Introduction to Machine Learning with Applications to Aeroheating Database Generation

Thermal & Fluids Analysis Workshop

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Goals of this short-course

1. **Provide a foundation in ML and resources for you to learn on your own**
    - Machine learning is a very broad field, impossible to teach everything here
    - Instead, introduce core principles and vocabulary
    - Resources for self-learning

2. **Demonstrate recent examples of ML in my daily work at NASA**
    - How to approach typical problems
    - Combine physical intuition and knowledge with ML principles
    - Gaussian Process regression

What do we mean by “learning”?

A formal definition: A computer program is said to ***learn*** from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience [1].

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- Machine learning is the science of designing computer algorithms that can <u>automatically</u> improve their performance at a given task, as additional data are provided to them

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Stockfish

Task:
Win chess match.

Performance Measure:
Number of wins

Experience:
Human logic and intuition.

AlphaZero

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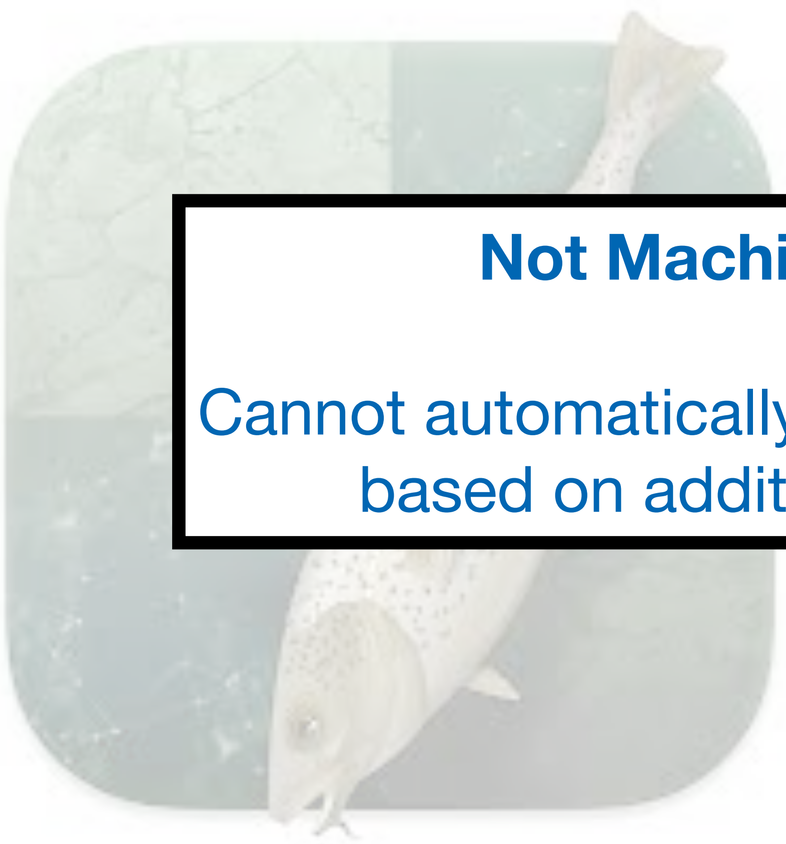

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Cannot automatically improve performance based on additional experience.

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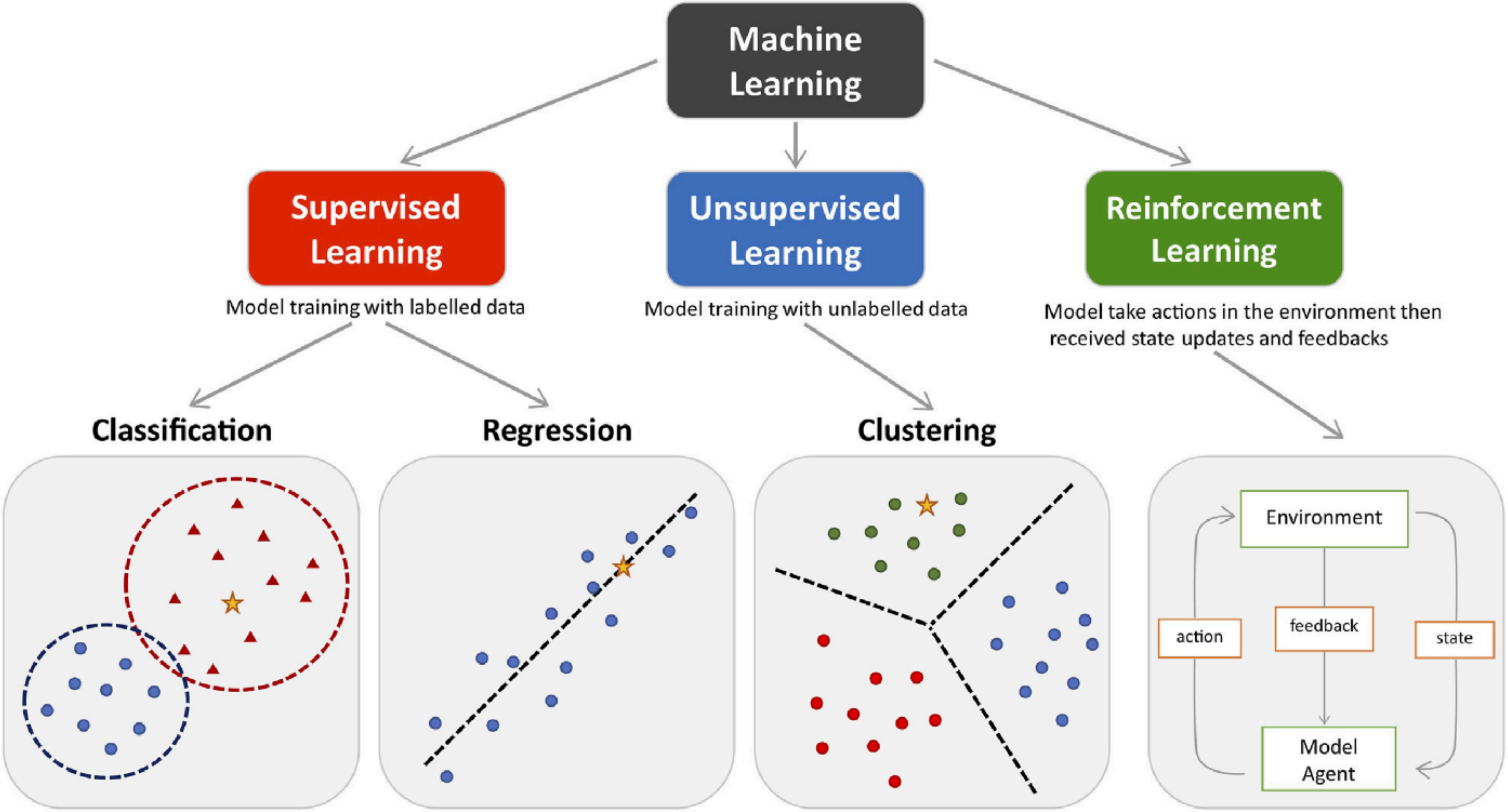
Types of learning problems



Peng, Jury, Donnes, Ciurtin. *Frontiers in Pharmacology* 12:720694, 2021.

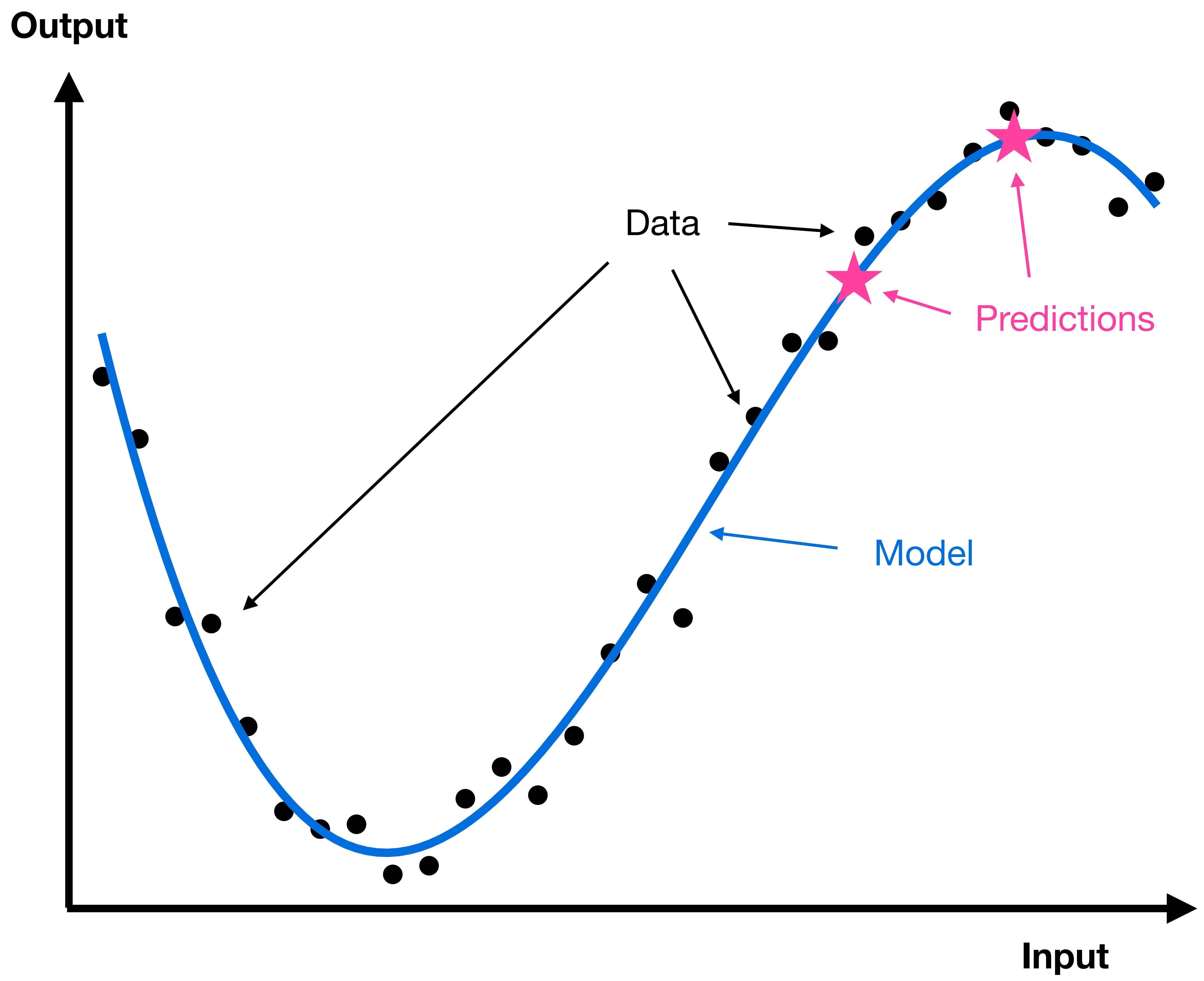
Regression in a nutshell

Learn a functional relationship (*model*) between data *inputs* and *outputs* to make *predictions* for unseen inputs

Supervised Learning Framework

- Given a *dataset*: $\mathscr{D} = \{(x_i, y_i) : x_i \in \Omega, \; y_i = f(x_i)\}$
- Given a (possibly *parametric*) model: $y = \hat{f}(x; \theta)$
- Find a model that best approximates the underlying relationship between inputs and outputs

$$\hat{f}(x; \theta^*) \approx f(x)$$



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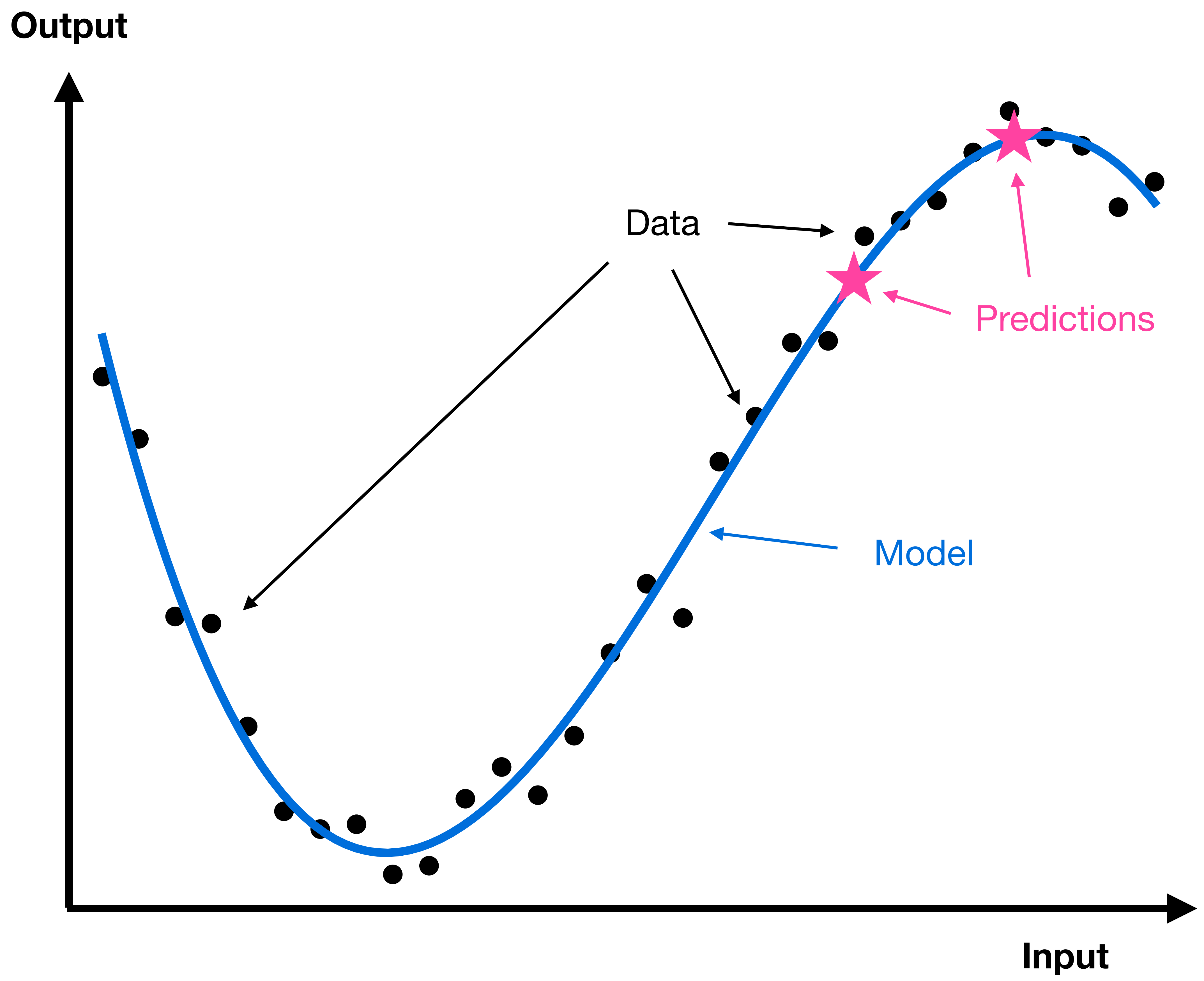
Key Questions

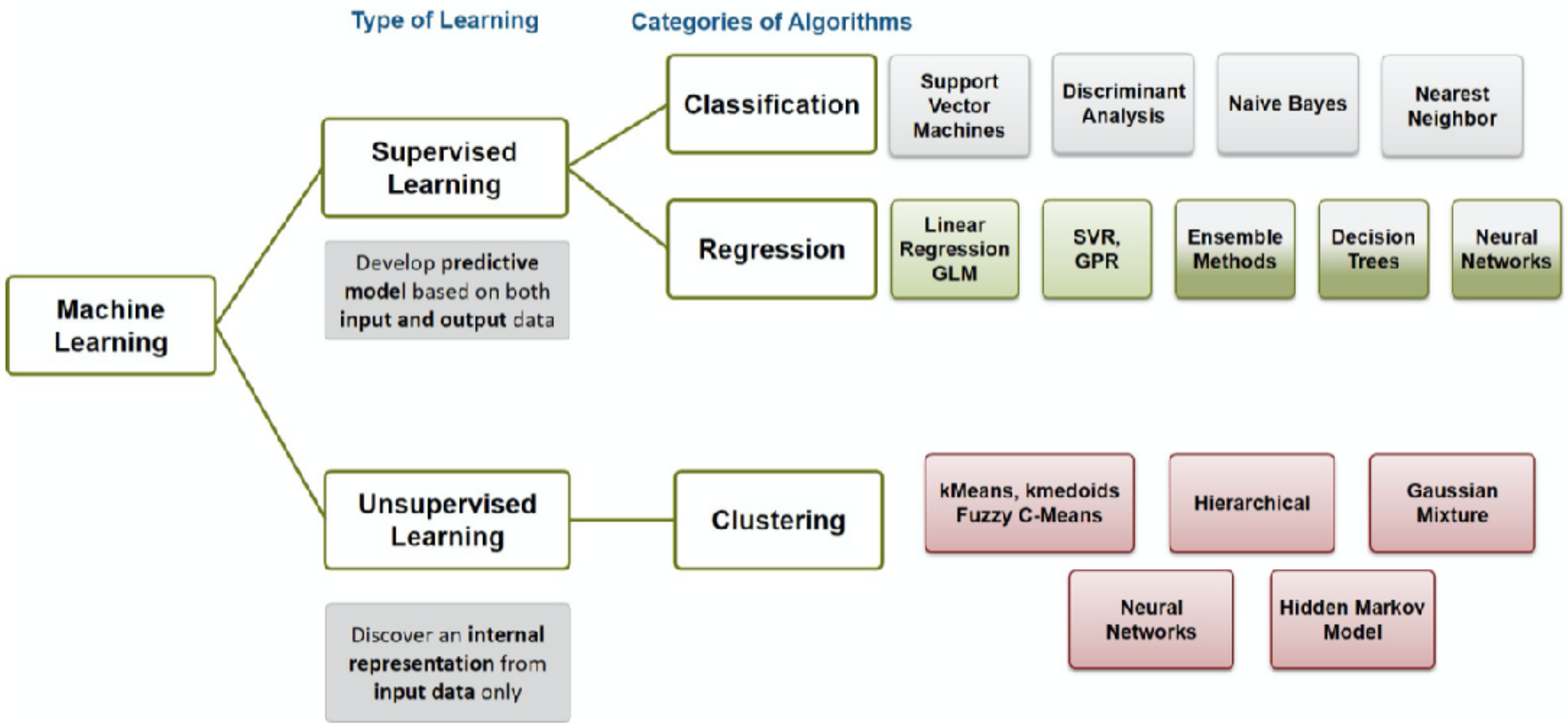
1. How do we know if a model is "good" (much less "best")?
2. What about noisy data?



Many models out there!

Examples:

- Linear Models
- Support Vector Machines
- Gaussian Processes
- Neural Networks
- Decision Trees



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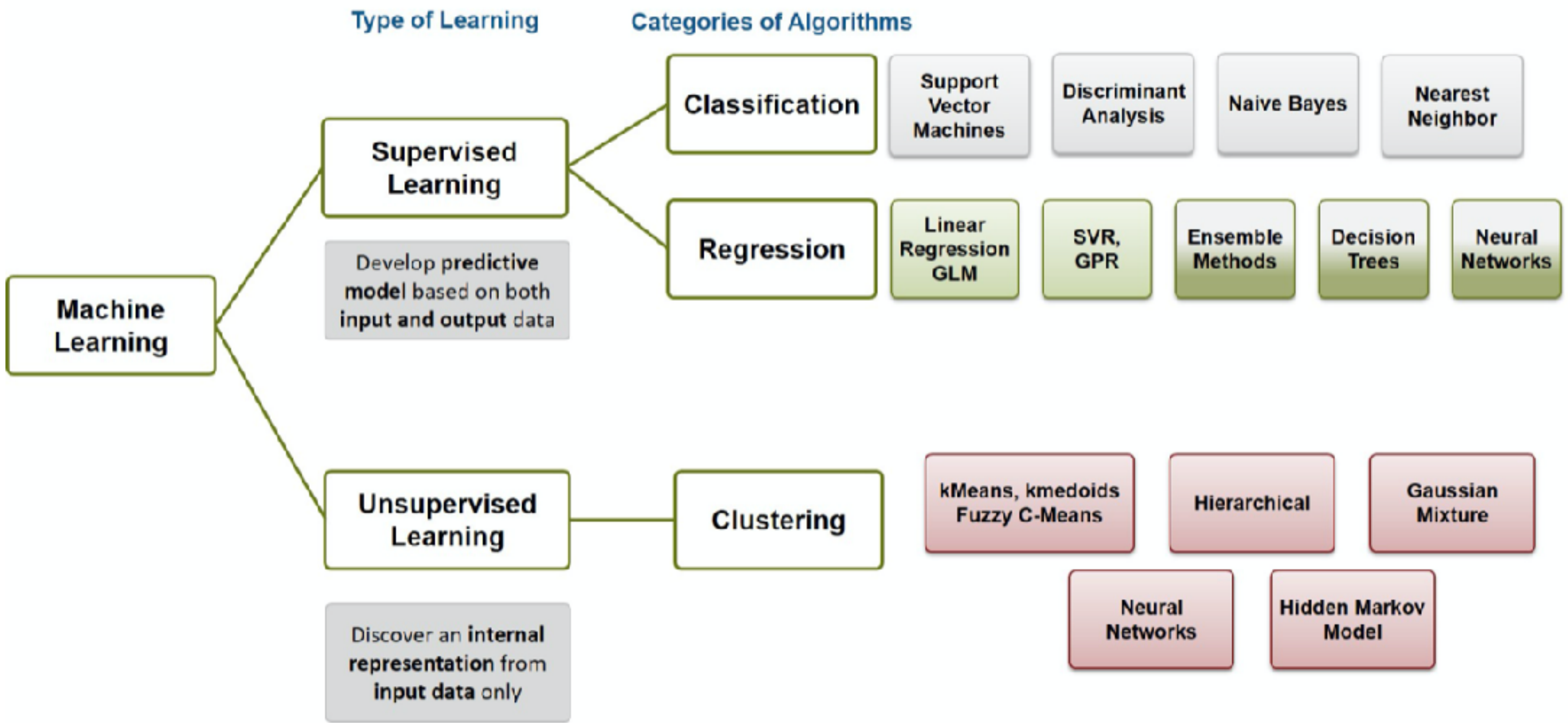


Choice depends on multiple factors:

- Training and evaluation cost
- Implementation and deployment
- Scalability
- Treatment of uncertainty

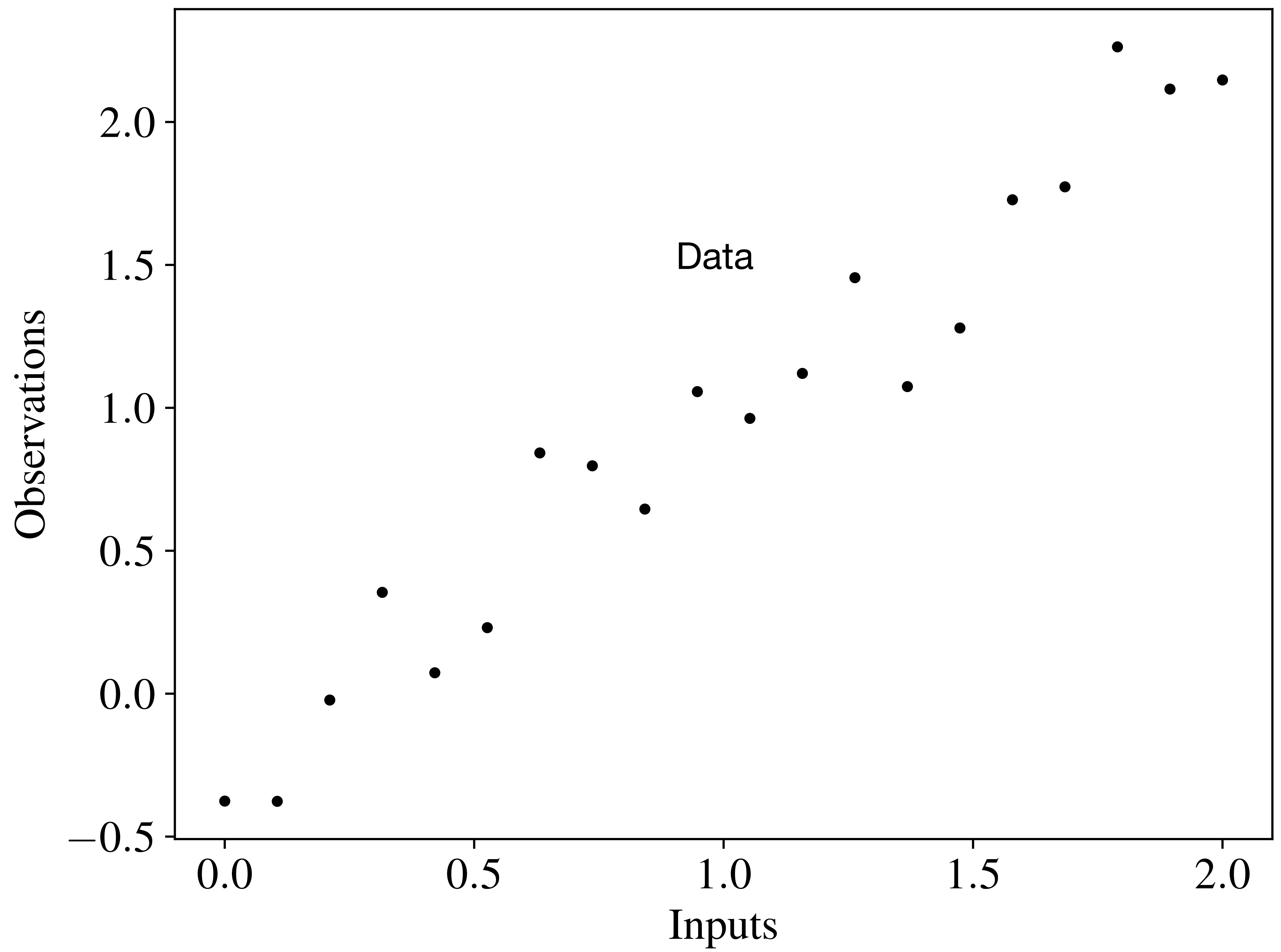
Linear regression

Given the data on the right, what are our initial thoughts?

- Observations generally increase with increasing input values
- Trend appears linear with a positive slope and negative intercept
- The trend is not perfect, noise or other unknown feature

Model assumption: response is linear with nonzero intercept

$$y = \hat{f}(x; w_0, w_1) = w_0 + w_1 x$$



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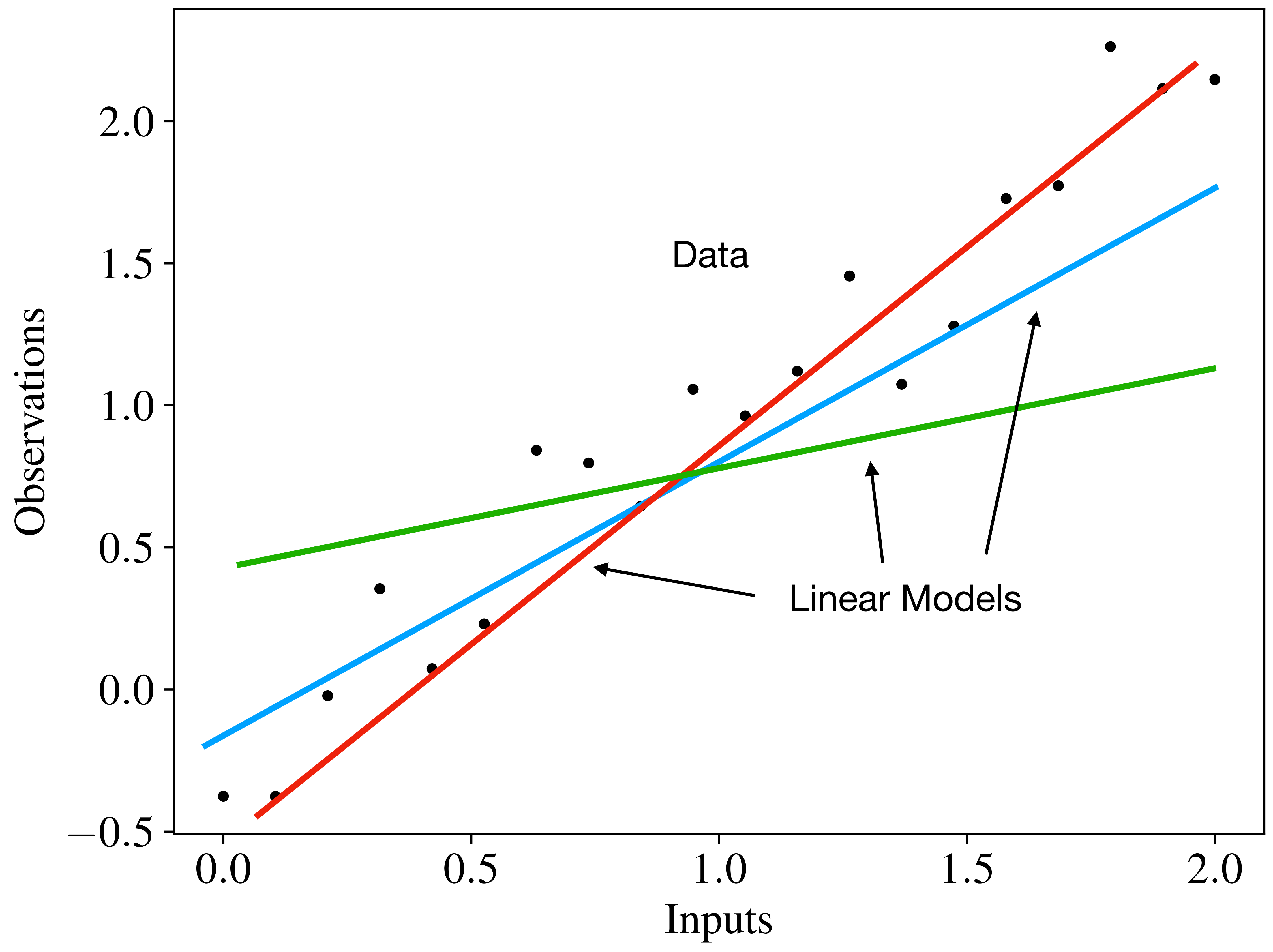

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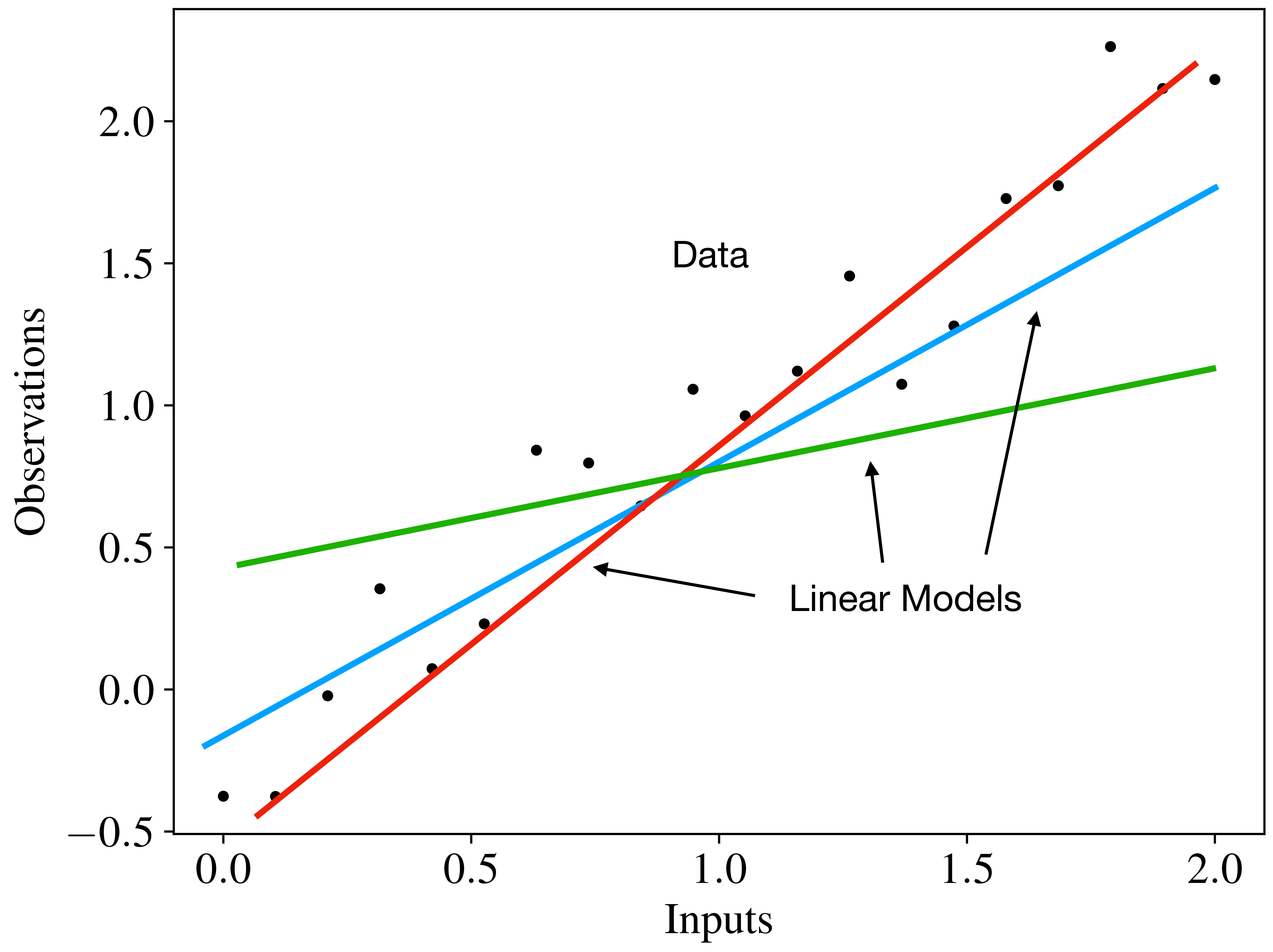

Loss functions

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In general, we can think of data as samples of an underlying joint probability density function $p(x, y) = p(y \mid x)\, p(x)$, where

$$p(y \mid x) = \begin{cases} 1, & y = f(x) \\ 0, & \text{otherwise} \end{cases}$$

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Loss as function of model parameters θ for given model $\hat{f}(x;\theta)$

Expected model error over the input probability distribution $p(x)$ for given error model l

Definition of the expectation of l on $p(x)$

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"Empirical" loss, evaluated on available dataset

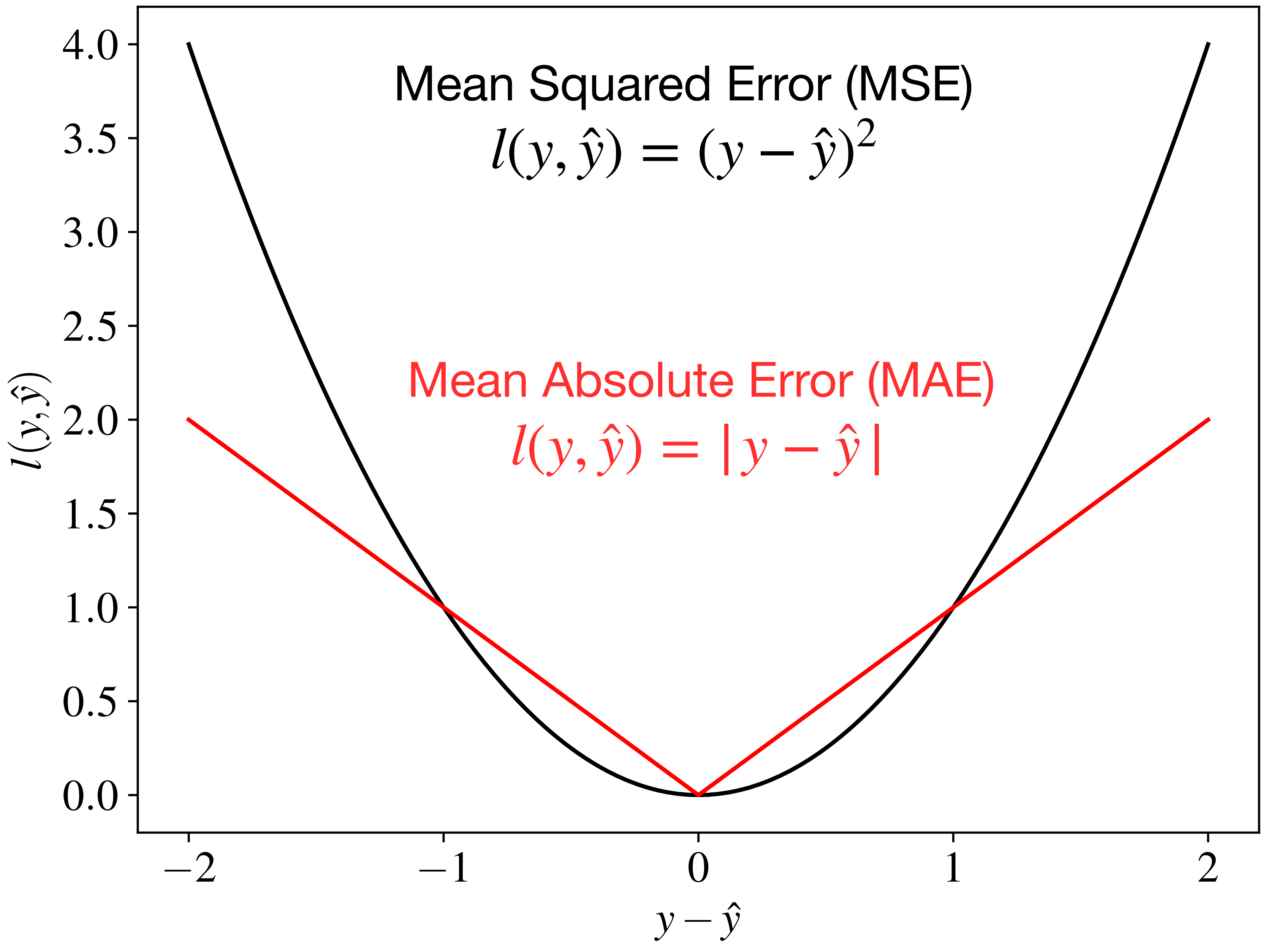
rely on approximate loss

$\boxed{\text{We generally don't know } p(x, y) \text{ because that's what we want to model!}}$

Example loss functions

Recall $\mathscr{L}(\theta)[\hat{f}] = \dfrac{1}{N} \sum_{(x_i, y_i) \in \mathscr{D}} l(y_i, \hat{f}(x_i; \theta))$

Model outputs are predicted values.



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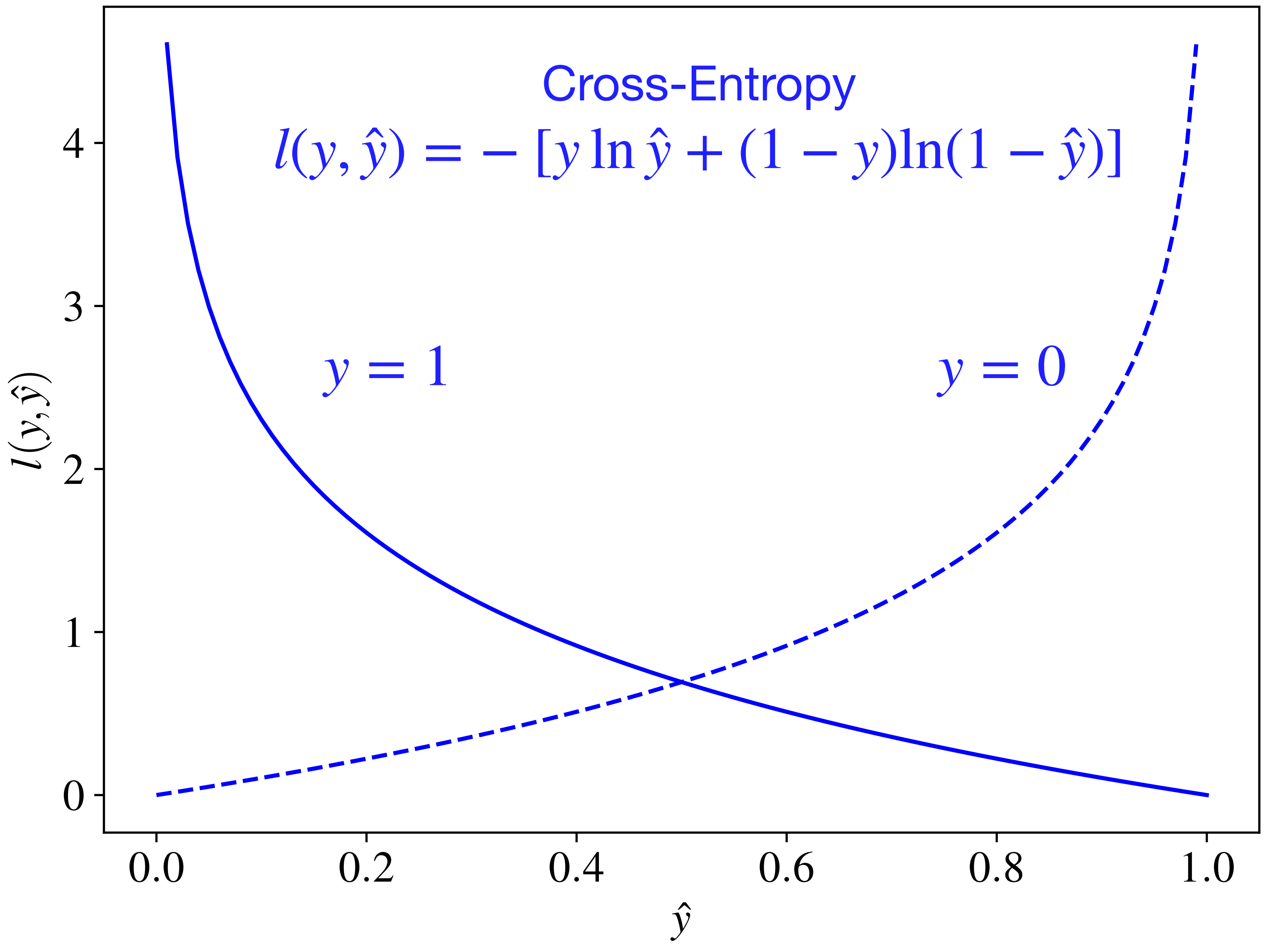

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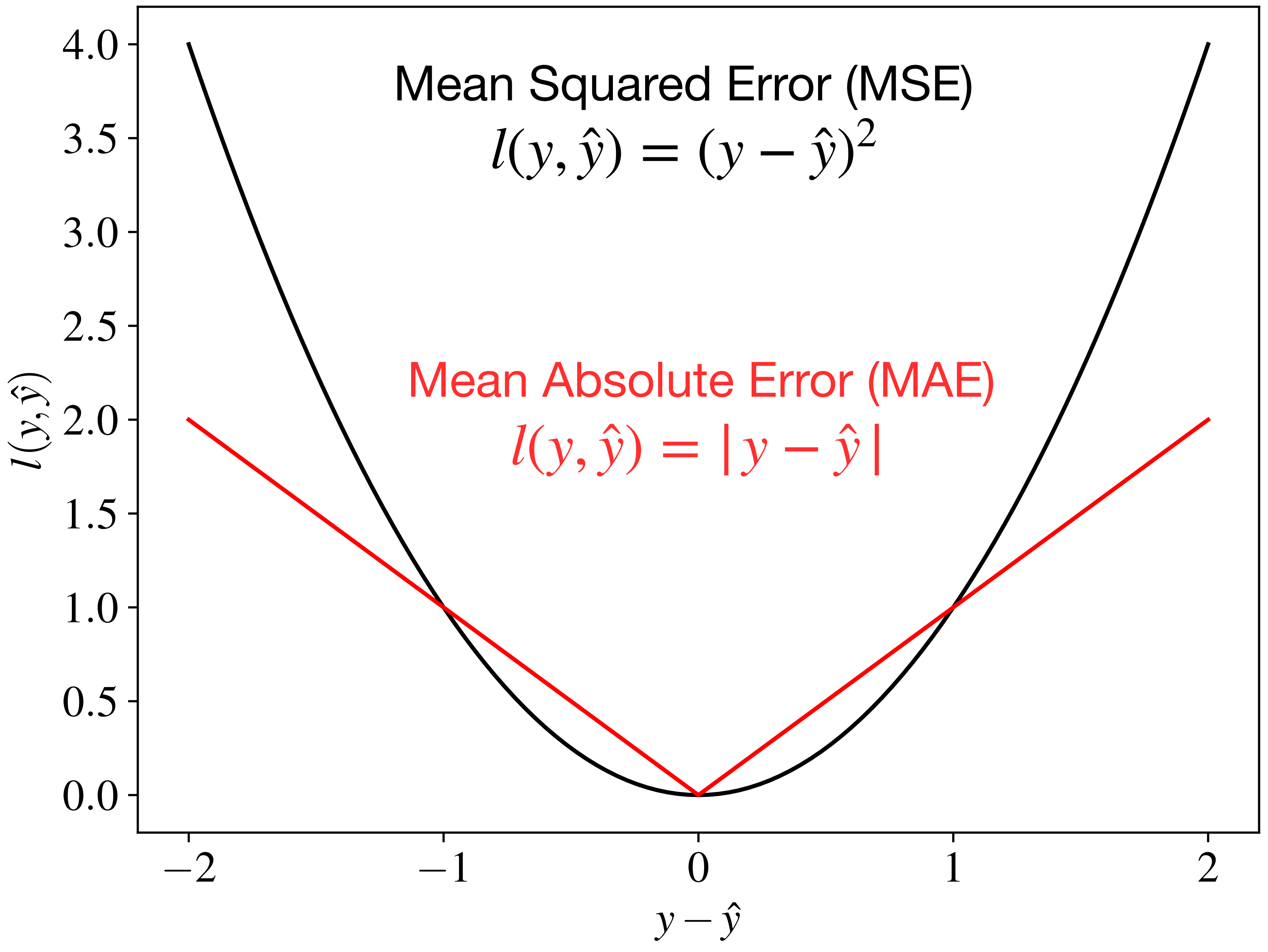

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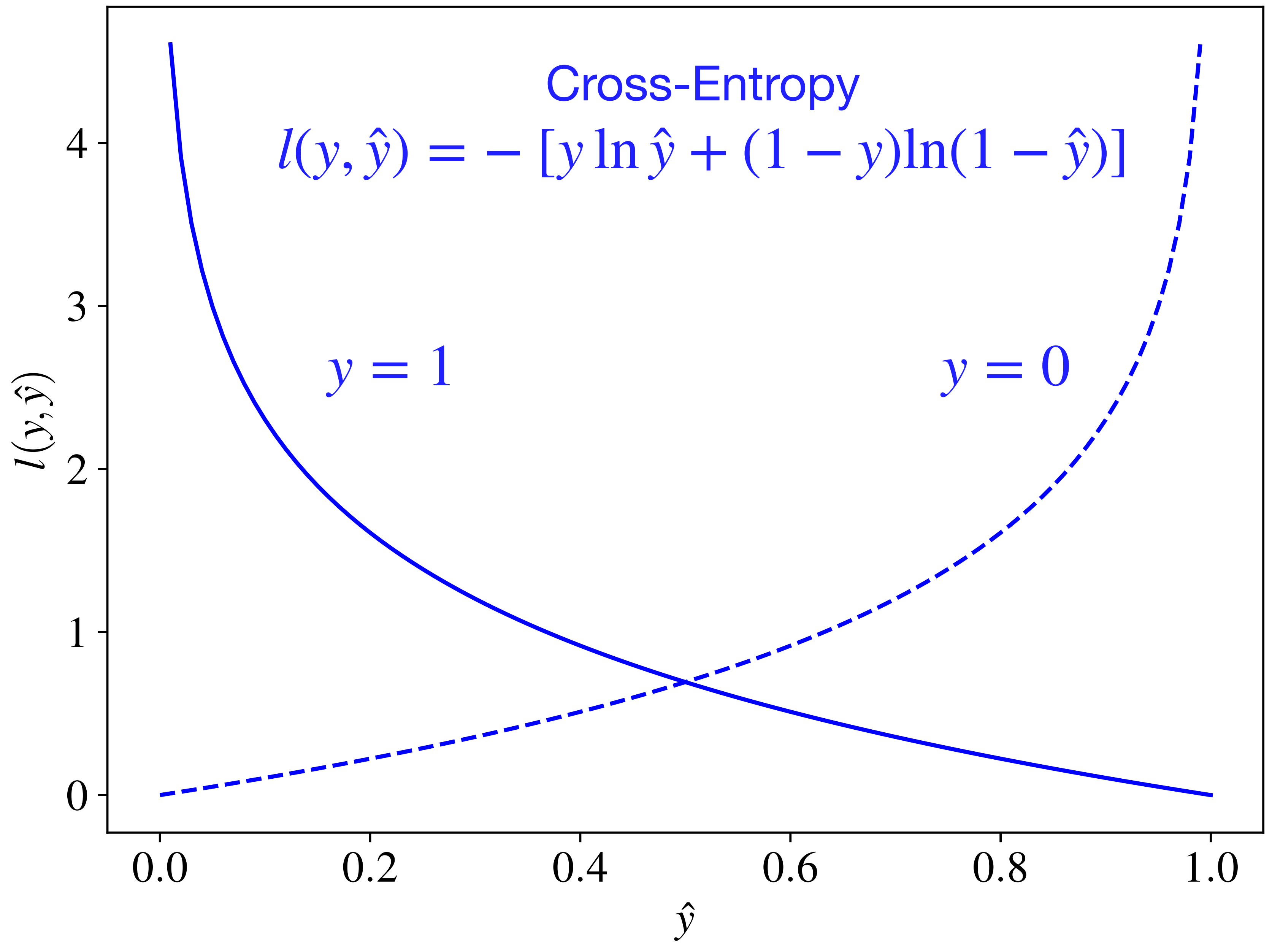

Choice depends on type of data and model.

