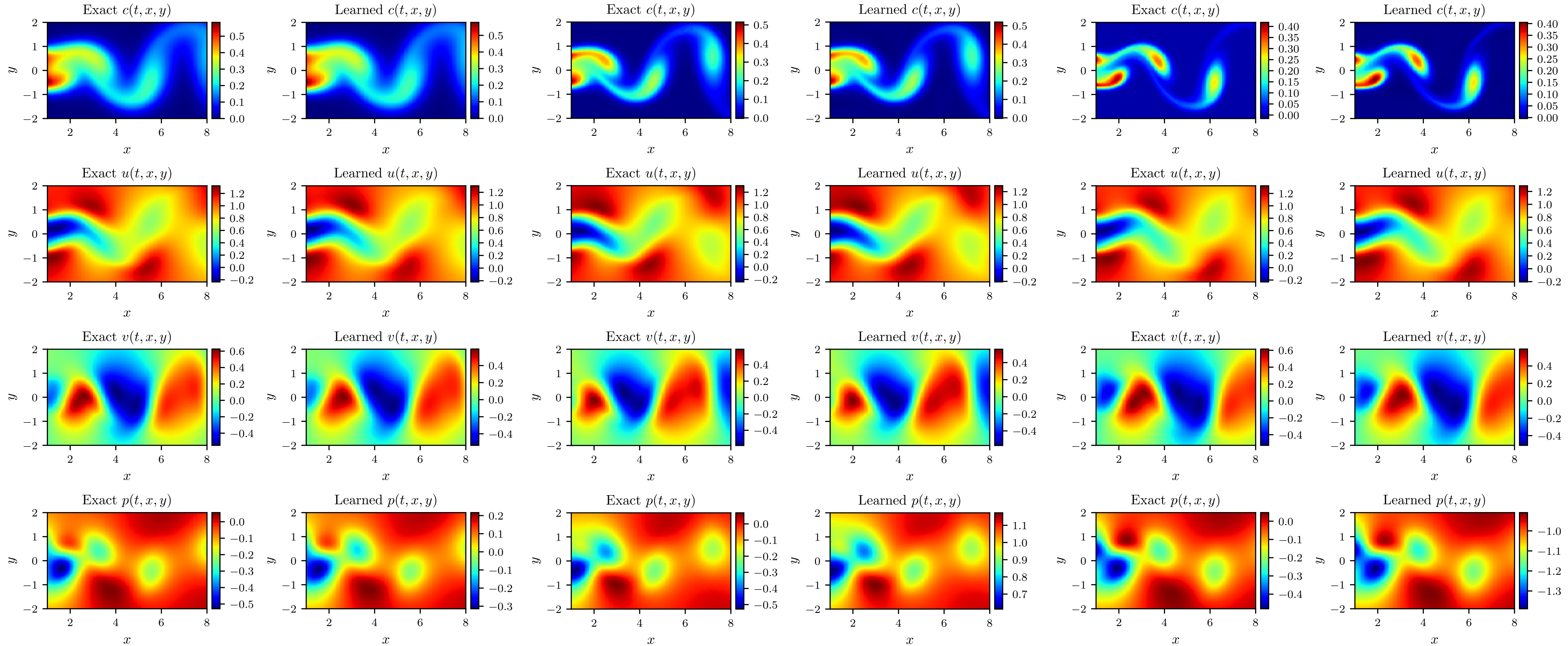
Exact pressure at time  $t = 0.00$ .



Learned pressure at time  $t = 0.00$ .



# Hidden Fluid Mechanics

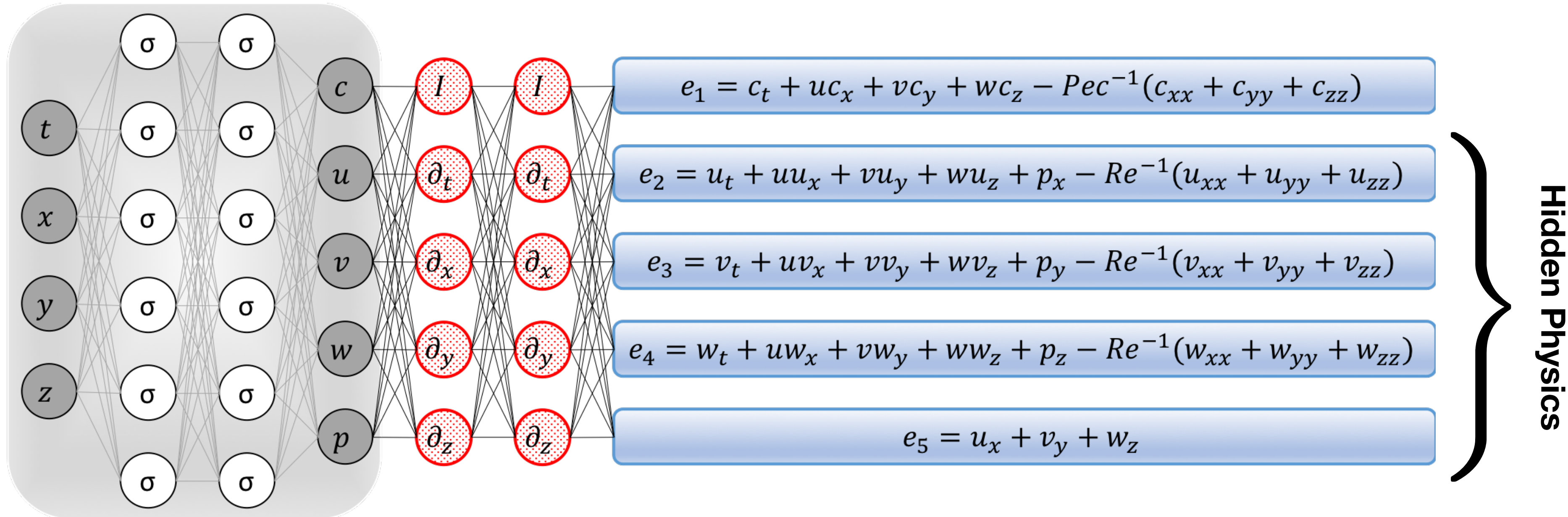


**Pec = 40**

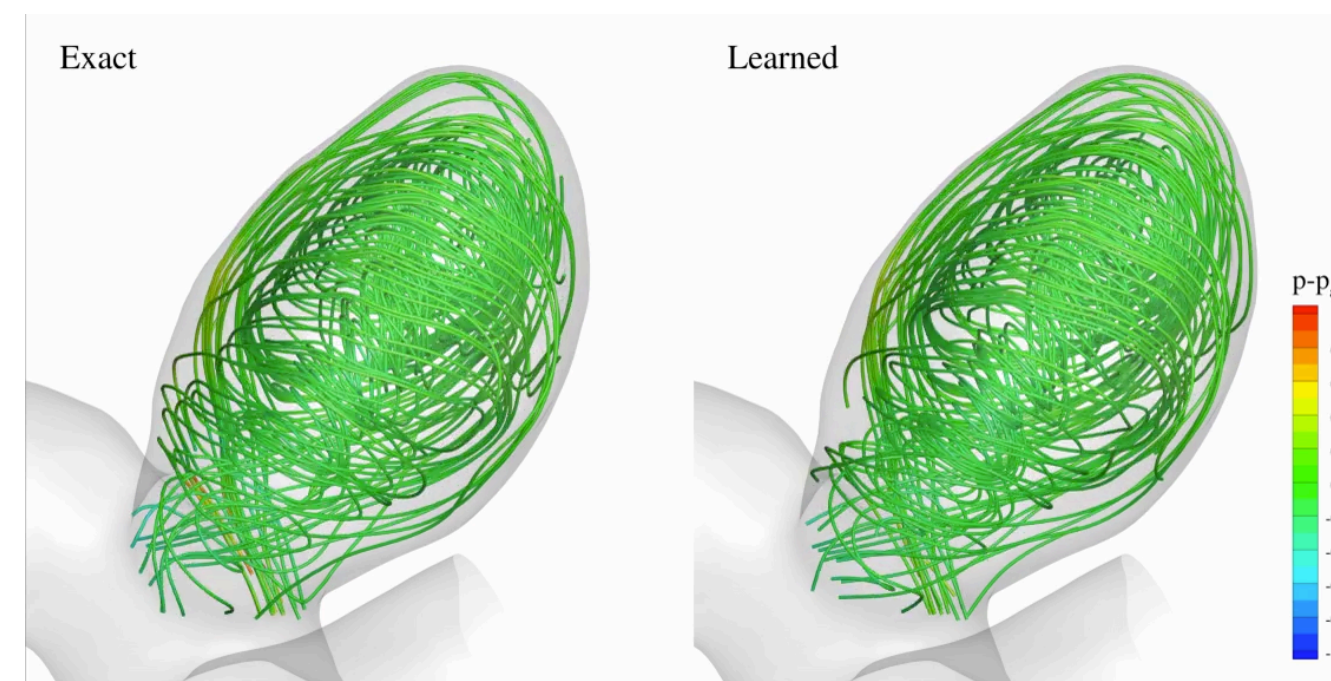
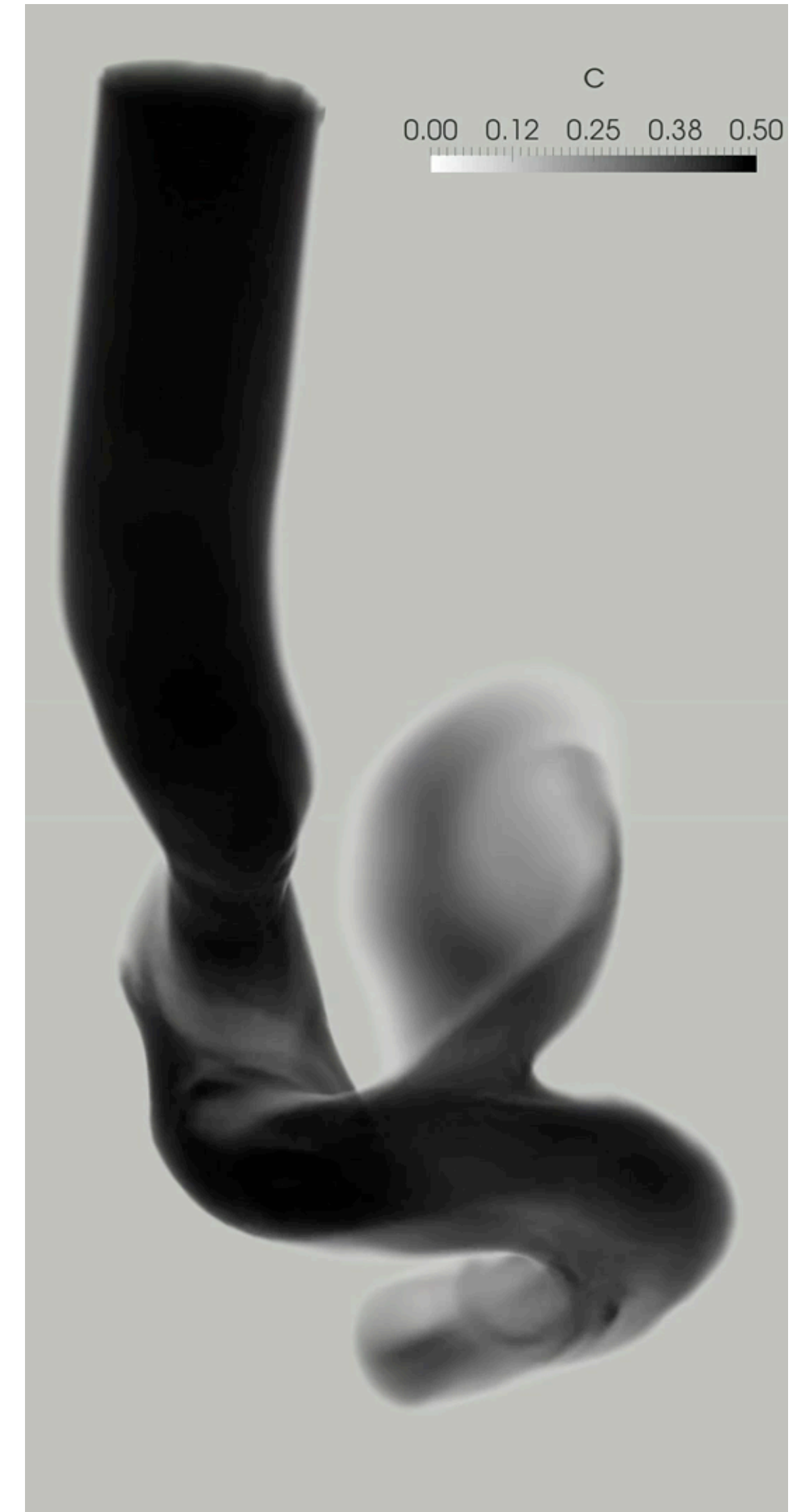
**Pec = 100**