Linear least squares regression

- Revisiting our linear model, the MSE loss is given as

$$\mathscr{L}(w_0, w_1) = \frac{1}{N}\sum_{i=1}^{N}[y_i - (w_0 + w_1 x_i)]^2$$

- Best model is one that minimizes the loss, can derive this analytically for linear least squares loss

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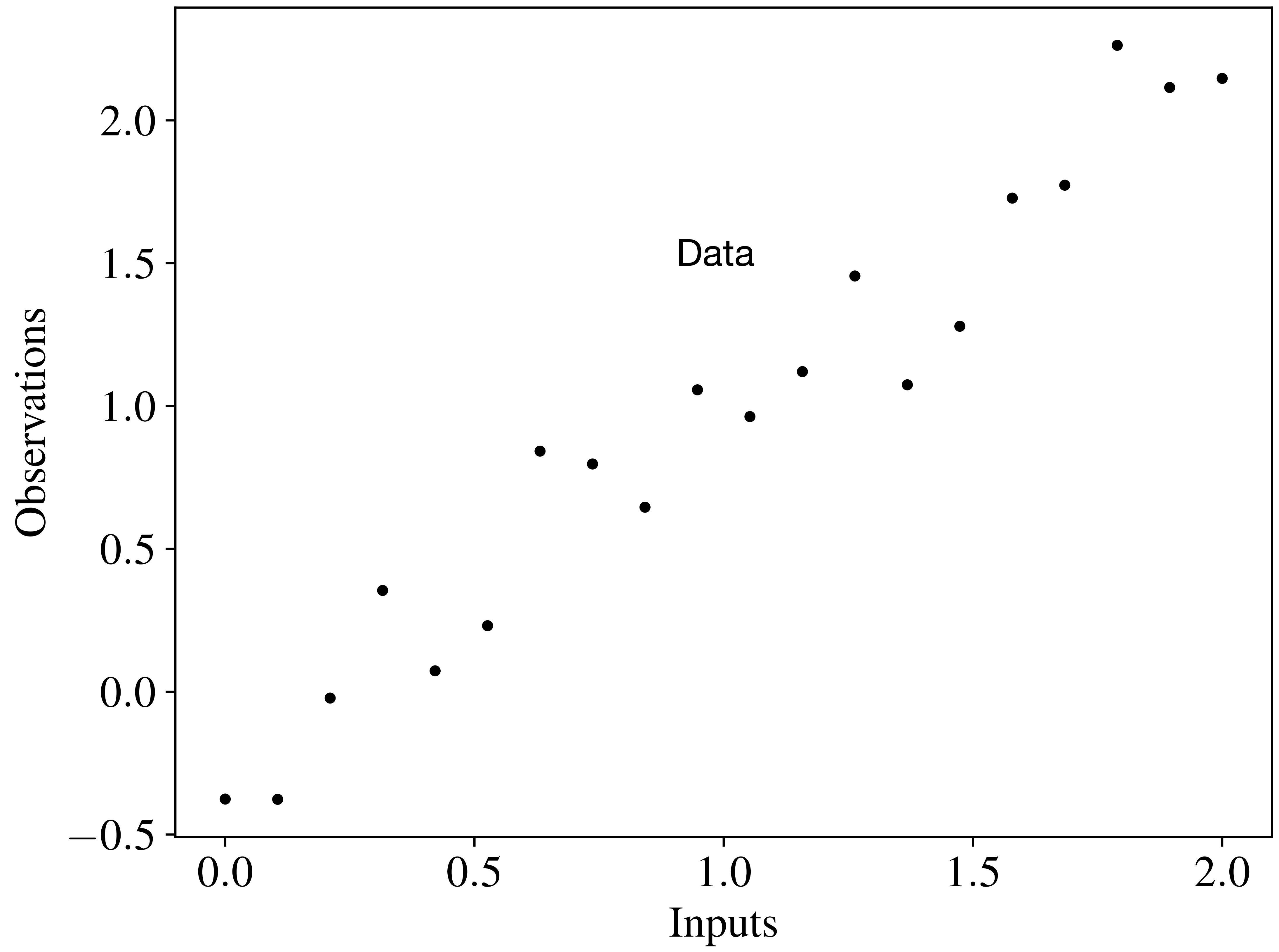

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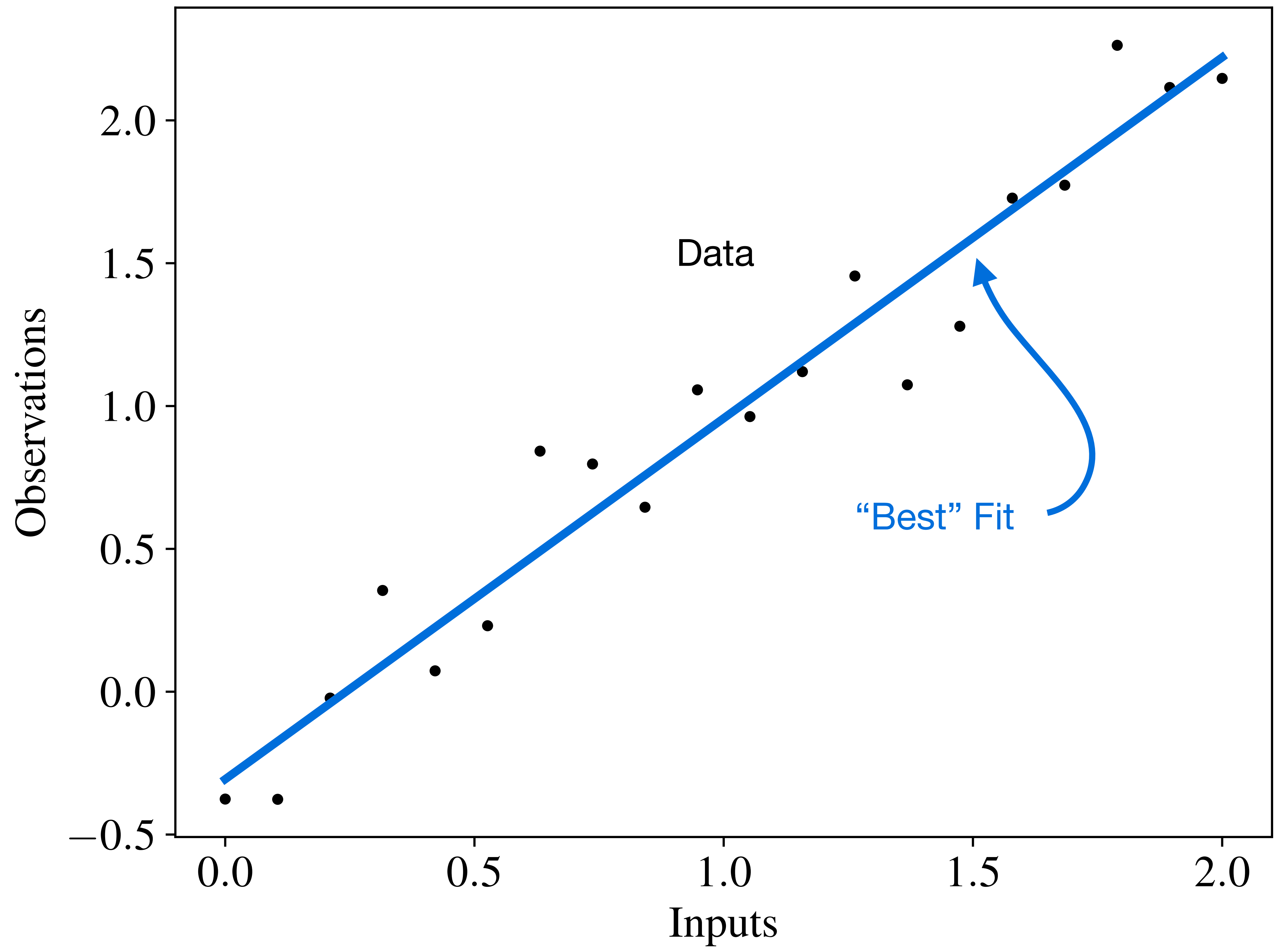


Learning nonlinear responses with linear model

- In general, linear model only needs to be linear in the parameters

$$\hat{f}(x) = w_0 h_0(x) + w_1 h_1(x) + w_2 h_2(x) + \dots$$

- We can write this compactly as

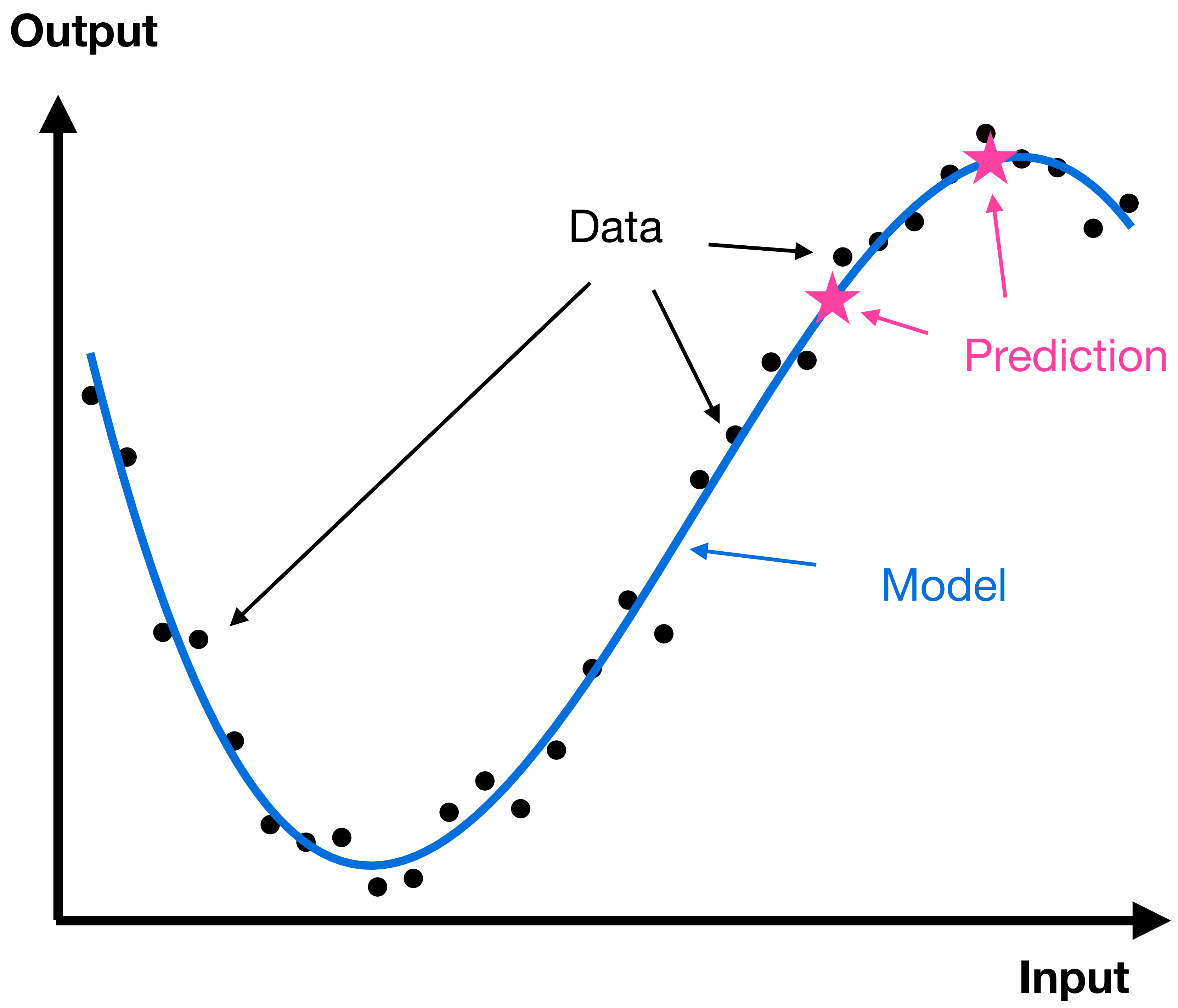
$$\hat{f}(x) = \mathbf{w} \cdot \mathbf{h}(x), \quad \mathbf{w} = [w_0, w_1, w_2, \dots]^T, \quad \mathbf{h}(x) = [h_0(x), h_1(x), h_2(x), \dots]^T$$

- This leads to a least-squares loss

$$\mathscr{L}(\mathbf{w}) = \frac{1}{N} \|\mathbf{y} - \mathbf{H}\mathbf{w}\|_2^2, \quad \mathbf{y} = [y_0, \dots, y_N]^T, \quad \mathbf{H} = [\mathbf{h}(x_0), \dots, \mathbf{h}(x_N)]$$

- Minimizing the loss leads to model of best fit

$$\mathbf{w} = (\mathbf{H}^T \mathbf{H})^{-1} \mathbf{H}^T \mathbf{y}$$



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- *Polynomial regression* is a linear problem!
  (think in terms of the weights)

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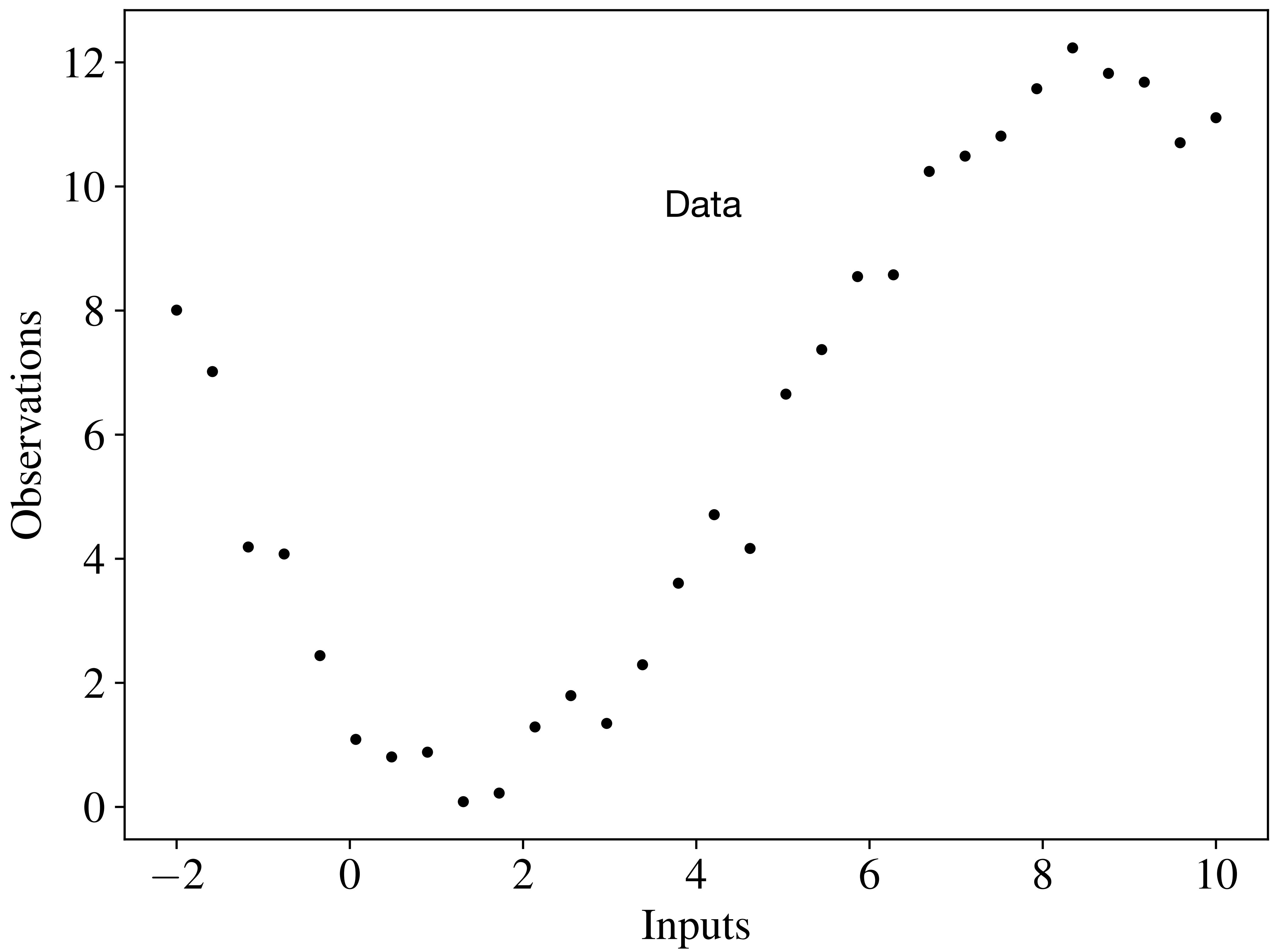

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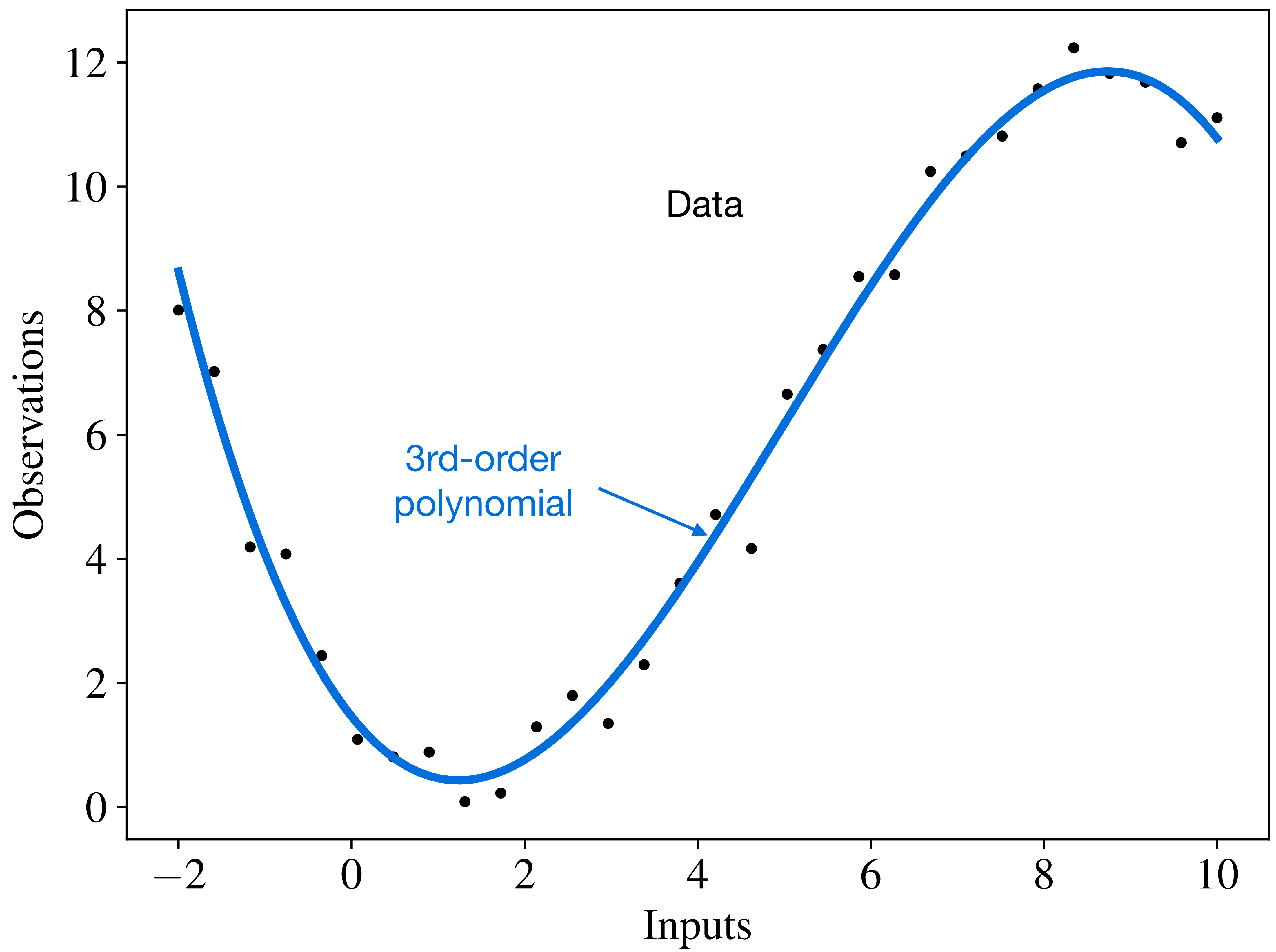

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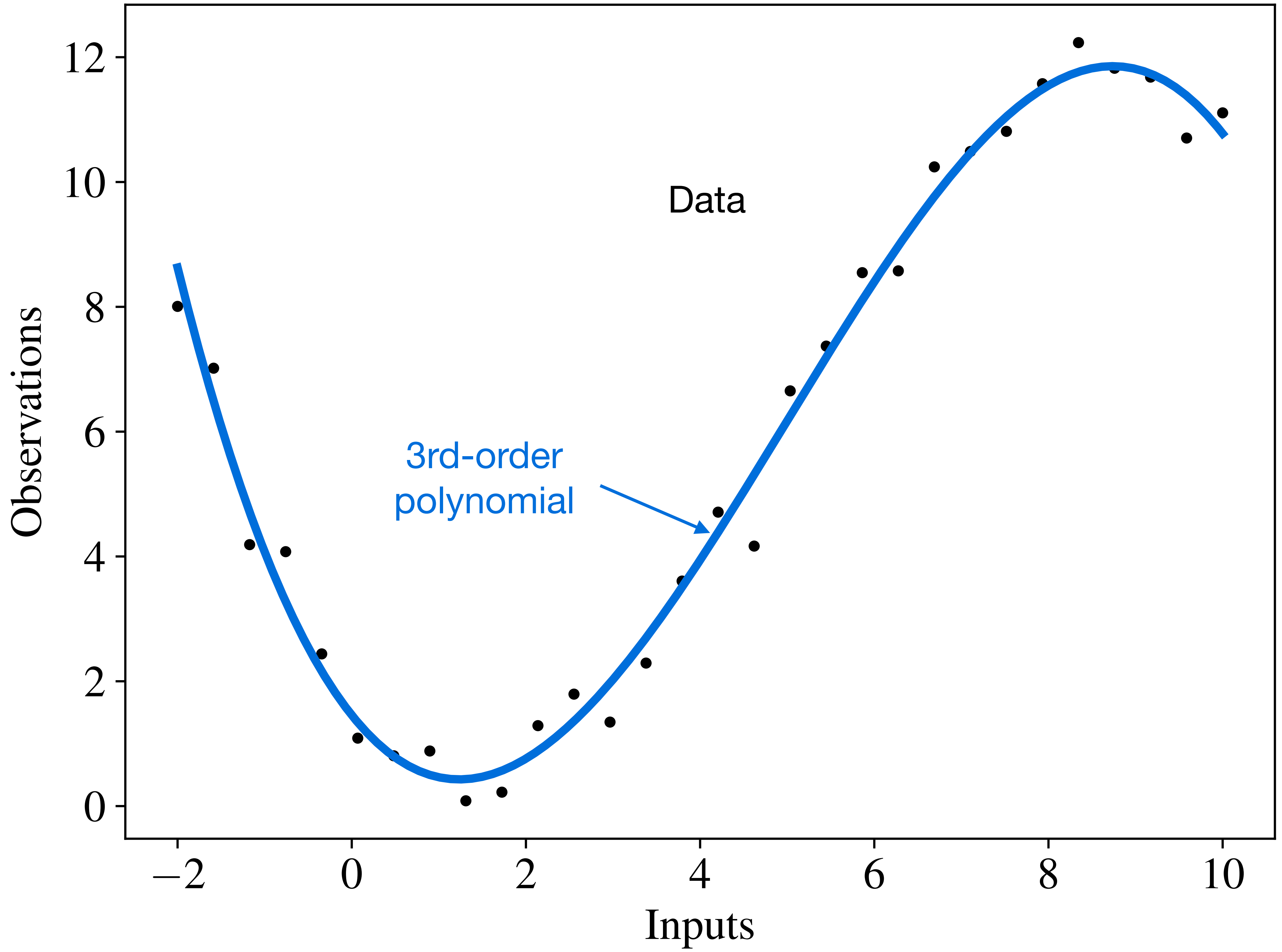

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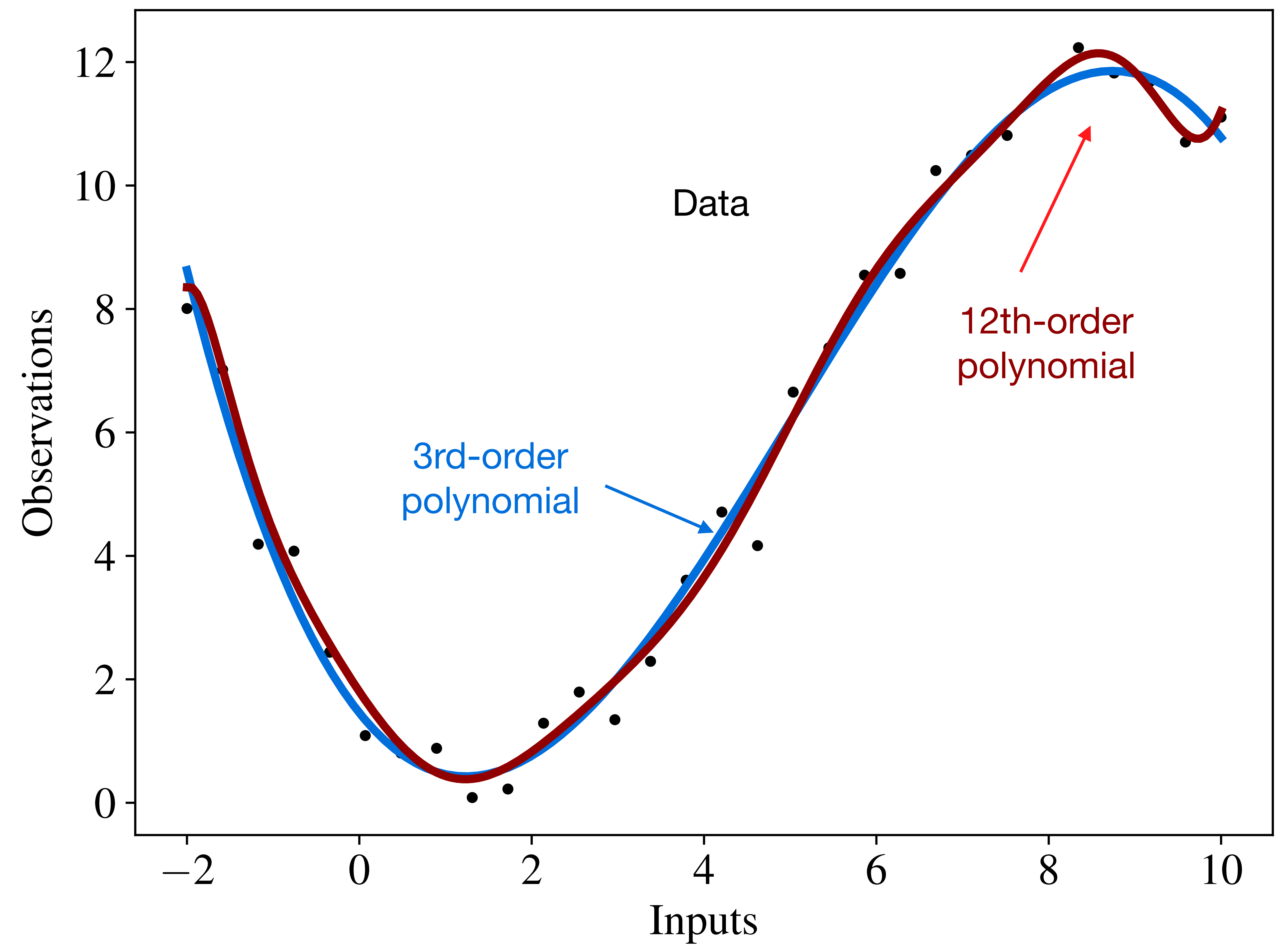
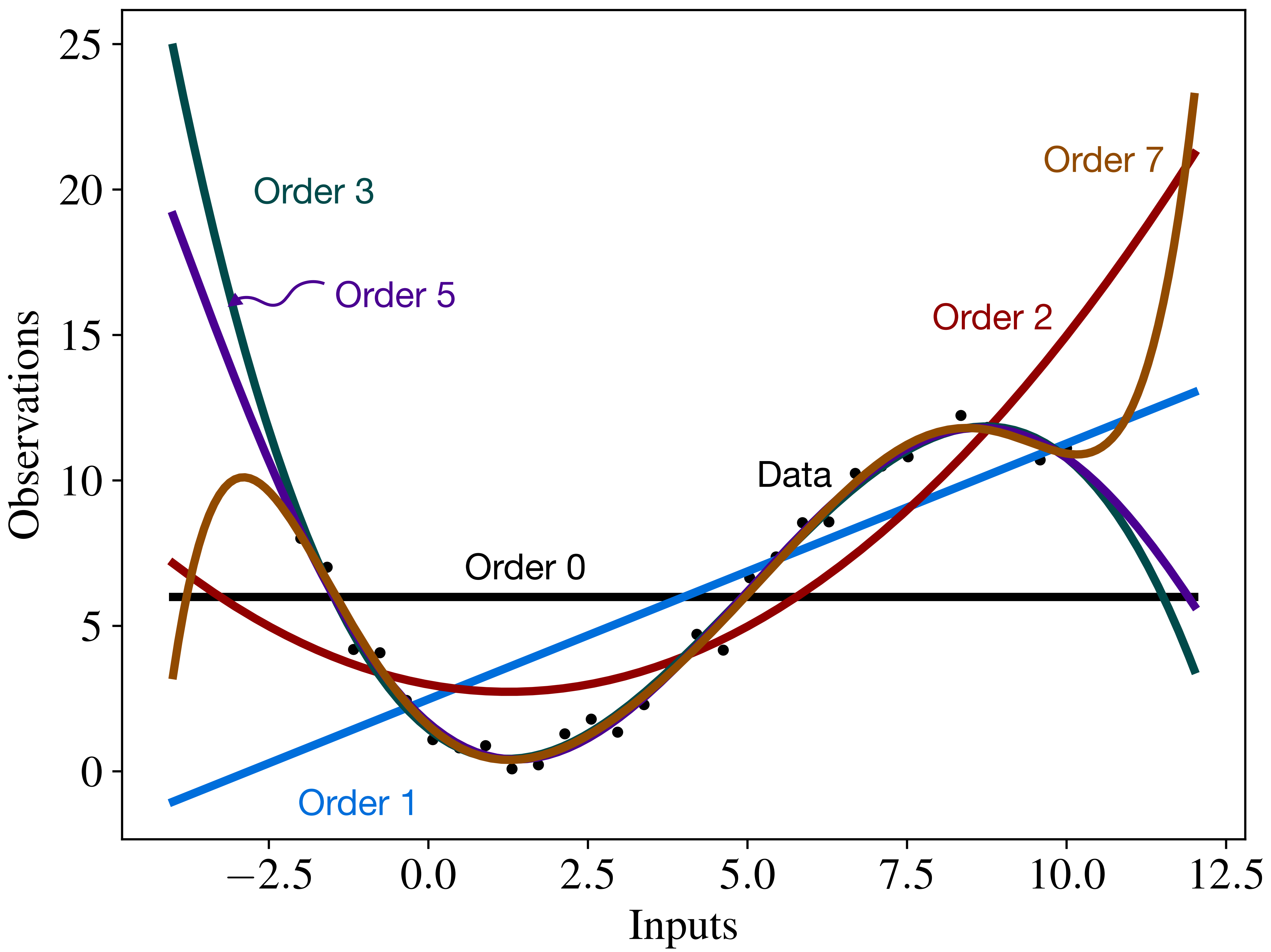
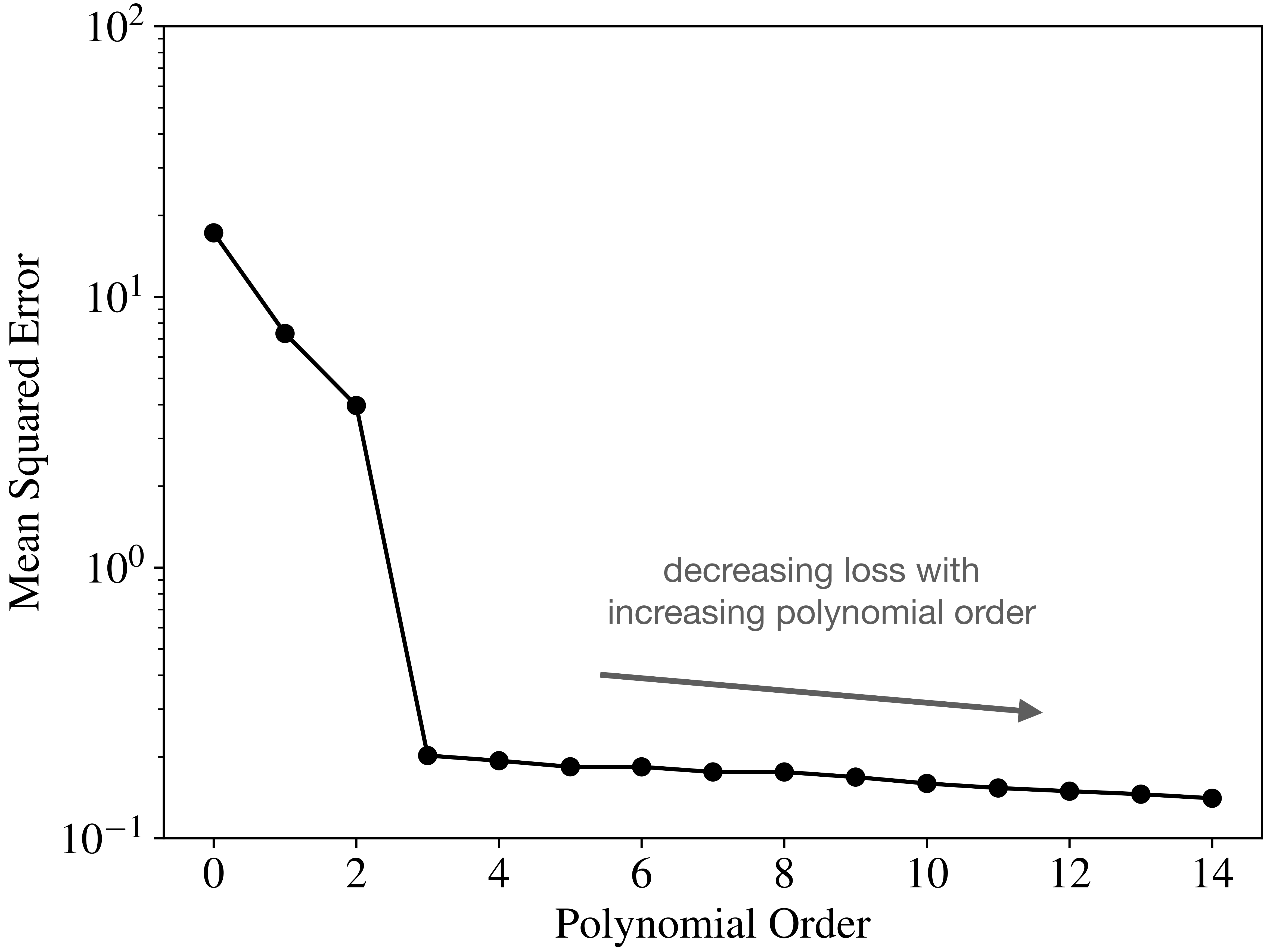


Generalization and overfitting

Least-squares loss favors model complexity over predictability!





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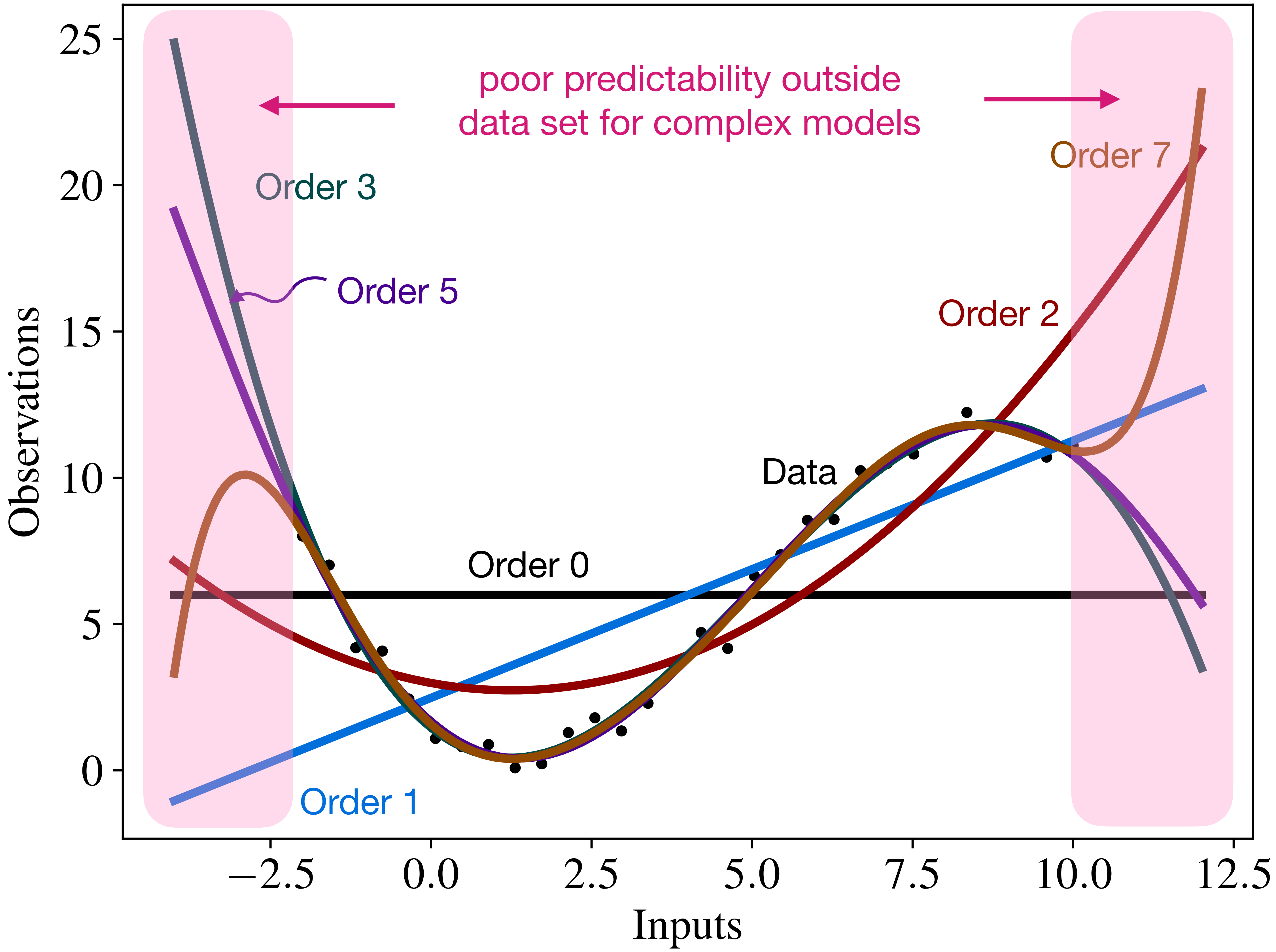