**Pec = 250**

# Hidden Fluid Mechanics



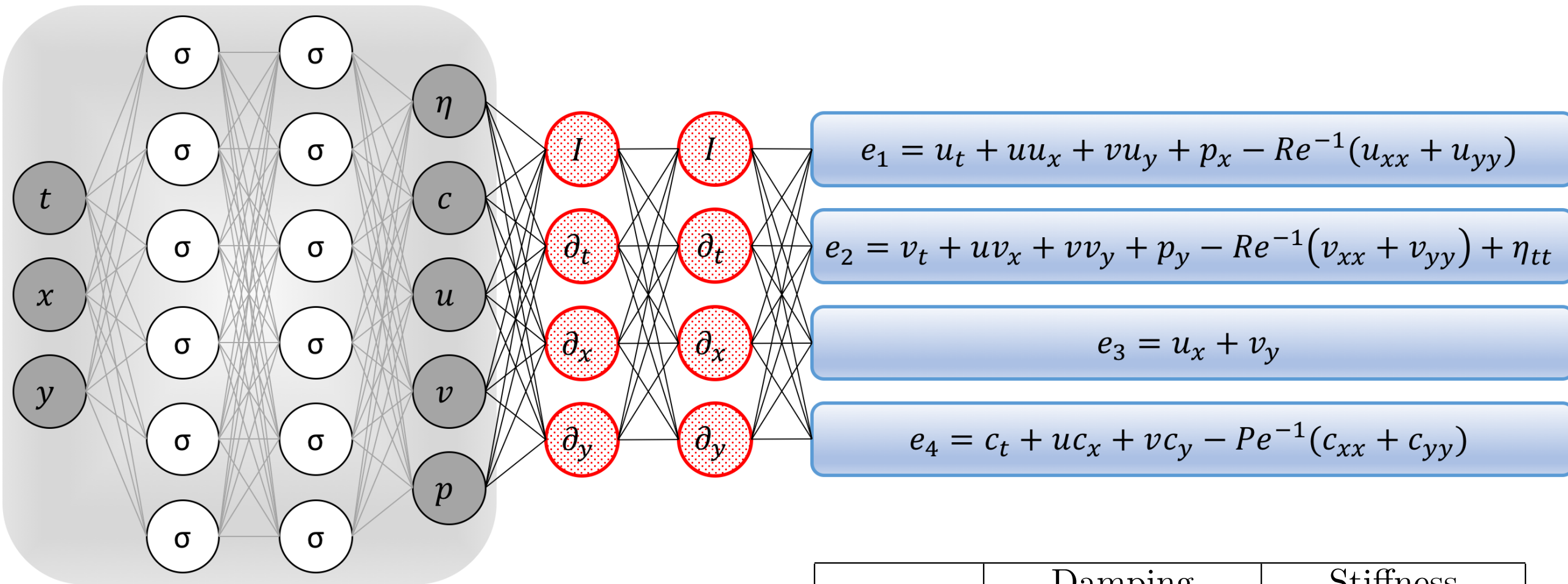
$$SSE = \sum_{n=1}^N |c(t^n, x^n, y^n, z^n) - c^n|^2 + \sum_{i=1}^5 \sum_{n=1}^N |e_i(t^n, x^n, y^n, z^n)|^2$$