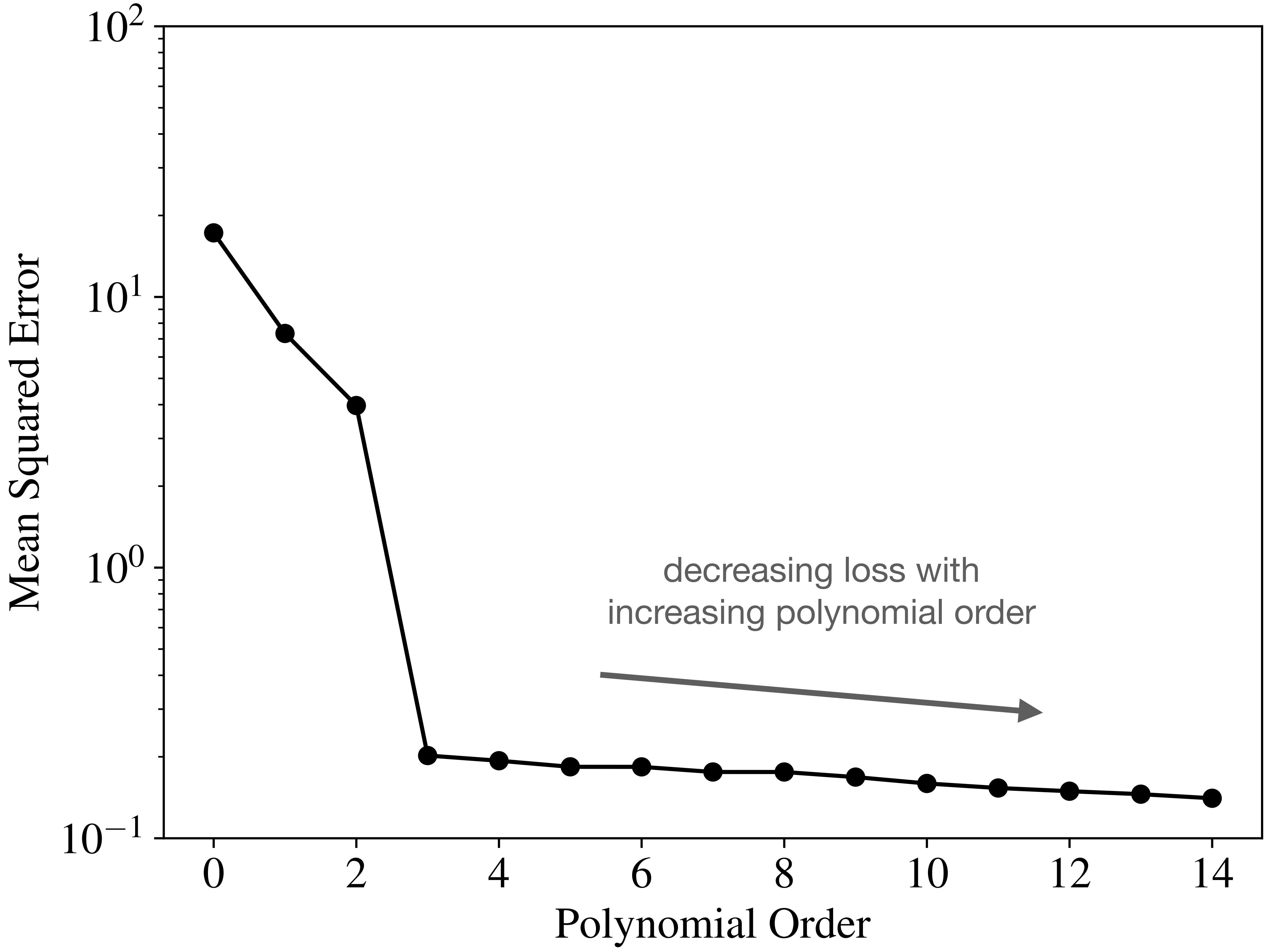

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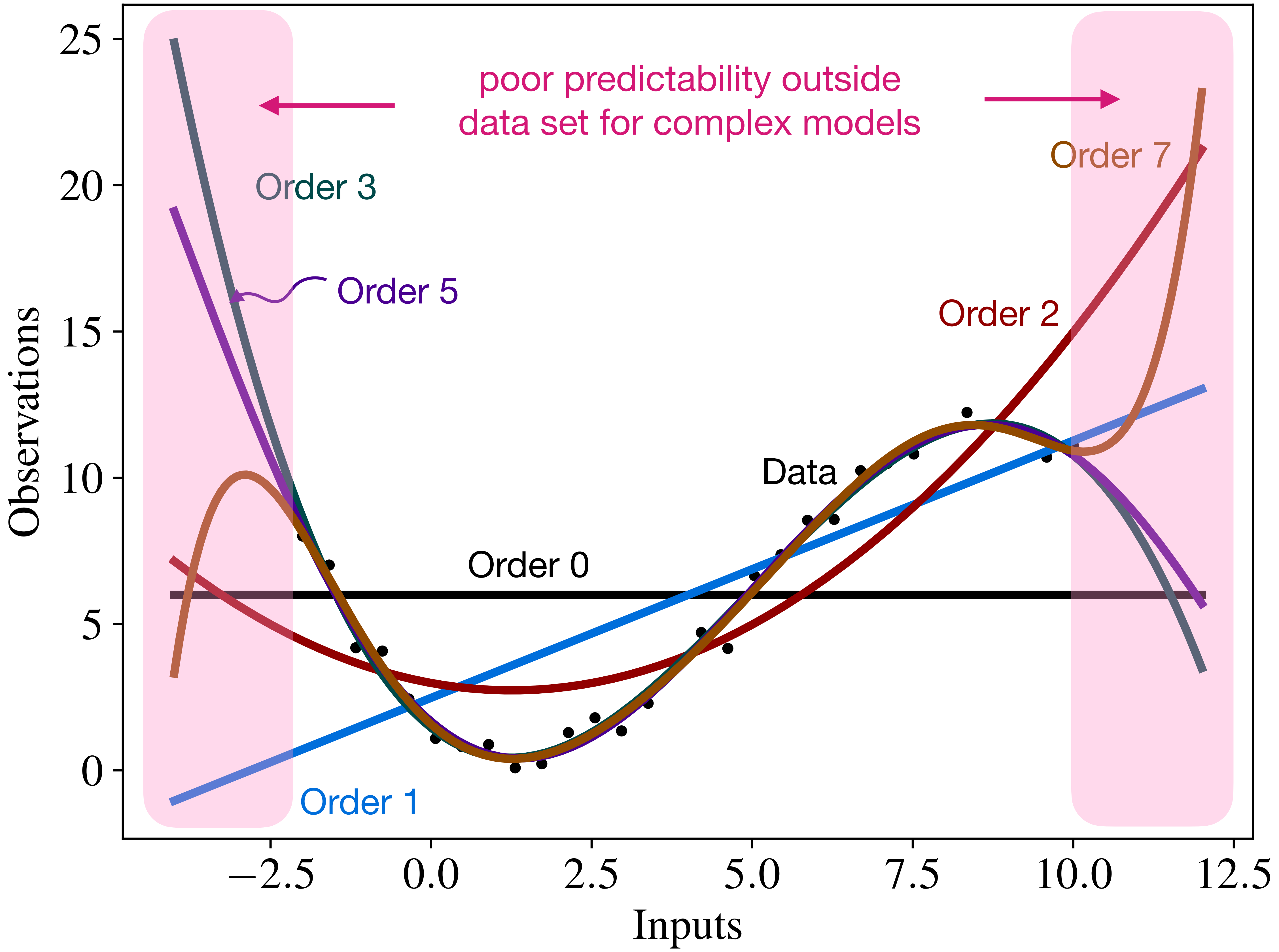
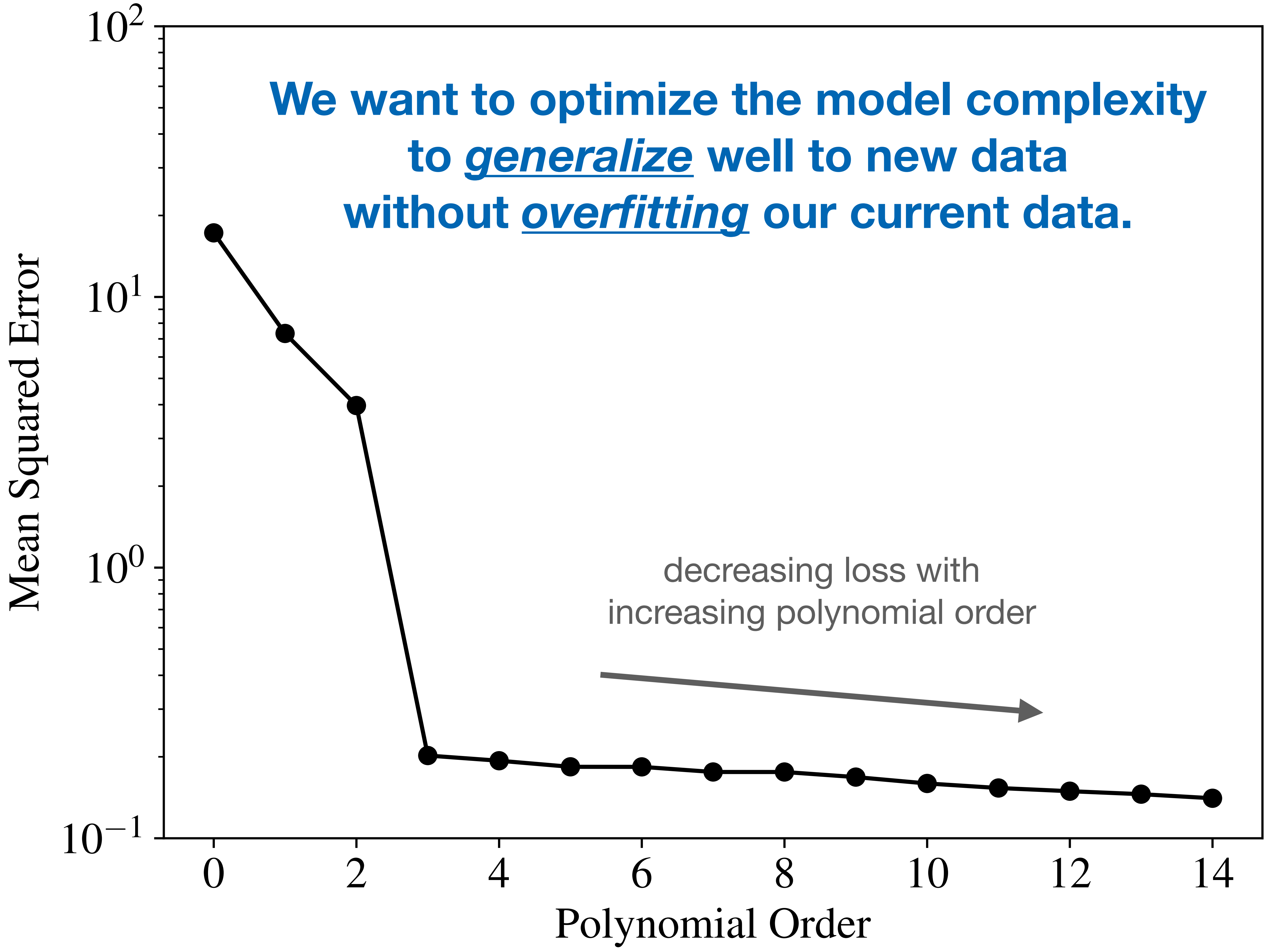
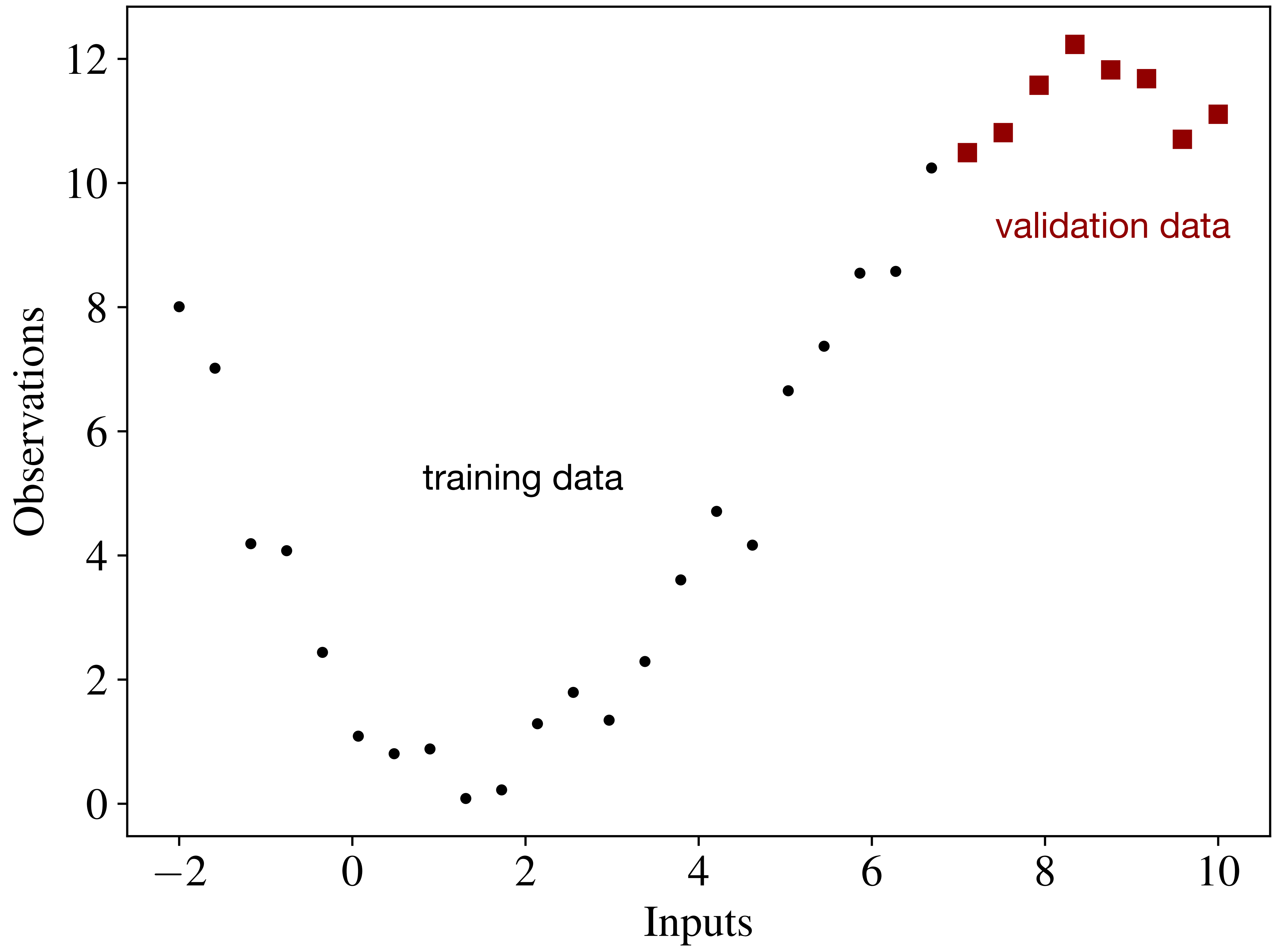
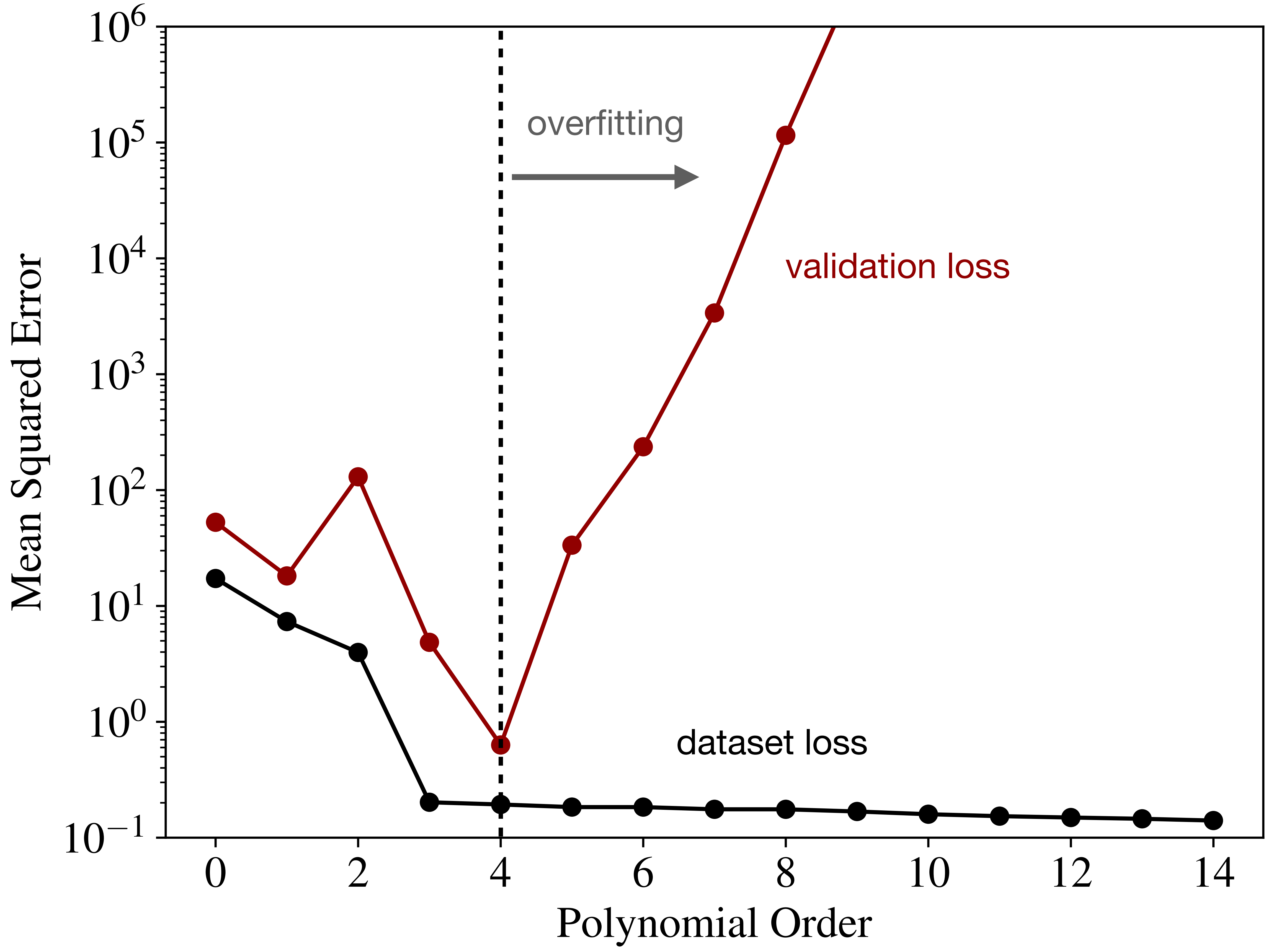




Validation data

Idea: hold back some *validation data* as a surrogate for unseen data to check model's generalizability





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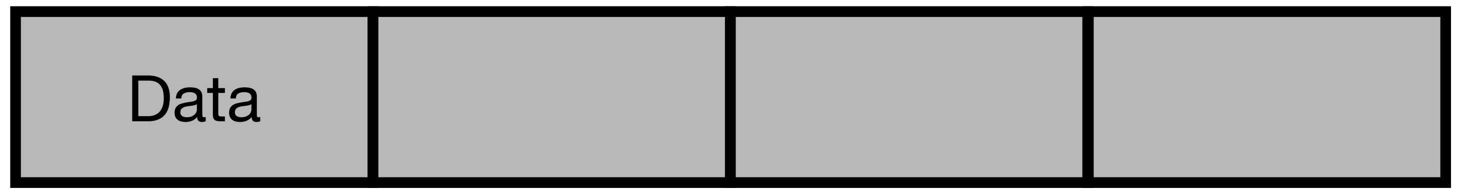

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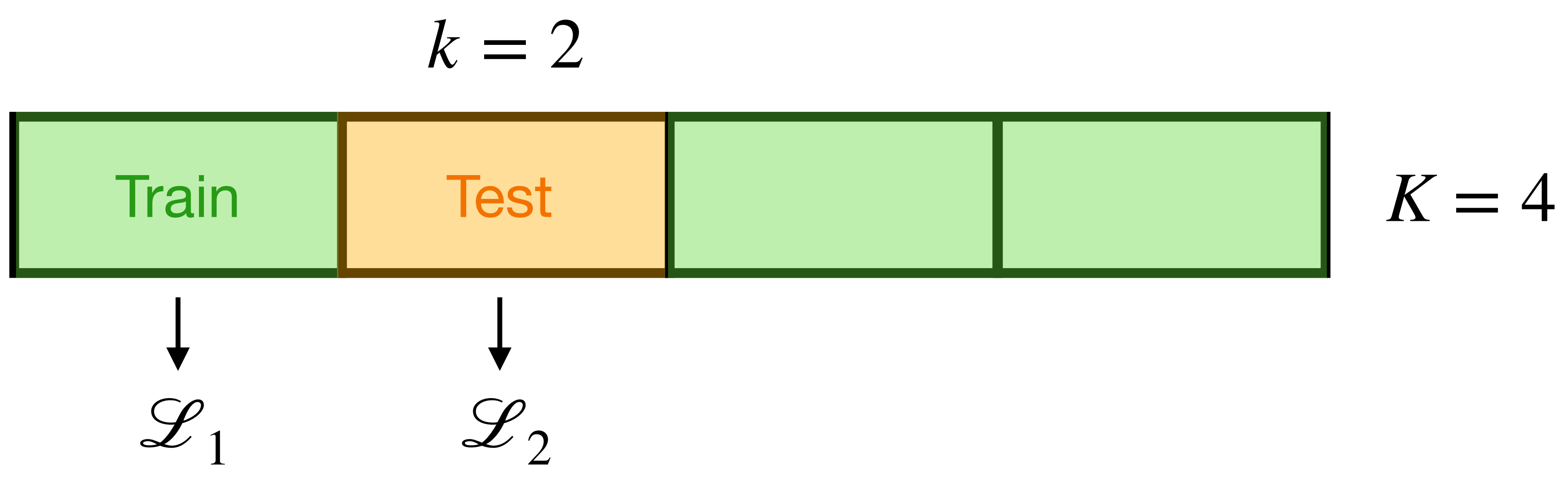

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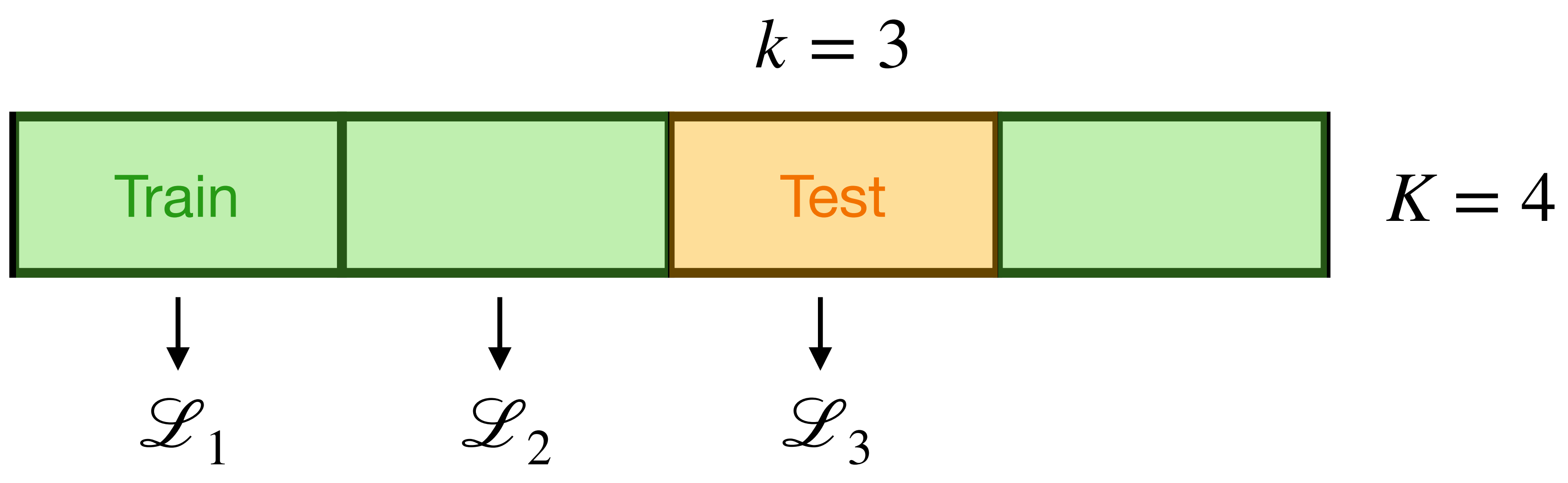

Cross-validation

- Validation loss is sensitive to which data we choose to hold back
- Can improve on this idea by taking the average validation loss over multiple choices of train/validation sets
- **K-Fold Cross-Validation (CV)**
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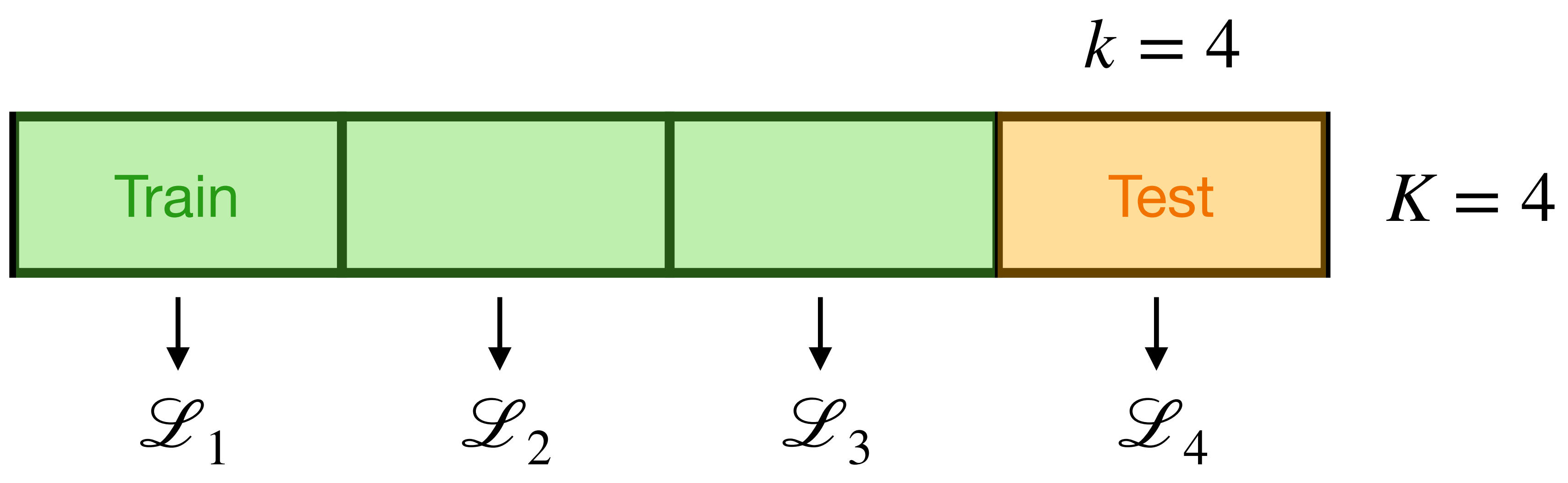

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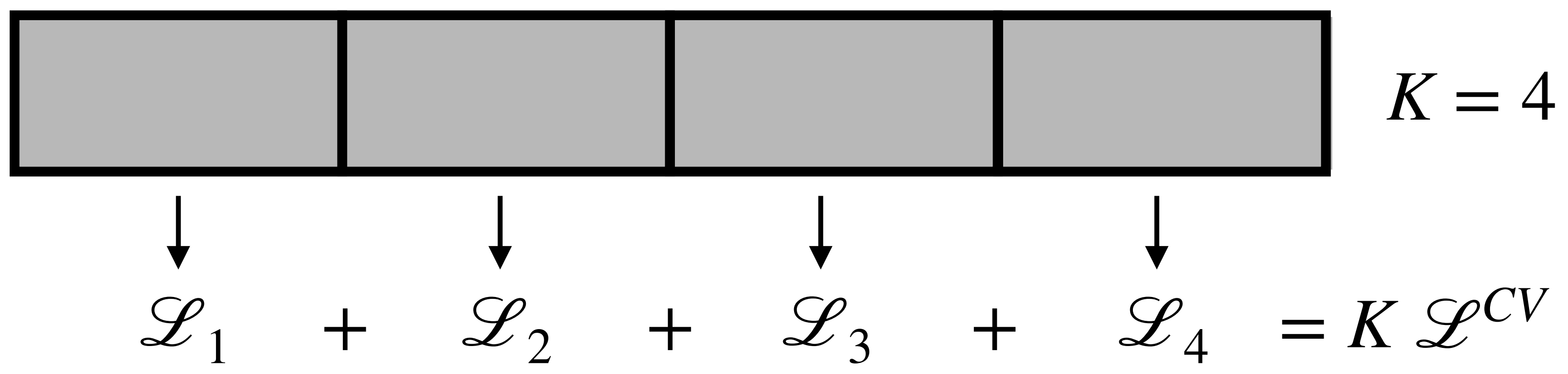

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  - Special case of K-Fold CV where K is number of data points

$$\mathscr{L}_1 + \mathscr{L}_2 + \mathscr{L}_3 + \mathscr{L}_4 = K\,\mathscr{L}^{CV}$$

$$\mathscr{L}^{CV} = \frac{1}{N}\sum_{i=1}^{N} l(y_i, \hat{f}(x_i; \theta^*_{-i}))$$

trained parameters on data without i^{th} point

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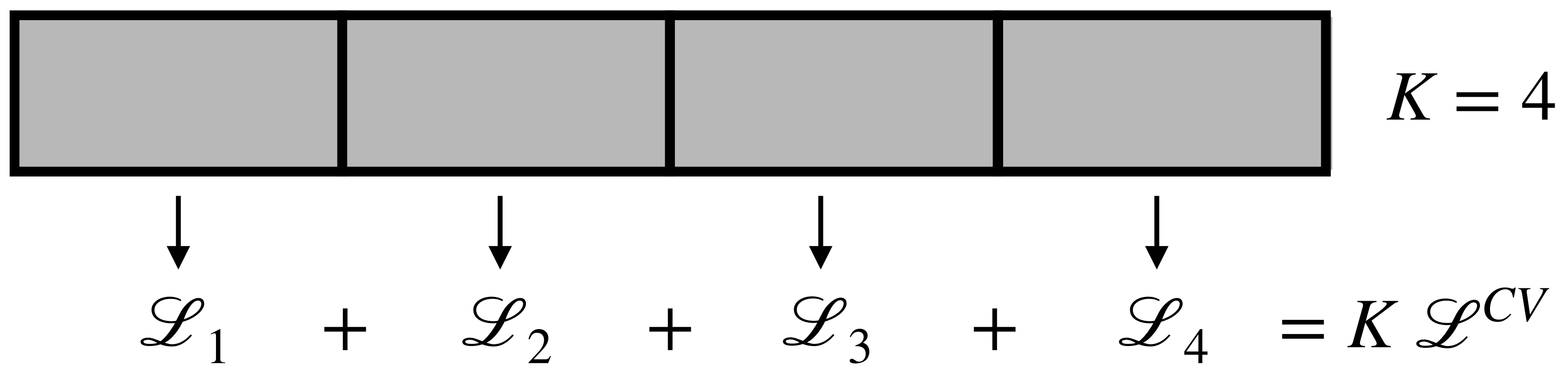

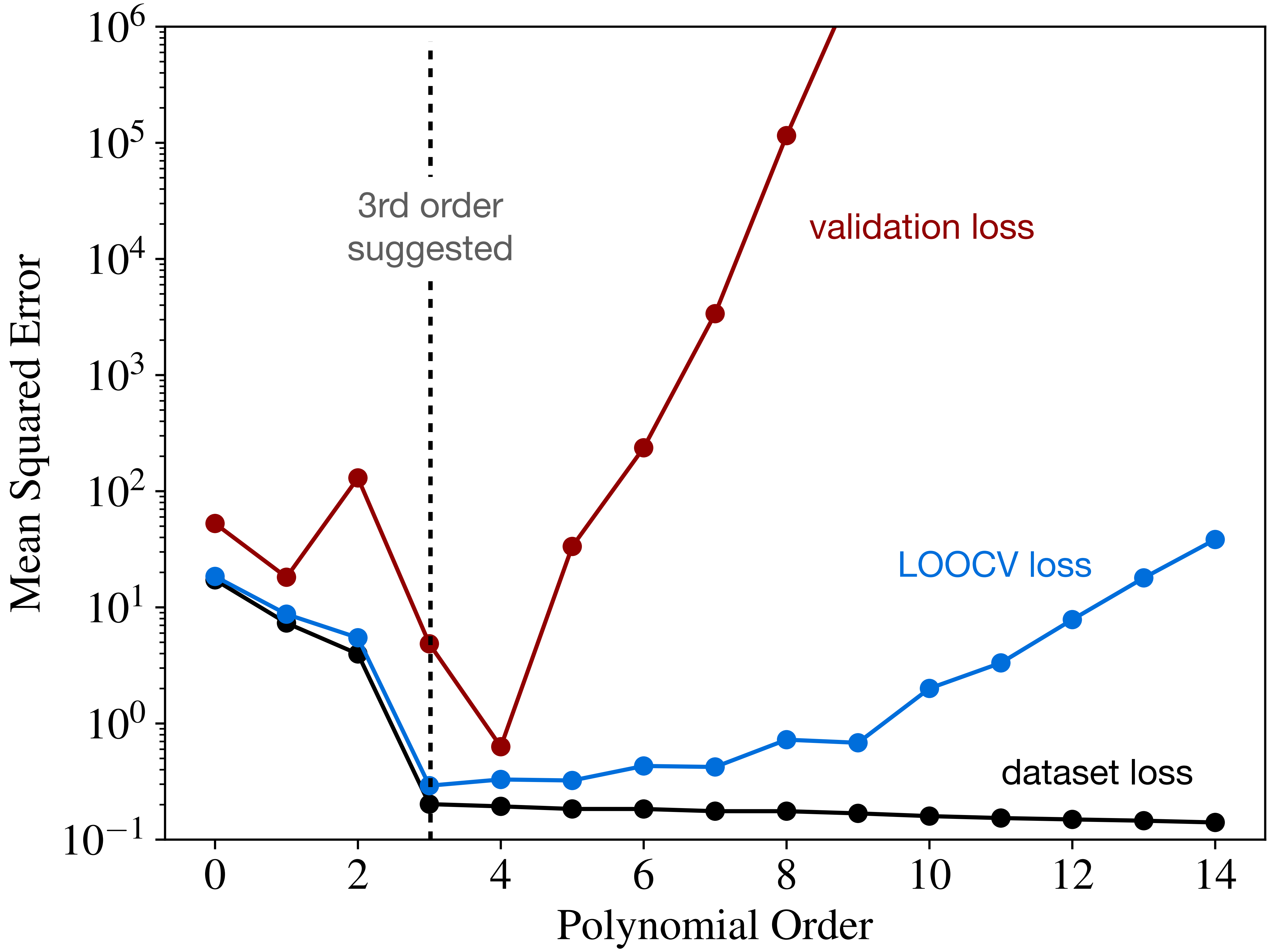

Regularization

Regularization **improves generalizability by penalizing model complexity in the loss function**

Regularized Linear Least-Squares

- Least complex model with $\mathbf{w} = \mathbf{0}$
- "Complexity" increases as parameters become more nonzero
- **Idea:** Add sum of parameters squared to loss

$$\mathscr{L}(\mathbf{w}) = \frac{1}{N}\|\mathbf{y} - \mathbf{H}\mathbf{w}\|_2^2 + \lambda \mathbf{w}^T\mathbf{w}, \quad \lambda \geq 0$$

least-squares loss

regularization

- Minimizing regularized loss leads to

$$\mathbf{w} = (\mathbf{X}^T\mathbf{X} + N\lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

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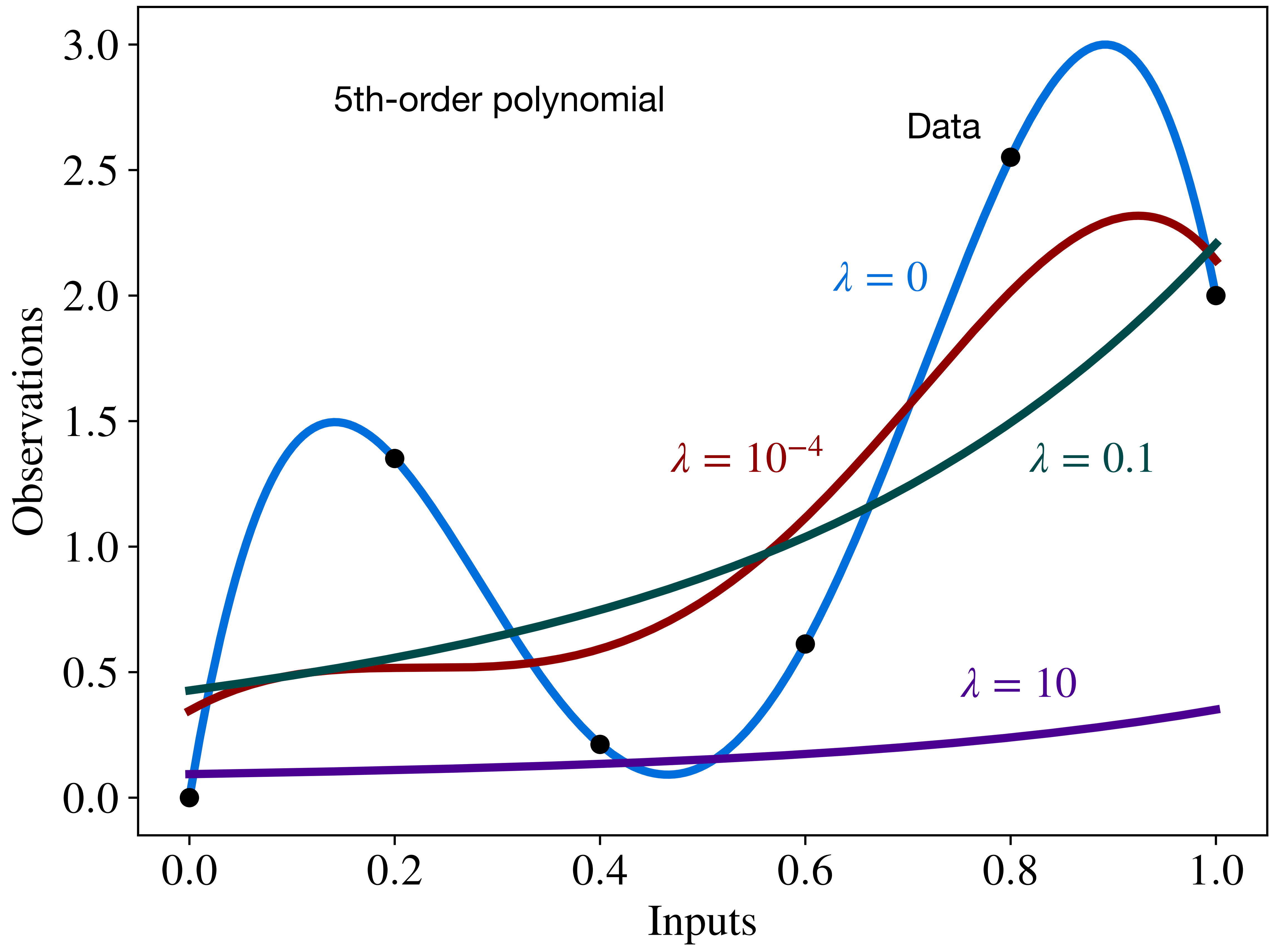

Normalization

Generally a good idea to *normalize* dataset prior to model training!

Examples:

- "Standard" normalization centers and scales to unit variance

$$\hat{x} = \frac{x - \bar{x}}{\sigma_x}$$

- "Min-Max" transforms data into range of [0,1]

$$\hat{x} = \frac{x - \min x}{\max x - \min x}$$

Notes:

- Choice depends on model, algorithm, data
- Perform on inputs and outputs
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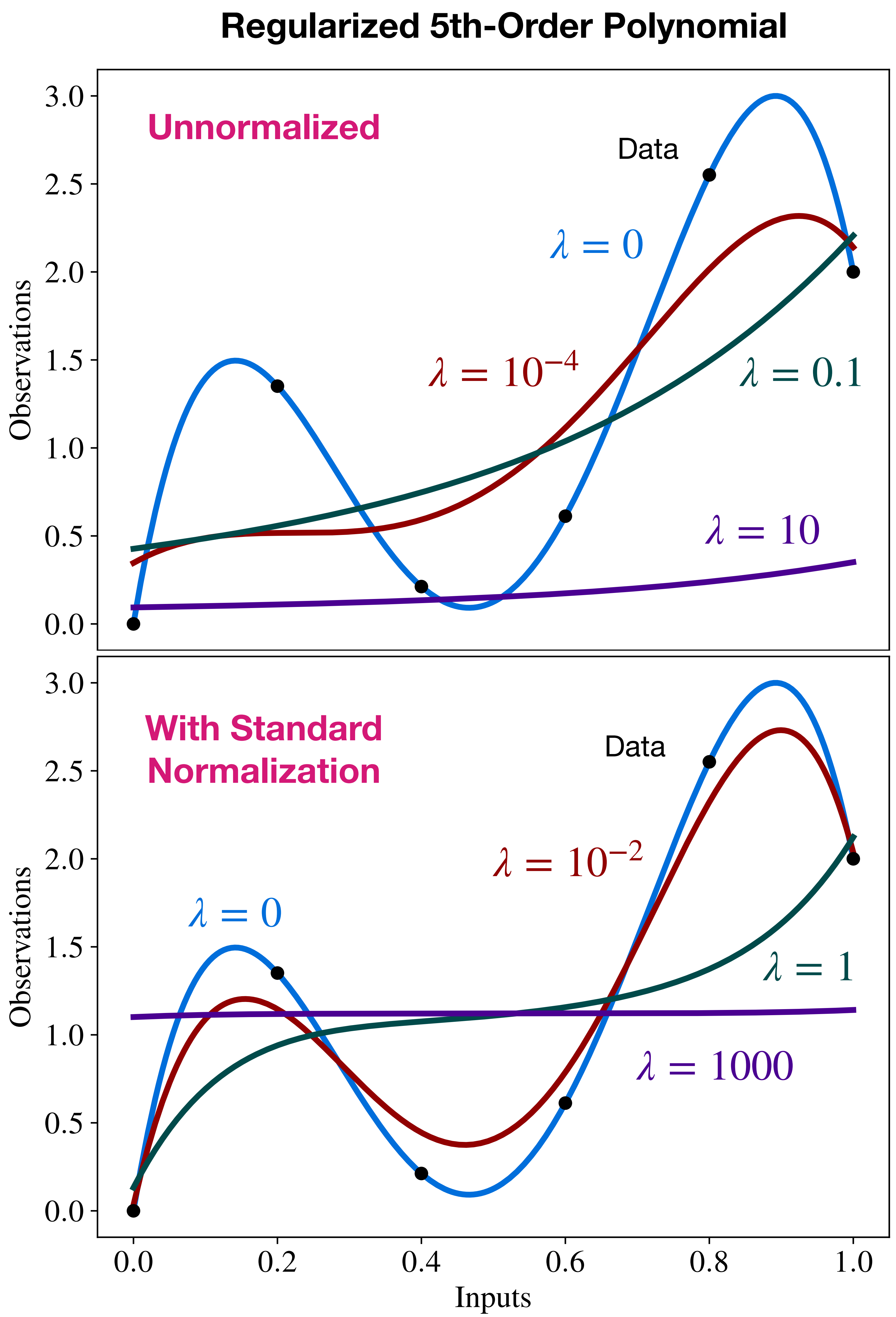
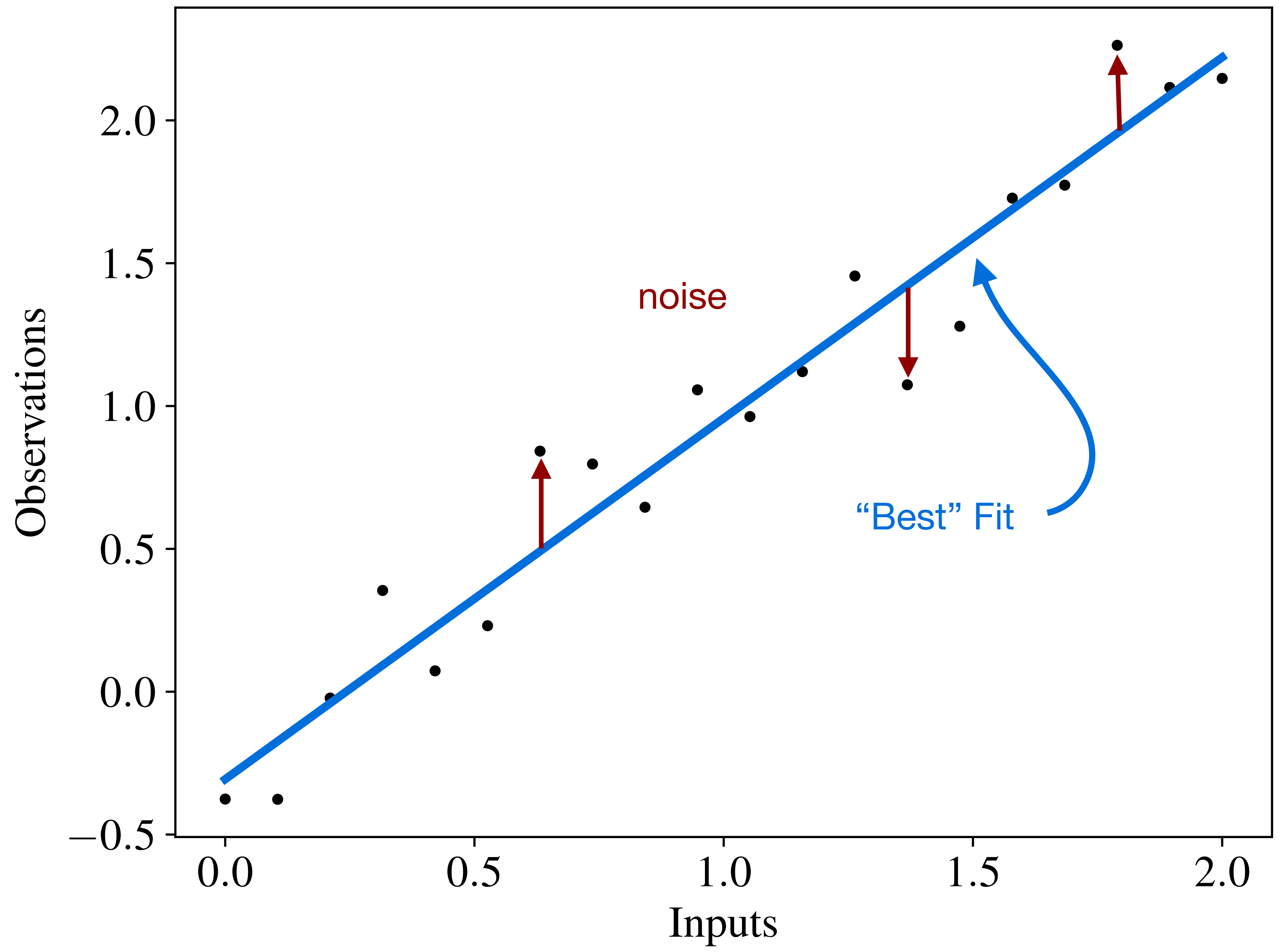


Summary of the basic ML pipeline

1. Gather data
    - Often the most challenging part of ML!
    - Study, plot, reason about, clean up, etc.
    - Ensure dataset covers all potential outcomes and is evenly weighted
2. Normalize dataset
3. Split into train, validation, and test datasets (shuffle)
4. Perform model selection / hyper parameter tuning
    - Look to maximize generalizability and prevent overfitting
    - Cross-validation
5. Train chosen model(s)
6. Deploy model
    - Monitor performance and go back to (1) if needed

What about noise?

- So far, we have neglected the *noise* in our data
- Noise represents *uncertainty* or *randomness* in the *generating process* used to create the data
  - *Latent* (hidden) variables
  - Measurement uncertainties
  - Model uncertainties (for derived data)
- From a modeling perspective, noise represents potential error in our model, because we are using imperfect data
- Interested in knowing the uncertainty in our model predictions
- **Not a course on *Uncertainty Quantification (UQ)*:** instead we will try to get a flavor of the ideas involved



Thinking generatively

Data generation is an inherently complex process!

- We can try to model this process by approaching the supervised learning task in a new way
    - Instead of looking for model that best fits the data,
    - Look for model that is most likely to generate that data
    - In general, these types of models are called _generative models_

How can build a model that can generate data that “looks” like ours?

- Obviously, we accept that this isn’t the real generating process
- However, this will be a useful strategy
- **Key Idea: Add randomness to our model that mimics the randomness present in the data**

A generative linear model

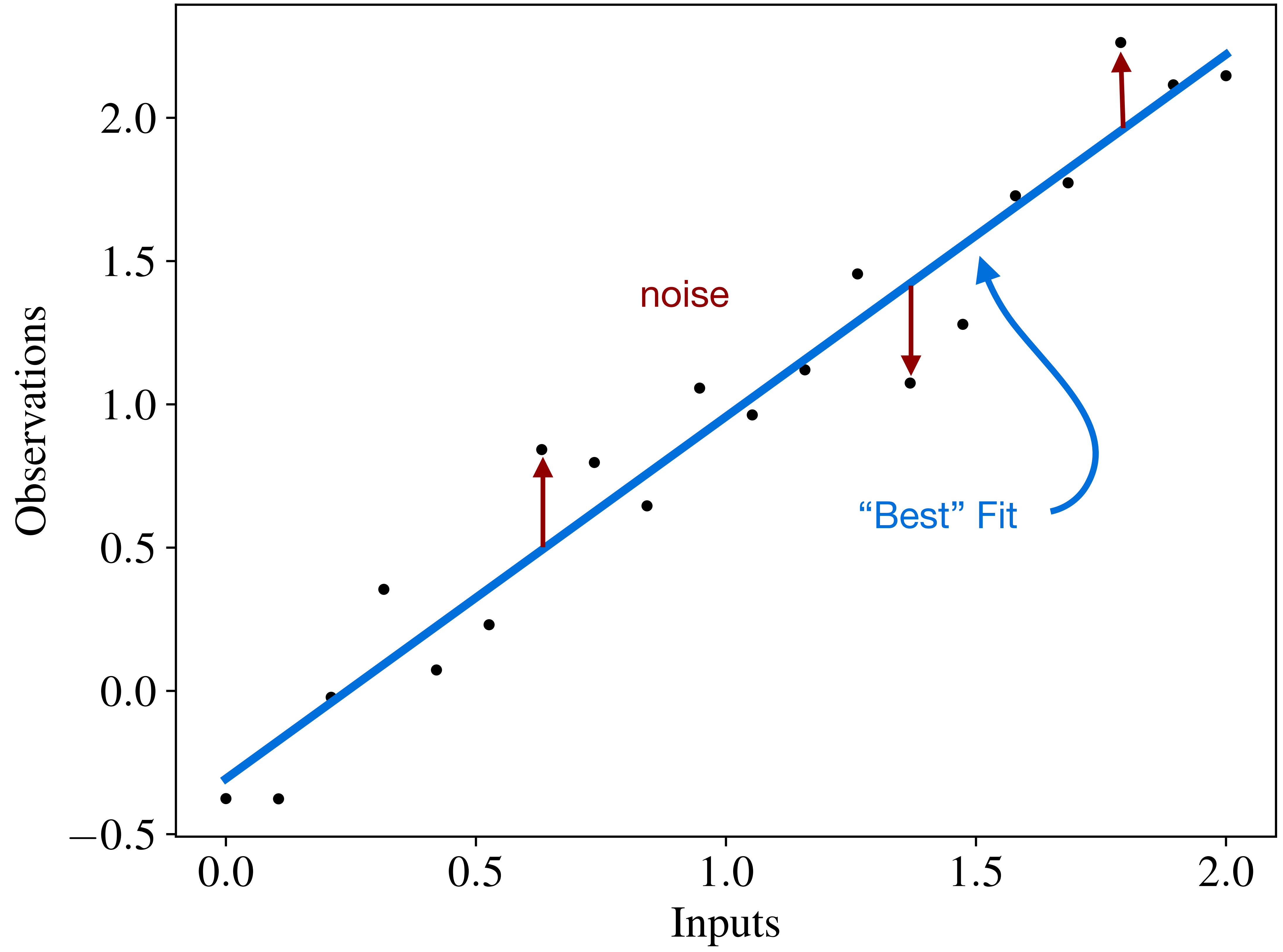
- Recall that our generalized linear model takes the form

$$\hat{f}(x) = \mathbf{w} \cdot \mathbf{h}(x)$$

- We can modify this by incorporating a random variable ε which represents the noise in our generative model

$$\hat{f}(x) = \underbrace{\mathbf{w} \cdot \mathbf{h}(x)}_{\text{deterministic}} + \underbrace{\varepsilon}_{\text{stochastic}}$$

- Note that the addition of ε into our linear model makes our model output random as well!
- Subtle point: we are implicitly assuming that the noise is independent of input location (not always true)
- **Left with 2 key problems:**
  1. What is the probability density of the stochastic component?
  2. How can we fit a random model to our data?



Choice of probability distribution $p(\varepsilon)$

In general, this will depend on your data and any knowledge you may have about the generating mechanism

- **For now, let's think of the key characteristics of our noise**
  - As written, it represents a deviation from the deterministic trend
  - Can be positive or negative
  - Likely to be closer to the nominal than far away
- These characteristics suggest that a Gaussian (normal) distribution with zero mean is a reasonable choice

$$p(\varepsilon) = \mathcal{N}(0, \sigma^2)$$

Likelihood

- Recall that our generative linear model is random, therefore, it has a probability density

$$\hat{y} = \hat{f}(x) = \mathbf{w} \cdot \mathbf{h}(x) + \varepsilon, \quad p(\varepsilon) = \mathcal{N}(0,\sigma^2)$$

- The probability density of the sum of a normally distributed random variable and a scalar shifts the mean

$$p(\hat{y} \,|\, \mathbf{w}, x, \sigma^2) = \mathcal{N}(\mathbf{w} \cdot \mathbf{h}(x), \sigma^2)$$

- The value of this distribution for a given set of parameters, input, and noise variance, is often called the *likelihood* because it represents how "likely" the model will output that particular value

- We can therefore define a *dataset likelihood* as the likelihood that our model will generate our particular dataset as

$$L = p(\mathbf{y} \,|\, \mathbf{x}, \mathbf{w}, \sigma^2) = \prod_{i=1}^{N} p(y_i \,|\, x_i, \mathbf{w}, \sigma^2) = \prod_{i=1}^{N} \mathcal{N}(\mathbf{w} \cdot \mathbf{h}(x_i), \sigma^2)$$

Maximum likelihood estimate

The *Maximum likelihood estimate* (MLE) maximizes the likelihood of generating the dataset with the model

- Specifically, we minimize the negative log dataset likelihood (NLL) for $\mathbf{w}$ and σ^2

$$\mathscr{L} = -\ln p(\mathbf{y} \,|\, \mathbf{x}, \mathbf{w}, \sigma^2) = -\frac{N}{2}\ln 2\pi - N\ln\sigma - \frac{1}{2\sigma^2}\sum_{i=1}^{N}(y_i - \mathbf{w}\cdot\mathbf{h}(x))^2$$

$$\frac{\partial \mathscr{L}}{\partial \mathbf{w}} = 0 \implies \mathbf{w} = (\mathbf{H}^T\mathbf{H})^{-1}\mathbf{H}^T\mathbf{y}$$

identical to our least-squares solution!

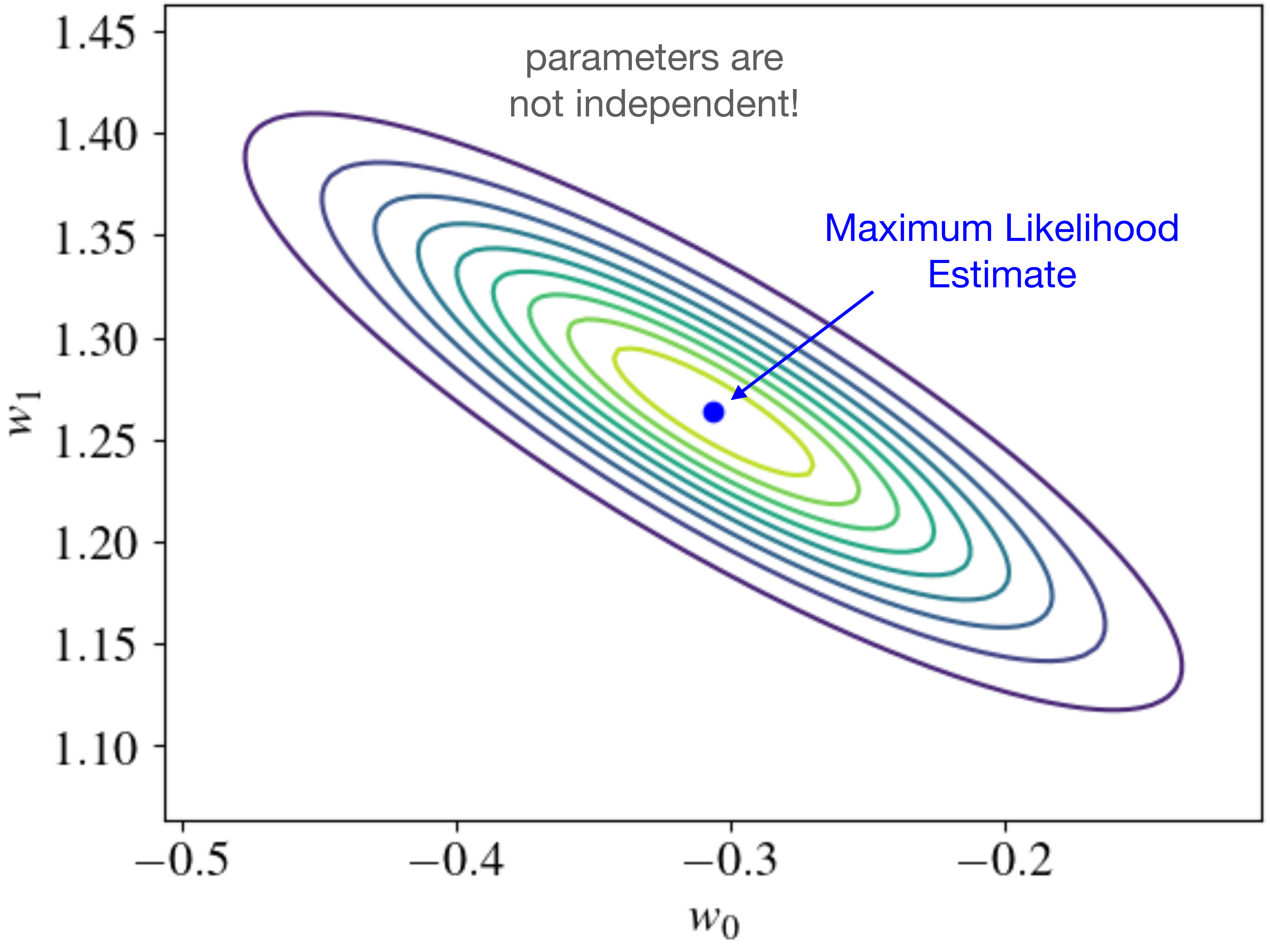
$$\frac{\partial \mathscr{L}}{\partial \mathbf{w}} = 0 \implies \sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(y_i - \mathbf{w}\cdot\mathbf{h}(x_i))^2$$

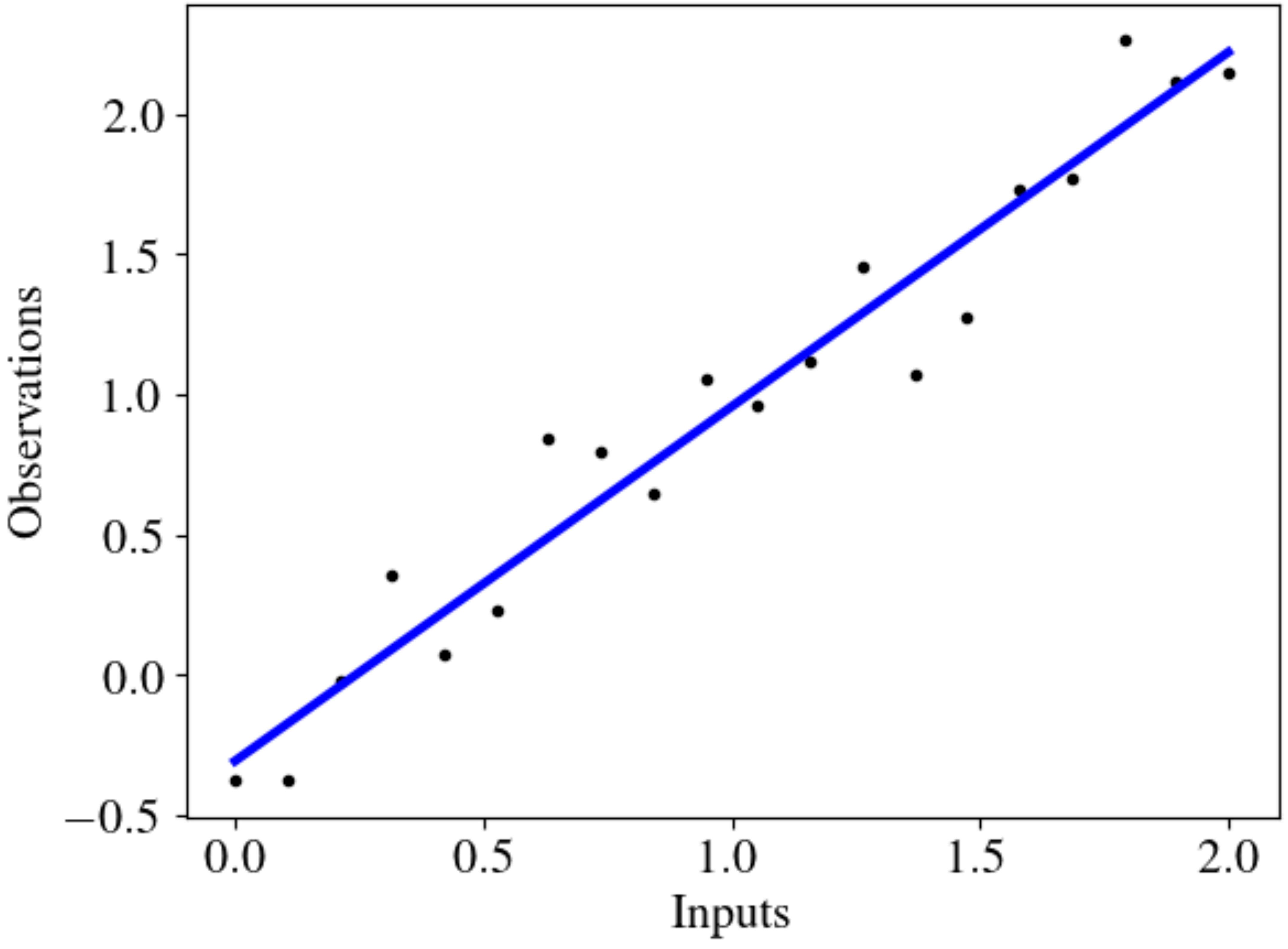
mean squared-error

Effect of noise on parameter estimates

Using our generative model, we can create fake datasets and see how our model parameters would be effected.

- For linear models, can derive analytical probability density of parameters, taking noise into account (give this a try!)
- Sampling from this distribution, provides a notion of predictive model uncertainty





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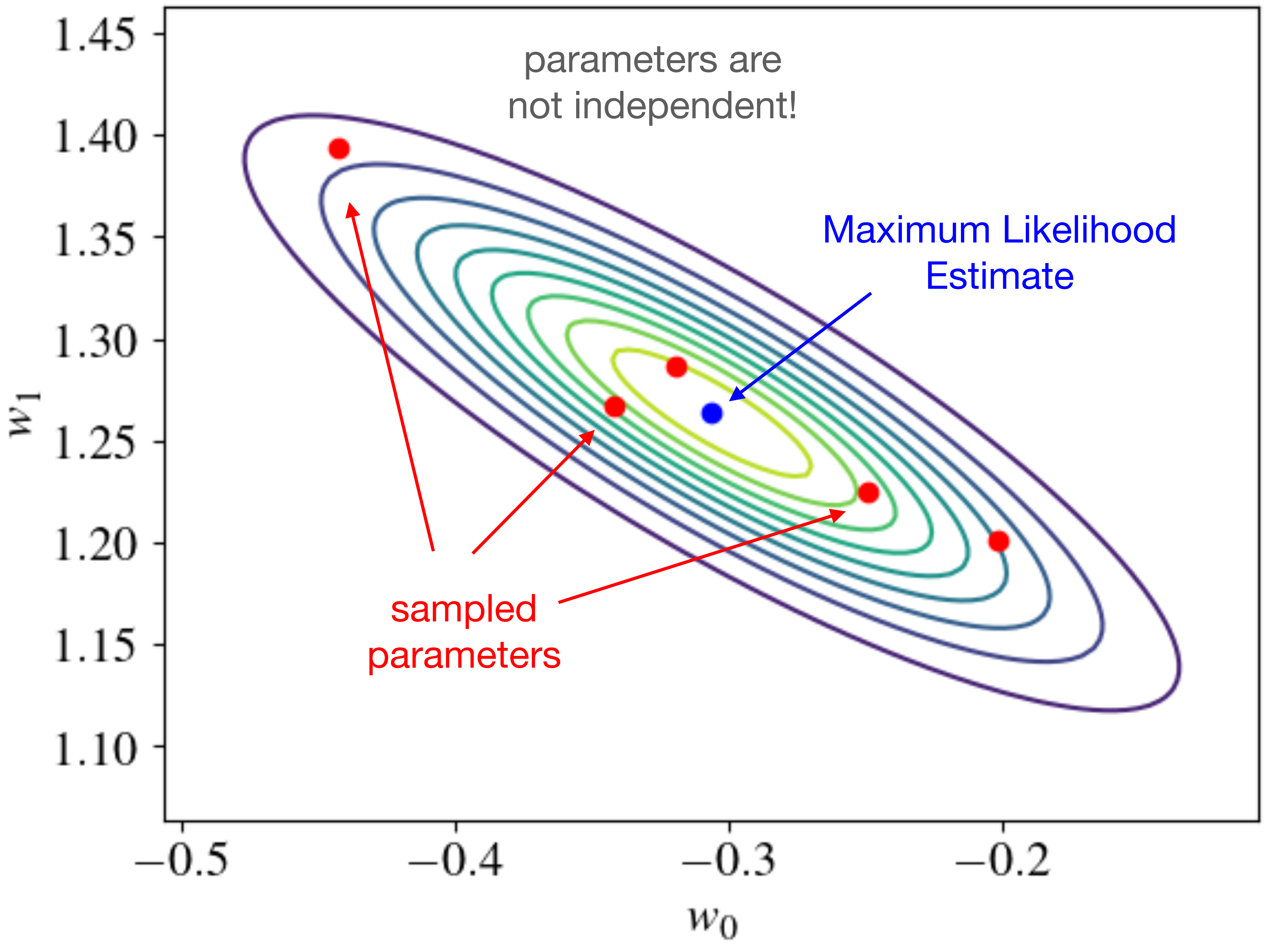
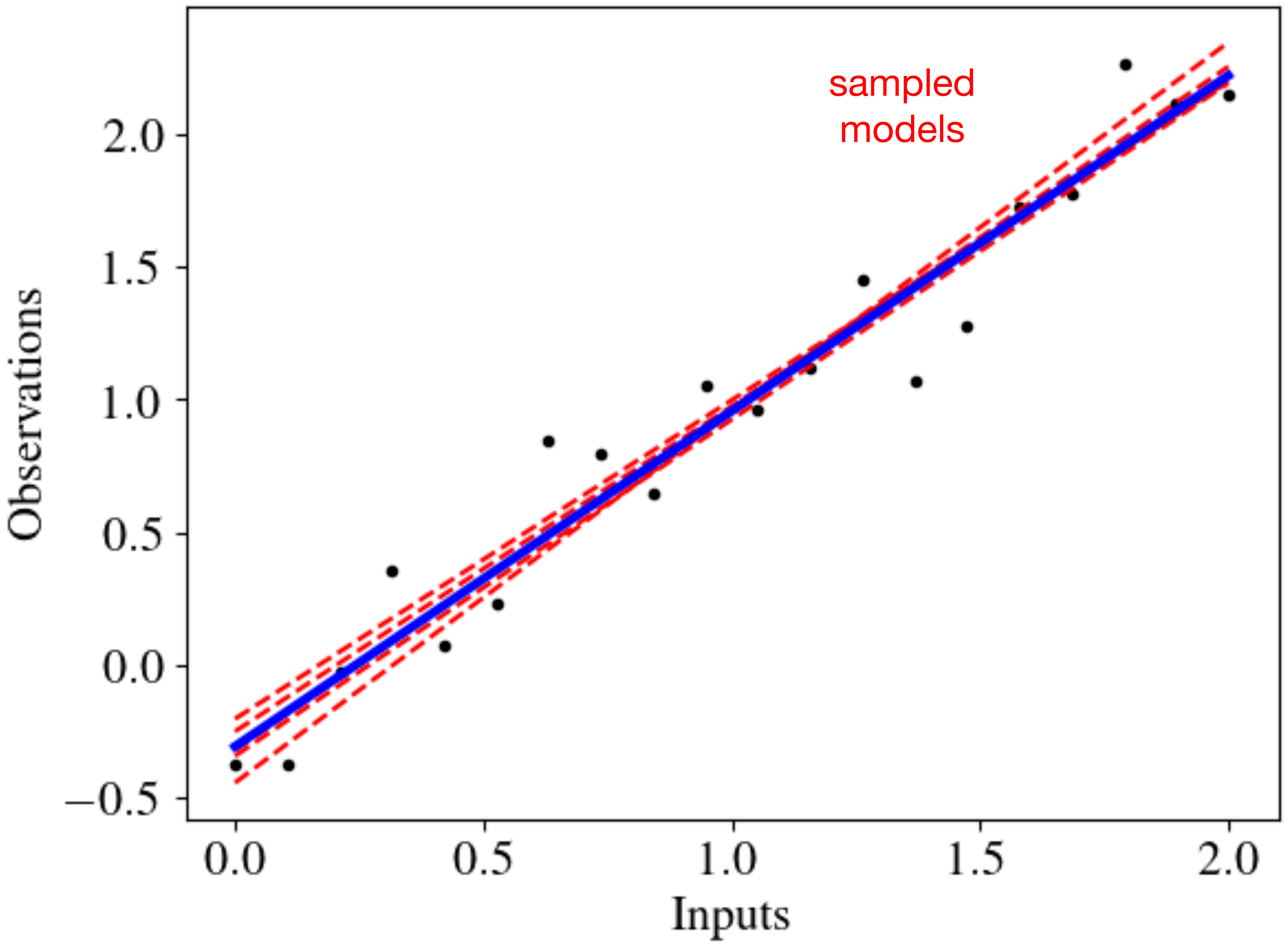


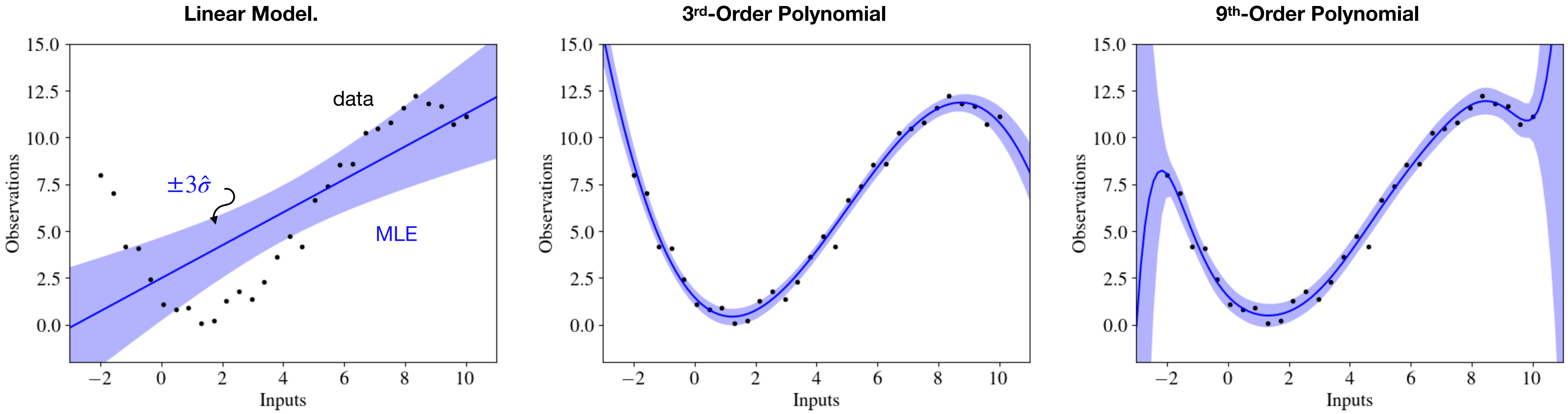


Predictive variance

- Summarizing prediction and variance for linear MLE model (skipping the details)

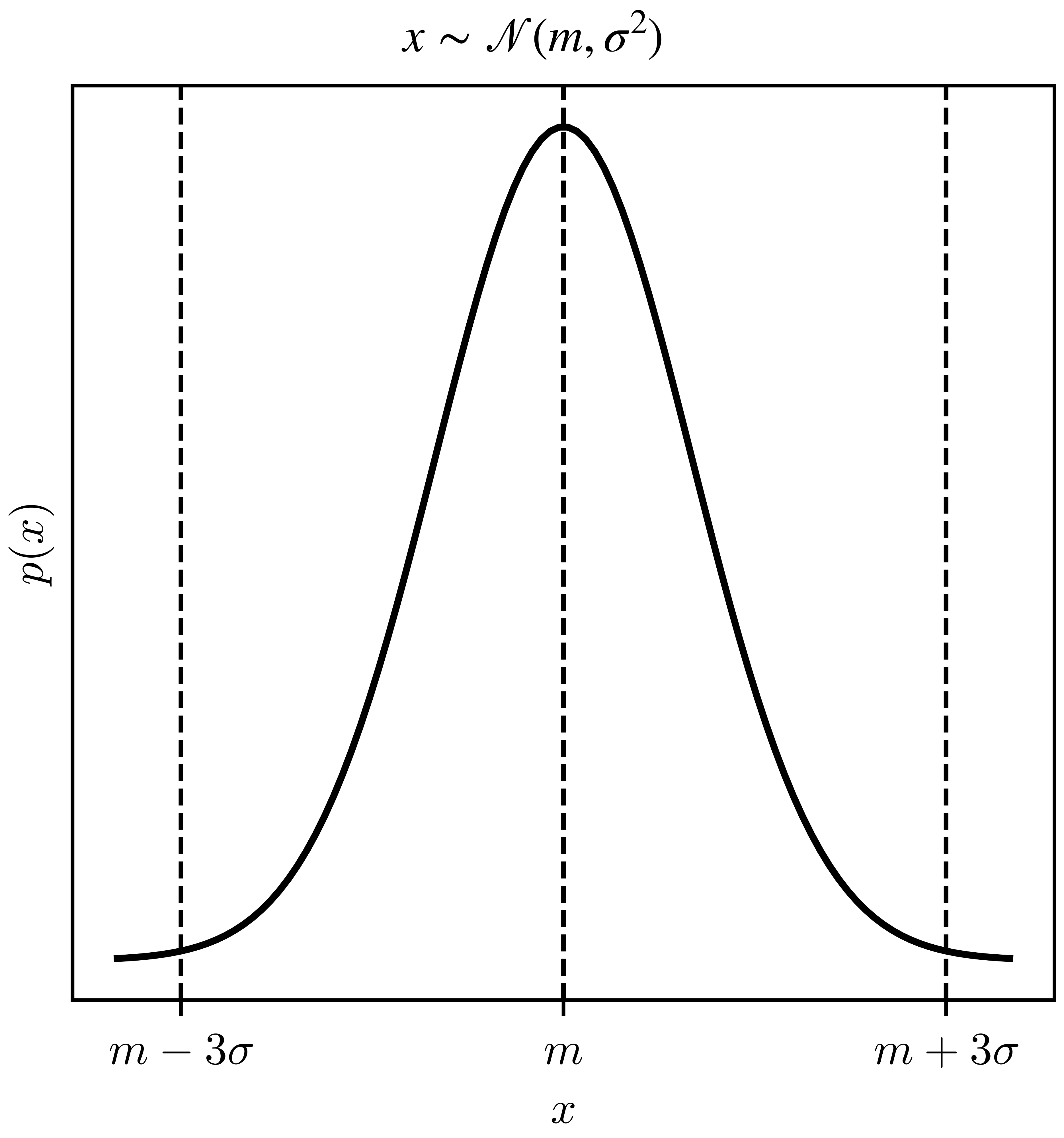
$$\hat{y} = \hat{f}(x) = \mathbf{h}(x)^T \mathbf{w} = \mathbf{h}(x)^T (\mathbf{H}^T \mathbf{H})^{-1} \mathbf{H}^T \mathbf{y}$$

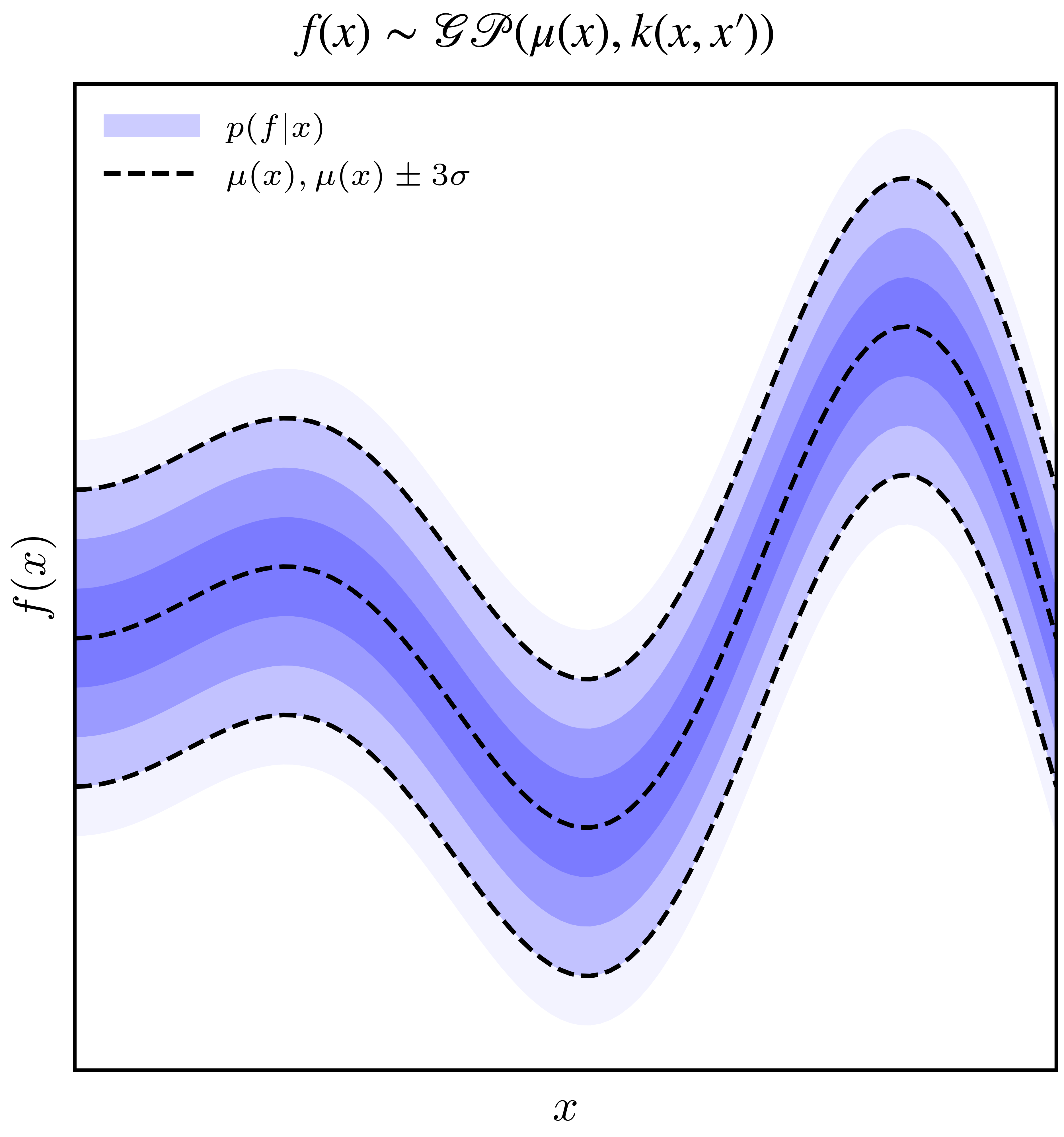
$$\hat{\sigma}^2(x) = \mathbf{h}^T(x) \, \text{cov}\{\mathbf{w}\} \, \mathbf{h}(x) = \sigma^2 \, \mathbf{h}^T(x) (\mathbf{H}^T \mathbf{H})^{-1} \mathbf{h}(x)$$



Gaussian Processes (GPs)

Generalization of the Gaussian distribution for random scalars to random functions





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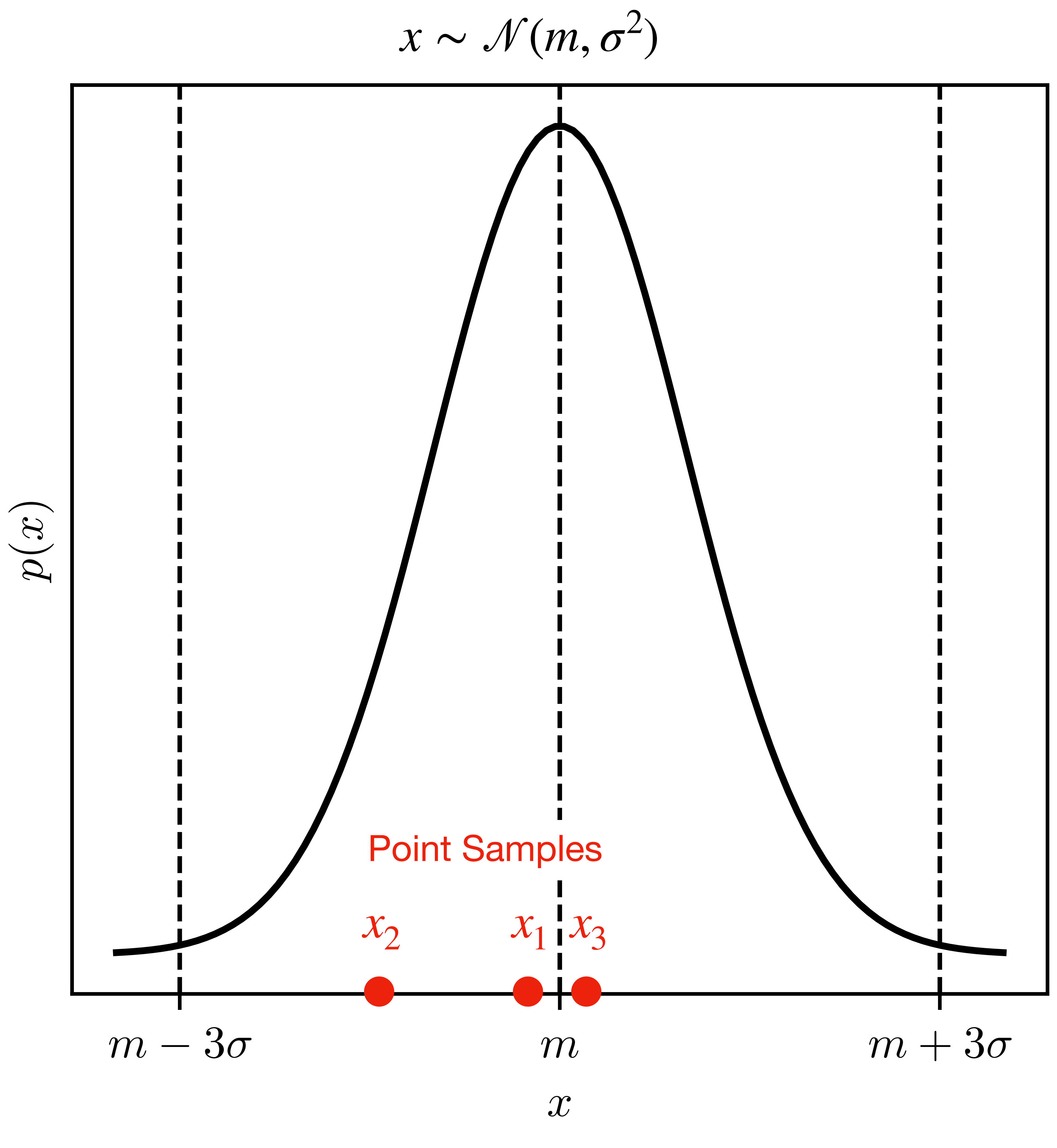

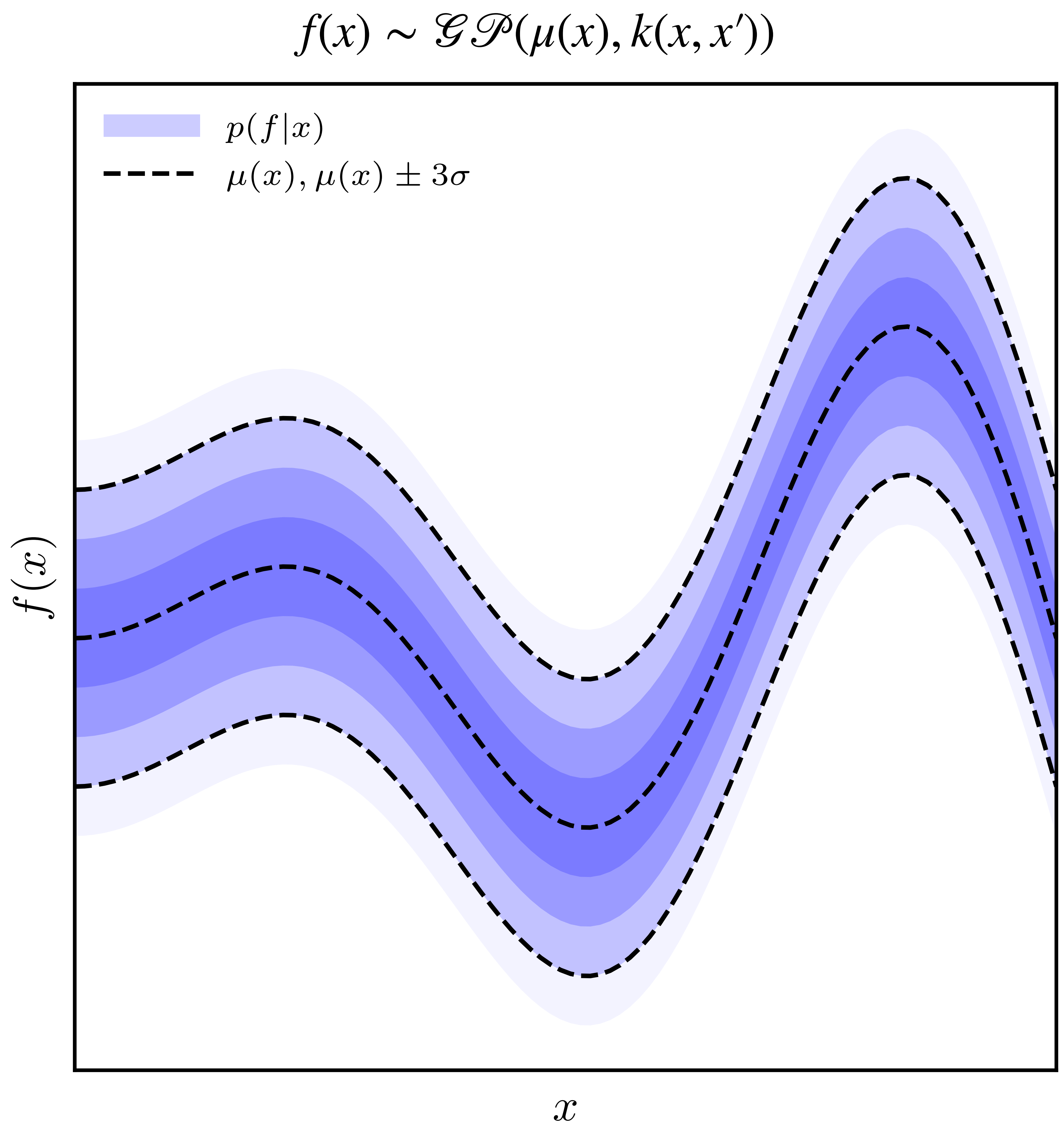

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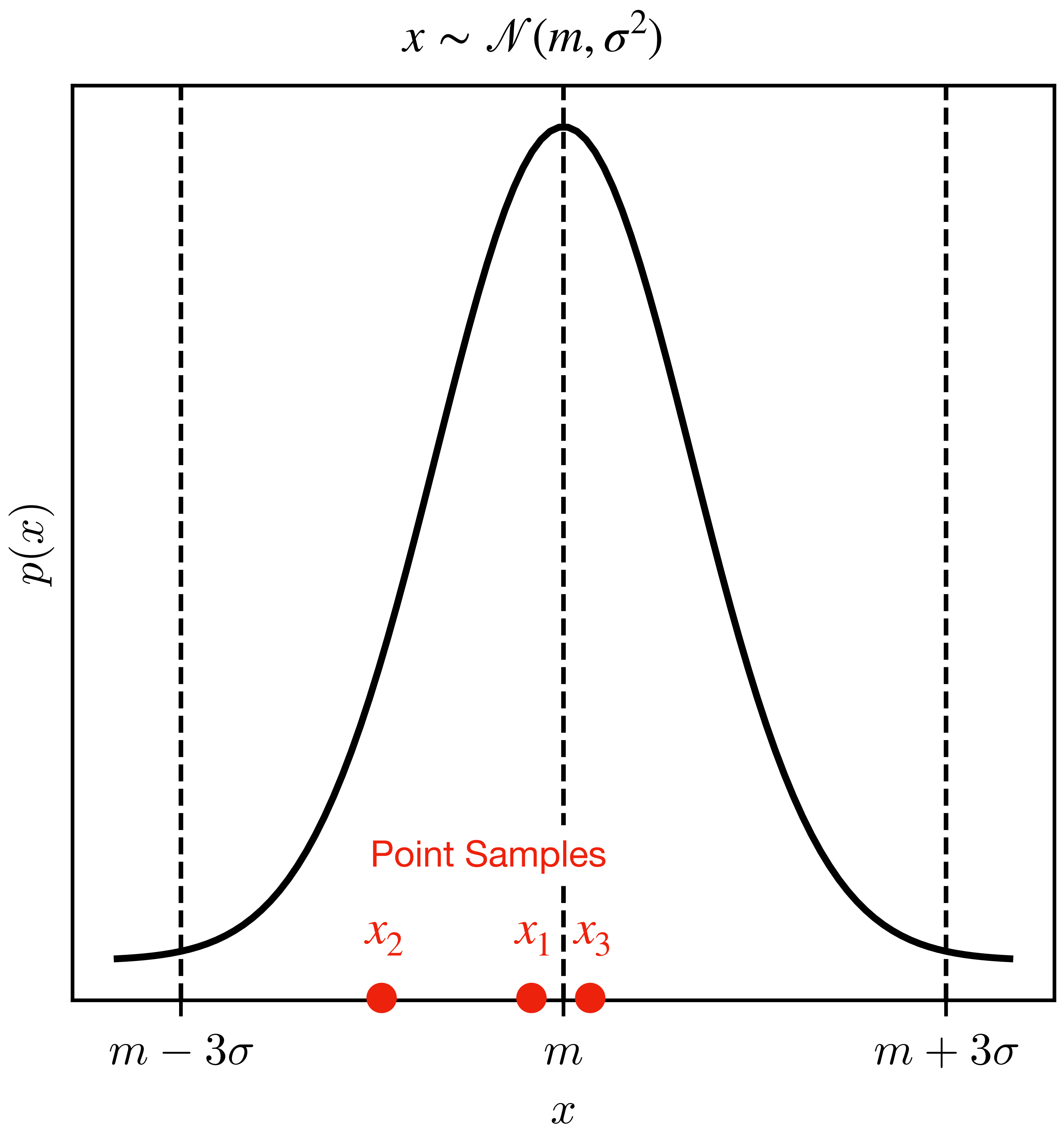
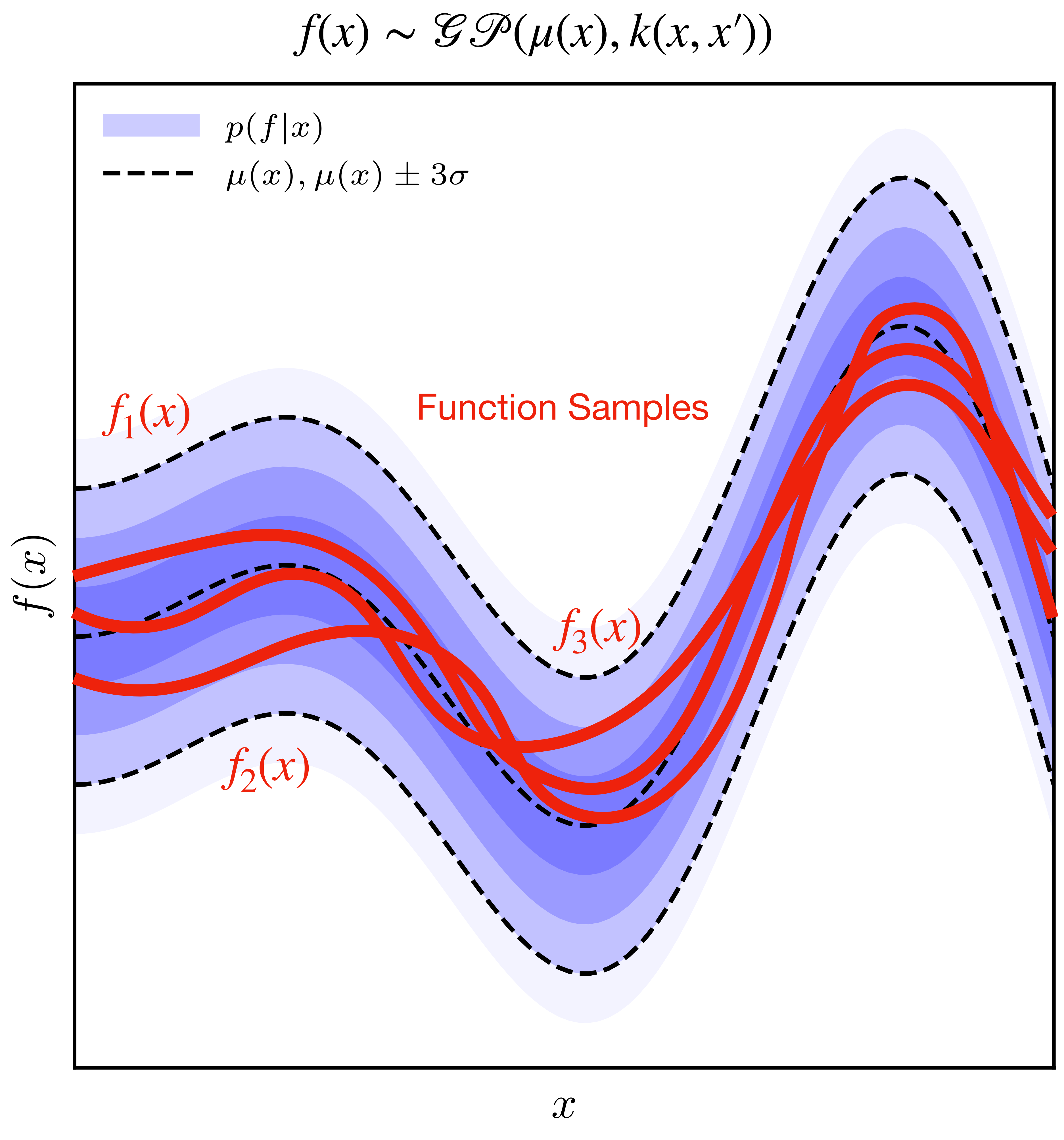




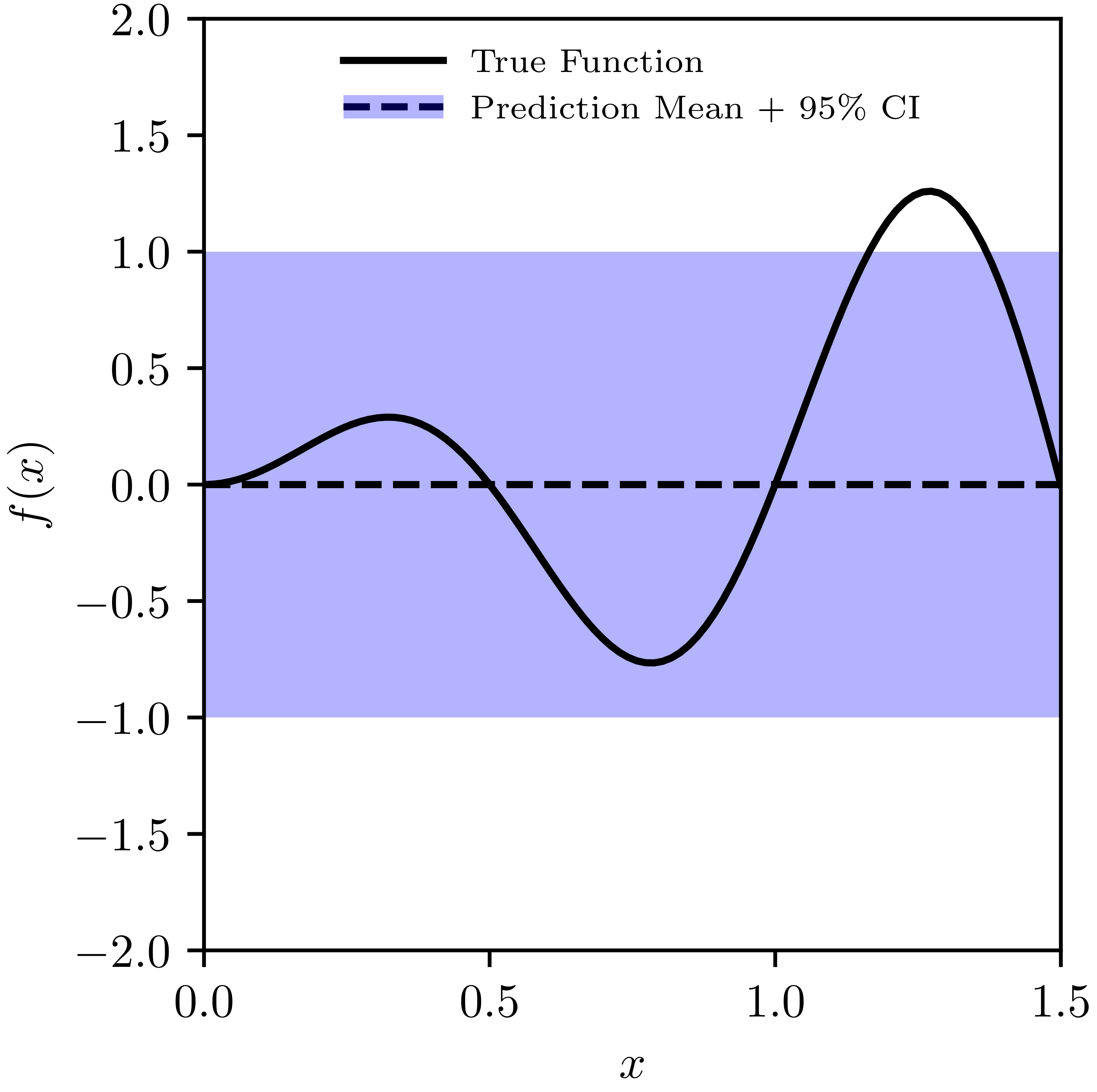
Gaussian Process Regression

Any finite set of index points $\{x_1, \ldots, x_n\}$ represents a multivariate Gaussian distribution for function values.

prior

$$f(x) \sim p(f \,|\, x) = \mathcal{GP}(\mu, k)$$

$$\implies \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu(x_1) \\ \mu(x_2) \\ \mu(x_3) \end{bmatrix}, \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) & k(x_1, x_3) \\ k(x_2, x_1) & k(x_2, x_2) & k(x_2, x_3) \\ k(x_3, x_1) & k(x_3, x_2) & k(x_3, x_3) \end{bmatrix} \right)$$



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Regression performed by conditioning the distribution on data
$\mathcal{D} = (X, f(X) = y)$

posterior

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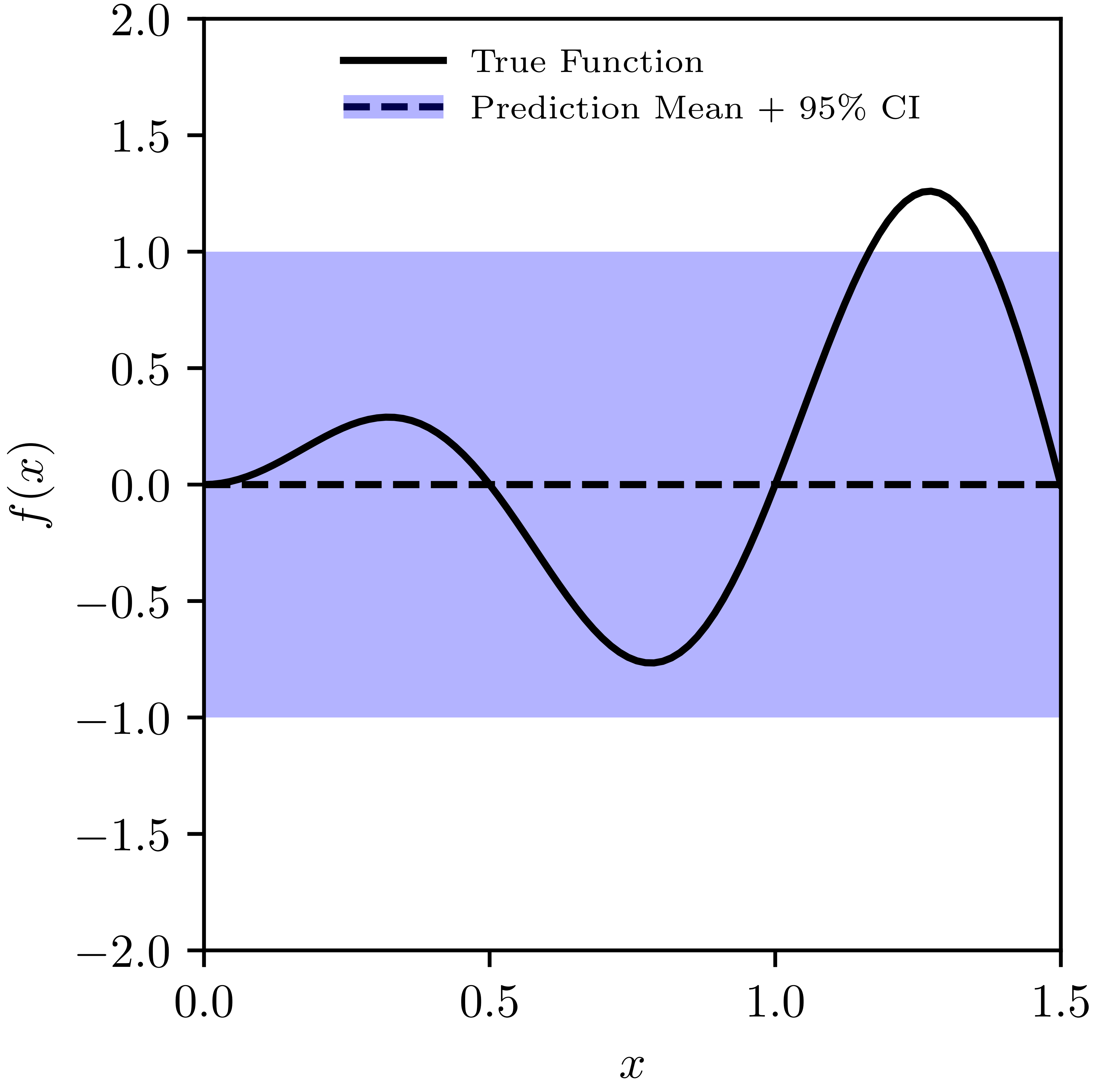