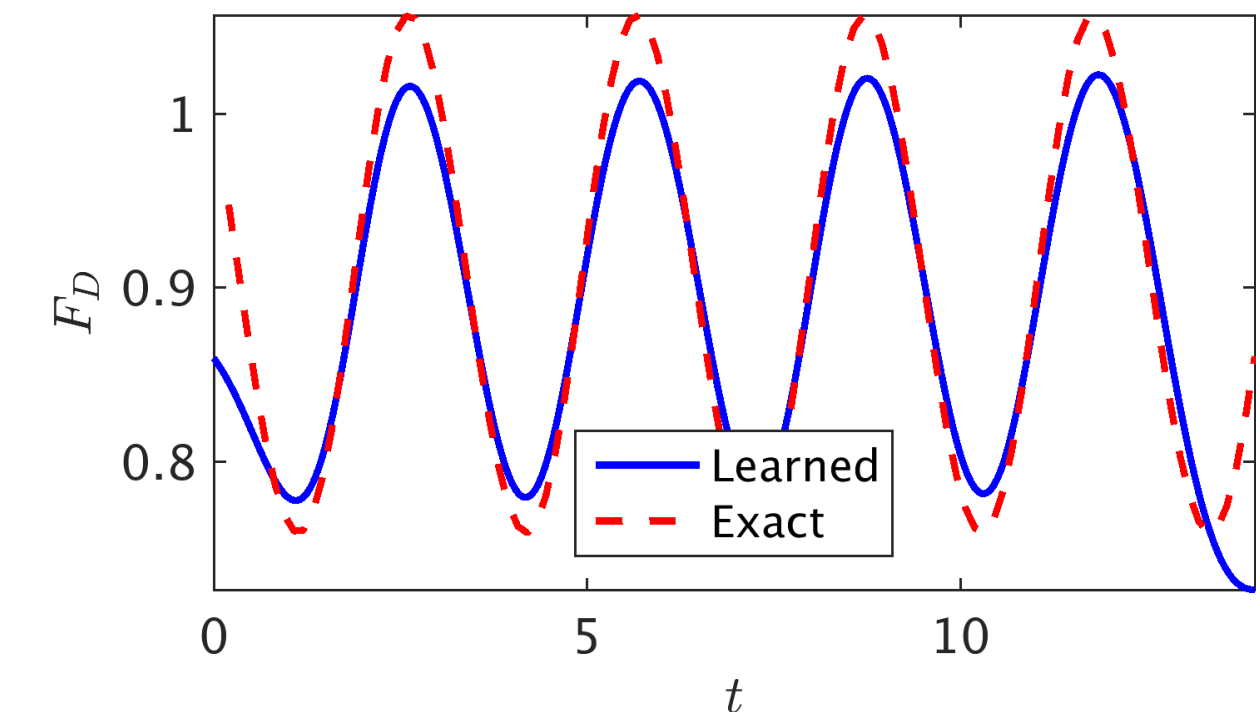
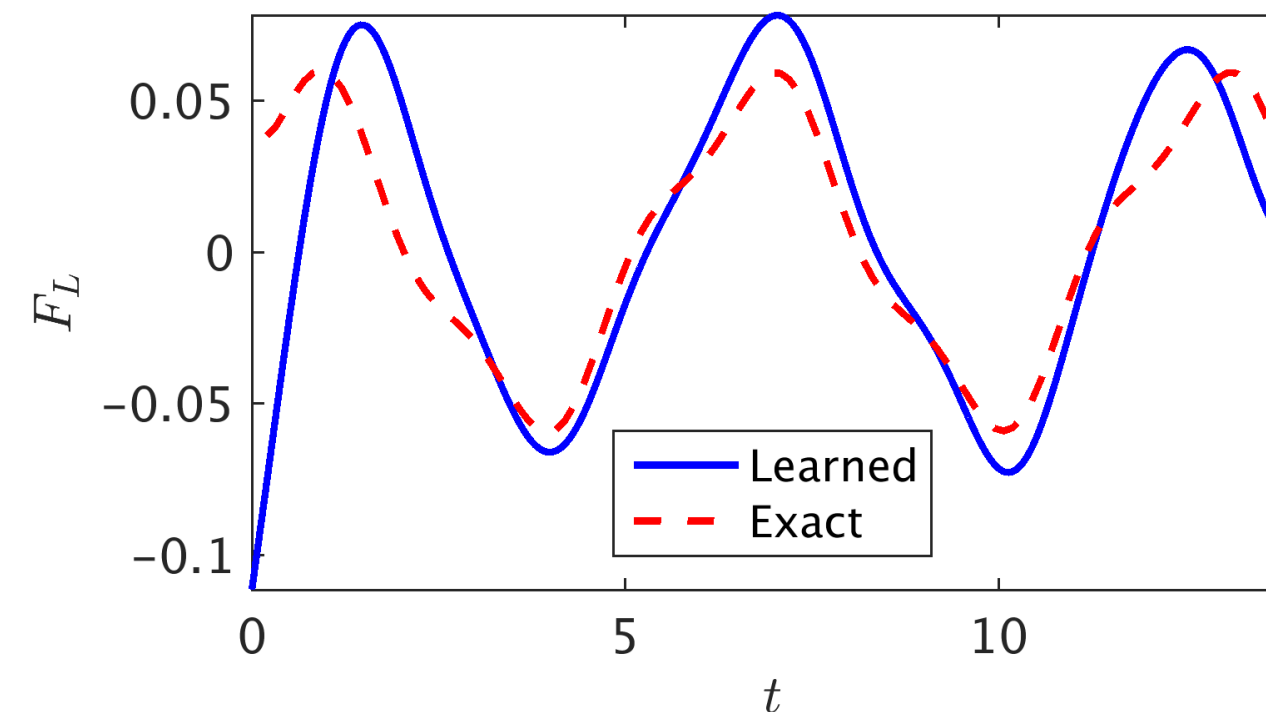
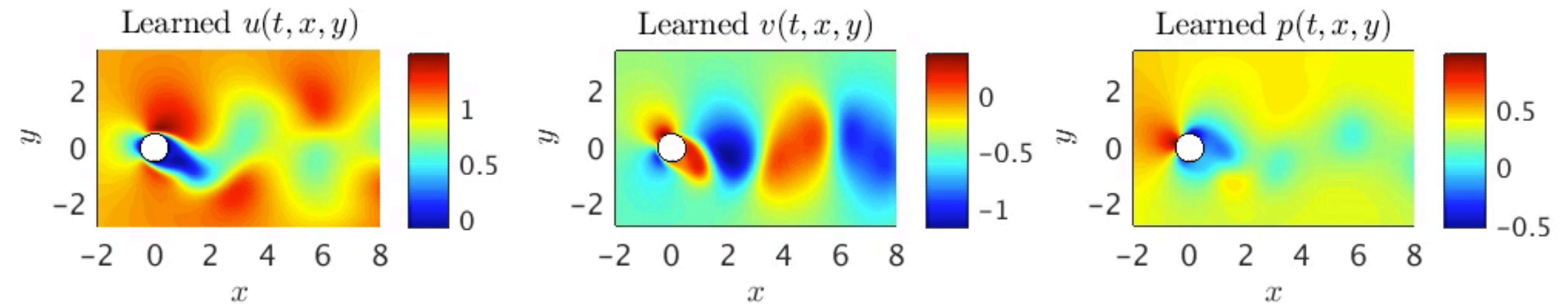
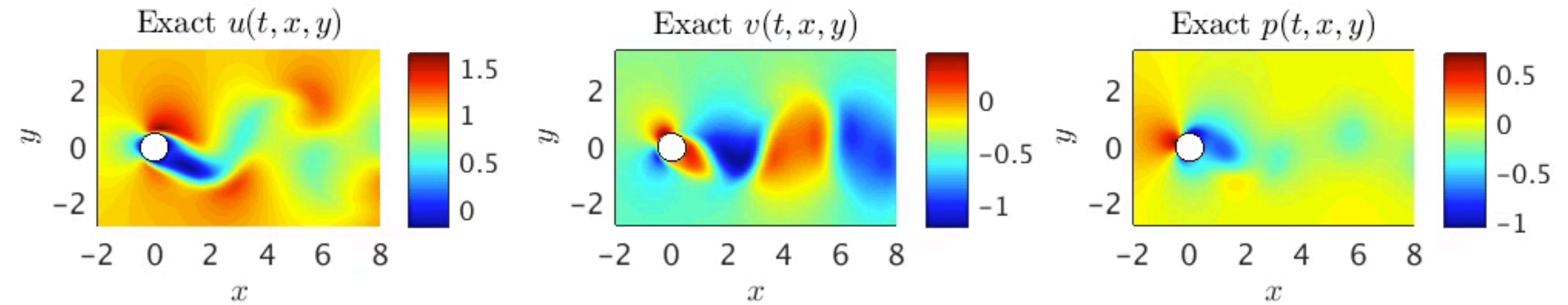
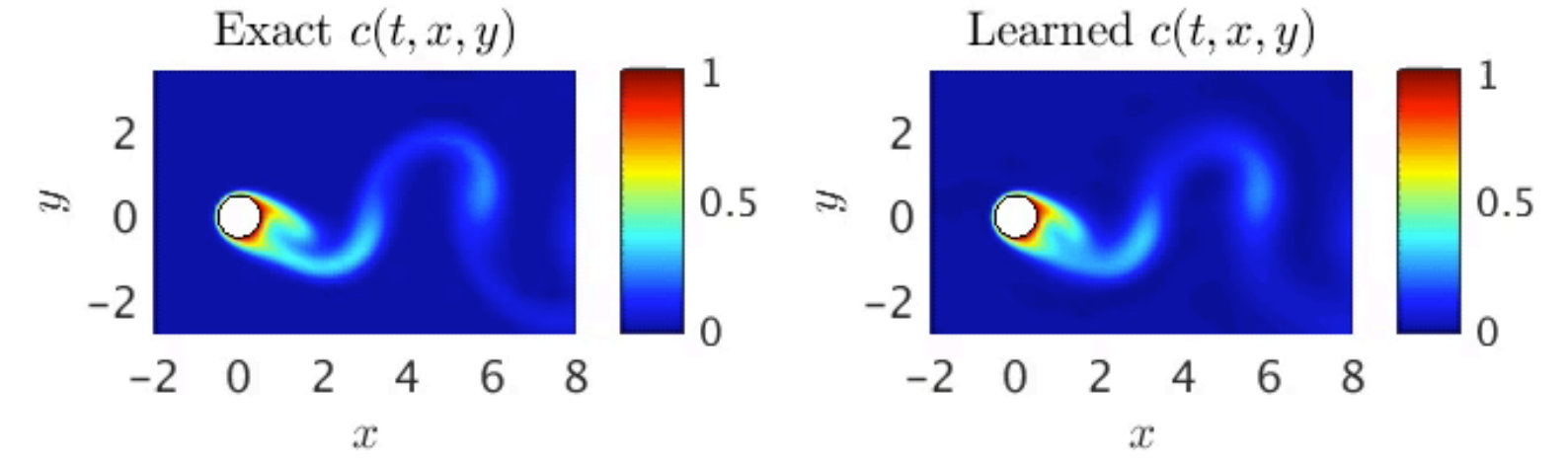
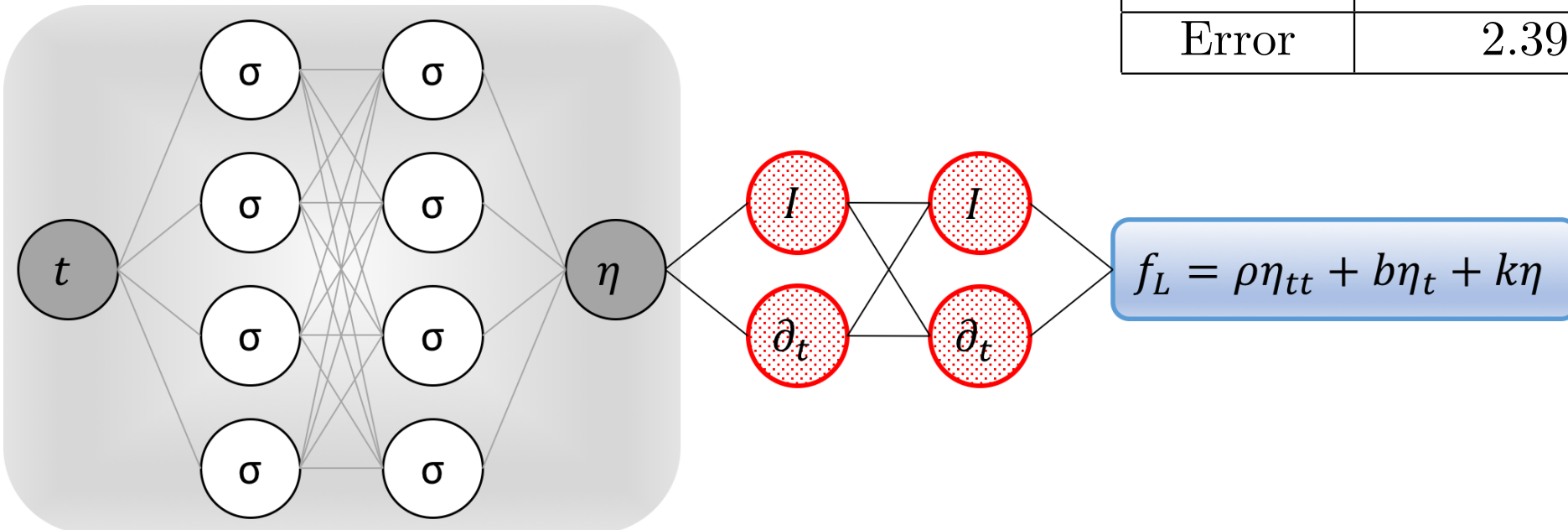
Raissi, Maziar, Alireza Yazdani, and George Em Karniadakis.  
 "Hidden fluid mechanics: Learning velocity and pressure fields  
 from flow visualizations." *Science* (2020).



# Deep Learning of Vortex Induced Vibrations

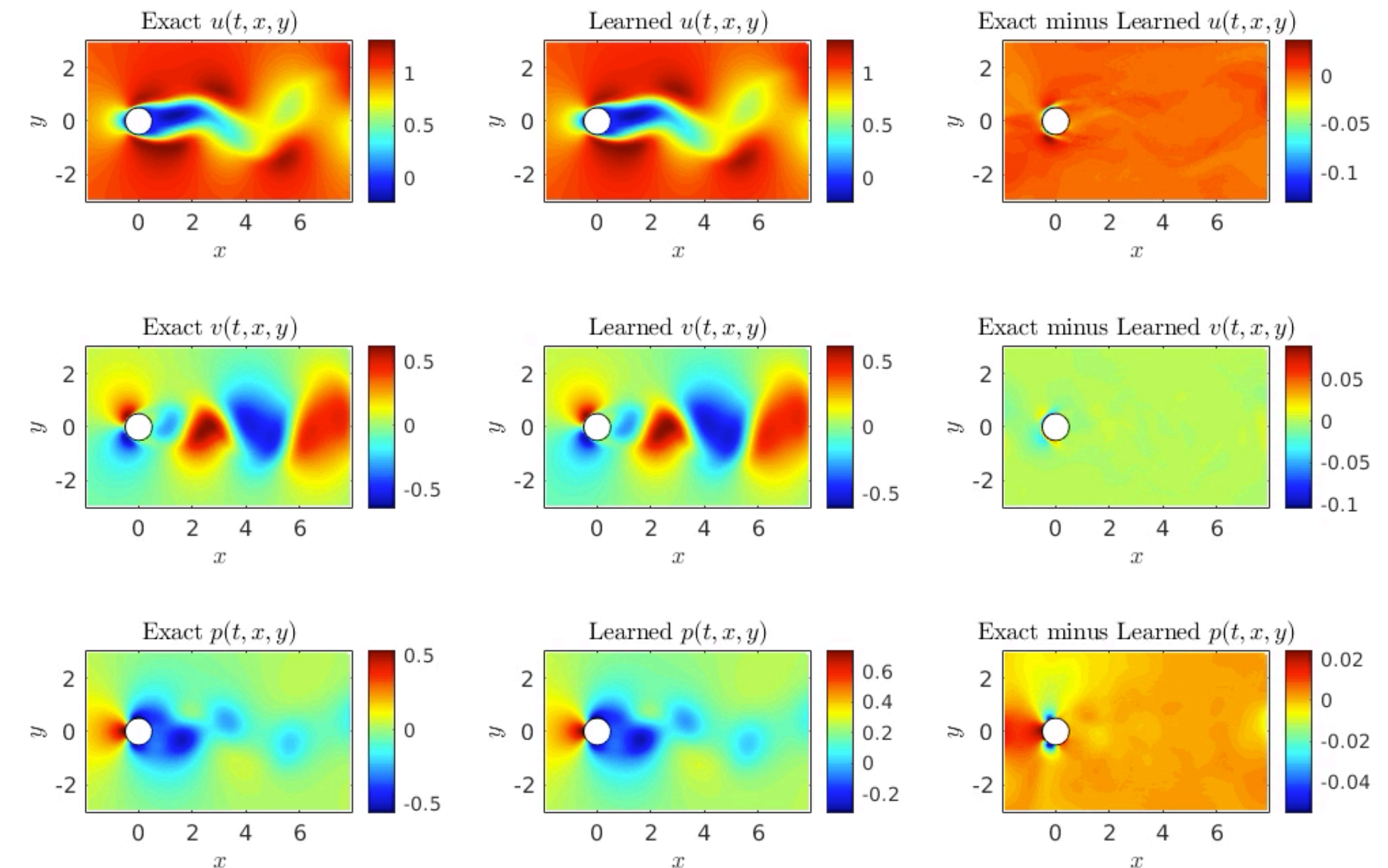
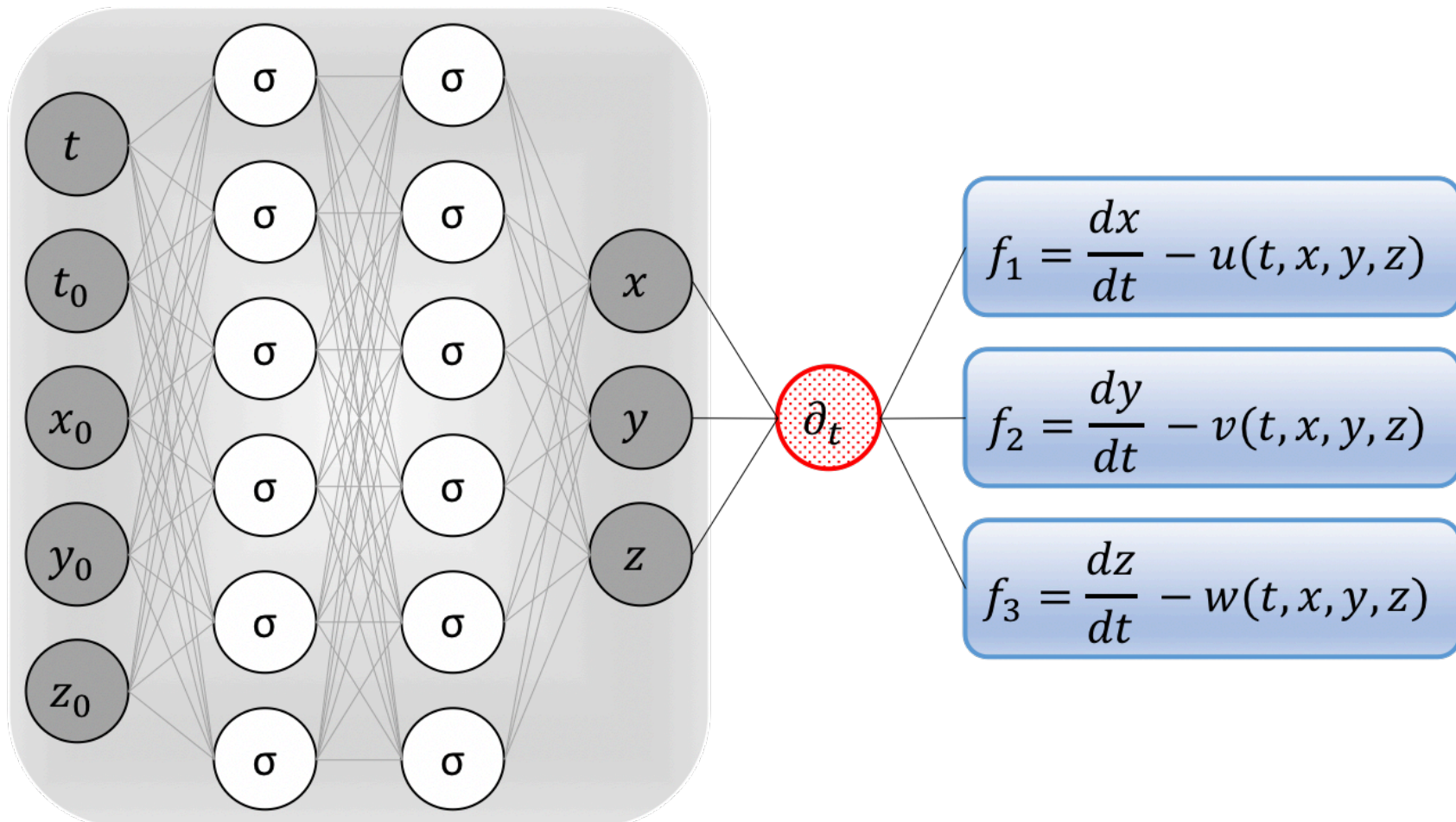
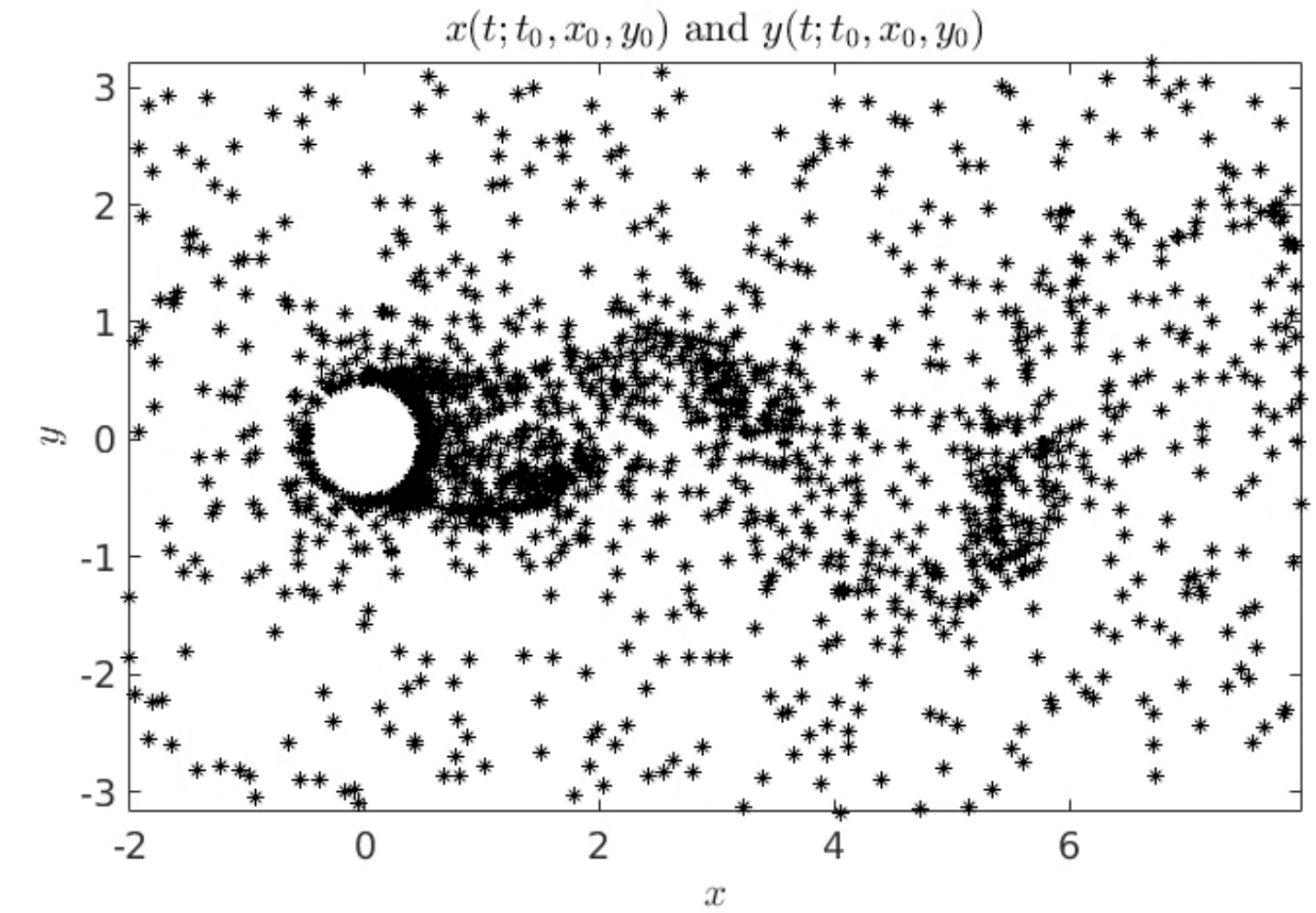
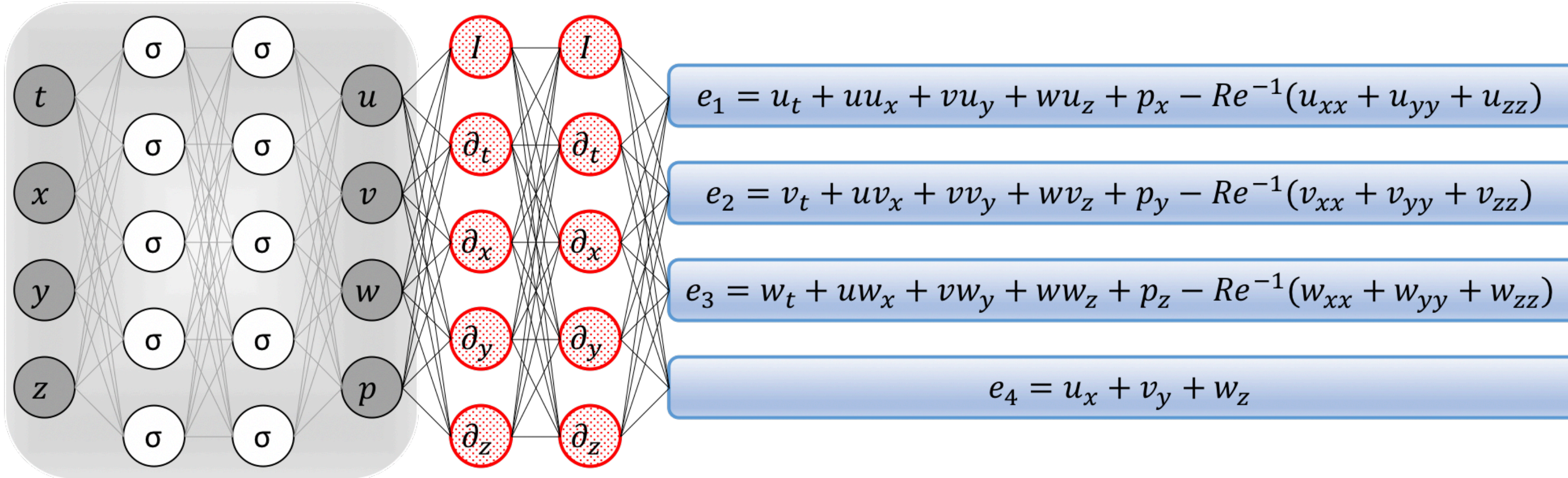