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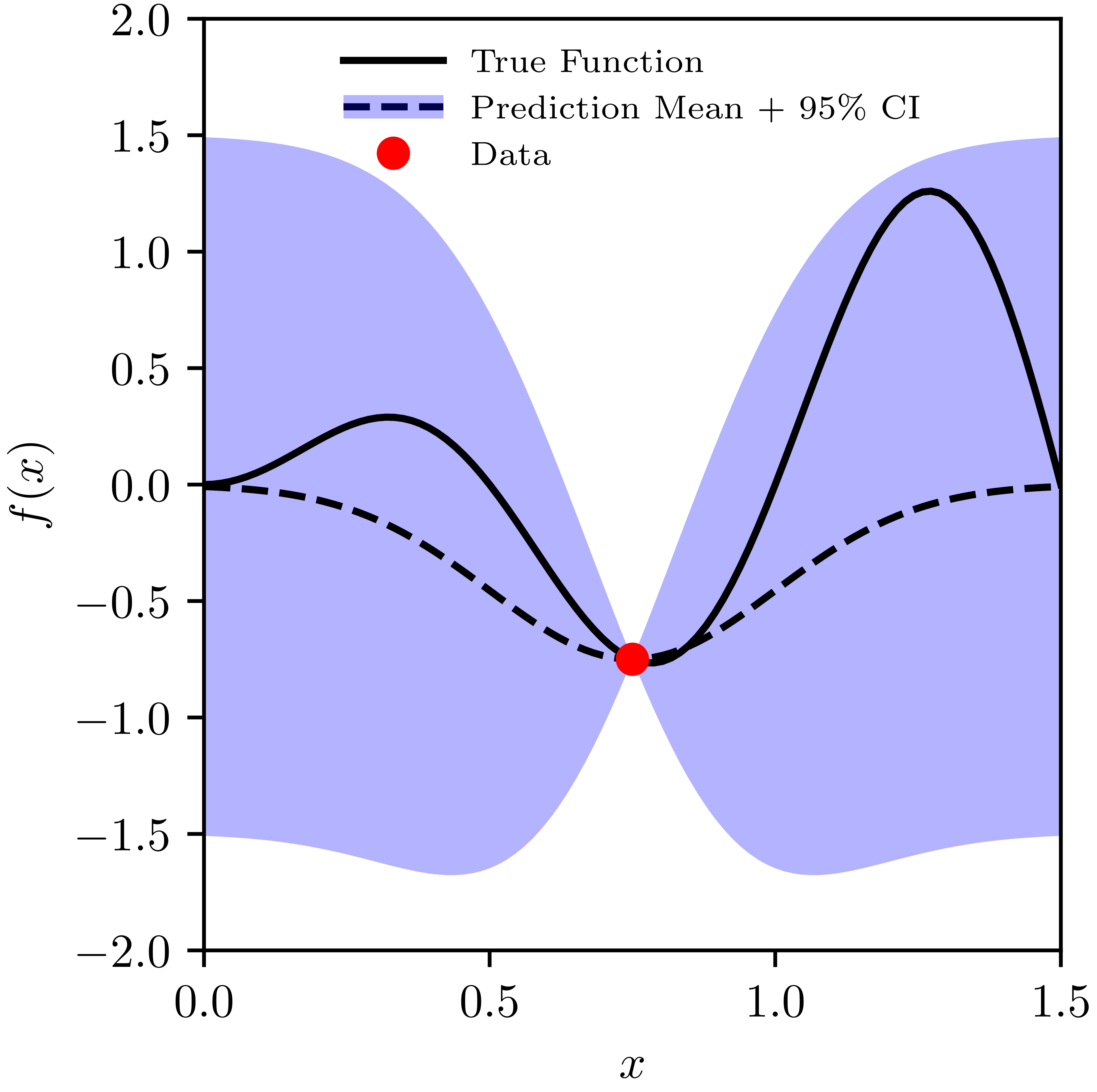

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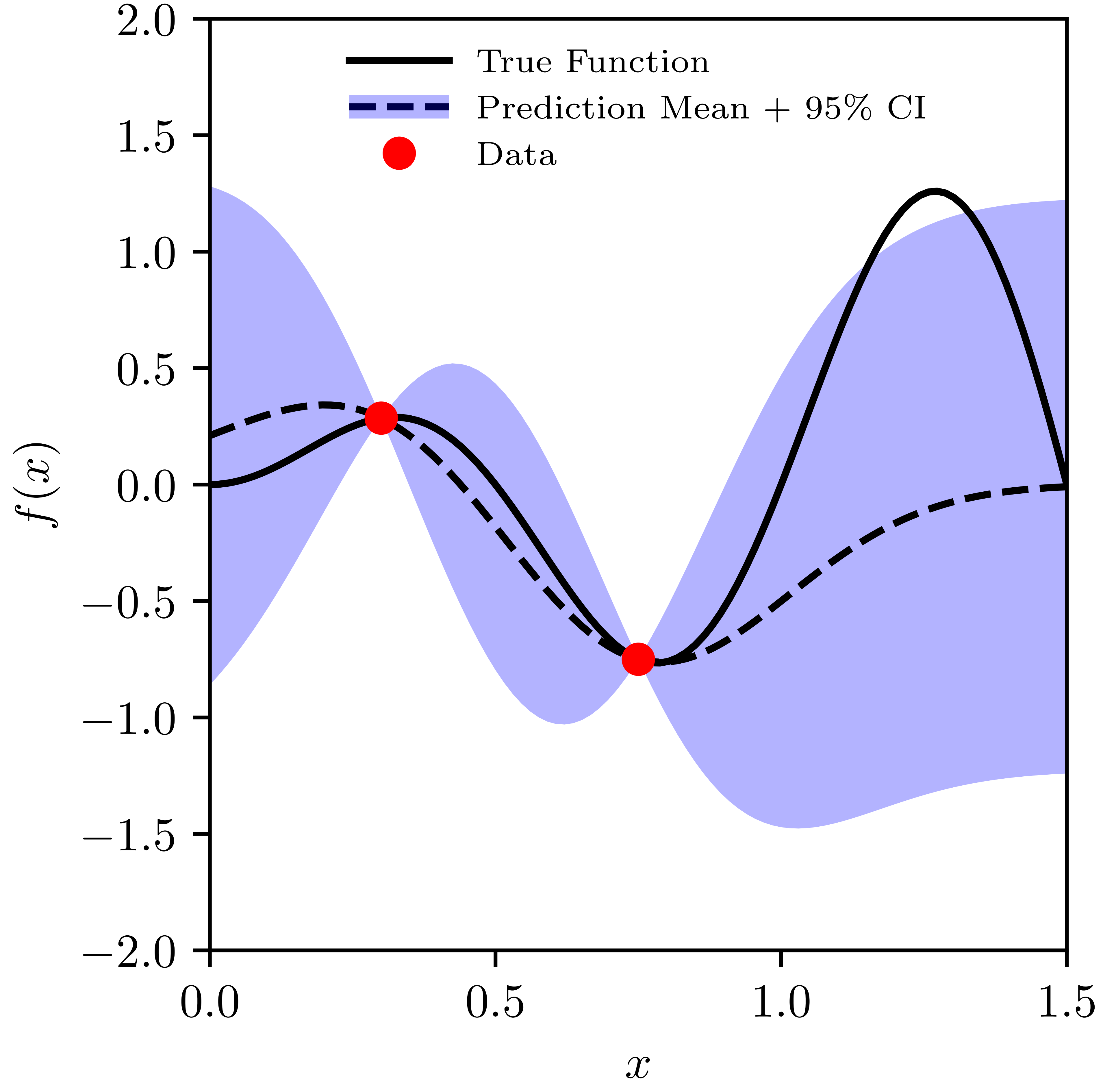

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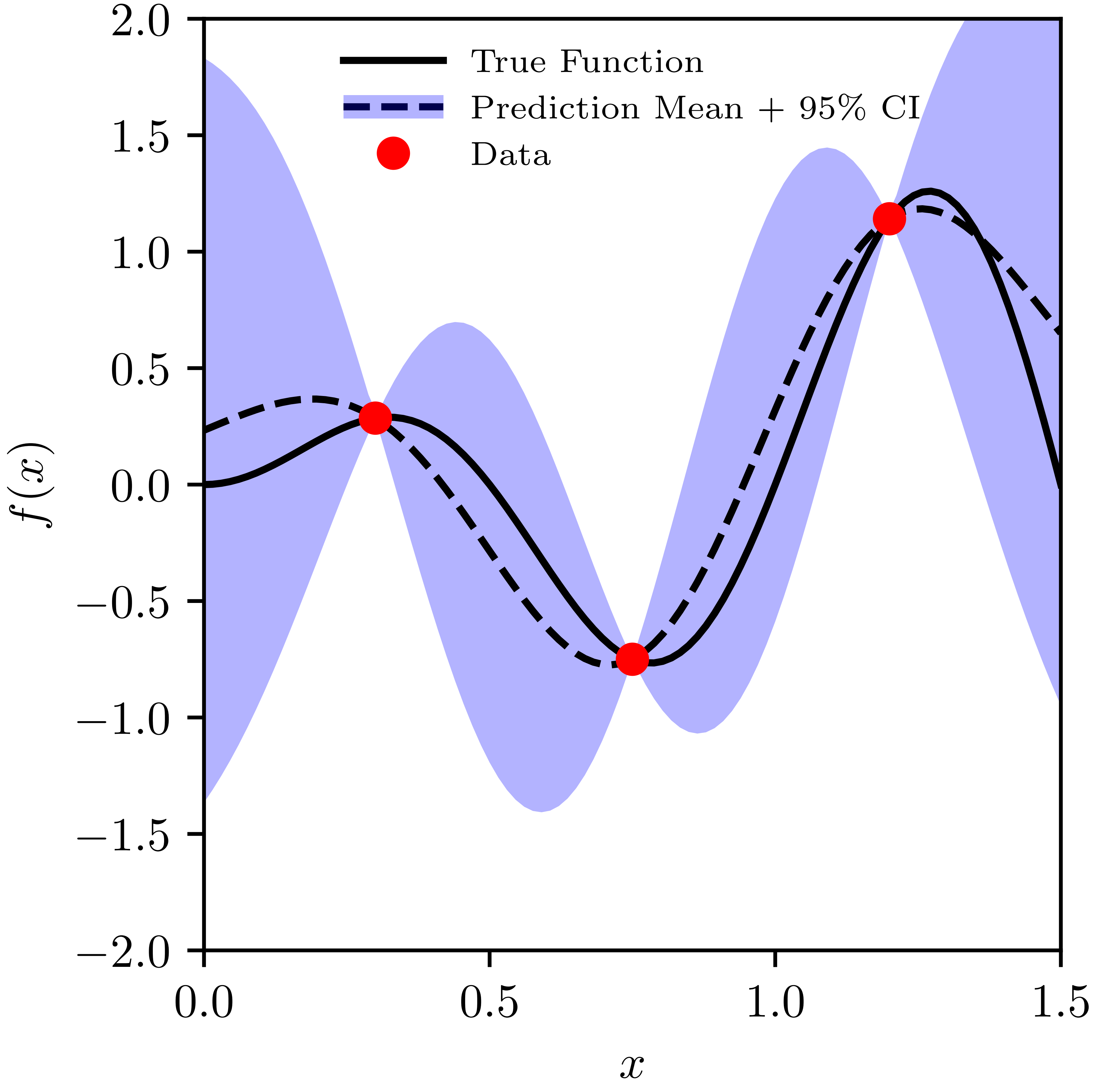
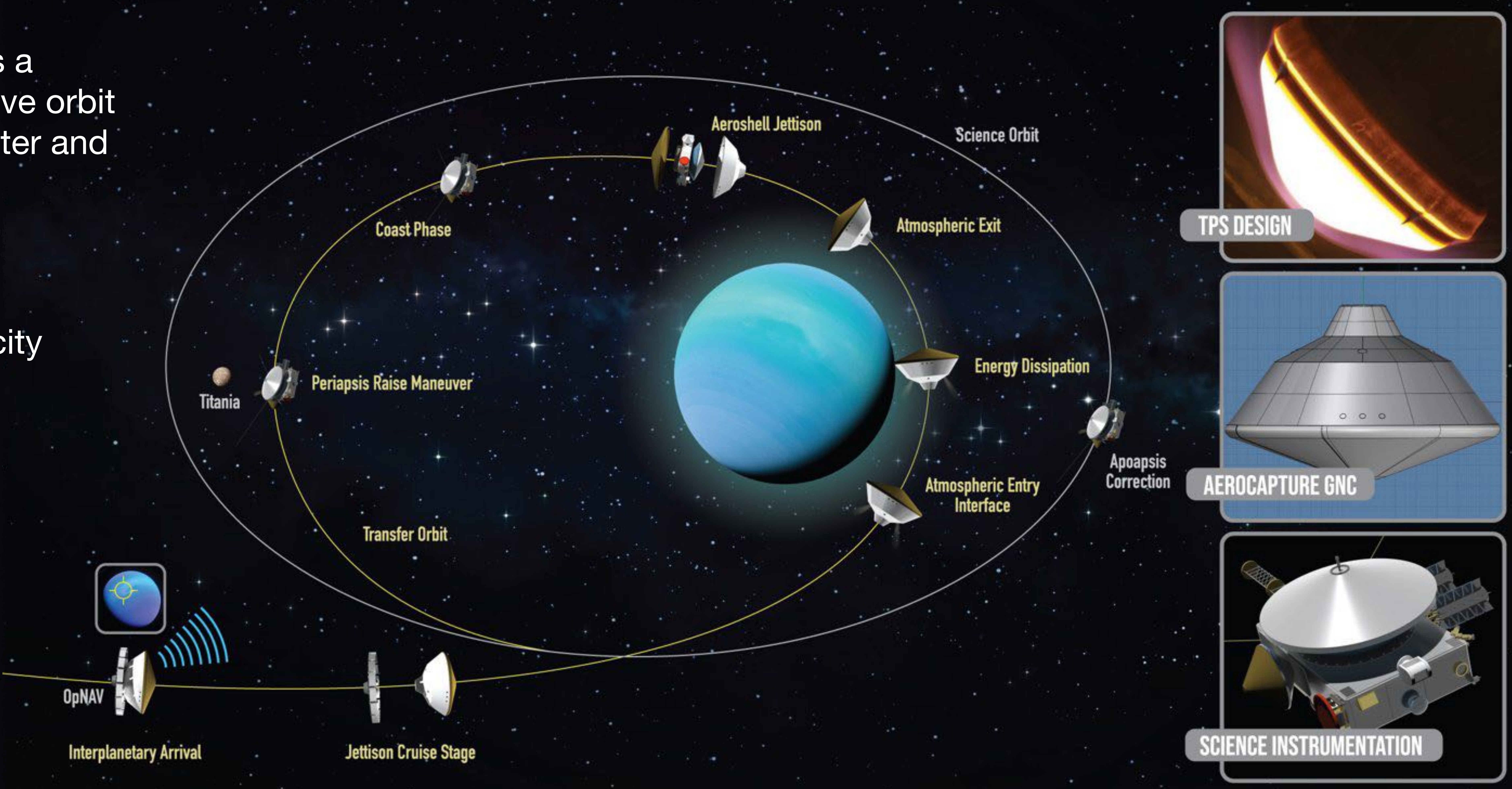


Example 1: Uranus Aerocapture

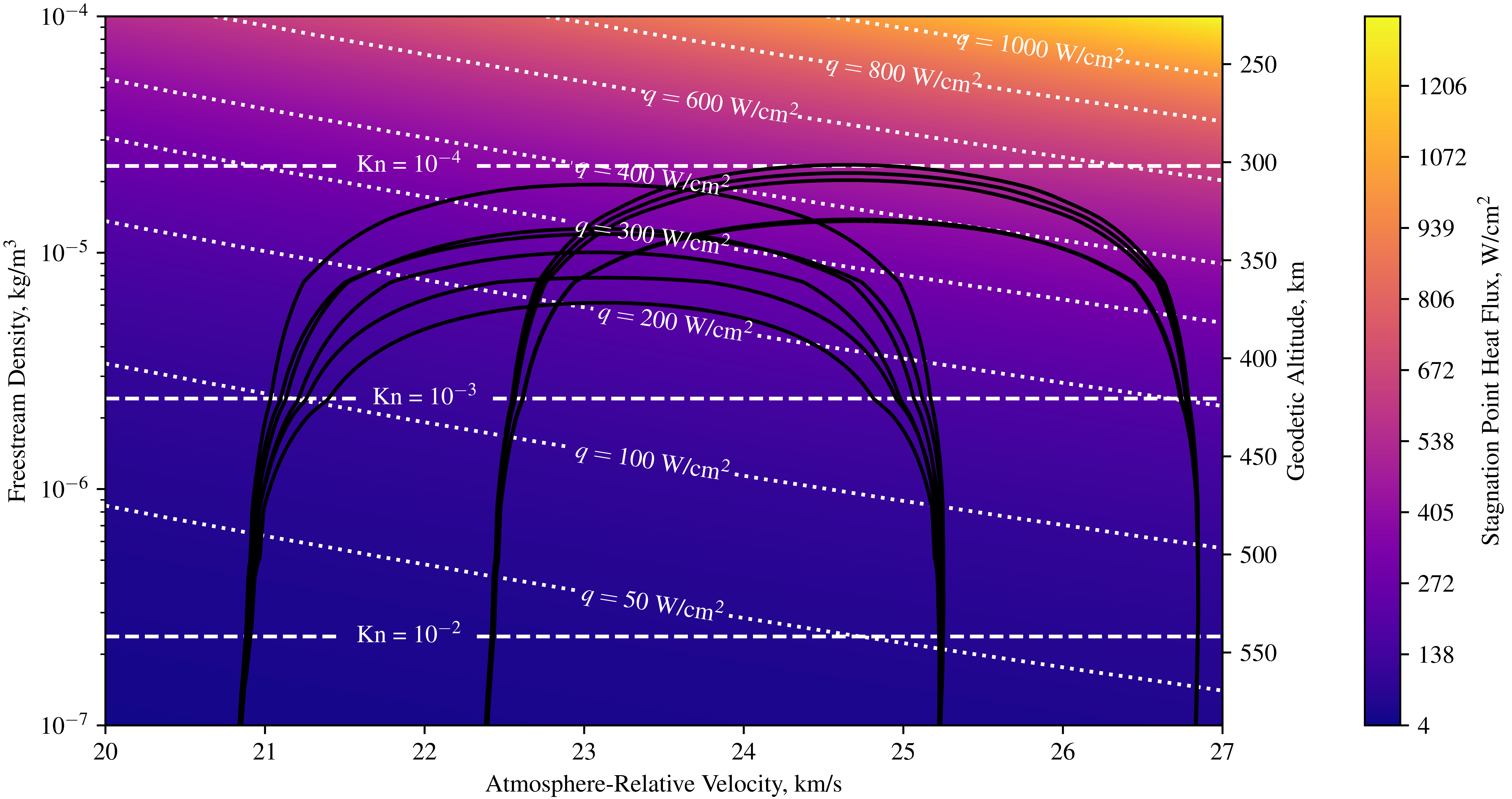
Early Career Initiative (ECI) Project

- Demonstrate *aerocapture* as a viable alternative to propulsive orbit insertions for Gas Giant orbiter and probe missions
- Benefits:
  - Increased payload capacity
  - Decrease cruise time



LaRC, ARC, JSC, JPL, Draper Laboratories, Booz Allen Hamilton, Intuitive Machines

Aeroheating database generation



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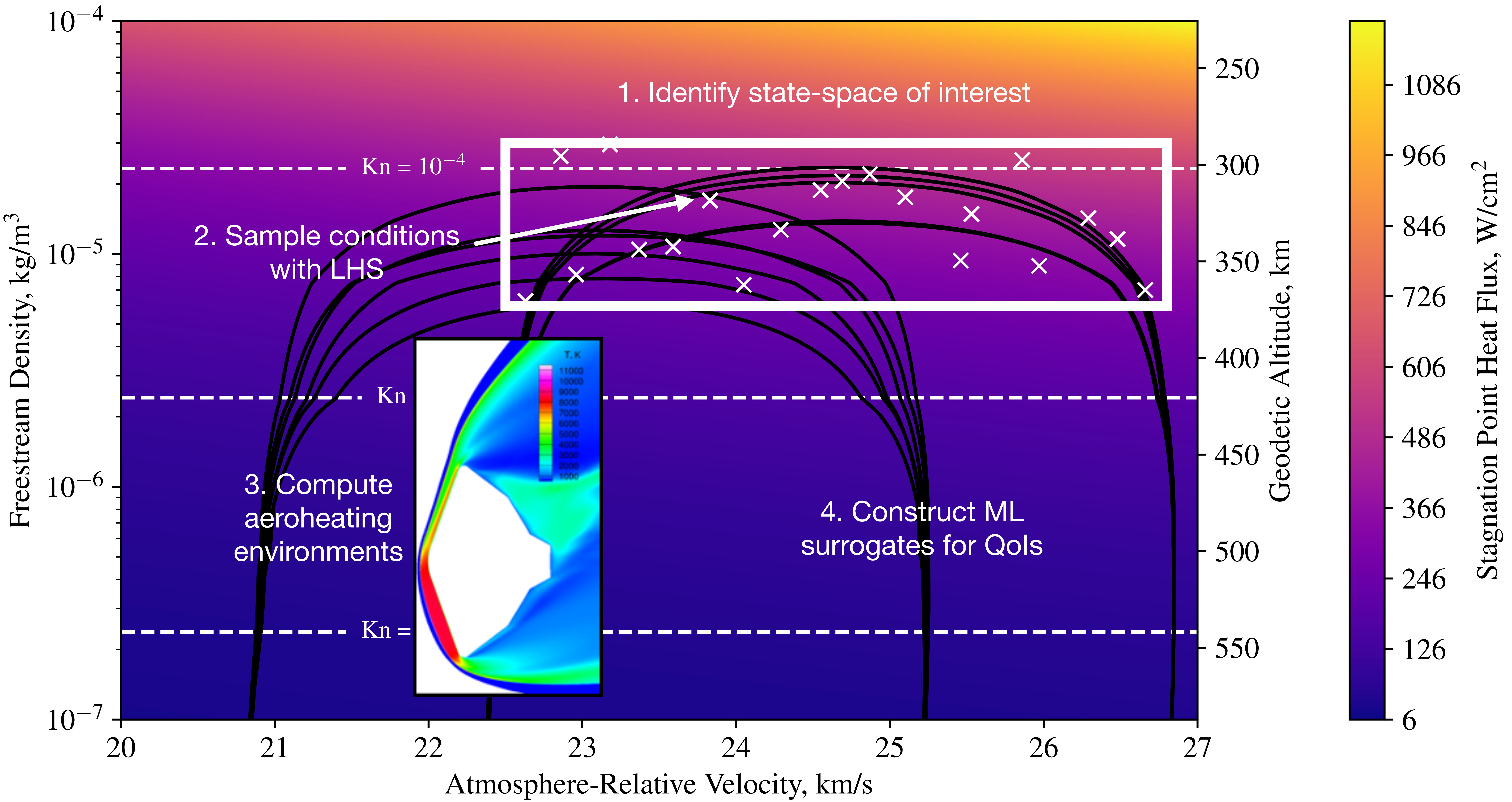


Axisymmetric forebody dataset

Conditions
X
Surface Points

Density	Velocity	Body Coordinate	Convective Heat Flux	Wall Pressure	Shear Stress
$\rho_{\infty 1}$	$V_{\infty 1}$	s_1	q_1	p_{w1}	τ_{w1}
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\rho_{\infty N}$	$V_{\infty N}$	s_N	q_N	p_{wN}	τ_{wN}

Axisymmetric forebody dataset

Conditions X # Surface Points

Input Data			Output Data		
Density	Velocity	Body Coordinate	Convective Heat Flux	Wall Pressure	Shear Stress
$\rho_{\infty 1}$	$V_{\infty 1}$	s_1	q_1	p_{w1}	τ_{w1}
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\rho_{\infty N}$	$V_{\infty N}$	s_N	q_N	p_{wN}	τ_{wN}

Axisymmetric forebody dataset

Input Data | **Output Data**

Conditions X # Surface Points

Density	Velocity	Body Coordinate	Convective Heat Flux	Wall Pressure	Shear Stress
$\rho_{\infty 1}$	$V_{\infty 1}$	s_1	q_1	p_{w1}	τ_{w1}
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\rho_{\infty N}$	$V_{\infty N}$	s_N	q_N	p_{wN}	τ_{wN}

Want to create surrogate models that fit the data and provide surface heat flux, pressure, and shear stress over entire state-space of interest in order to provide estimates over computed trajectories

- Maintain physical scaling when making predictions outside of the dataset range
- Estimate model uncertainties

Dataset normalization

- Good opportunity to ask “What do I know about my data?”
  - Dimensionality reduction, known scaling laws or engineering correlations, limits or bounds?
  - Sutton-Graves model for max convective heating:

$$q_{conv}^{max} = K\sqrt{\frac{\rho_\infty}{R_n}}V_\infty^3$$

  - Newtonian pressure theory:

$$C_p^{max} = \frac{p_{max} - p_\infty}{\frac{1}{2}\rho_\infty V_\infty^2} \approx 2 \implies p_{max} \approx A\rho_\infty V_\infty^2$$

  - Suggests that maximum value of QoIs for each freestream condition follow generalized Sutton-Graves relation

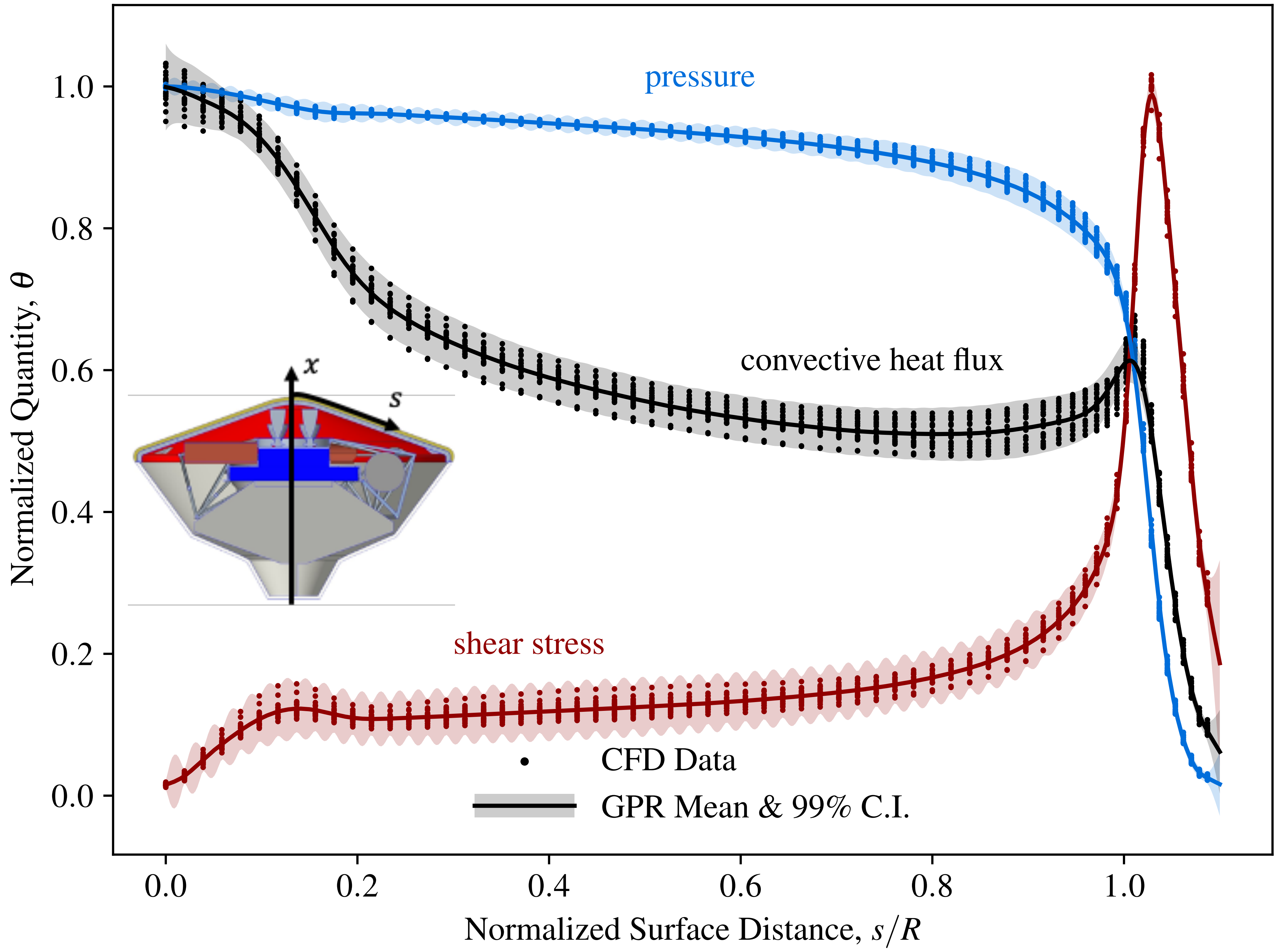
$$\theta_{max} = C_\theta\, \rho_\infty^{m_\theta}\, V_\infty^{n_\theta}$$

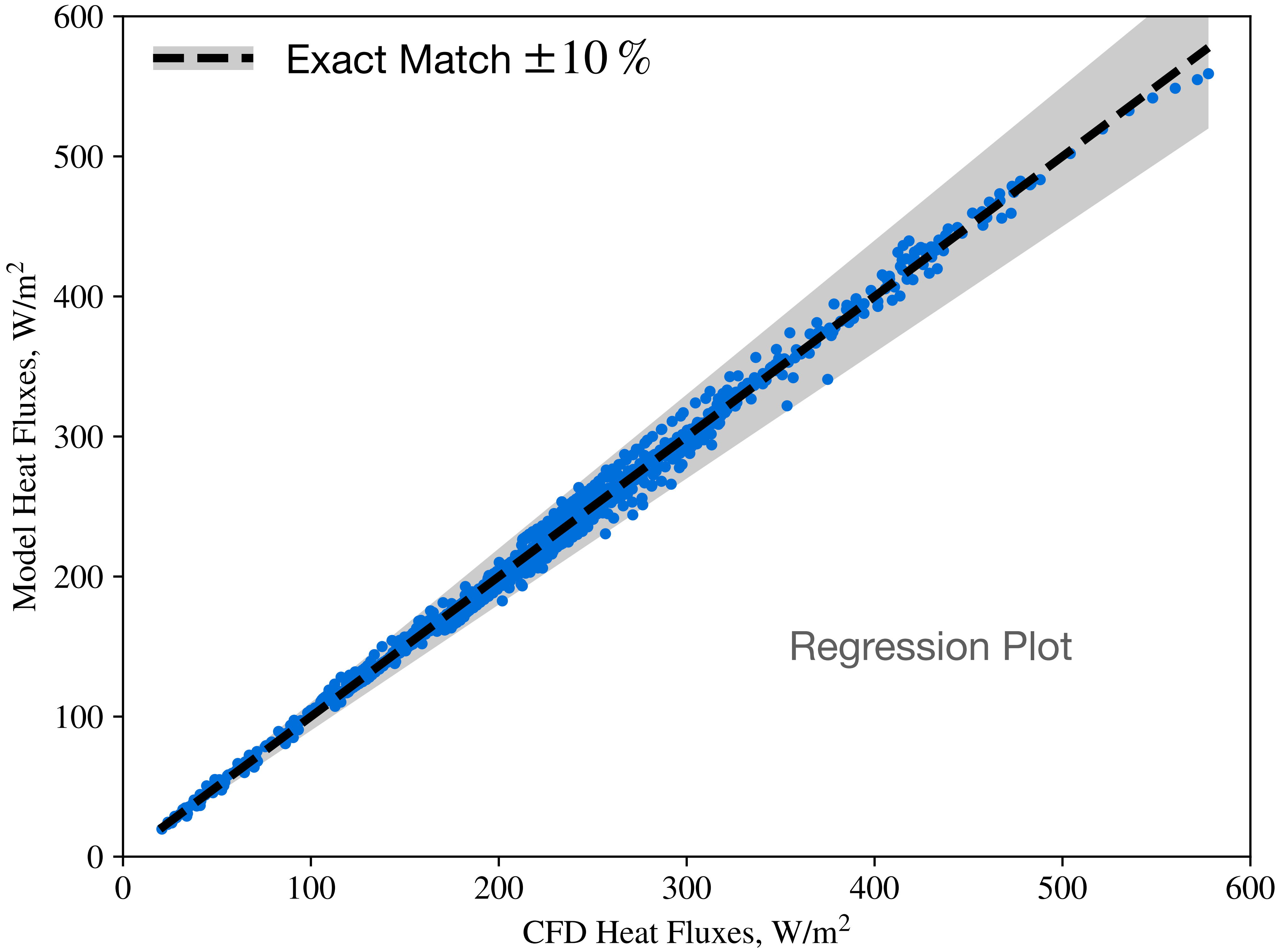
Linear models to rescue

- The generalized Sutton-Graves model is linear in it's parameters with appropriate transformation!

$$\theta_{max} = C_\theta\, \rho_\infty^{m_\theta}\, V_\infty^{n_\theta} \implies \ln \theta_{max} = \ln C_\theta + m_\theta \ln \rho_\infty + n_\theta \ln V_\infty$$

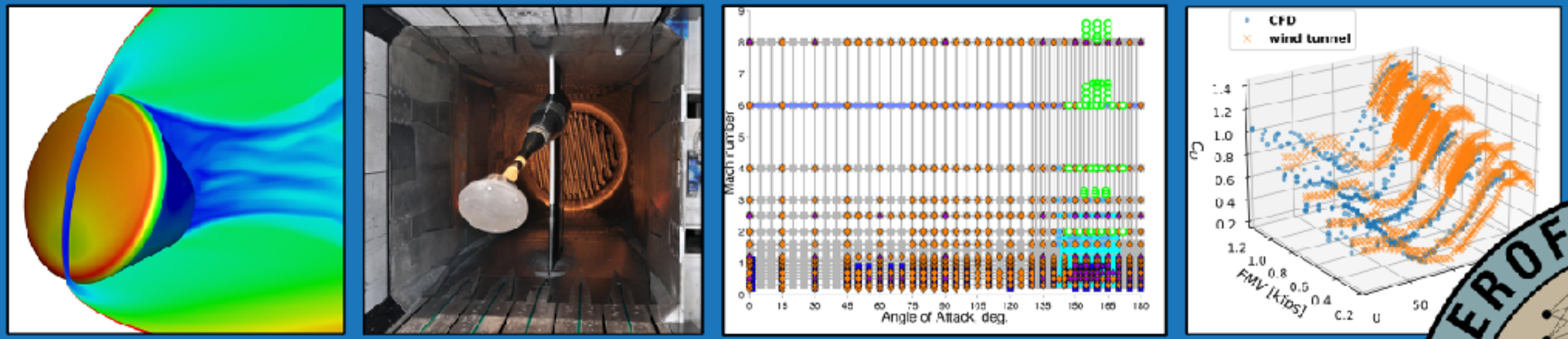
- Normalizing all the data by our new fits reduces the dimensionality of the problem to the body coordinate



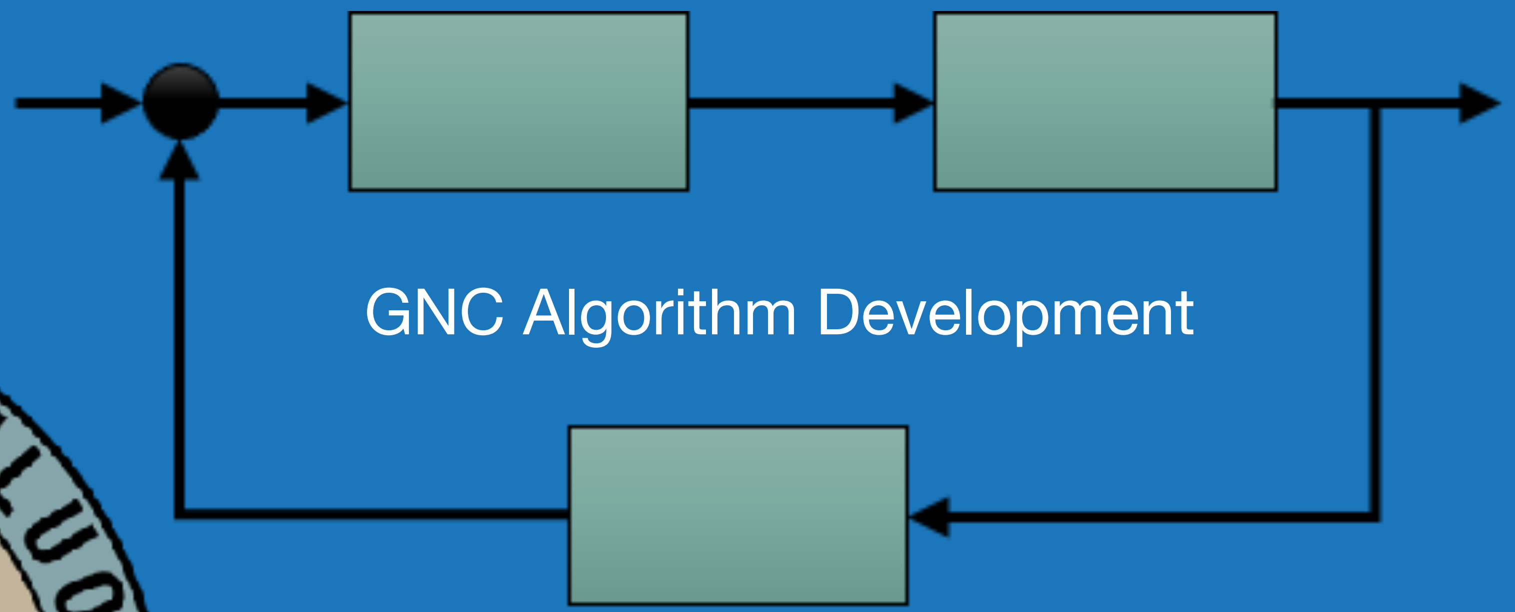


Example 2: Aerofusion Early Career Initiative

CFD Solutions and Wind Tunnel Tests

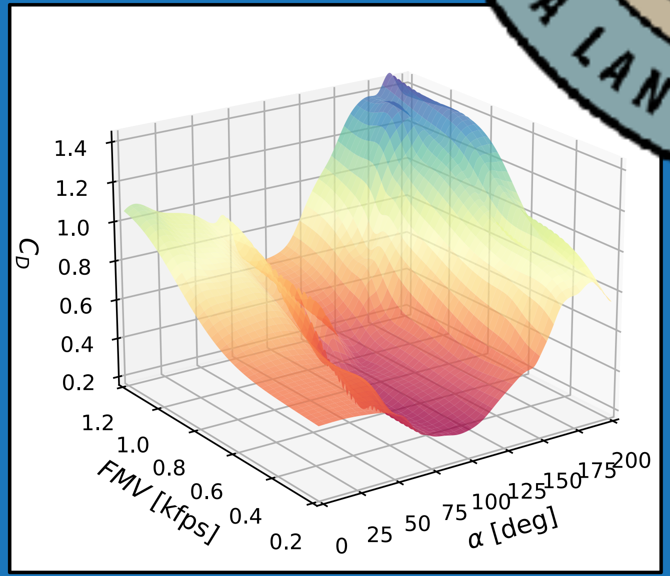


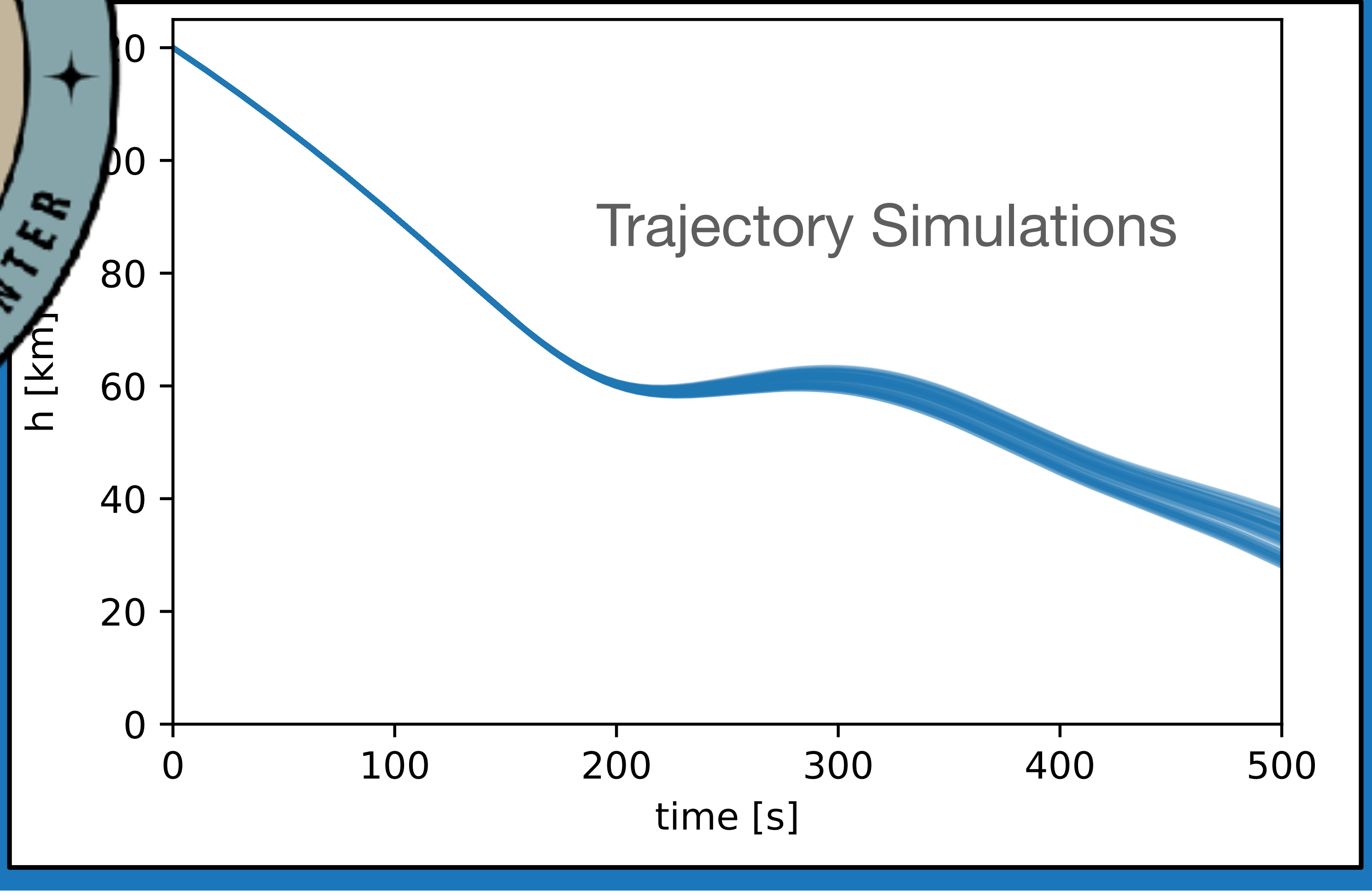
Engineering and Mission Design



Aerodynamic Database Construction

$$\begin{bmatrix} \text{FMV} & \text{Mach or Velocity} \\ \alpha & \text{Angle of Attack} \\ \beta & \text{Side-slip Angle} \\ \text{Re} & \text{Reynolds Number} \\ \vdots & \end{bmatrix} \Longrightarrow \begin{bmatrix} C_L & \text{Lift Coef.} \\ C_D & \text{Drag Coef.} \\ C_m & \text{Pitching Coef.} \\ \vdots & \end{bmatrix}$$





See recent publications for more details about the project:

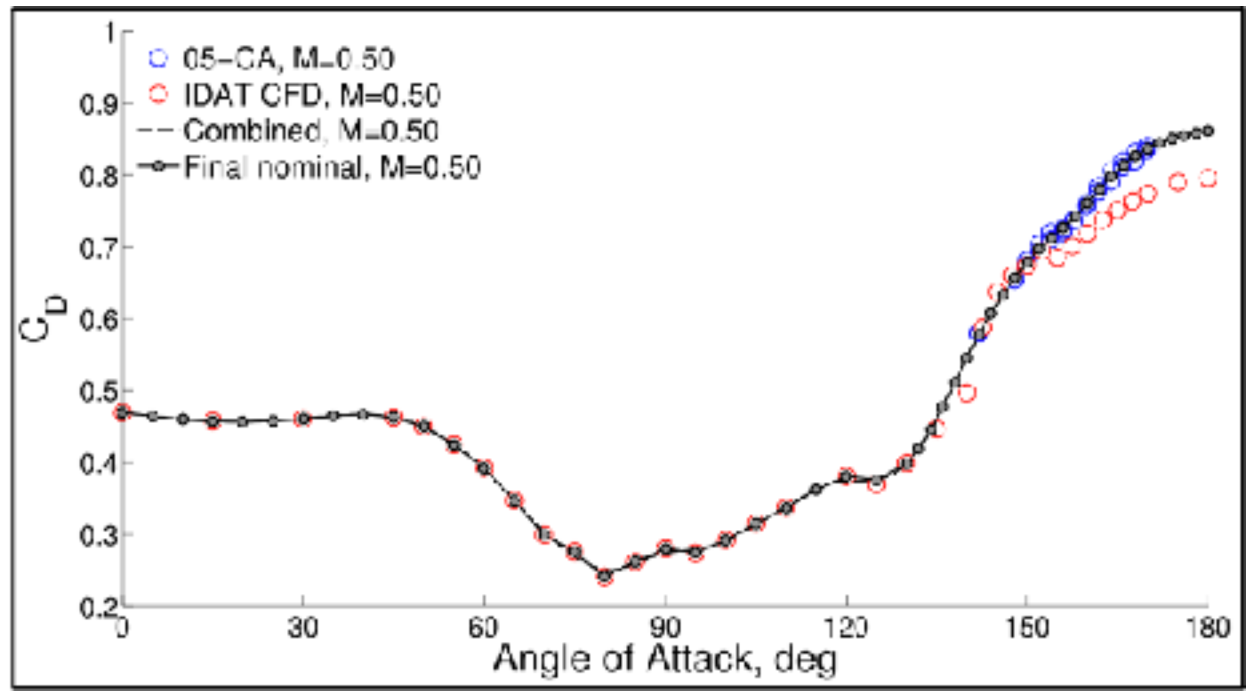
- Snyder et al. "AeroFusion: Data Fusion and Uncertainty Quantification for Lander Vehicles." *SciTech 2023.* AIAA 2023-1182.
- Scoggins et al. "Multi-hierarchy Gaussian Process Models for Probabilistic Aerodynamic Databases using Uncertain Nominal and Off- Nominal Configuration Data." *SciTech 2023*. AIAA 2023-1185.

Data fusion with uncertainties

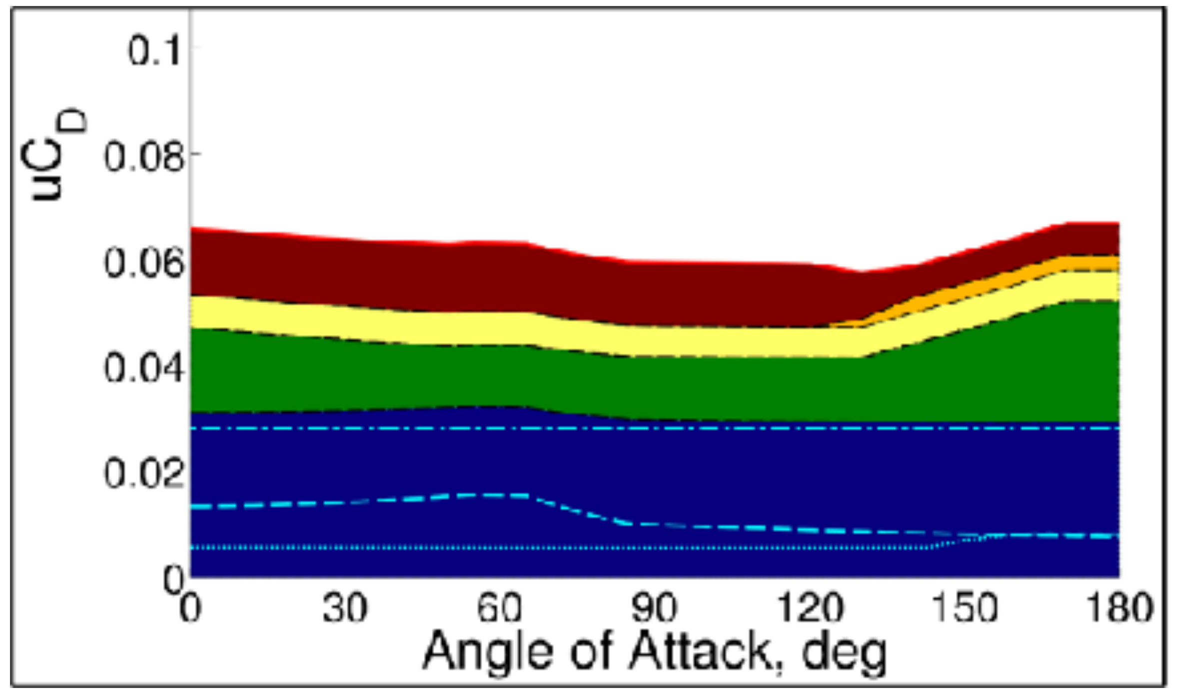
Typical data is noisy, with varying degrees of fidelity to flight vehicle

- Data continuously updated as design matures
- Different levels of fidelity in computational tools
- Wind tunnel models approximate vehicle geometry and roughness
- Wind tunnels cannot always reproduce flight conditions

Current state of the practice: “UQ by Inspection”



Nominal aerocoefficients constructed using expert judgment, given multiple sources of data.