	Damping	Stiffness
Exact	$b = 0.084$	$k = 2.2020$
Learned	$b = 0.08600664$	$k = 2.2395933$
Error	2.39%	1.71%

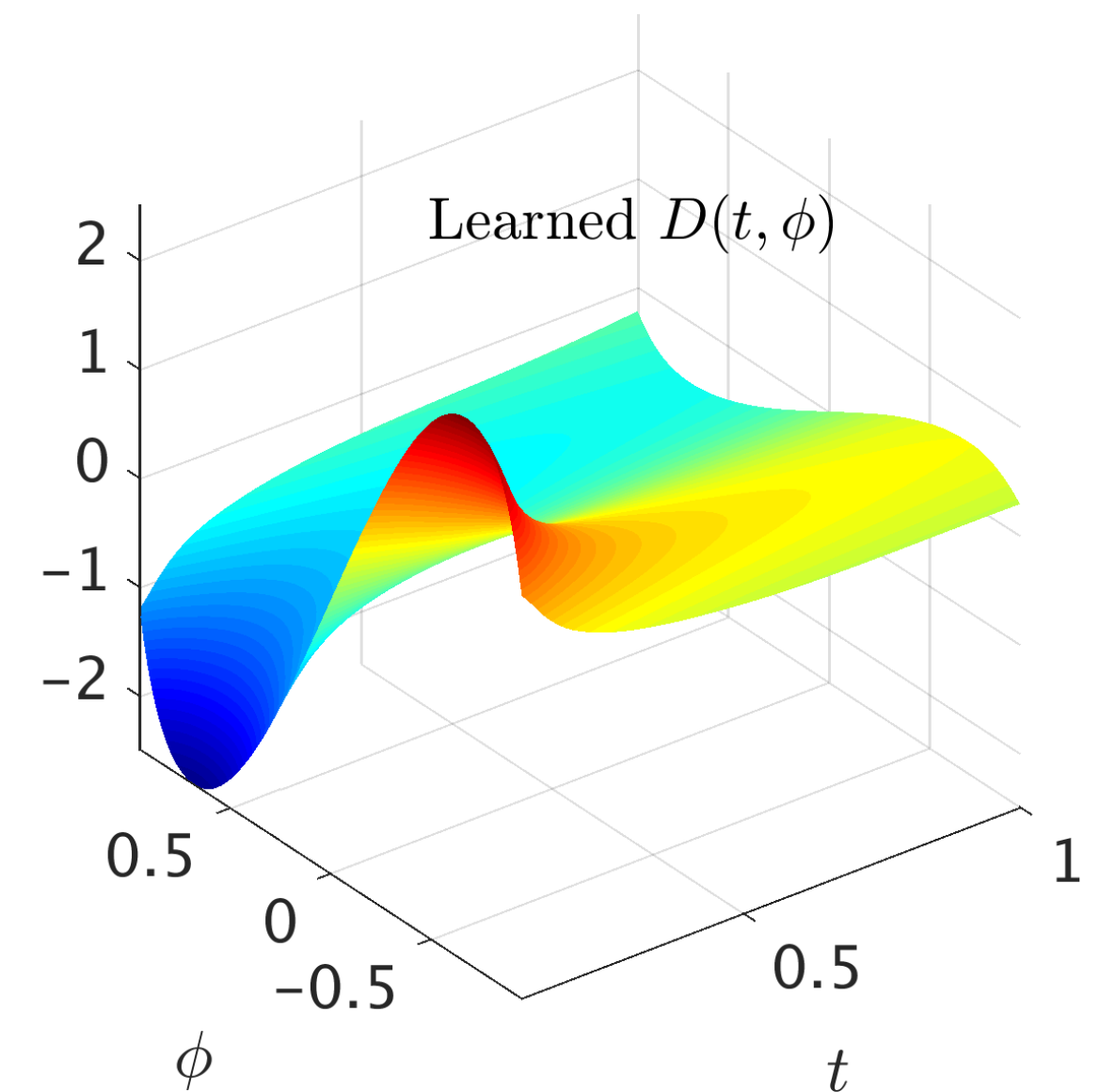
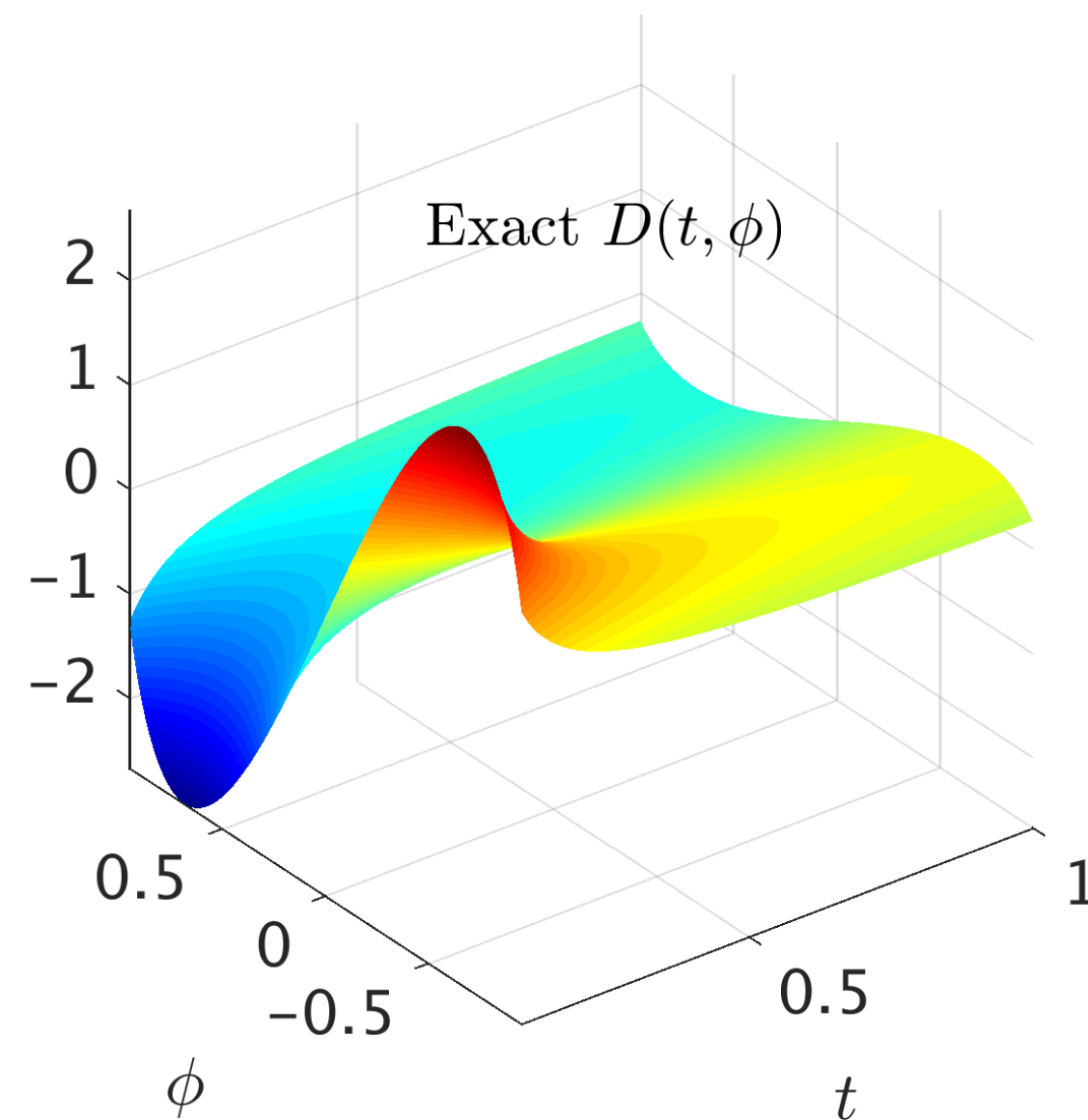
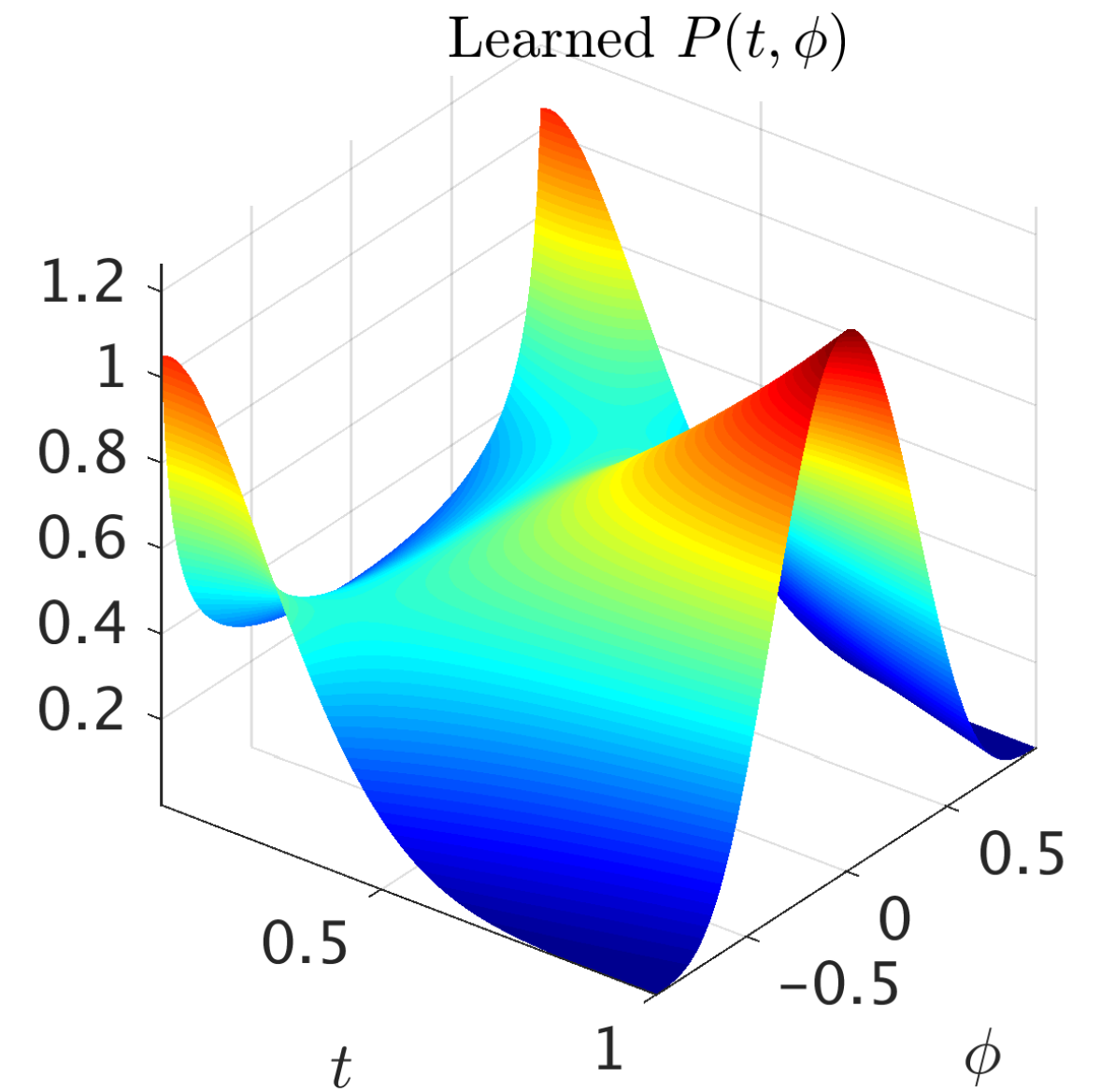
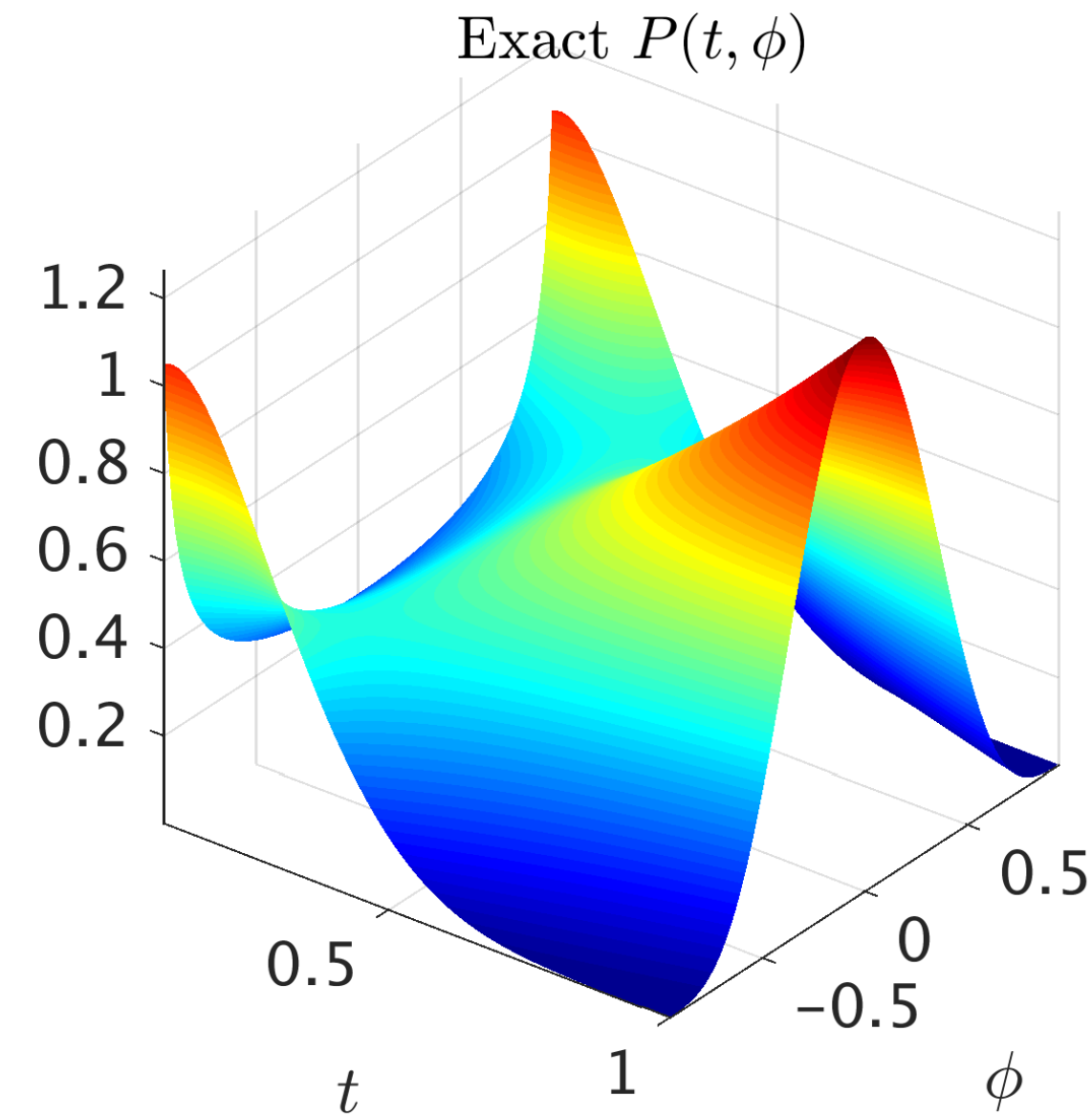
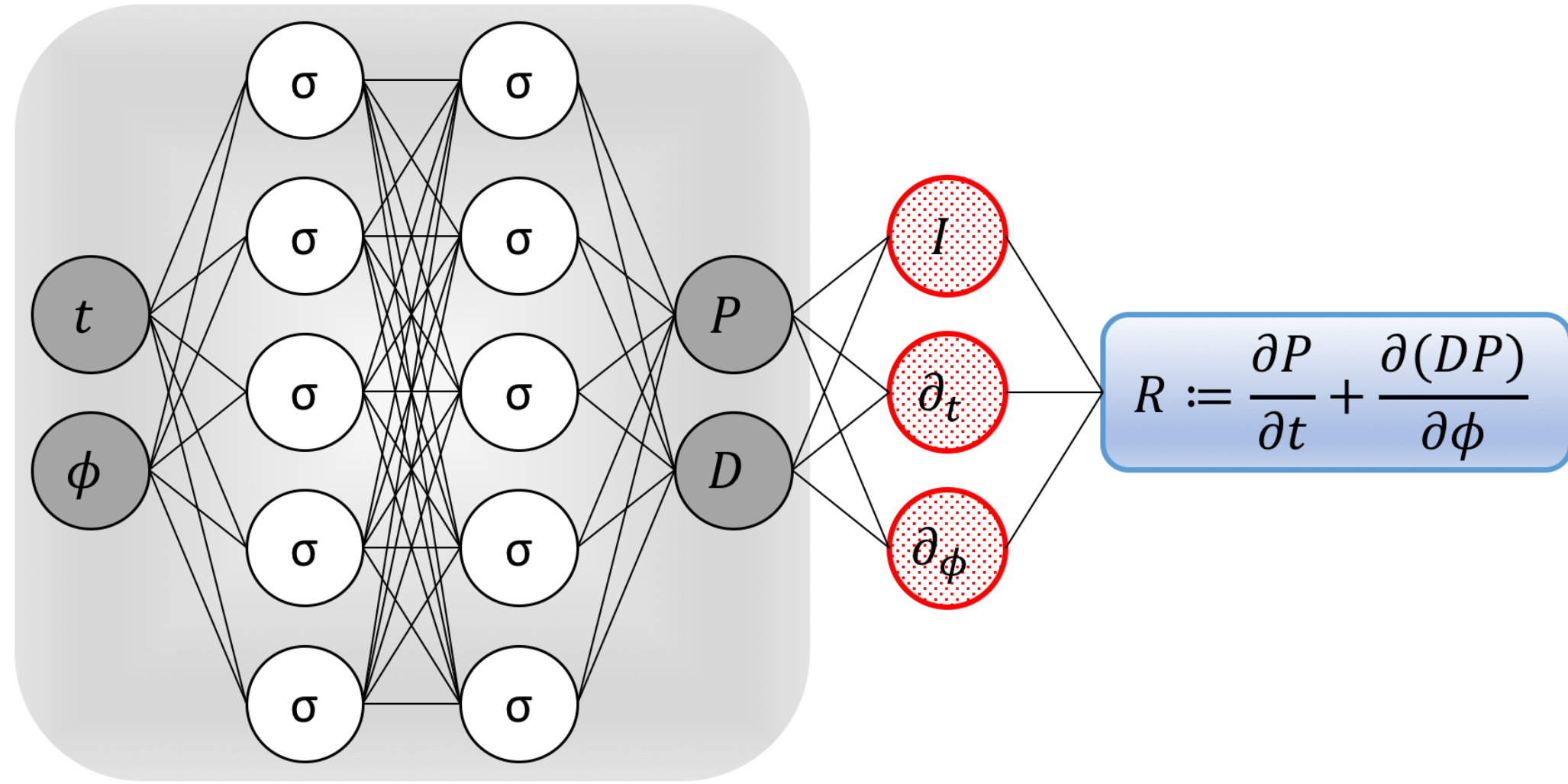


Raissi, Maziar, Zhicheng Wang, Michael S. Triantafyllou, and George Em Karniadakis. "Deep Learning of Vortex Induced Vibrations." *Journal of Fluid Mechanics* (2018).