Uncertainty buildup based on dispersion factors, tuned to cover varying data sources.

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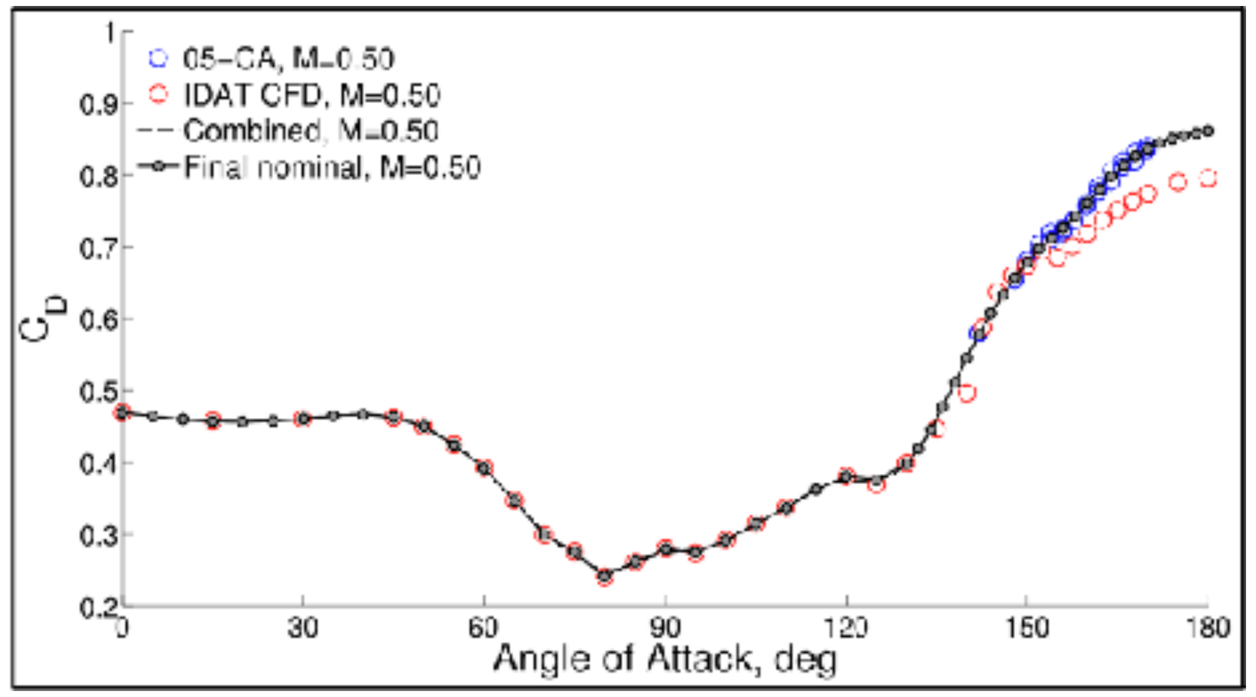

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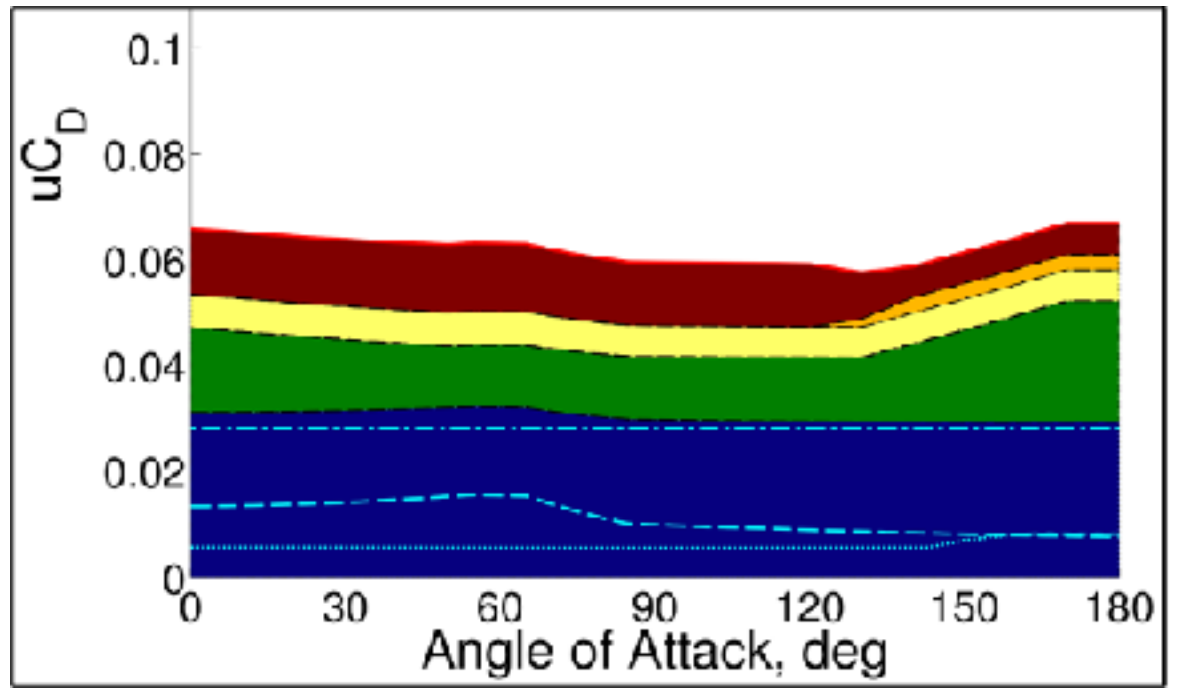
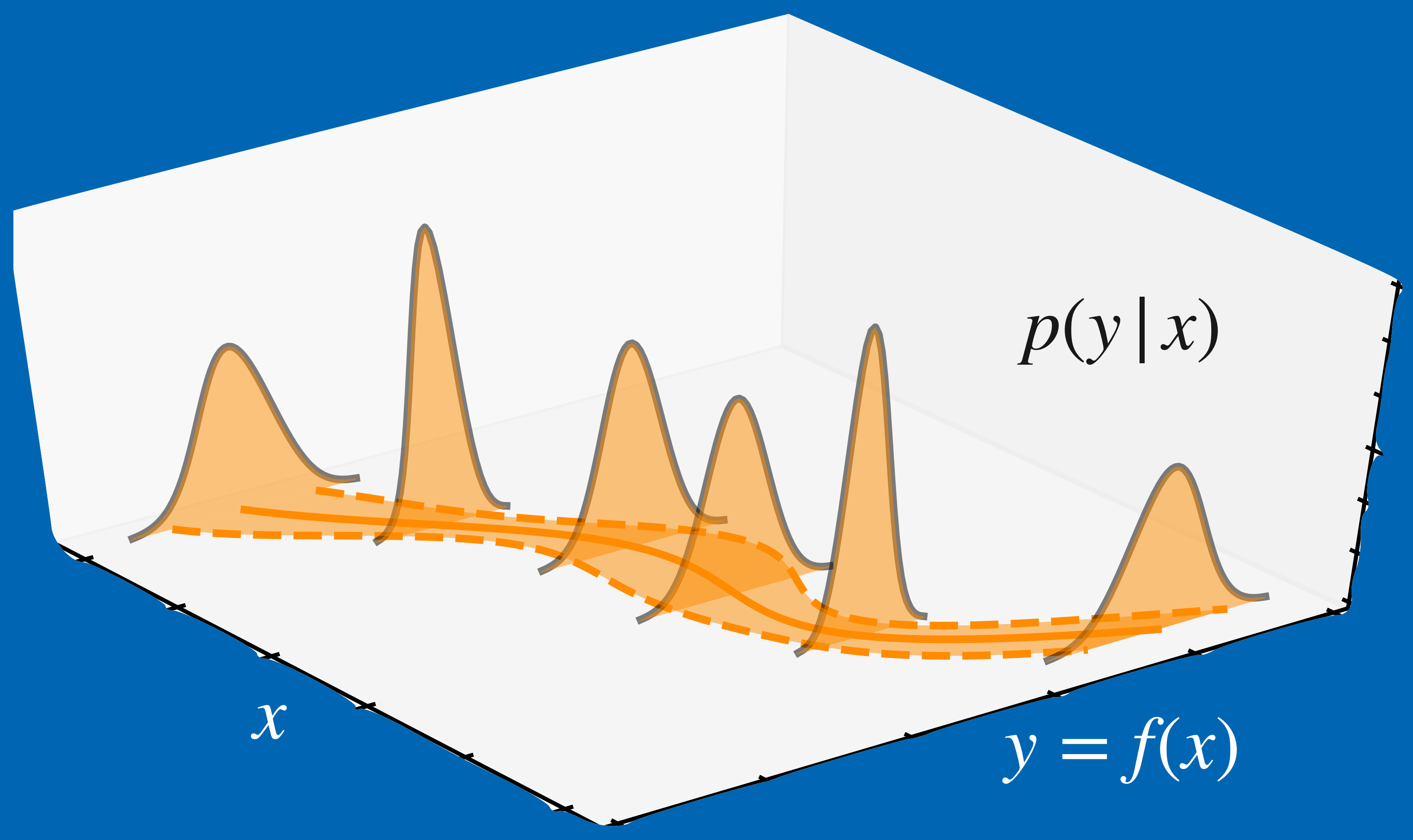


Uncertainty buildup based on dispersion factors, tuned to cover varying data sources.

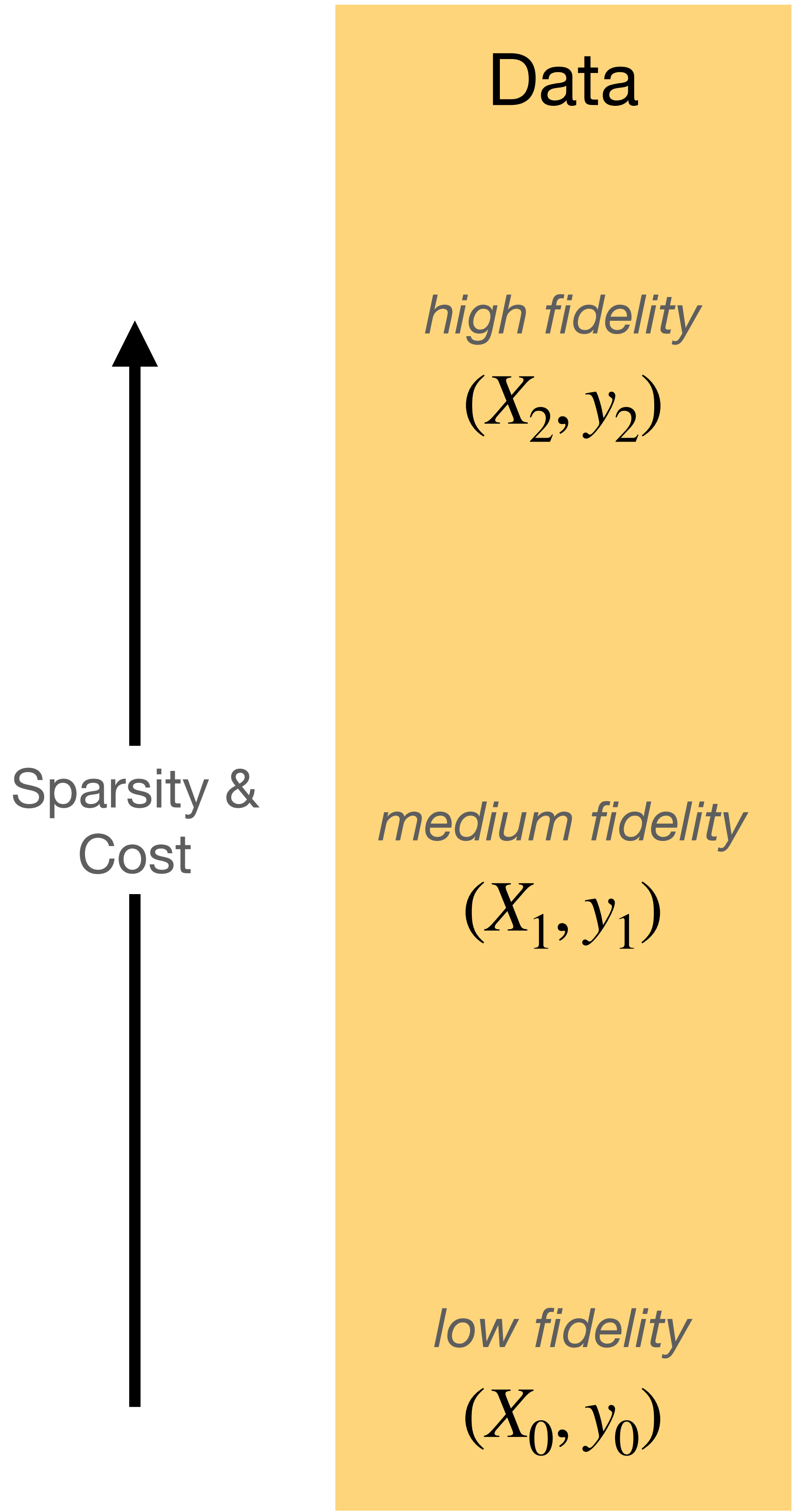
<u>Want to "learn" a surrogate conditional probability distribution, given all data sources</u>



- $p(y\,|\,x)$ defines the "probability of outcome y given x"
- surrogate model is "stochastic" but not "random"

Multifidelity Gaussian Process Regression

- Multiple sources of data of increasing fidelity
  - Increasing CFD mesh resolutions
  - Heat flux correlations and 3D CFD solutions
  - CFD solutions and wind tunnel data



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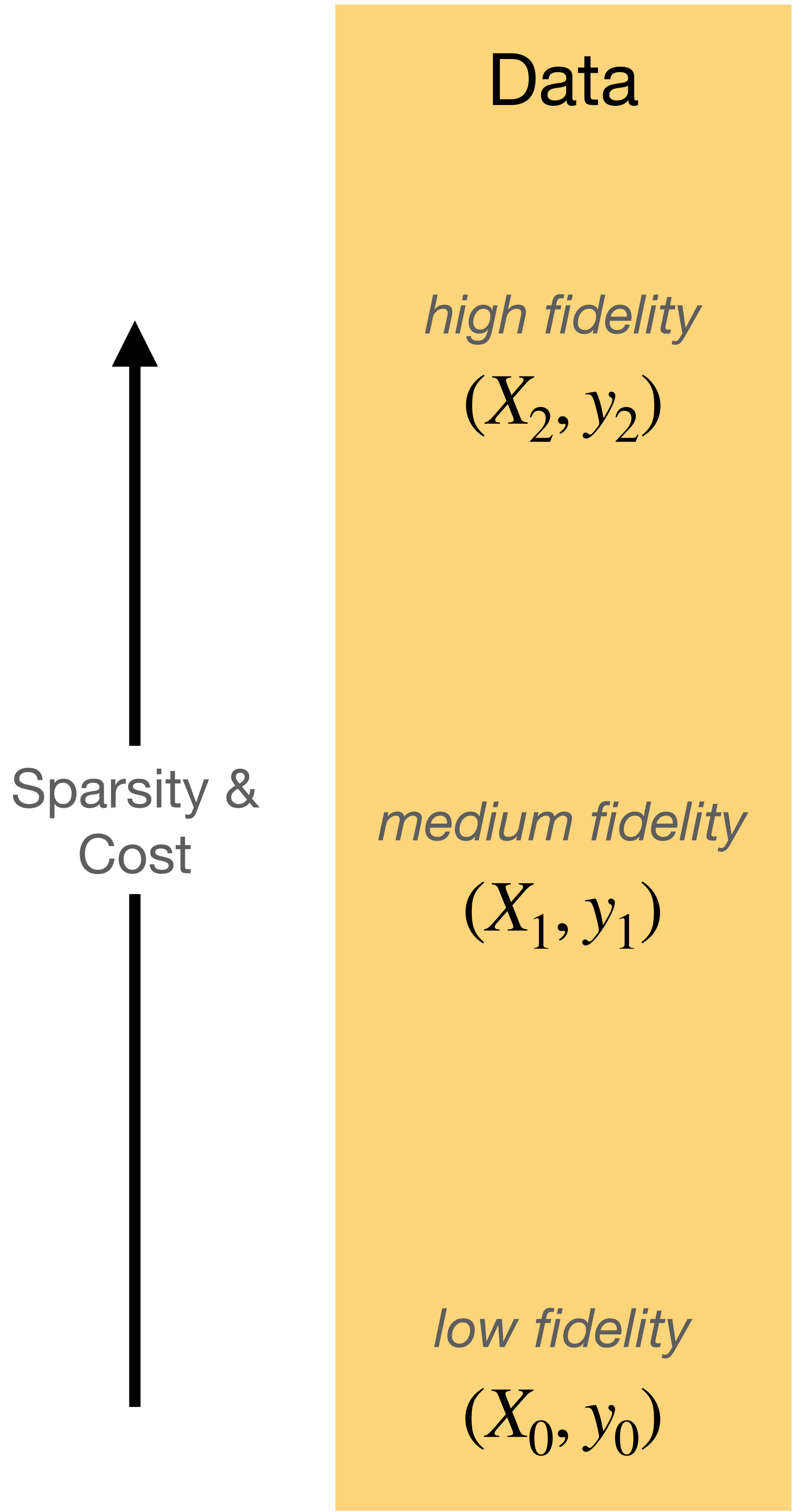

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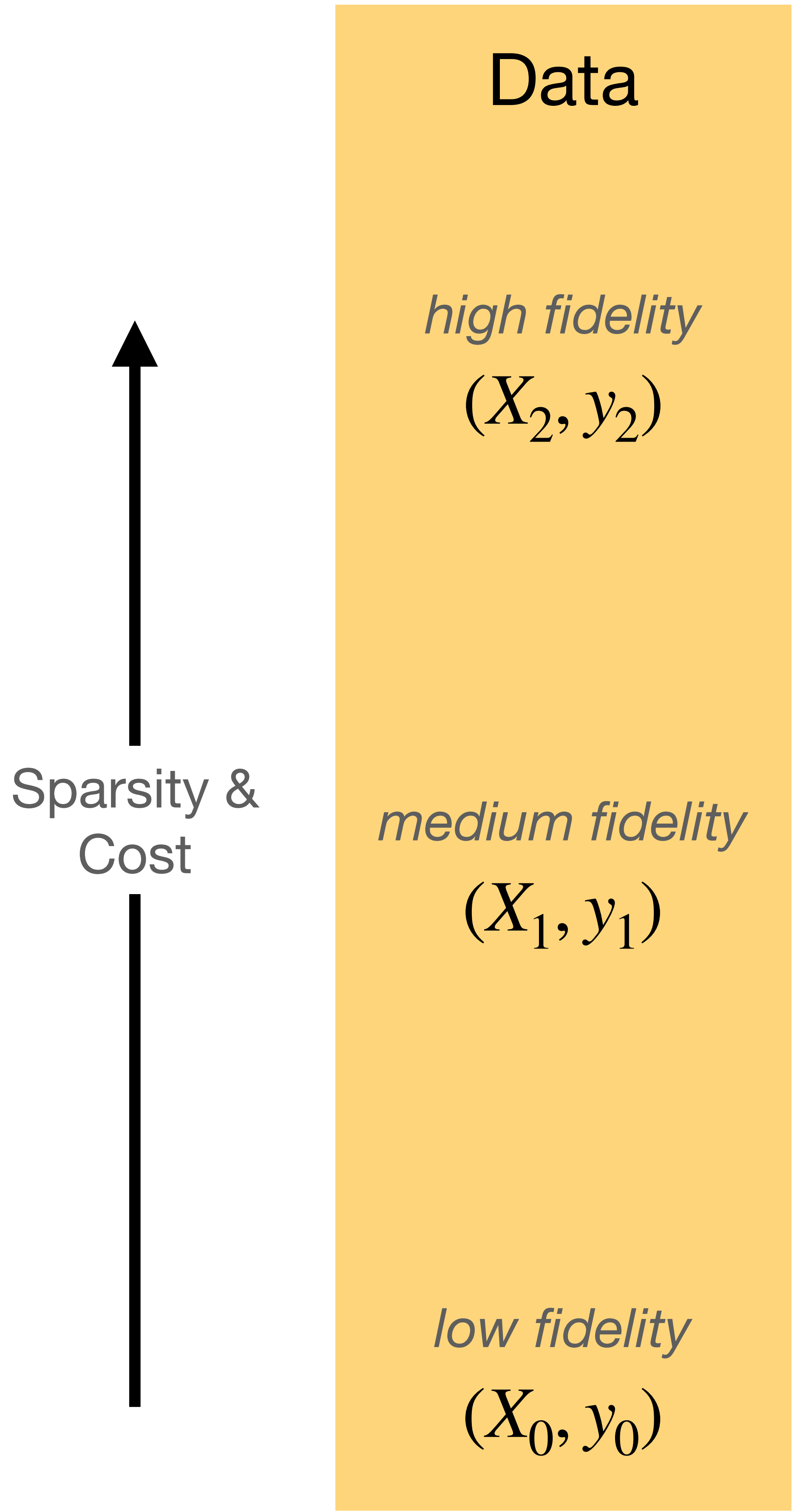

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$$f_k(x) = \rho_k f_{k-1}(x) + \delta_k(x)$$

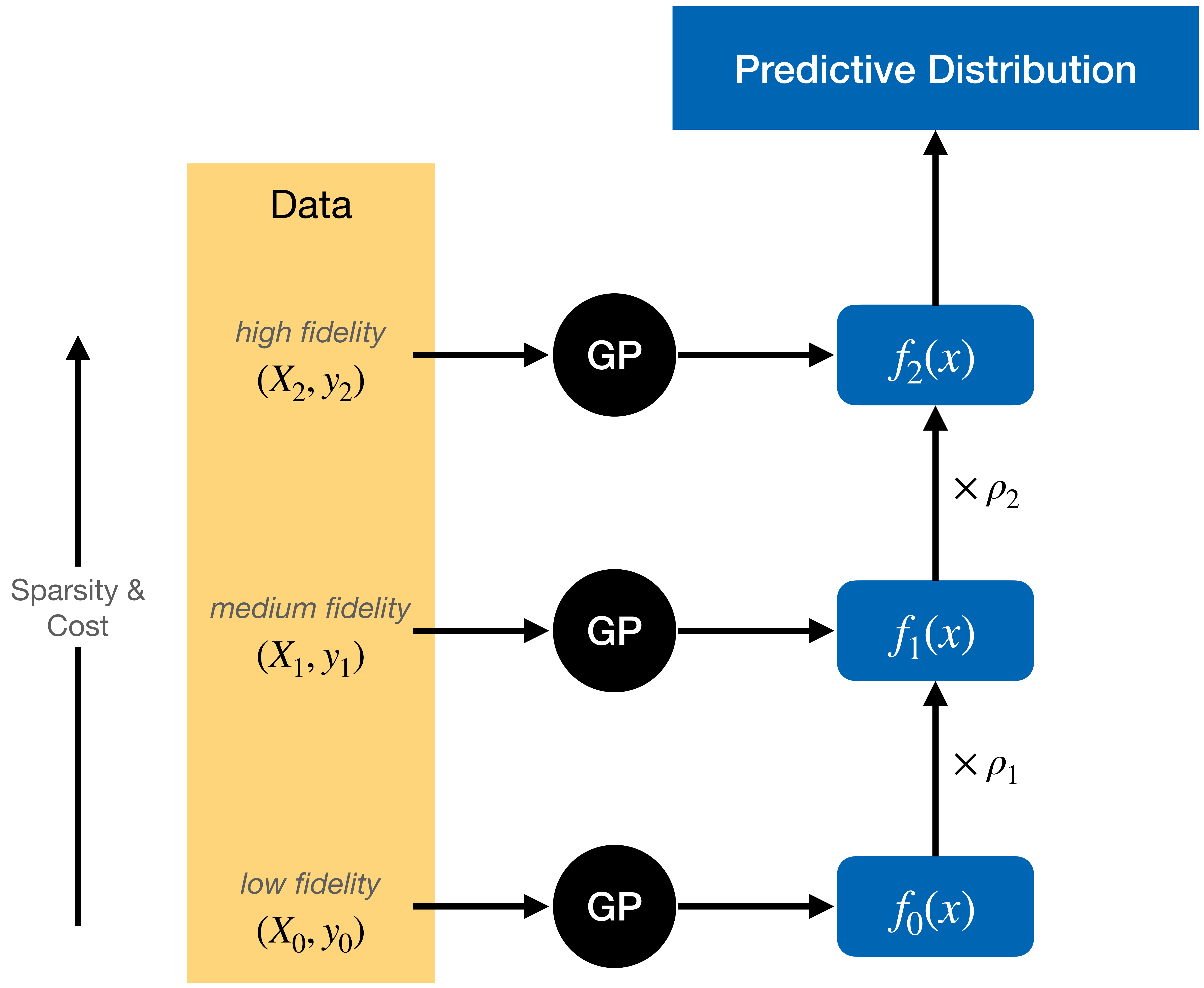

Diagram of the AR1 multifidelity GP model.

[1] Kennedy and O'Hagan. *Biometrika* 87:1-13, 2000.

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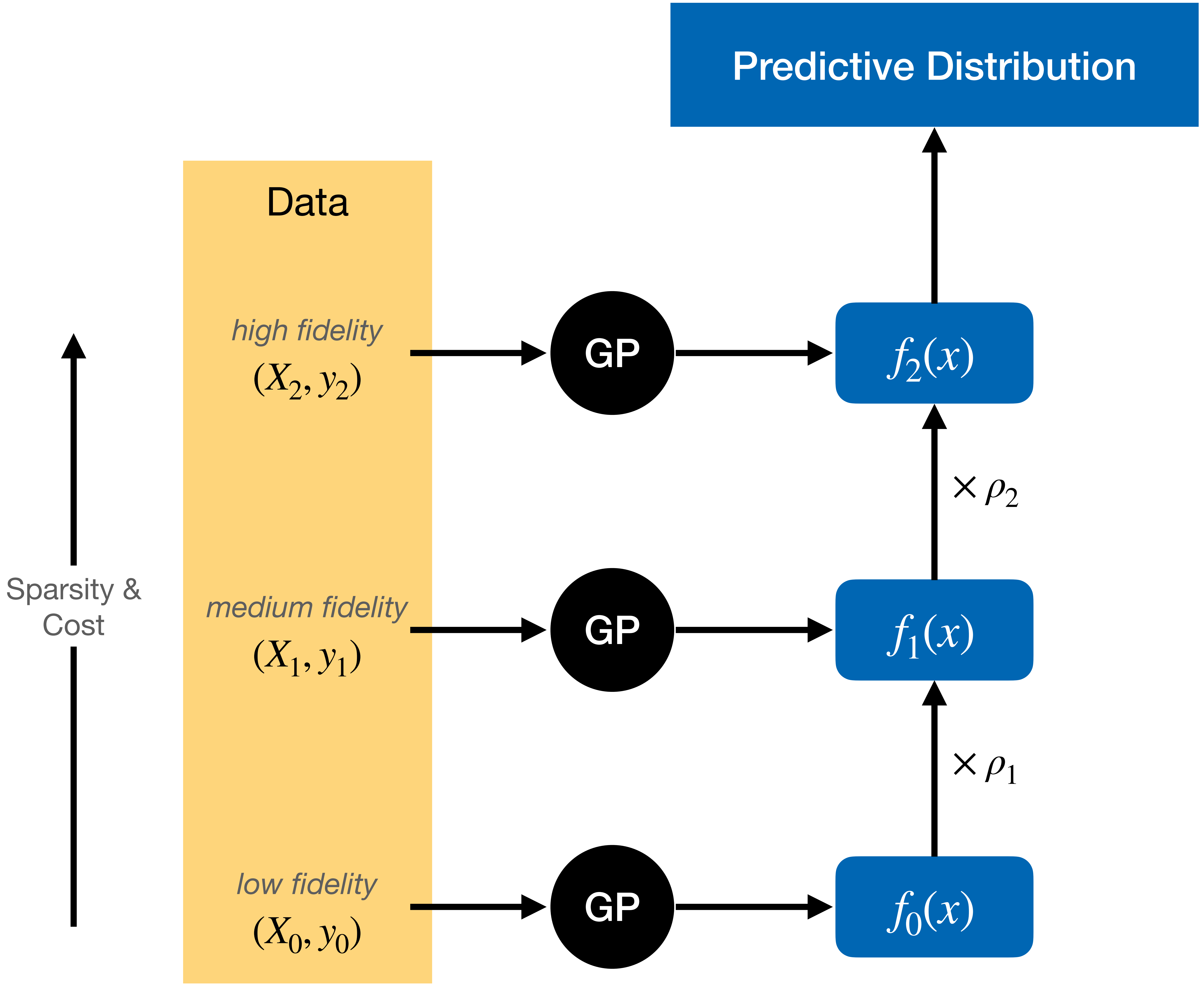
- **Requires an obvious hierarchy of fidelity levels!**



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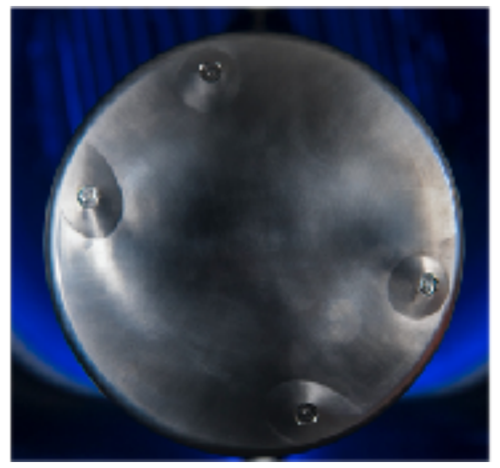
Multihierarchy Gaussian Process Regression

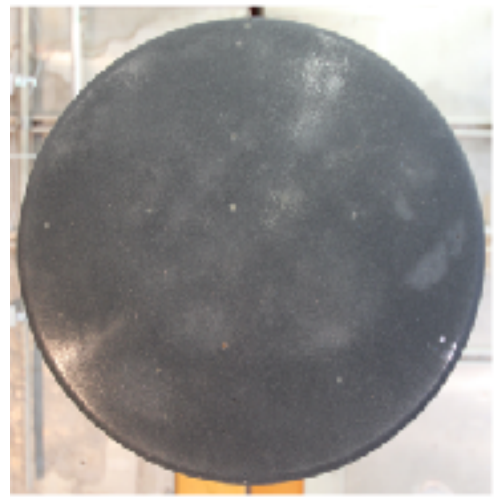
- Real world data typically cannot be organized into hierarchy of fidelity levels with single "truth"
- Easier to categorize "nominal" and "off-nominal" data

Orion heatshield models used in 133-CA test campaign in the National Transonic Facility

Asymmetric, Smooth



Symmetric, Rough



Symmetric, Smooth

Data

+ second effect

(X_2, y_2)

+ first effect

(X_1, y_1)

nominal

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Predictive Distribution

$$f(x) = f_0(x) + w_1 \Delta f_1(x) + w_2 \Delta f_2(x)$$

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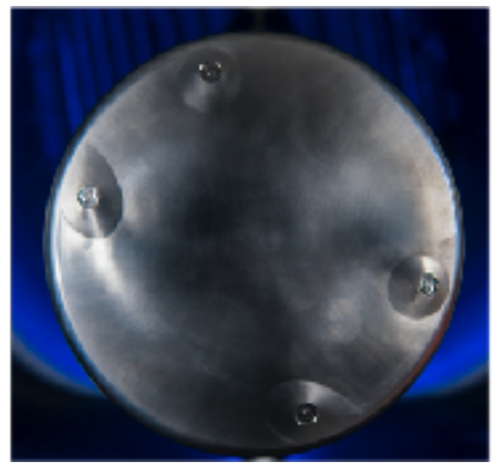

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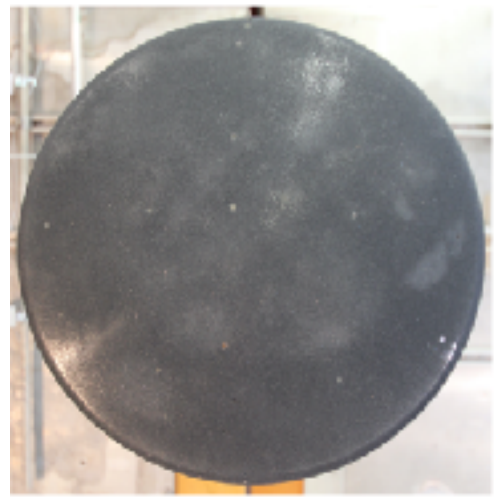

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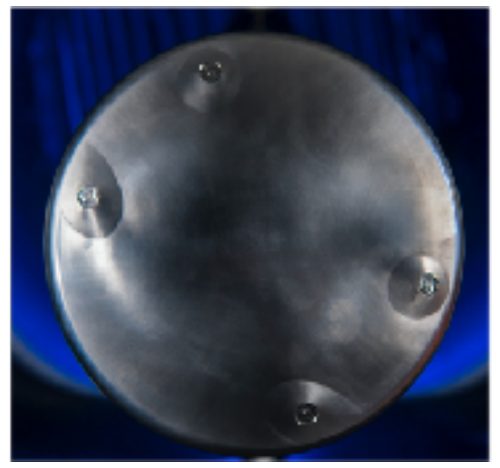

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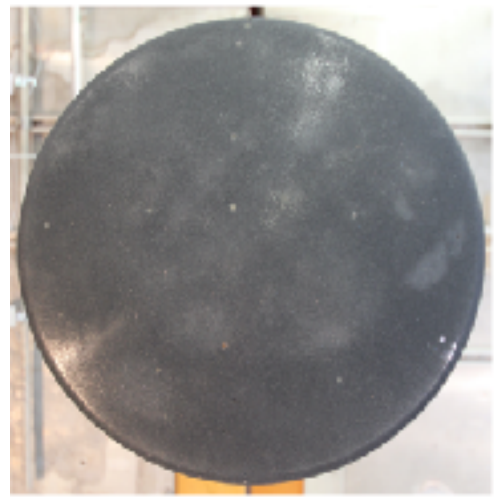

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GP

$f_0(x)$

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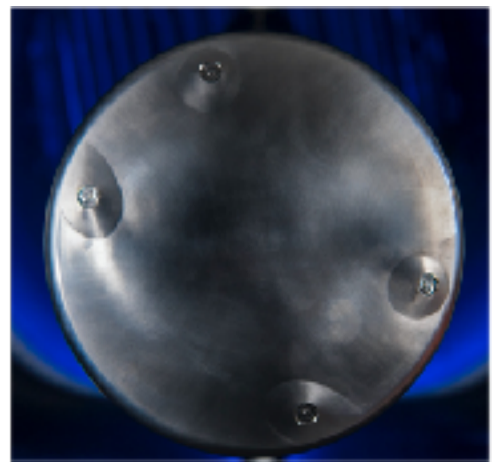

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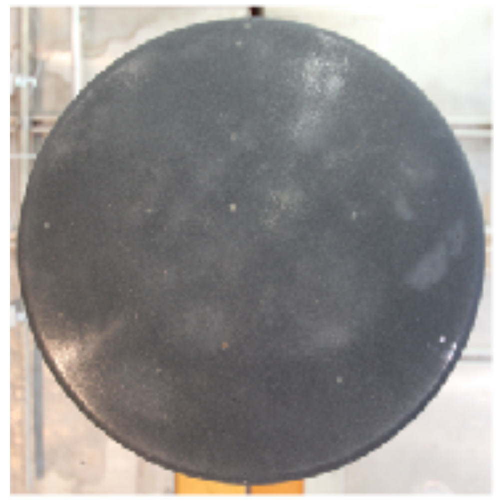

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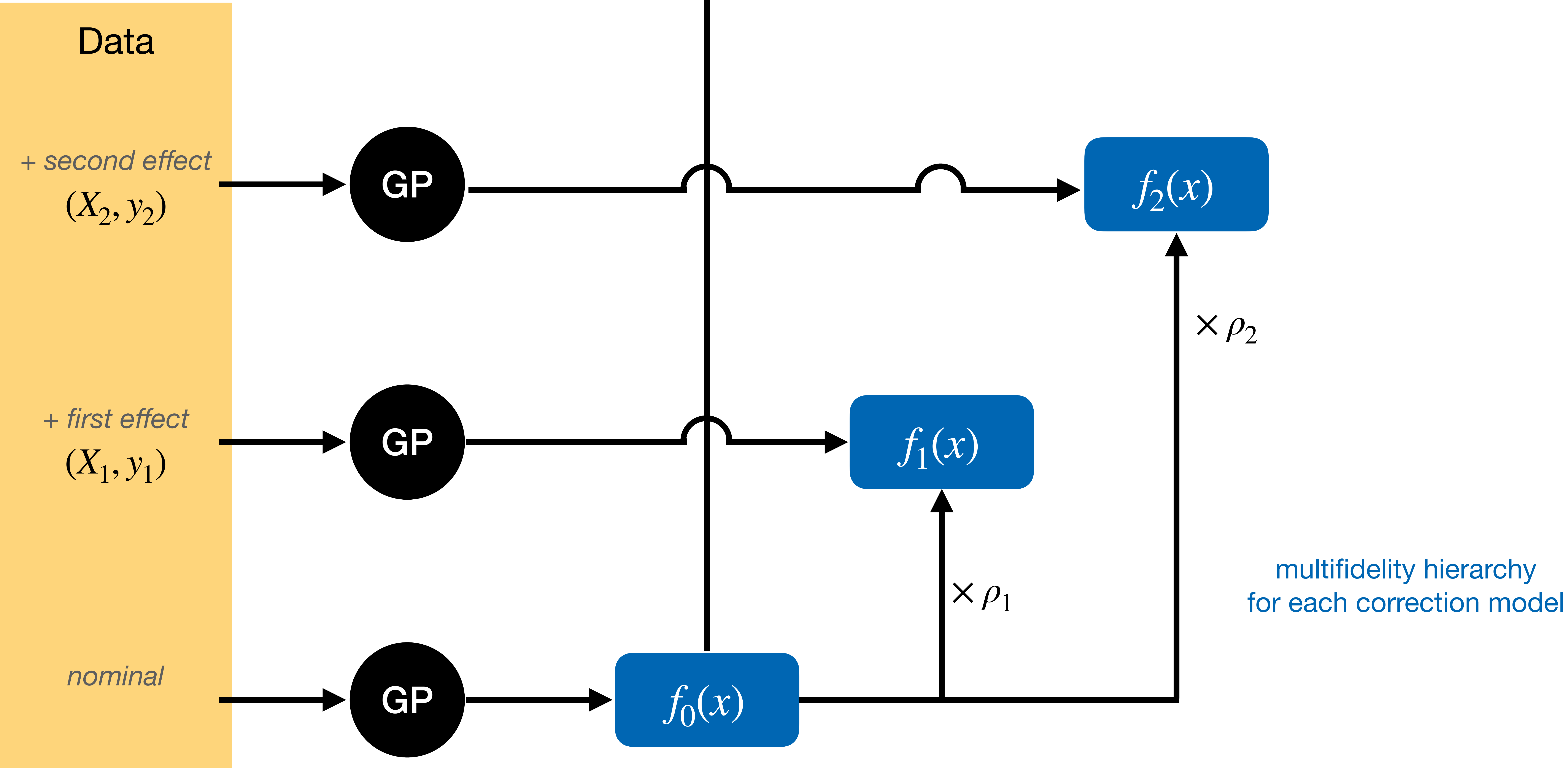

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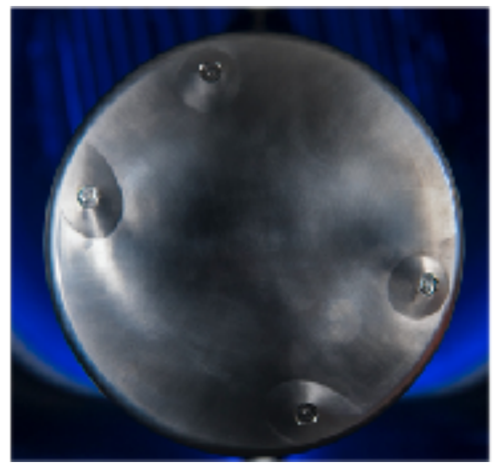

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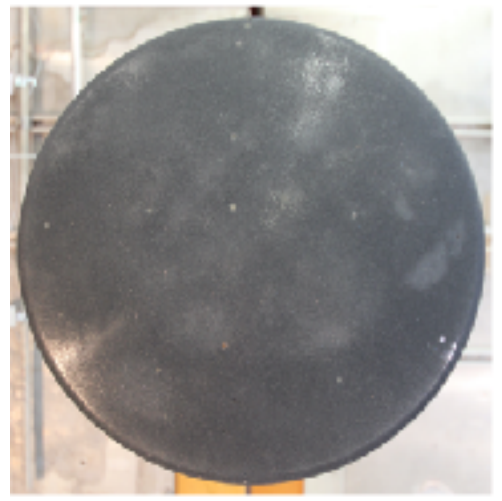

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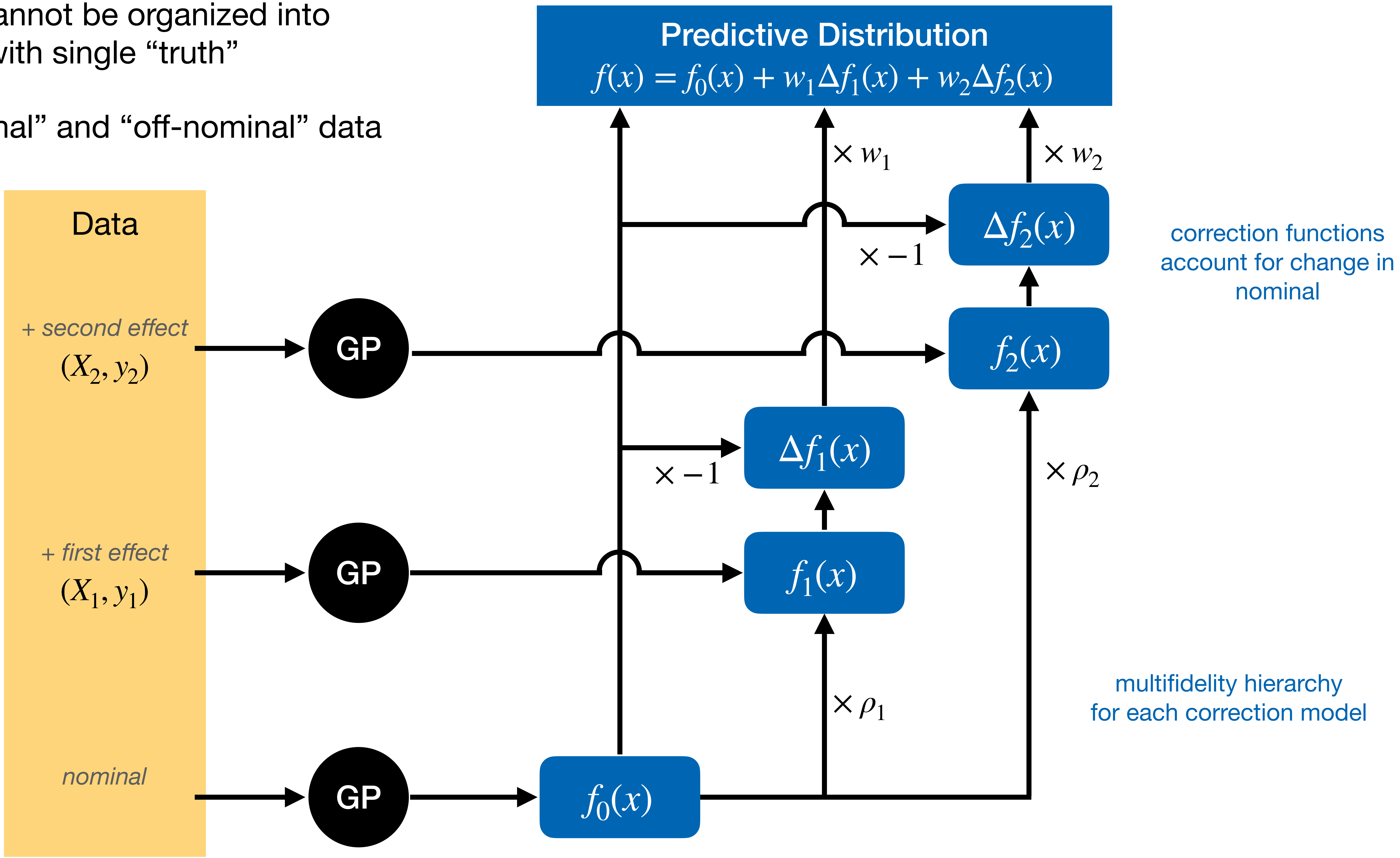

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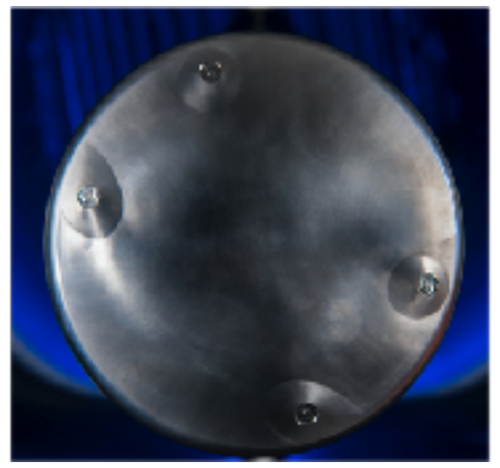

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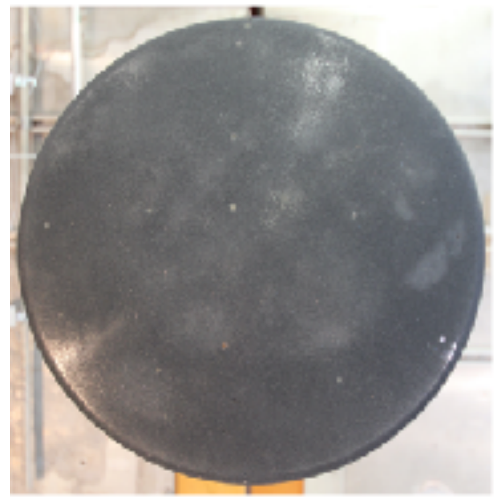

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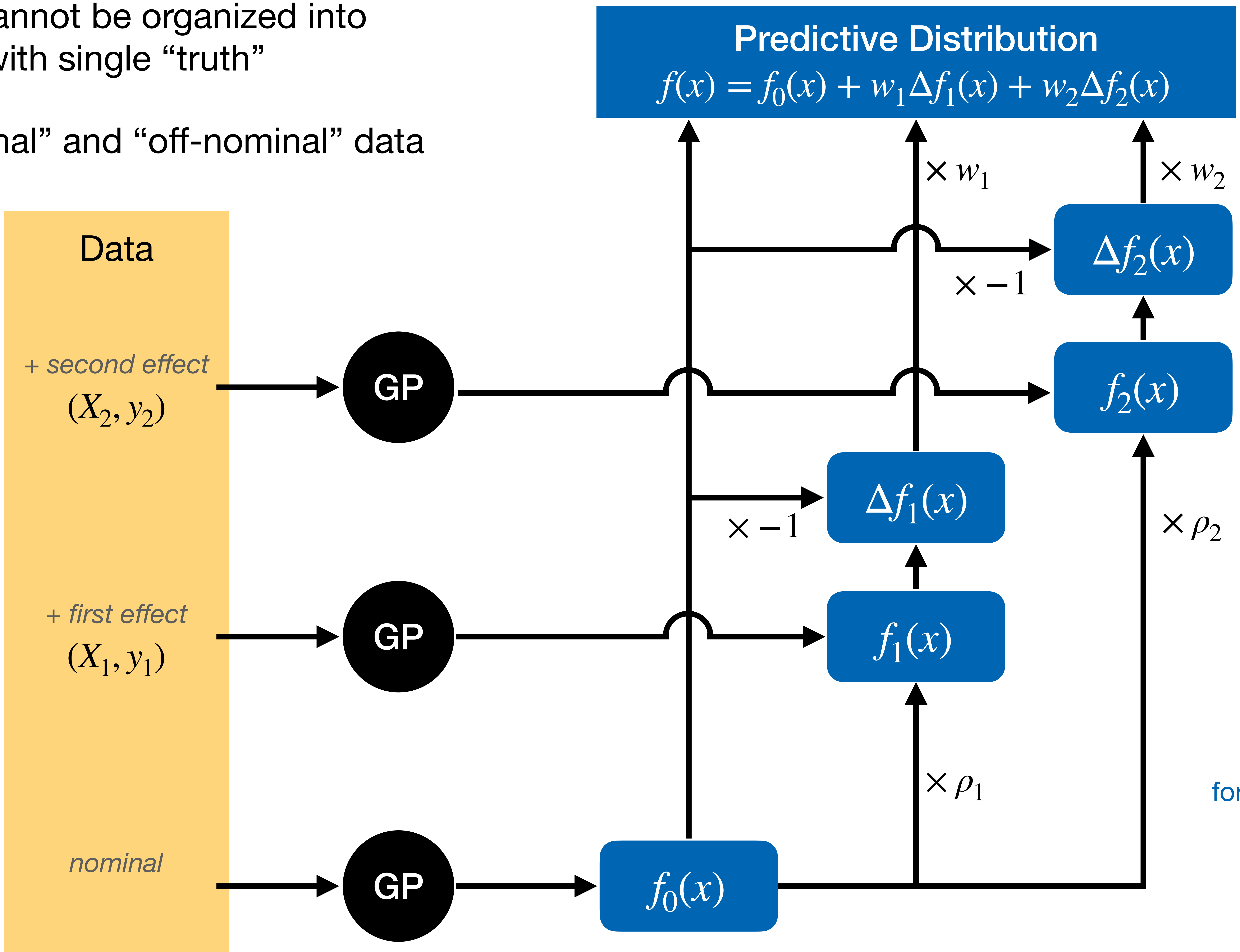


no assumed truth!
weight parameters learned from flight data or estimated from previous vehicles