# Eulerian-Lagrangian Neural Networks



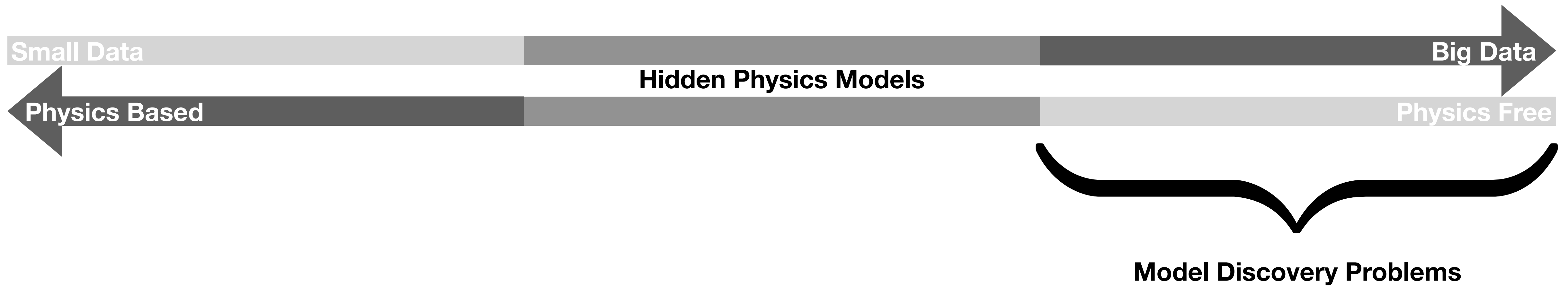
# Deep Learning of Turbulent Scalar Mixing



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



# Model Discovery Problems

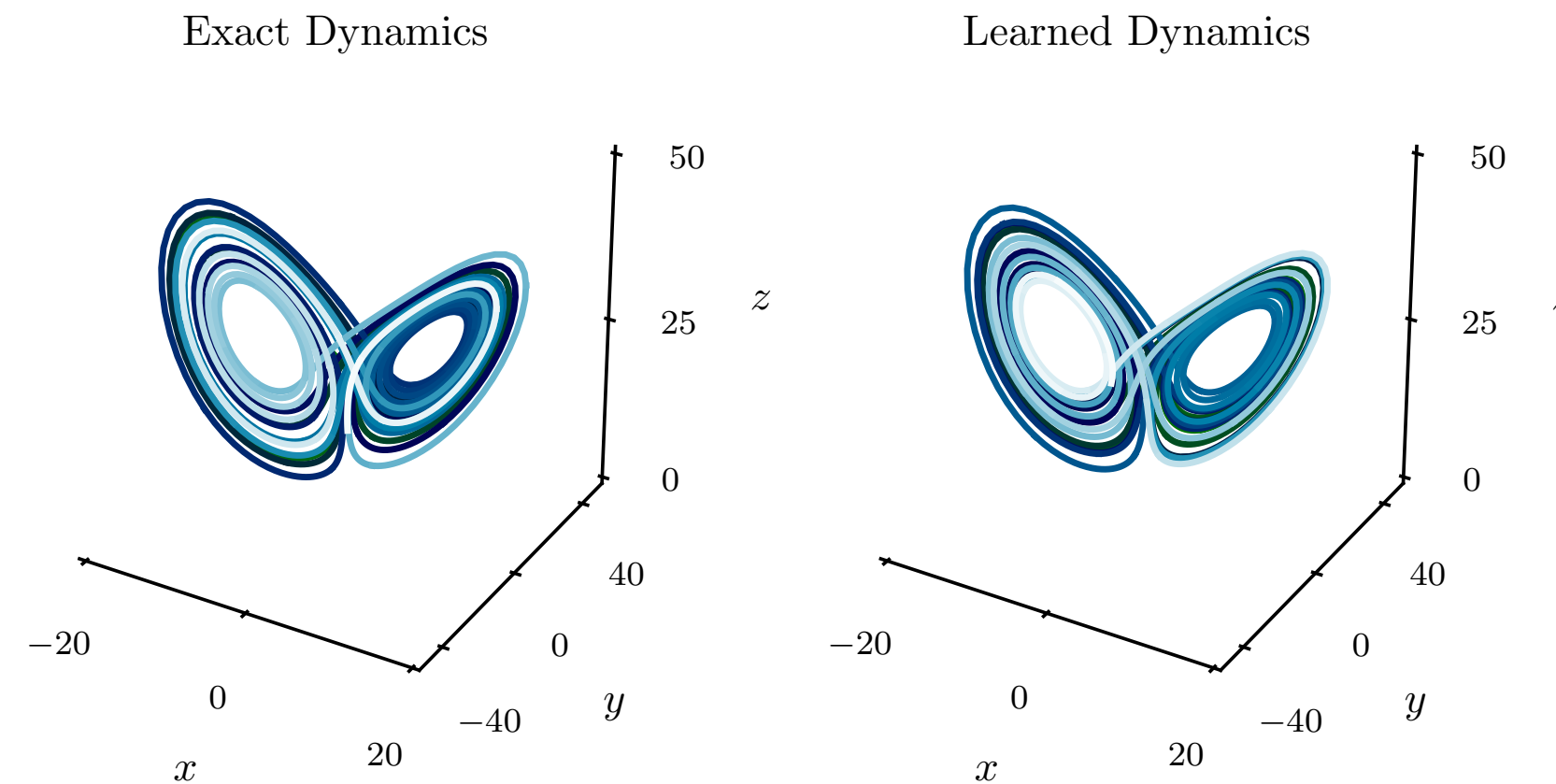


# Multi-step Neural Networks

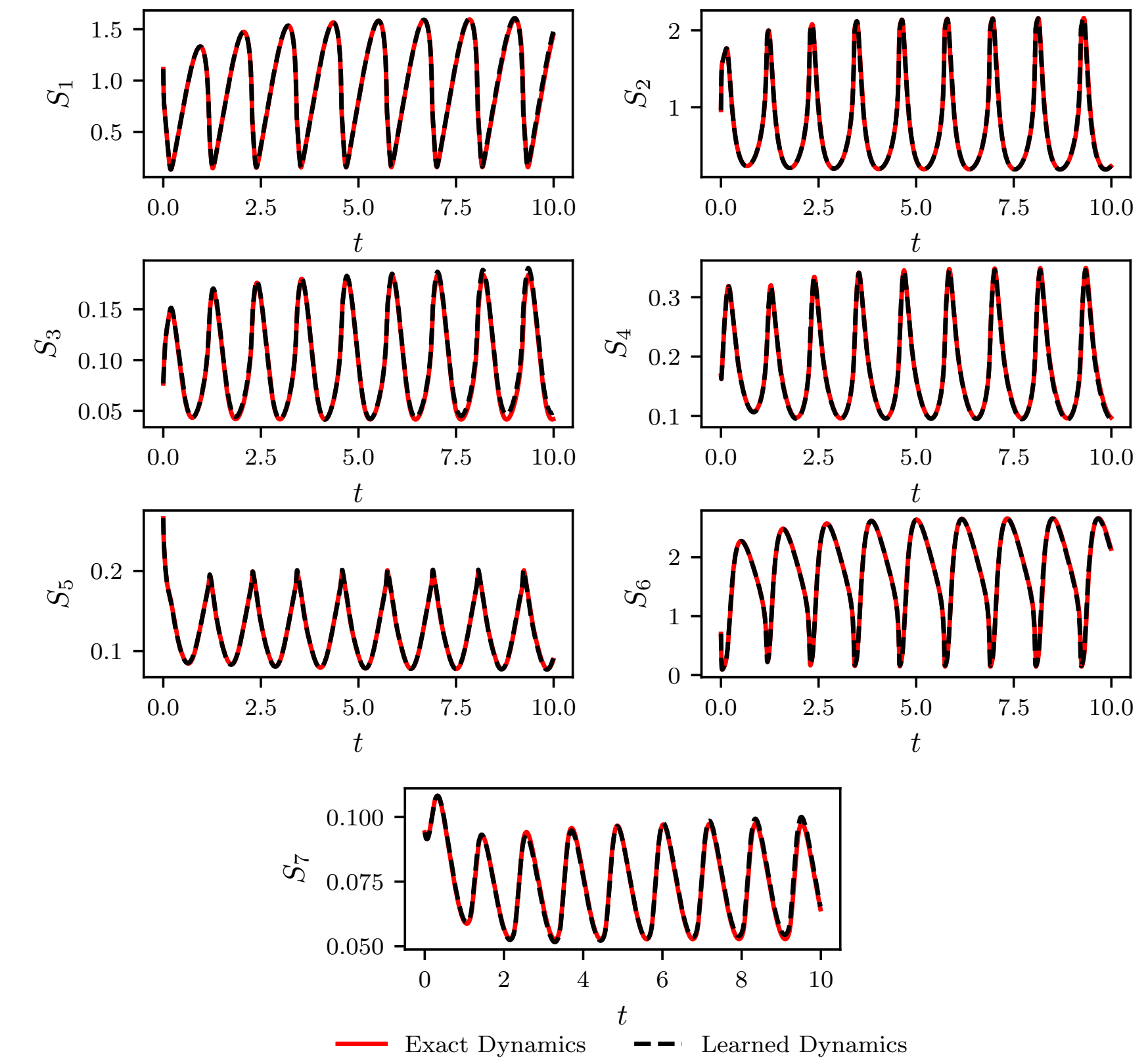
$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$$