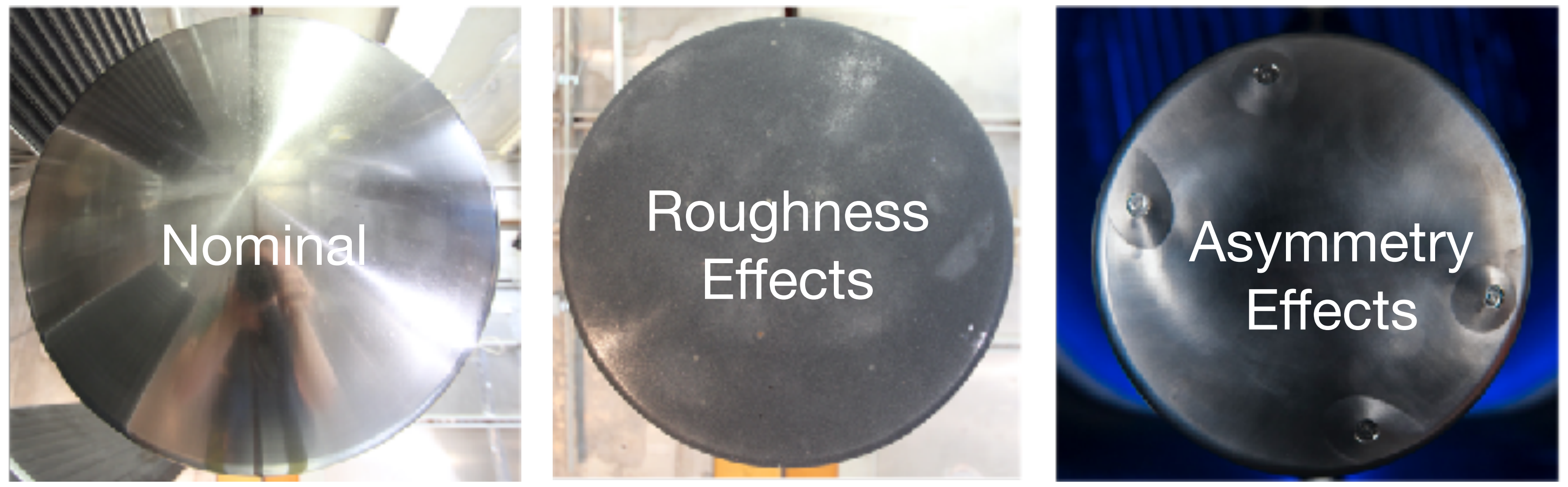
correction functions account for change in nominal

multifidelity hierarchy for each correction model

Example Orion NTF data

- All reported results based on Orion 133-CA test campaign performed in the National Transonic Facility at NASA LaRC [1]

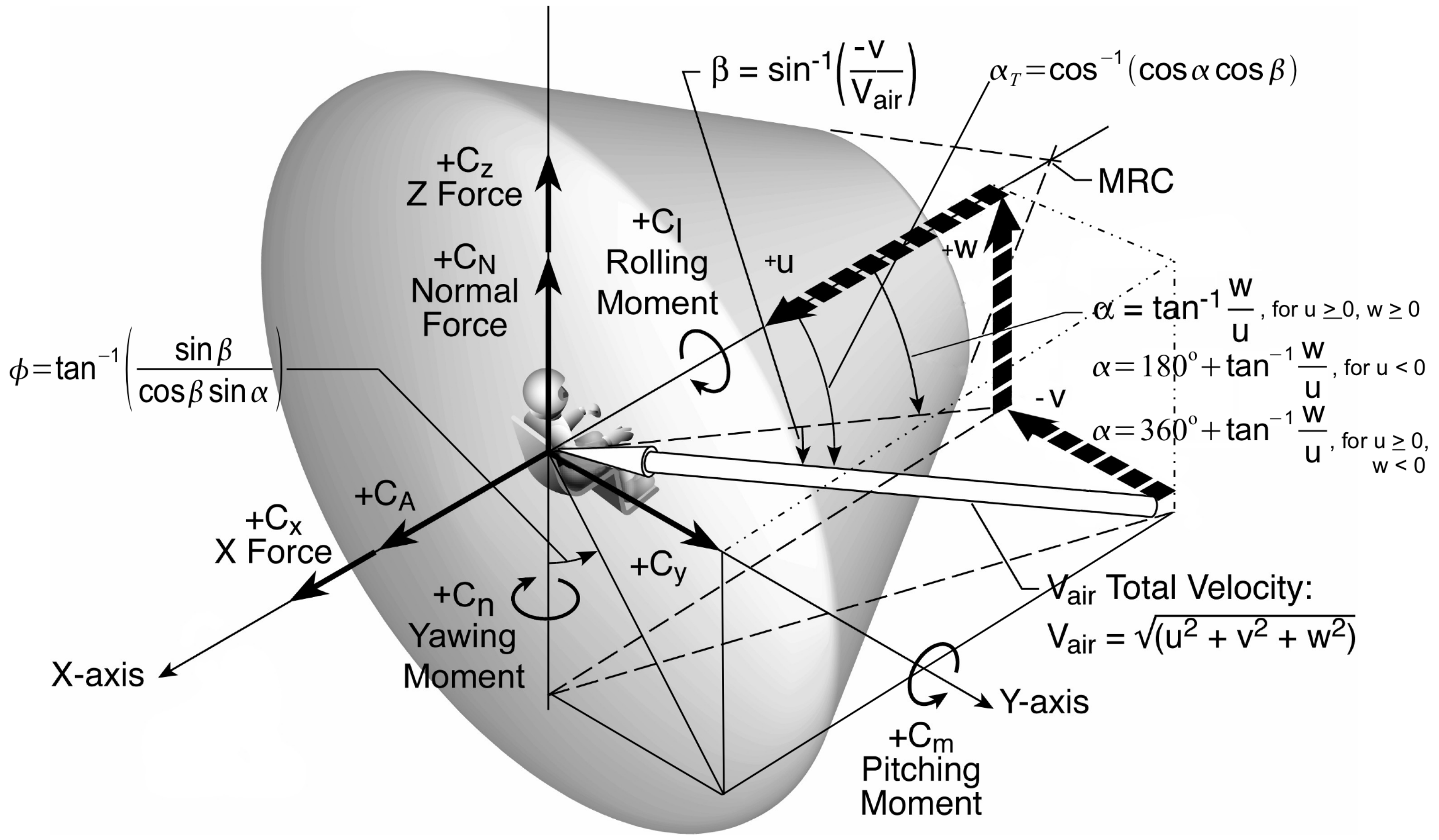
Train



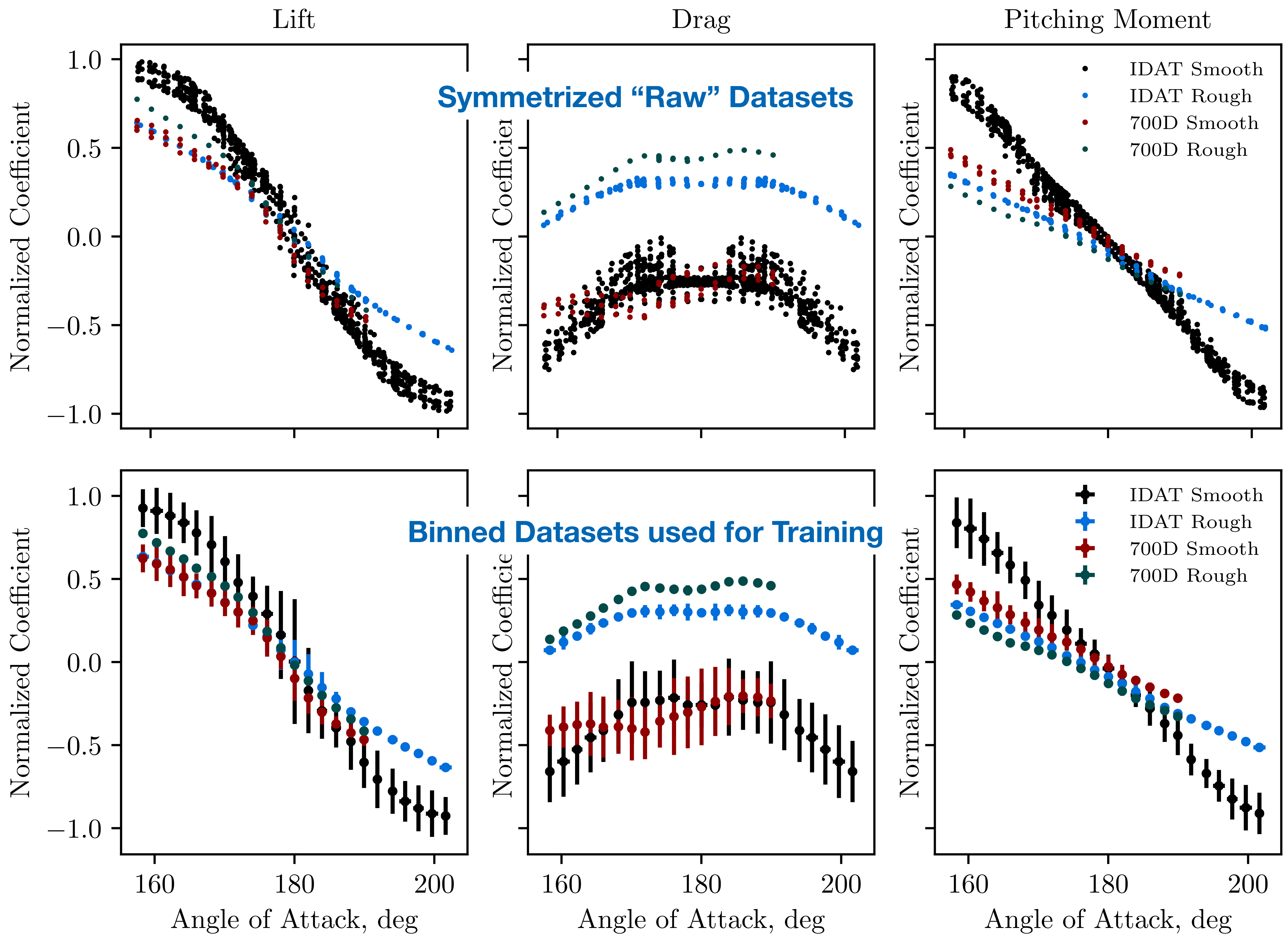
IDAT Smooth | IDAT 240 Grit | 700D Smooth

700D Fenced + 240 Grit

Test



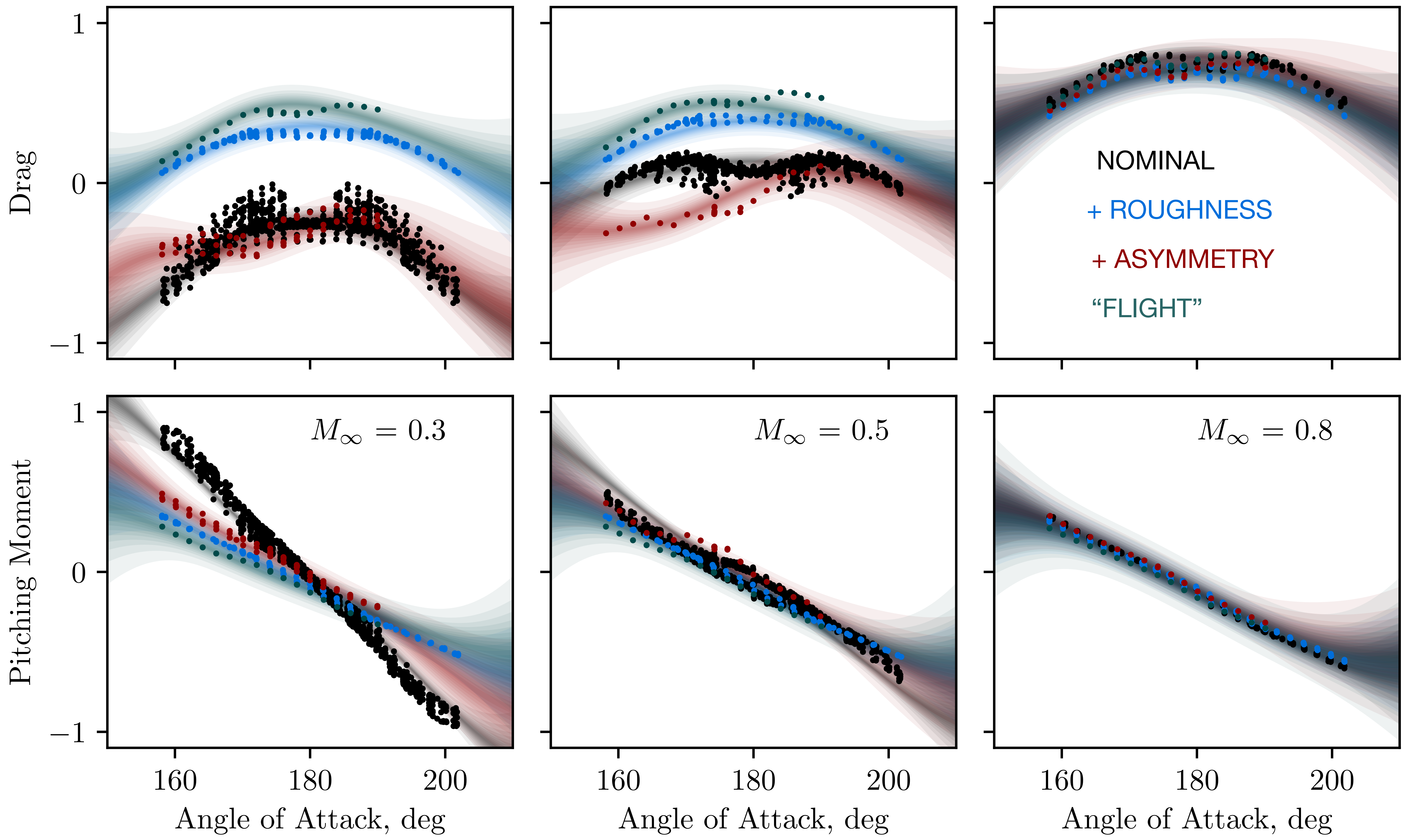
Orion "IDAT" Geometry with coordinates, forces, and moments.



Slices of data around Mach 0.3 and Reynolds 7.5x10⁶.

[1] Brauckmann. *CAP WTT Report EG-CAP-12-65*, NASA LaRC, 2022 (under preparation).

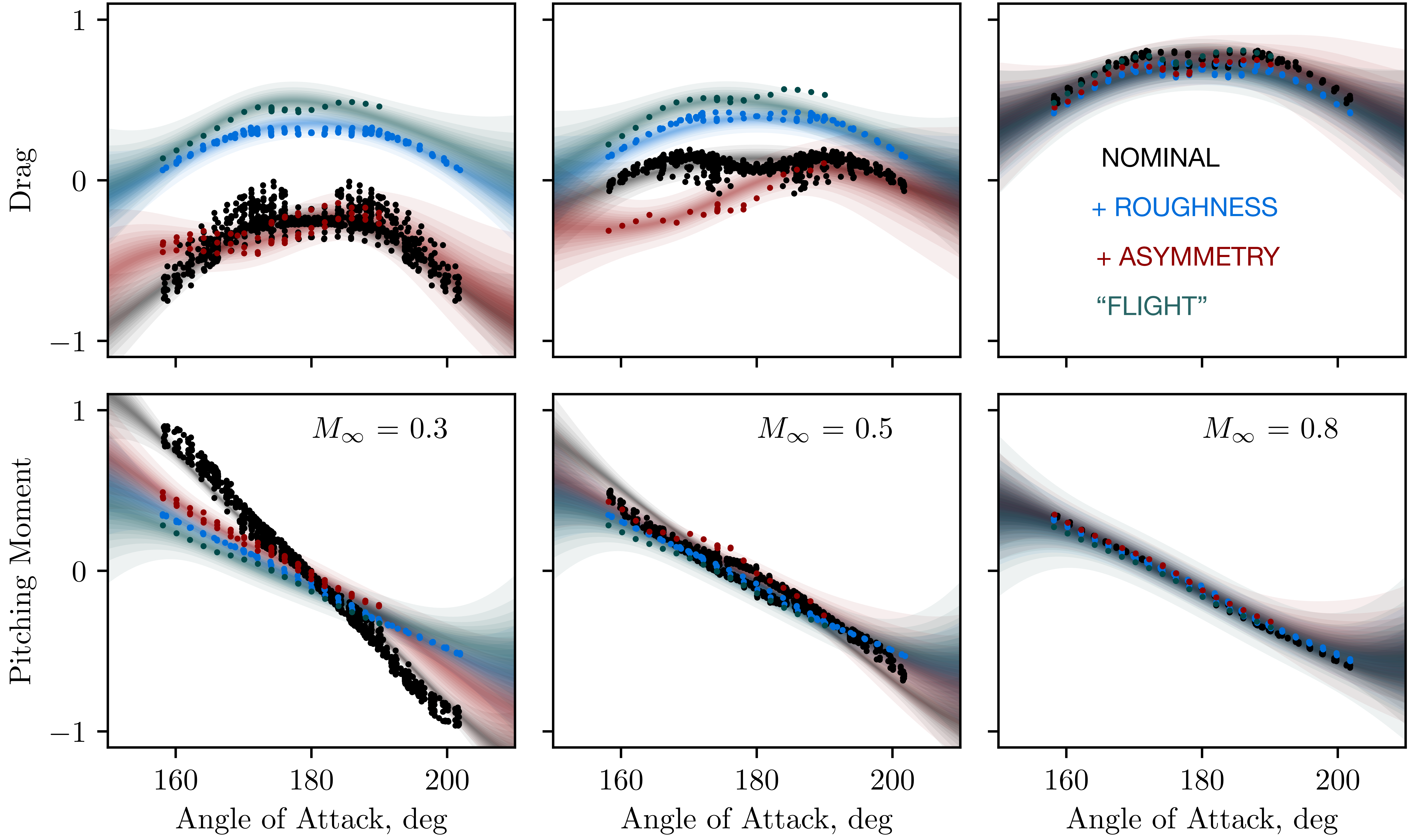
Model distributions compared to data



Normalized aerodynamic coefficient function distributions at 3 Mach numbers and Reynolds 7.5x10^6.

Model distributions compared to data

excellent agreement with “noisy” data



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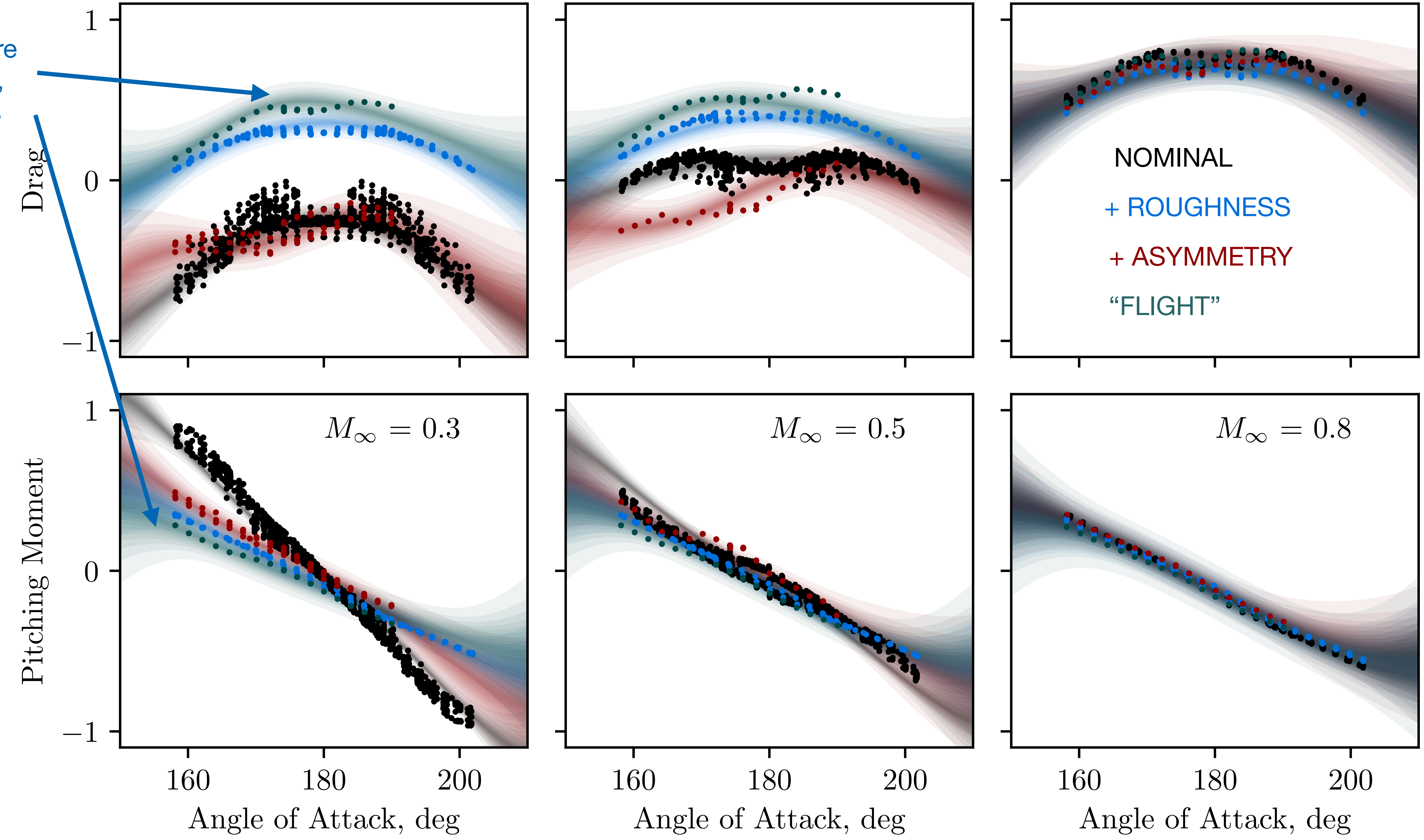

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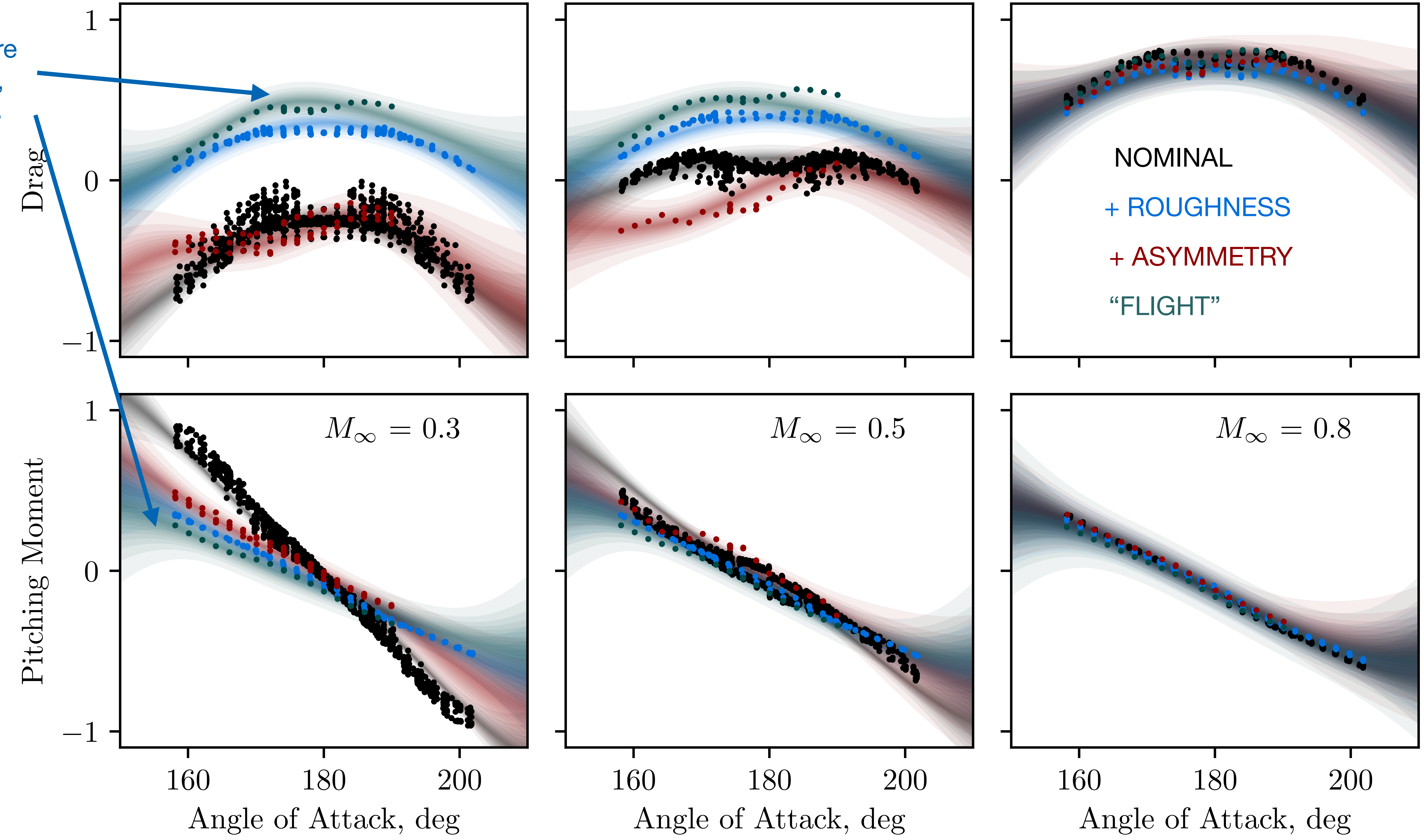
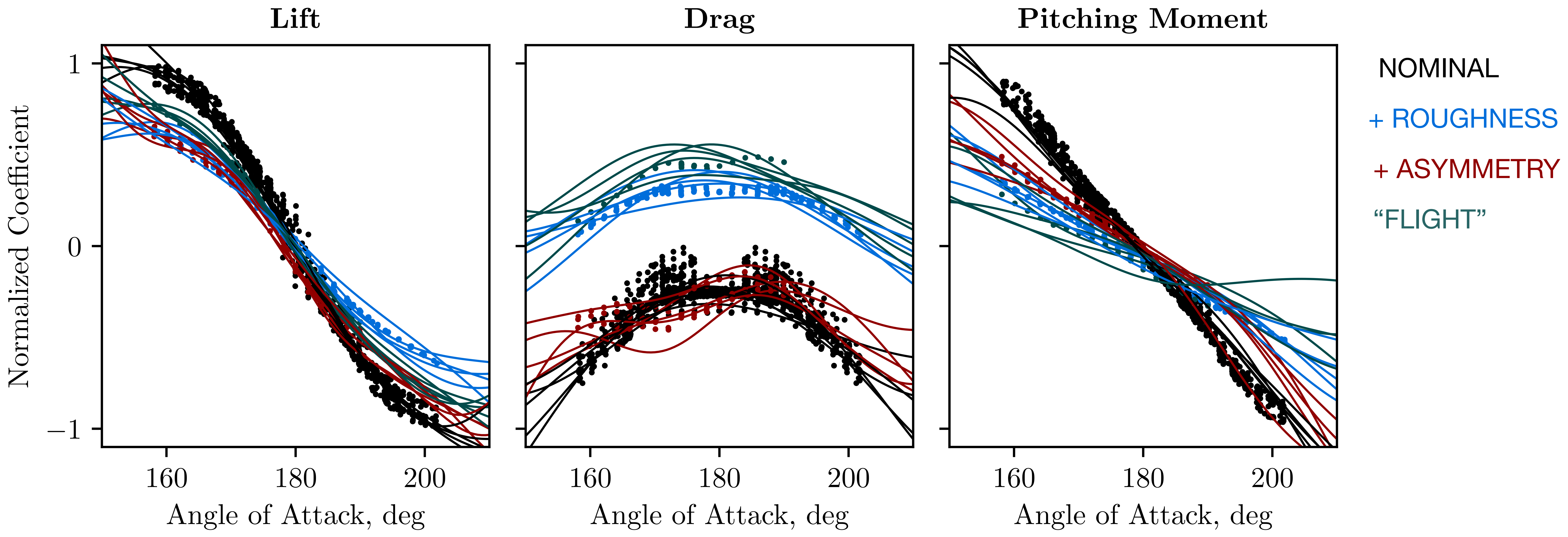


“out-of-distribution” uncertainty in regions of no data

Normalized aerodynamic coefficient function distributions at 3 Mach numbers and Reynolds 7.5x10⁶.

Function sampling from model distributions

- State-of-the-practice uses random dispersion offsets from the nominal for Monte Carlo trajectory simulations
- Proposed approach allows for function sampling that is more consistent with underlying conditional distribution
- **Each function is a plausible explanation of the data, reproduces conditional distribution in aggregate**



Aerodynamic coefficient function samples at Mach 0.5 and Reynolds 7.5x10^6.

Probability distributions for derived quantities

Model distributions can be used to obtain conditional distributions on derived quantities of interest

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- **Example:** trim angle of attack found using *Bayes' Theorem*

$$p(\alpha = \alpha_{\text{trim}}) = p(\alpha \,|\, C_{\text{m,cg}} = 0) \propto p(C_{\text{m,cg}} = 0 \,|\, \alpha)\; p(\alpha)$$

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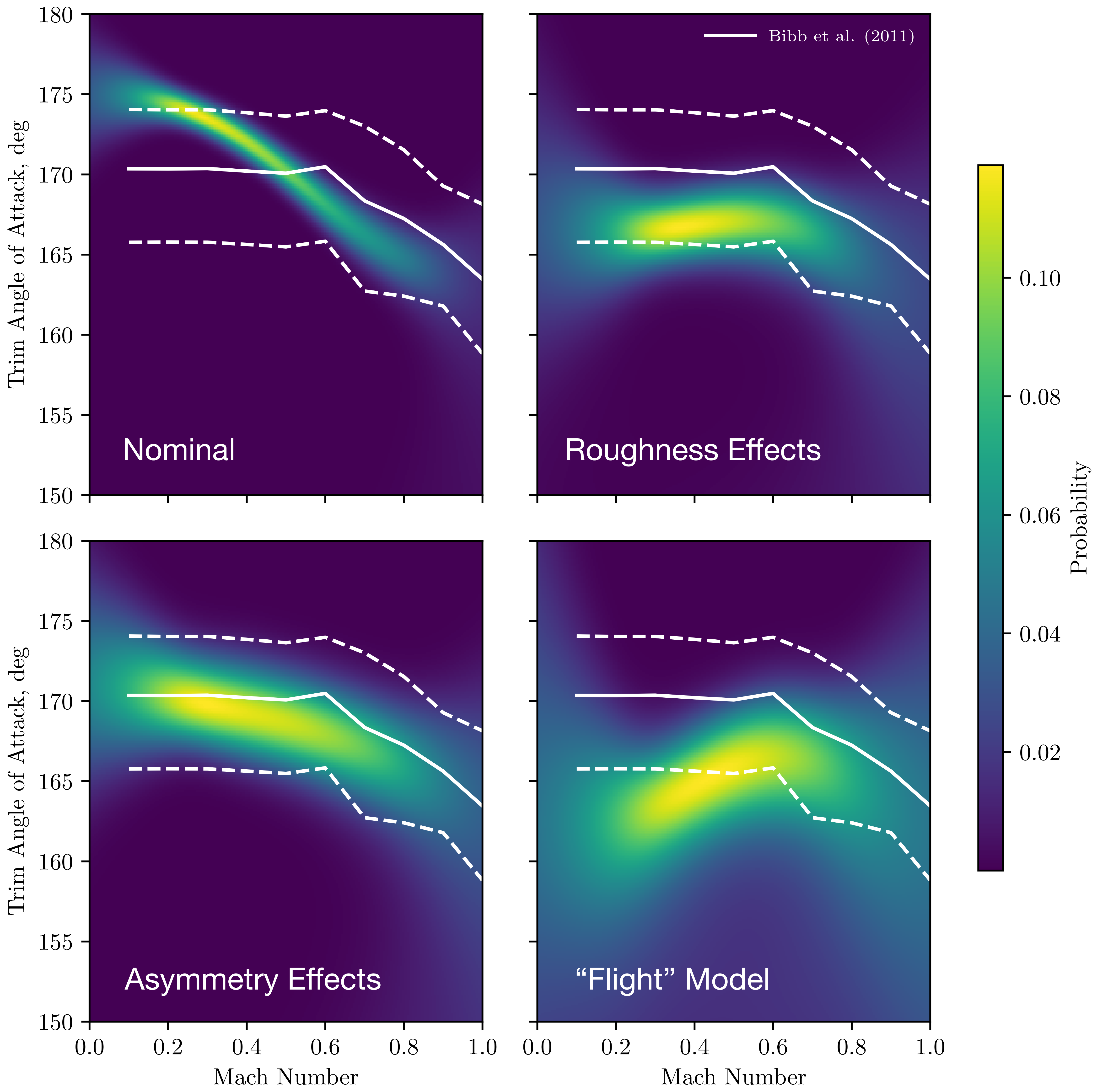

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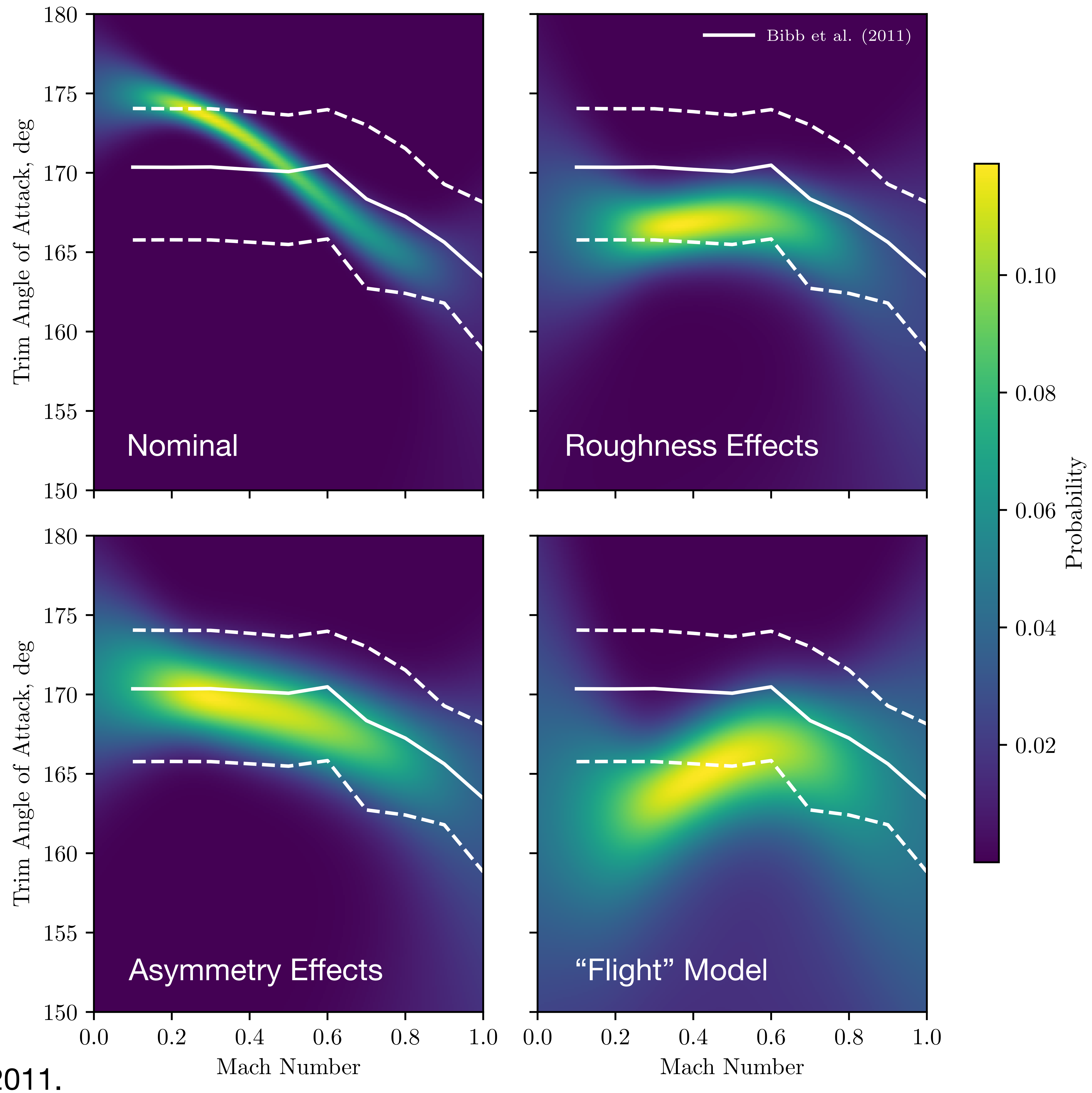
- Orion v0.60 DB nominal and 100% CI bounds [1] provided for comparison



[1] Bibb, Walker, Brauckmann, Robinson. *29th AIAA Applied Aero. Conf.,* No. 2011-3507, 2011.

Questions?

Where to find additional resources:

- **Books I recommend**
  - I. Goodfellow, Y. Bengio, A. Courville. *Deep Learning*. MIT Press, 2016. (www.deeplearningbook.org)
  - C.E. Rasmussen, C.K.I. Williams. *Gaussian Processes for Machine Learning*. MIT Press, 2006. (gaussianprocess.org/gpml)
  - S. Rogers, M. Girolami. *A First Course in Machine Learning, 2nd Ed.* CRC Press, 2017.
  - D.S. Sivia. *Data Analysis: A Bayesian Tutorial*. Oxford University Press, 2006.
  - R.B. Gramacy. *Surrogates: Gaussian Process Modeling, Design, and Optimization for the Applied Sciences*. CRC Press, 2020. (bobby.gramacy.com/surrogates)
- **Free online courses**
  - Stanford CS230: Deep Learning. Video lectures available at cs230.stanford.edu/lecture.
  - MIT 6.036: Introduction to Machine Learning. Course notes and lectures at openlearninglibrary.mit.edu/courses/course-v1:MITx+6.036+1T2019.
- **Python packages**: scikit-learn, Pytorch, Tensorflow, JAX, GPy, …

Backup

Physics Informed Neural Networks

- Networks are trained with/without data, but regularized using physical laws
- Loss function constructed from data term and residuals of governing equations
- Boundary conditions treated like data (constrained) or enforced by construction (unconstrained) of the neural network

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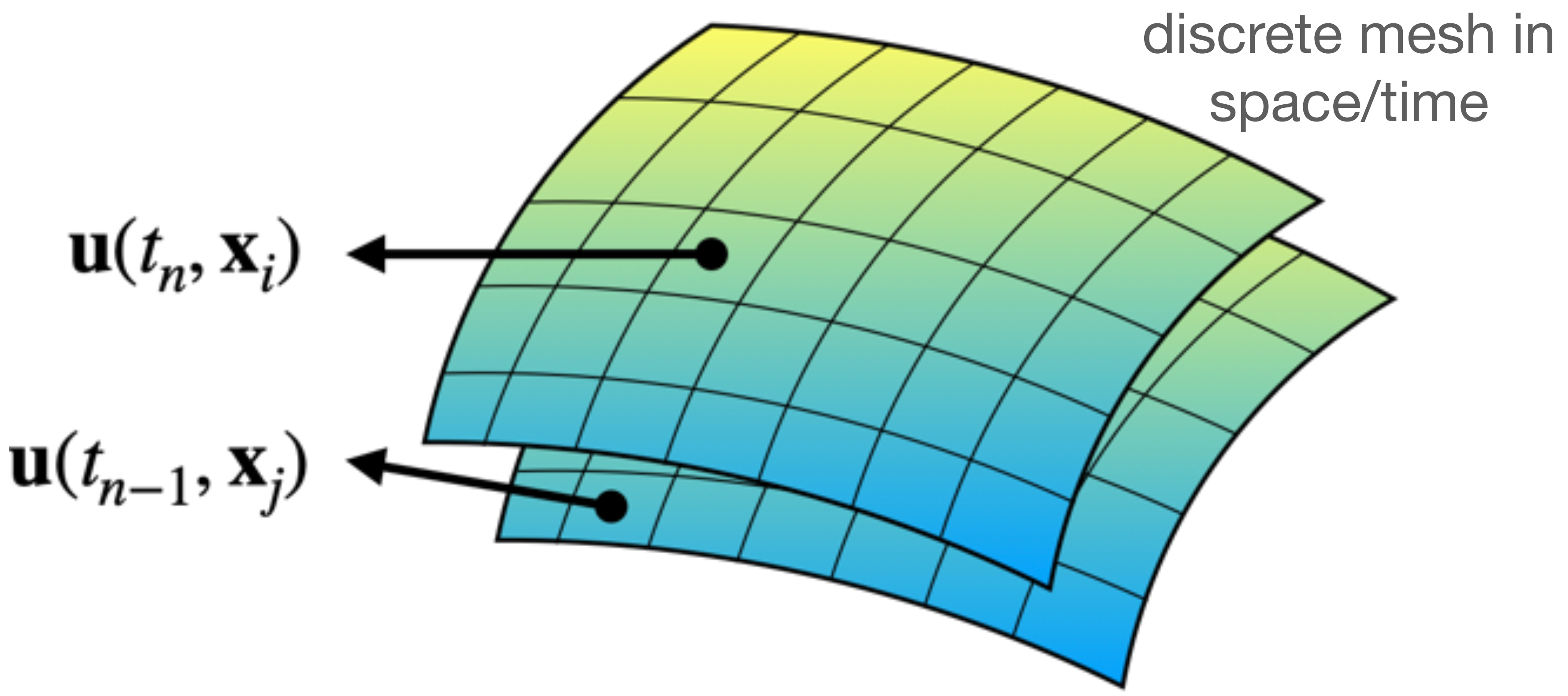
Conventional Discretization Approaches (CFD)



- Space discretization leads to large system of ODEs
- Solution defined and dependent on mesh discretization
- Solution satisfies system of PDEs in a weak sense
- Rigorous theory for convergence and stability

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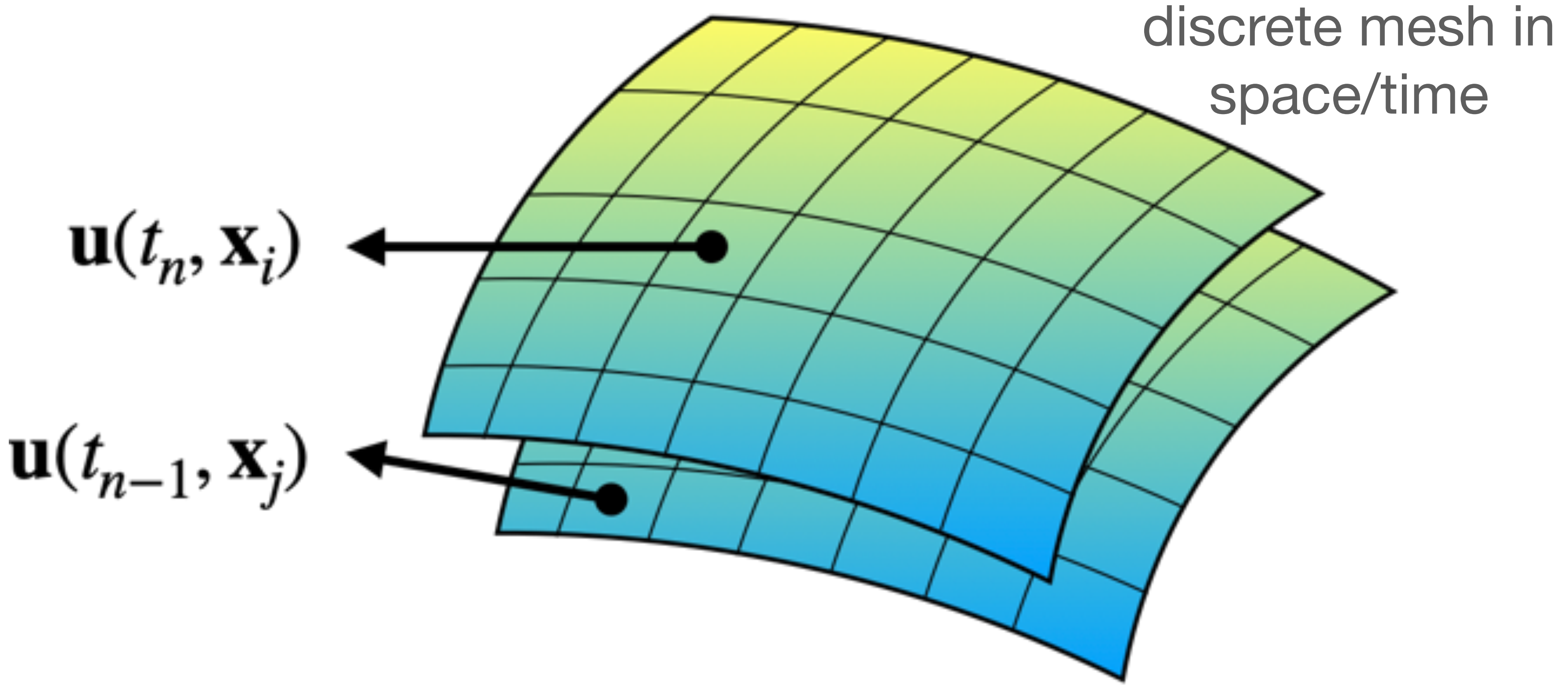

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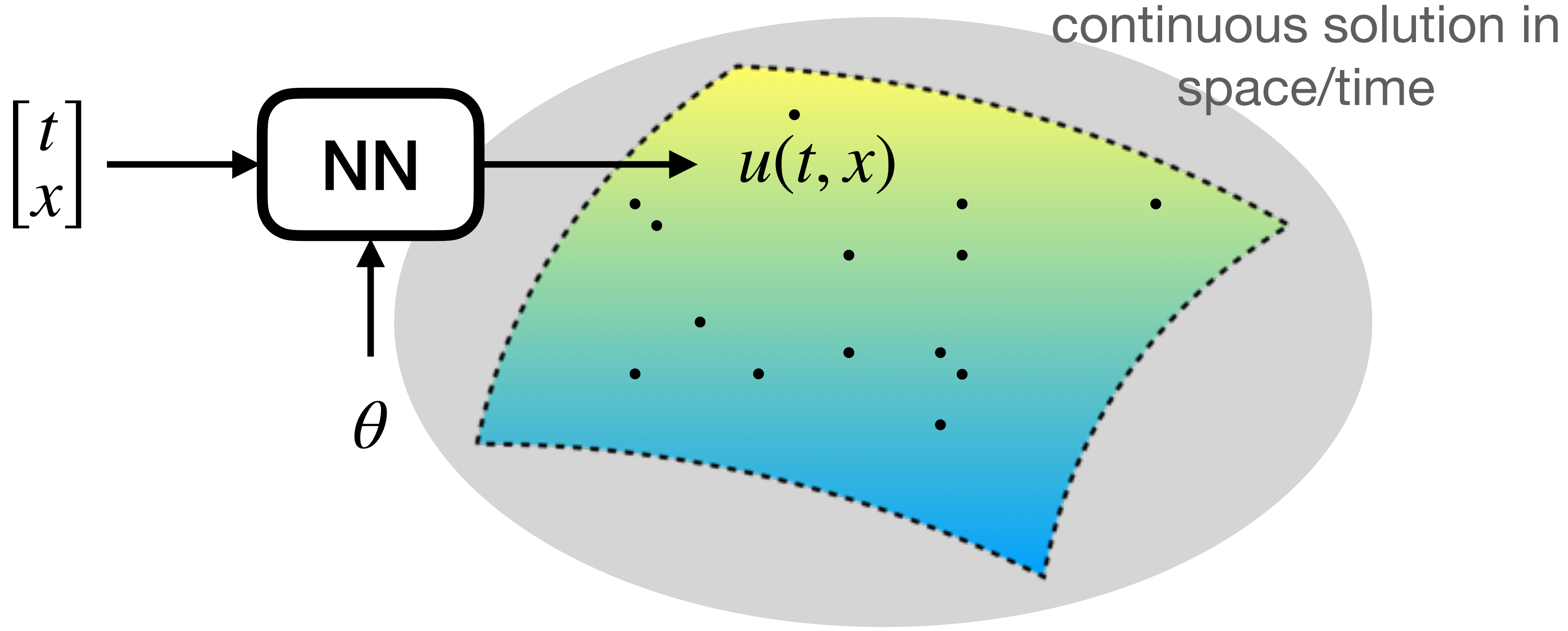
Deep-Learning Approach

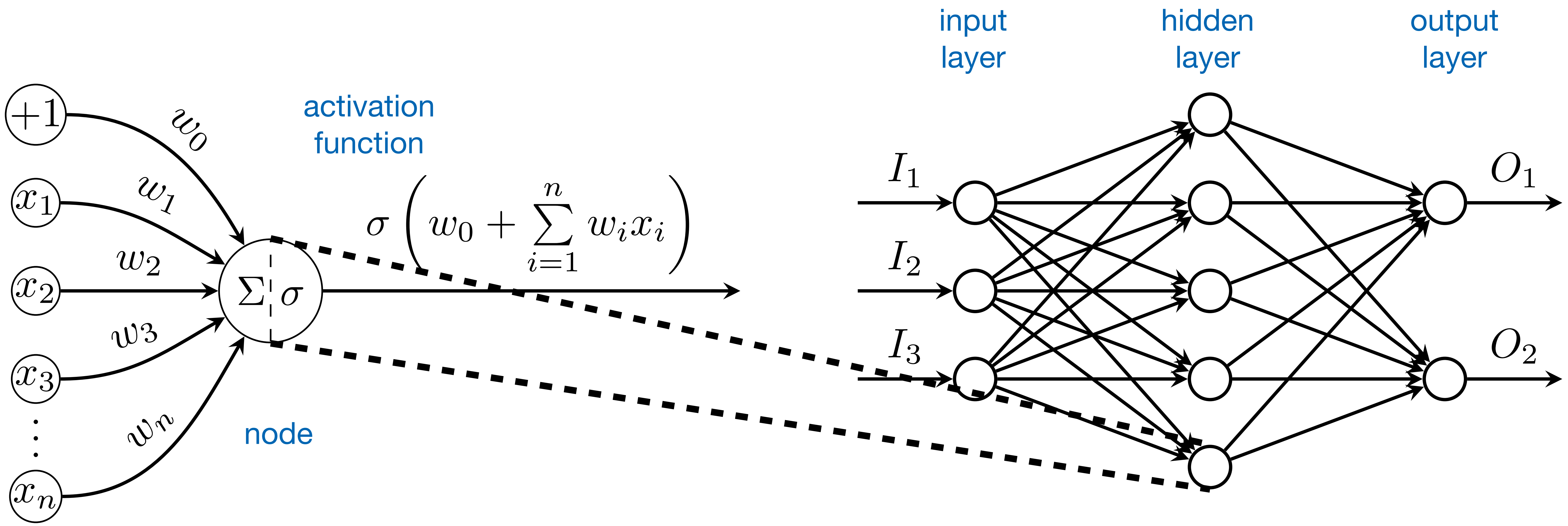


- PDEs converted into large optimization problem on params.
- Solution dependent on training points, defined everywhere
- Solution satisfies system of PDEs in a continuous sense
- Convergence and stability are active fields of research

What's a Neural Network?