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

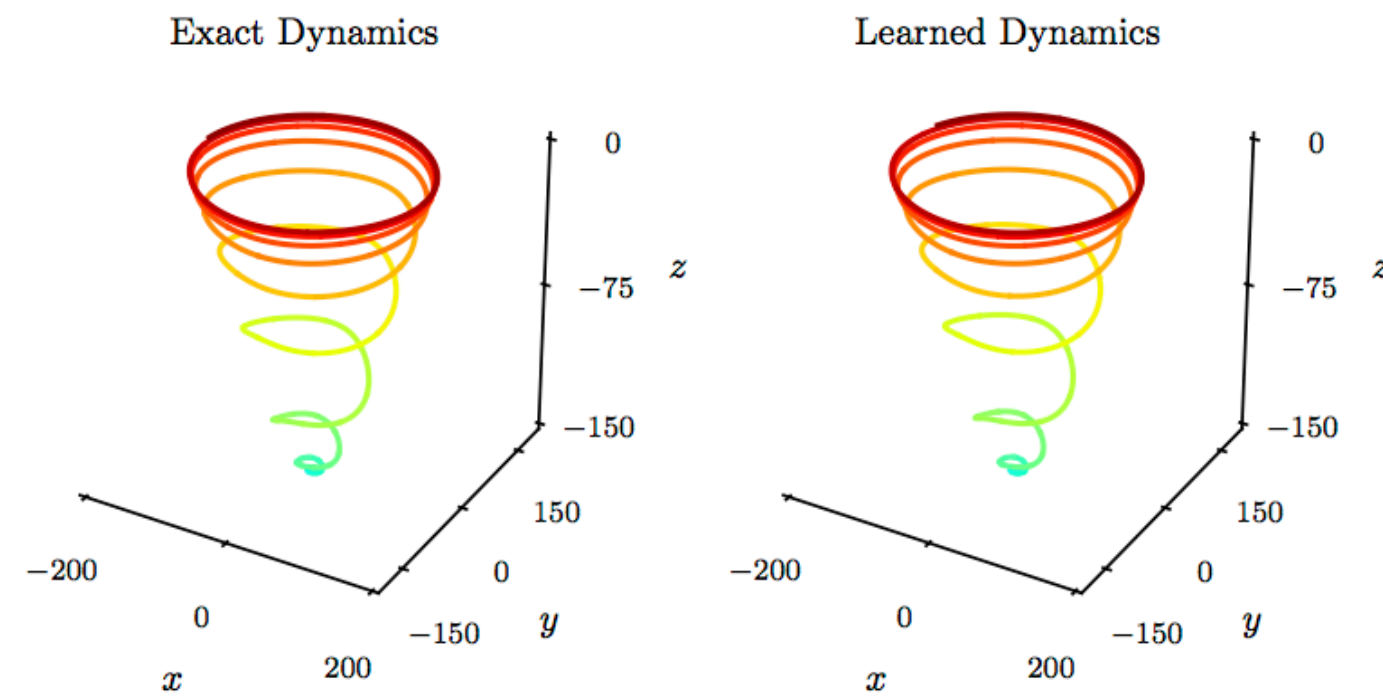
## Lorenz System



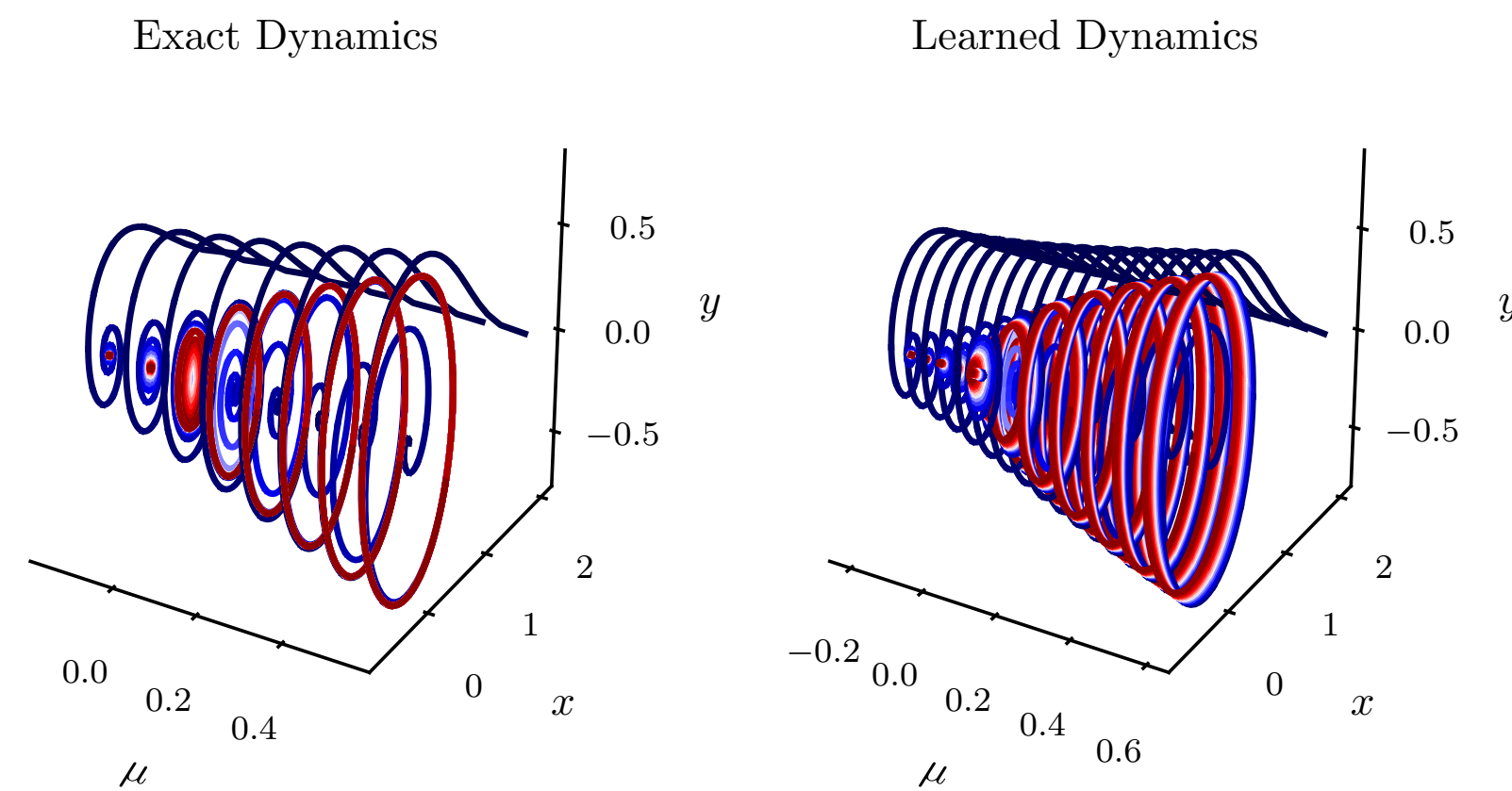
## Glycolytic Oscillator



## Navier-Stokes Equations

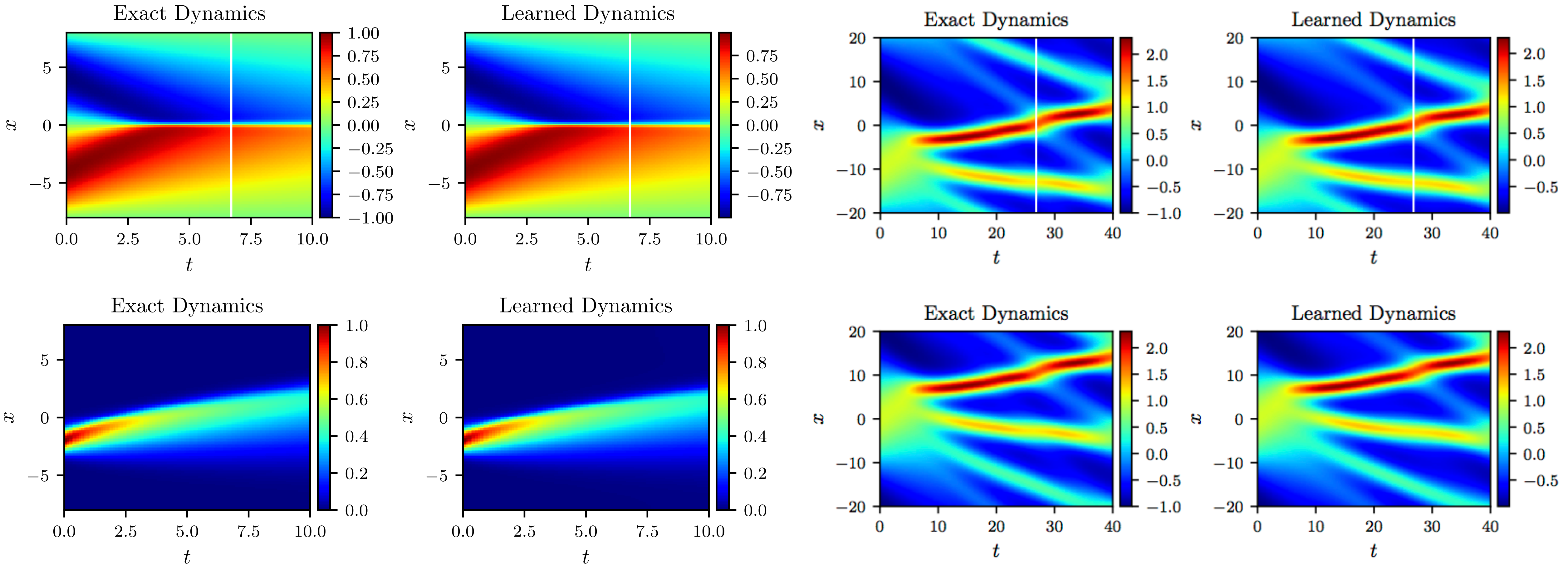


## Hopf Bifurcation



# Deep Hidden Physics Models

$$u_t = \mathcal{N}(t, x, u, u_x, u_{xx}, \dots) \quad f = u_t - \mathcal{N}(t, x, u, u_x, u_{xx}, \dots) \quad \sum_{i=1}^N |u(t_i, x_i) - u_i|^2 + |f(t_i, x_i)|^2$$





# Hidden Physics Models

## Thank you!

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### 📄 NumericalGP

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

● MATLAB ☆ 35 🍷 28

### 📄 HPM

Hidden physics models: Machine learning of nonlinear partial differential equations

● MATLAB ☆ 66 🍷 47

### 📄 ParametricGP

Parametric Gaussian Process Regression for Big Data

● Python ☆ 29 🍷 14

### 📄 DeepHPMs

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

● Python ☆ 161 🍷 119

### 📄 PINNs

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

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

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