- Nothing more than a function mapping an input space to an output space via a series of linear/nonlinear transformations

Conceptional View



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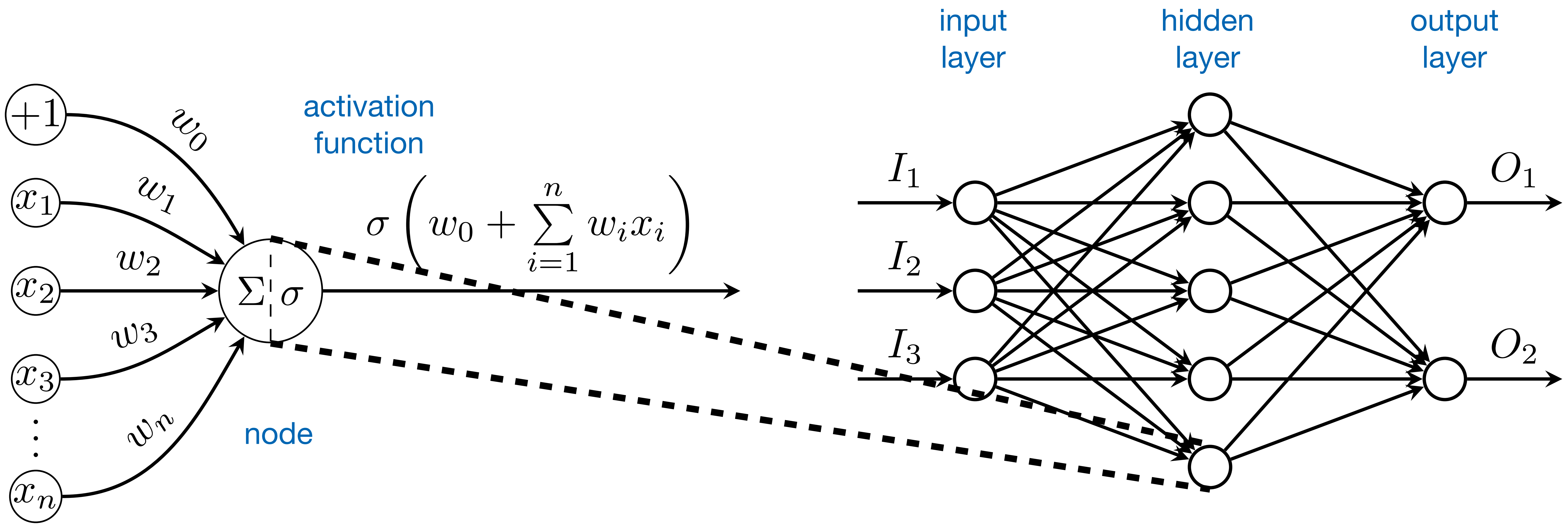
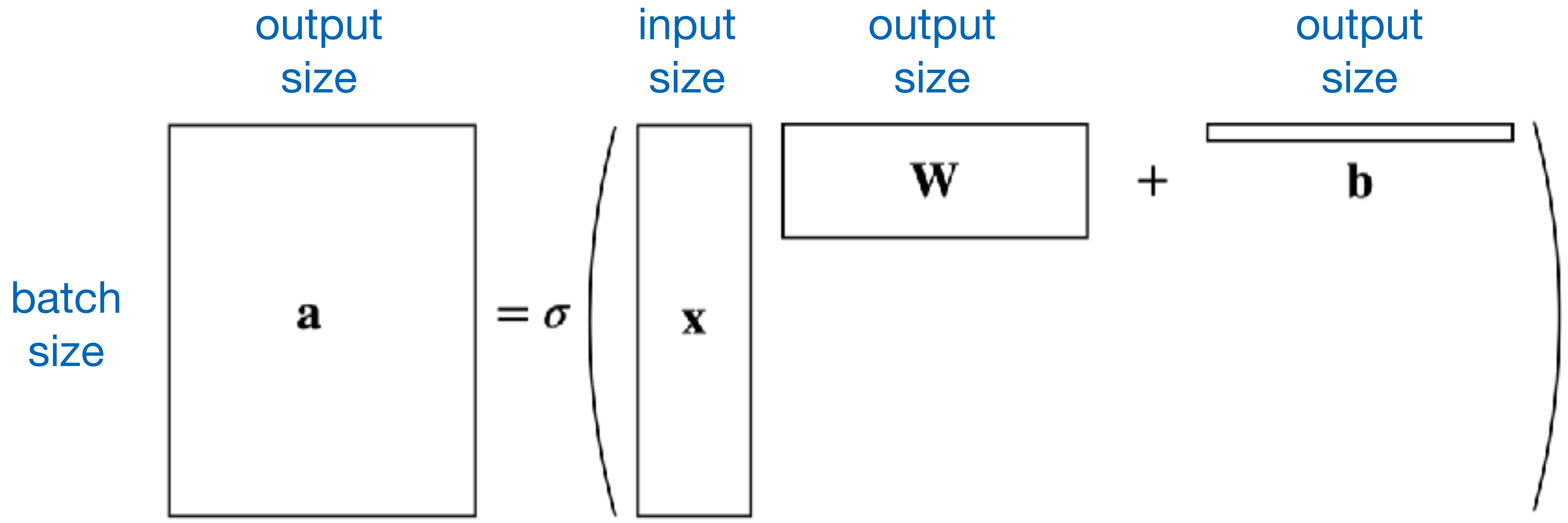


Practical Layerwise Implementation



But seriously, how do we learn equations?

1. **Consider the general PDE:**

$$\mathfrak{F}[u](x) = 0, \quad x \in \Omega$$
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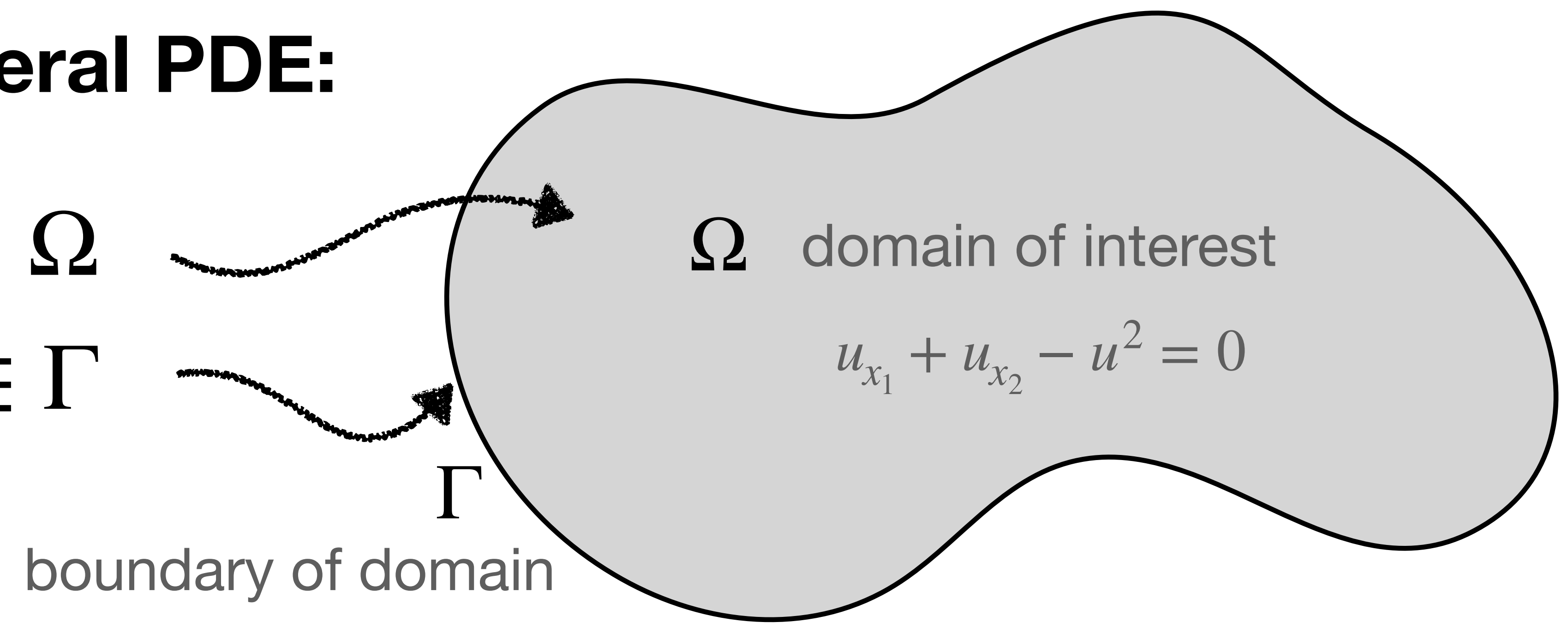

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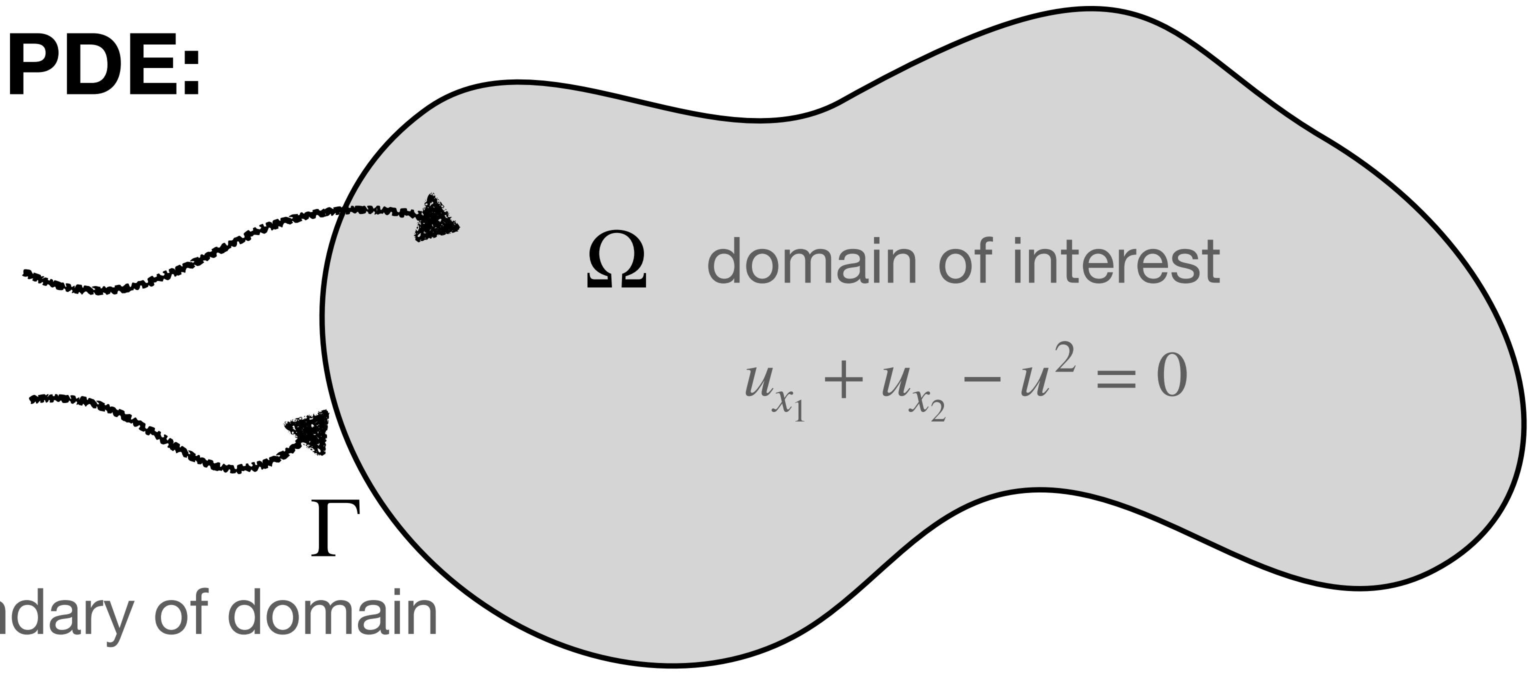

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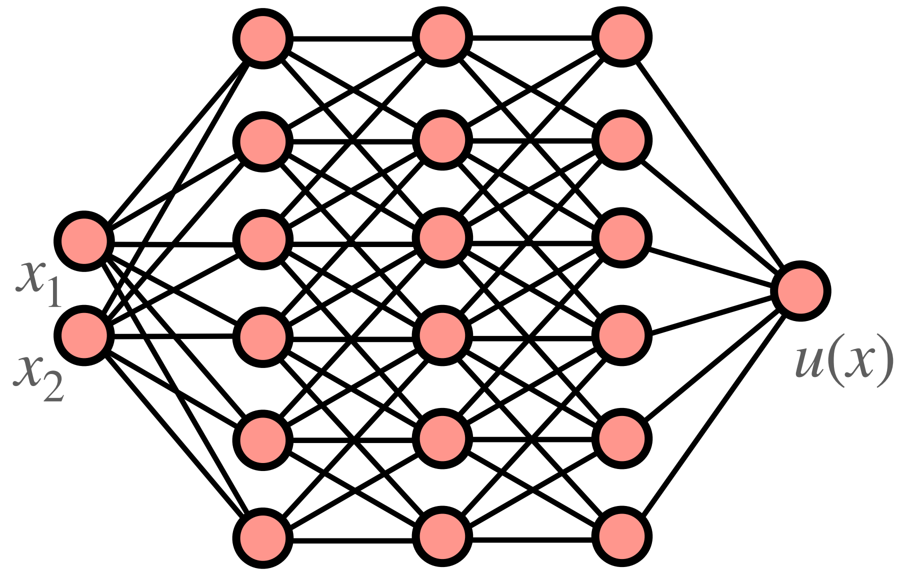
$$\hat{u}(x;\theta) \approx u(x)$$



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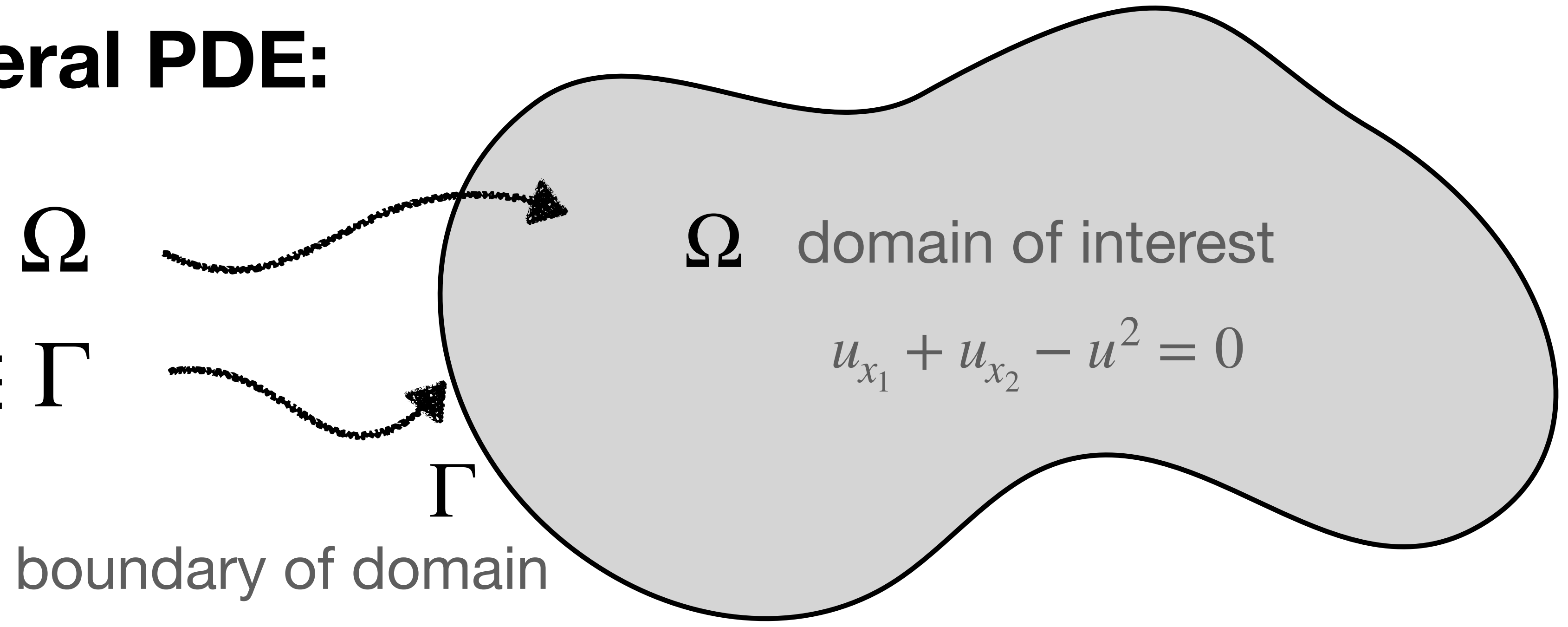

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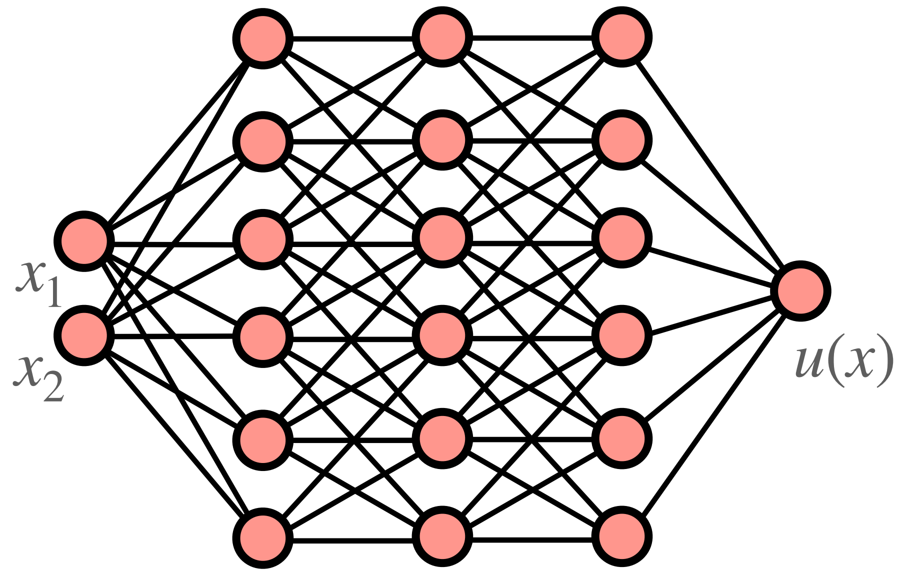

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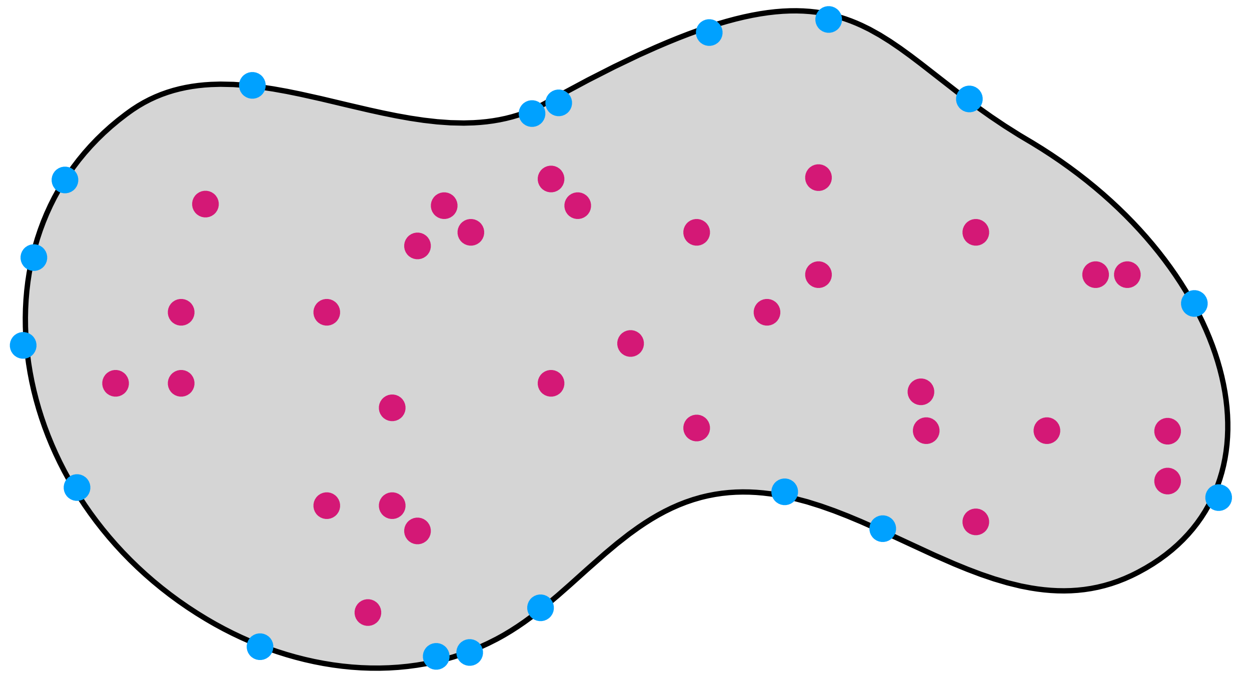

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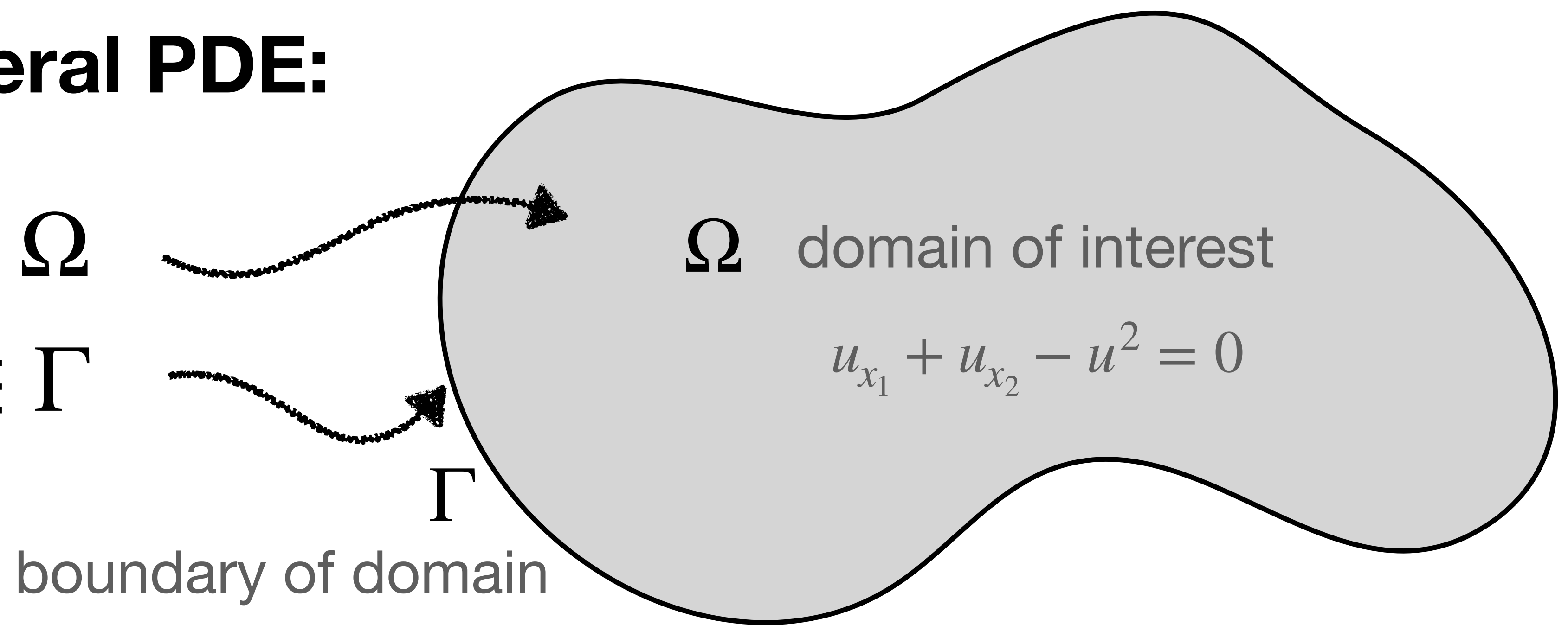

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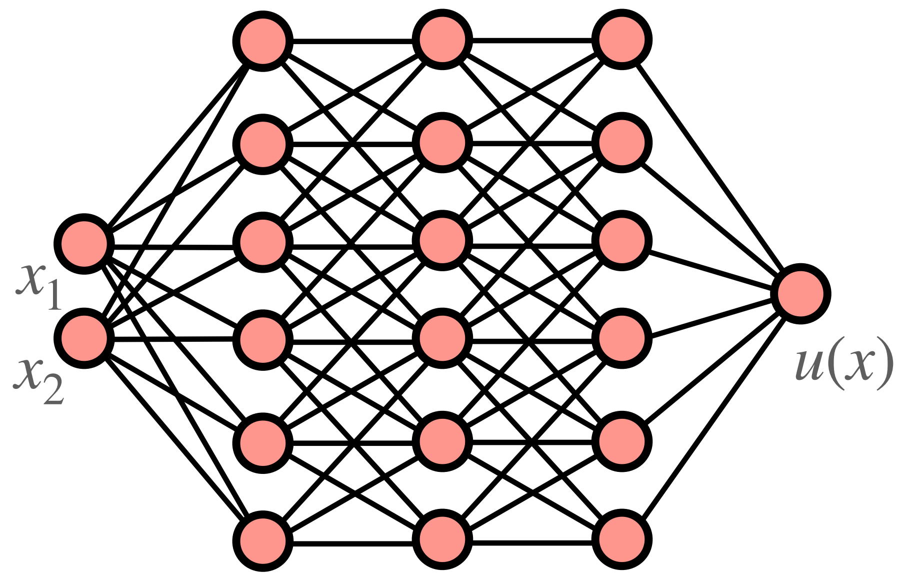

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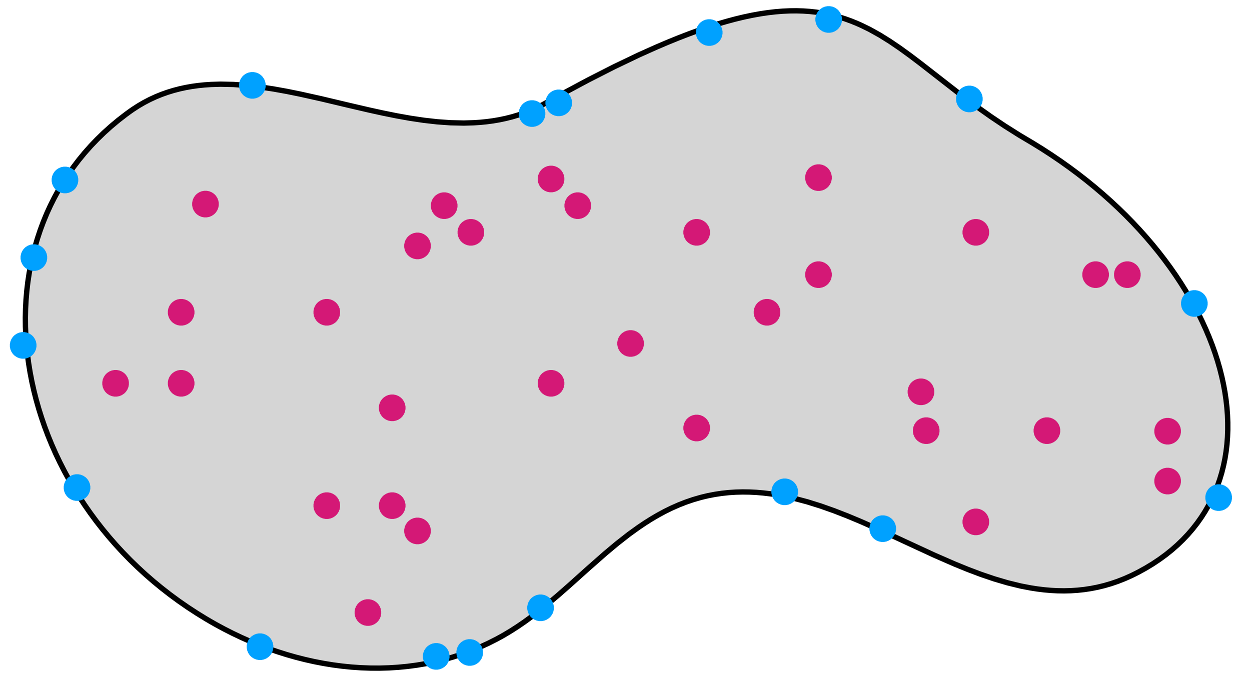

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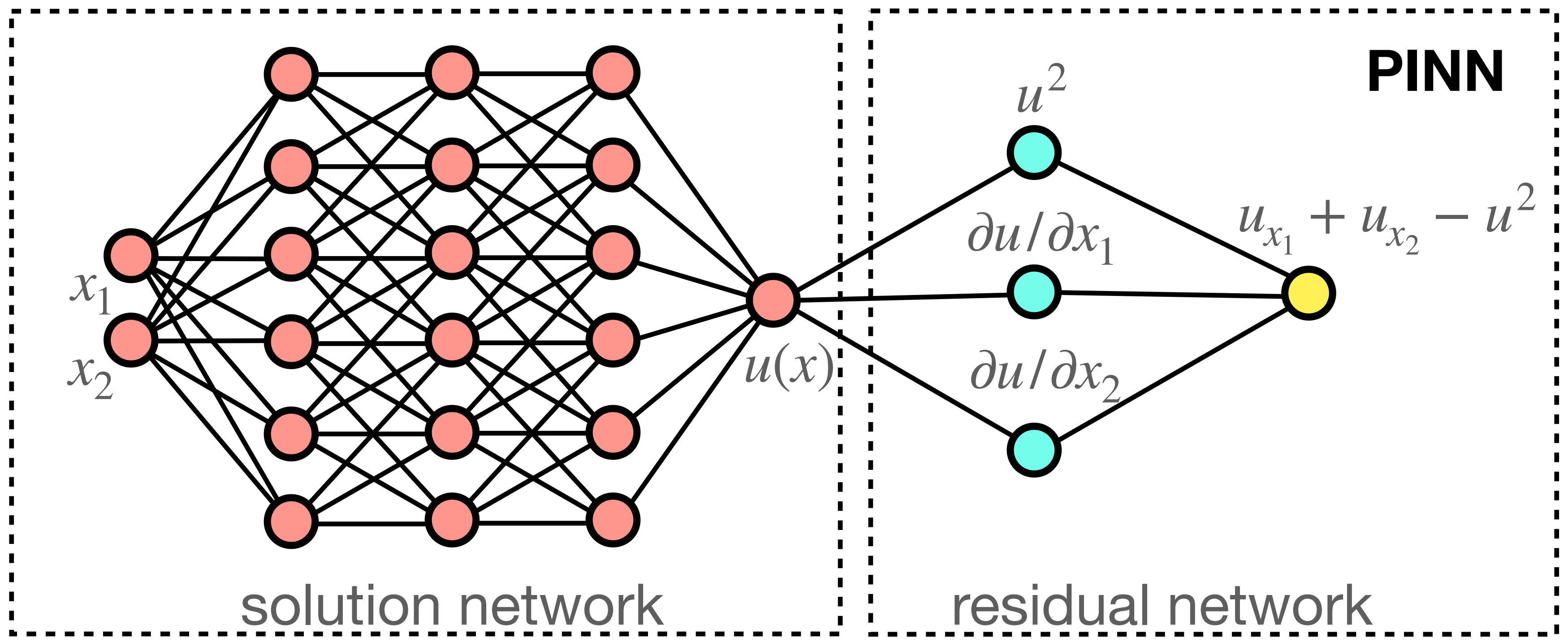
$$\mathscr{L}(\theta) = \frac{1}{|\hat{\Omega}|}\sum_{x_i \in \hat{\Omega}} |\mathfrak{F}[\hat{u}](x_i;\theta)|^2 + \frac{\eta}{|\hat{\Gamma}|}\sum_{x_i \in \hat{\Gamma}} |\mathfrak{B}[\hat{u}](x_i;\theta)|^2$$



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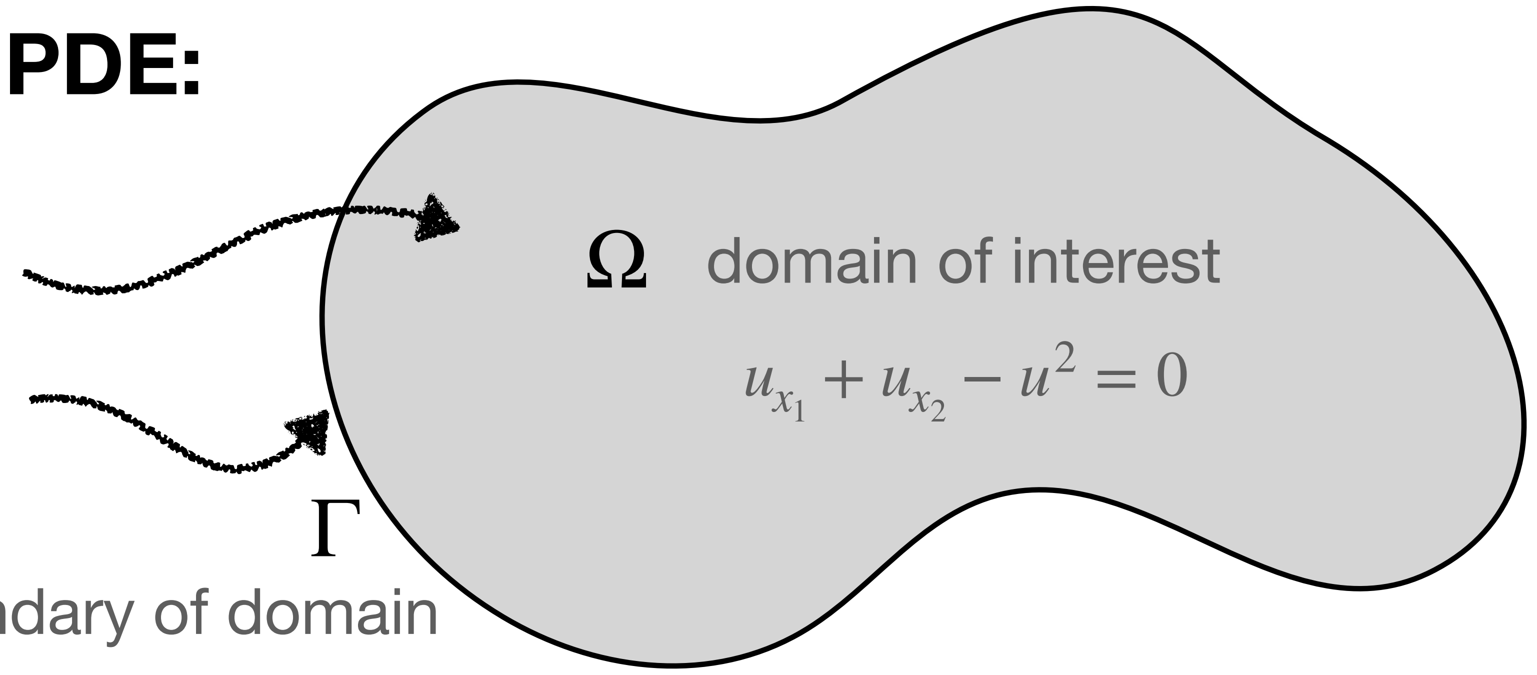

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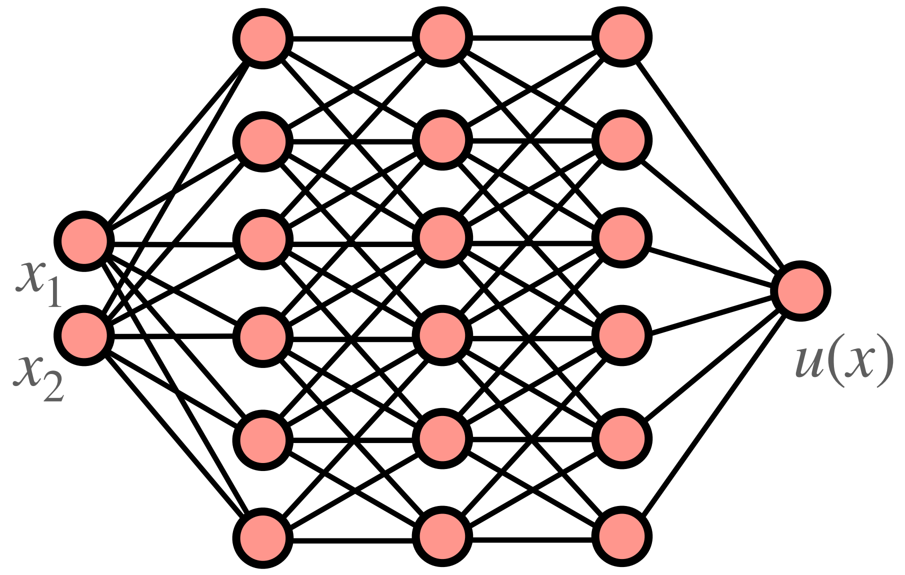

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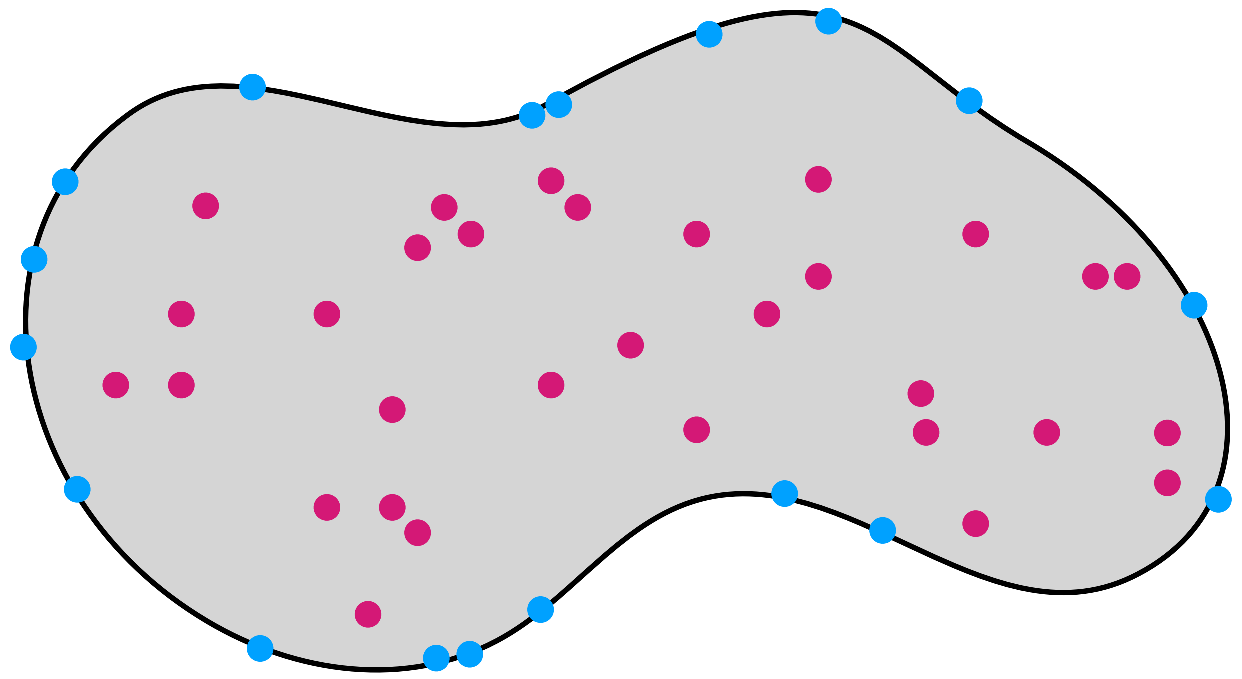

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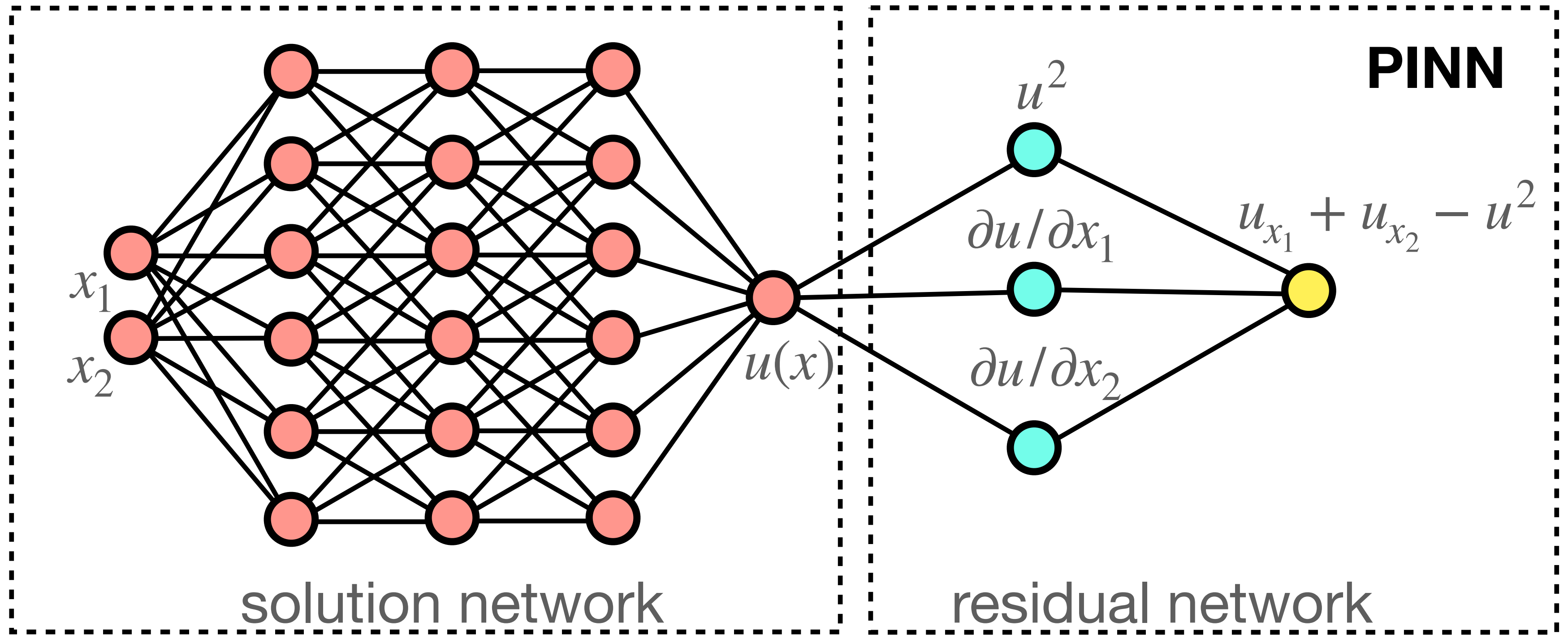


5. **Minimize the loss function with respect to network parameters**

$$\hat{u} = \hat{u}(x;\theta^*), \quad \underset{\theta}{\operatorname{argmin}}\, \mathscr{L}(\theta)$$

Navier-Stokes equations for perfect gas

- Interested in assessing the heating predictions obtained with neural networks in “simple” configurations at high speed
- Previous literature is not concerned with heating

Governing equations.

$$\frac{\partial \boldsymbol{U}}{\partial t} + \frac{\partial \boldsymbol{F}}{\partial x} + \frac{\partial \boldsymbol{G}}{\partial y} = \frac{\partial \boldsymbol{F}^v}{\partial x} + \frac{\partial \boldsymbol{G}^v}{\partial y}, \quad \forall (x, y) \in \boldsymbol{\Omega}$$

$$\boldsymbol{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{bmatrix}, \quad \boldsymbol{F} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ \rho u H \end{bmatrix}, \quad \boldsymbol{G} = \begin{bmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ \rho v H \end{bmatrix}, \quad \boldsymbol{F}^v = \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ \tau_{xx} u + \tau_{xy} v - q_x \end{bmatrix}, \quad \boldsymbol{G}^v = \begin{bmatrix} 0 \\ \tau_{yx} \\ \tau_{yy} \\ \tau_{yx} u + \tau_{yy} v - q_y \end{bmatrix}$$

$$p = \frac{\rho T}{\gamma M_\infty^2}, \quad E = \frac{1}{\gamma - 1}\frac{p}{\rho} + \frac{u^2 + v^2}{2}$$

$$\tau_{xx} = \hat{\mu}\left(\frac{4}{3}\frac{\partial u}{\partial x} - \frac{2}{3}\frac{\partial v}{\partial y}\right), \quad \tau_{yy} = \hat{\mu}\left(\frac{4}{3}\frac{\partial v}{\partial y} - \frac{2}{3}\frac{\partial u}{\partial x}\right), \quad \tau_{xy} = \tau_{yx} = \hat{\mu}\left(\frac{\partial v}{\partial x} + \frac{\partial u}{\partial y}\right), \quad q_x = -k\frac{\partial T}{\partial x}, \quad q_y = -k\frac{\partial T}{\partial y}$$

$$\hat{\mu} = \frac{1}{\mathrm{Re}_\infty}\frac{C + T_\infty}{C + T_\infty T} T^{3/2}, \quad k = \frac{\hat{\mu}}{(\gamma - 1) M_\infty^2 \mathrm{Pr}}$$

Loss function in Python code.

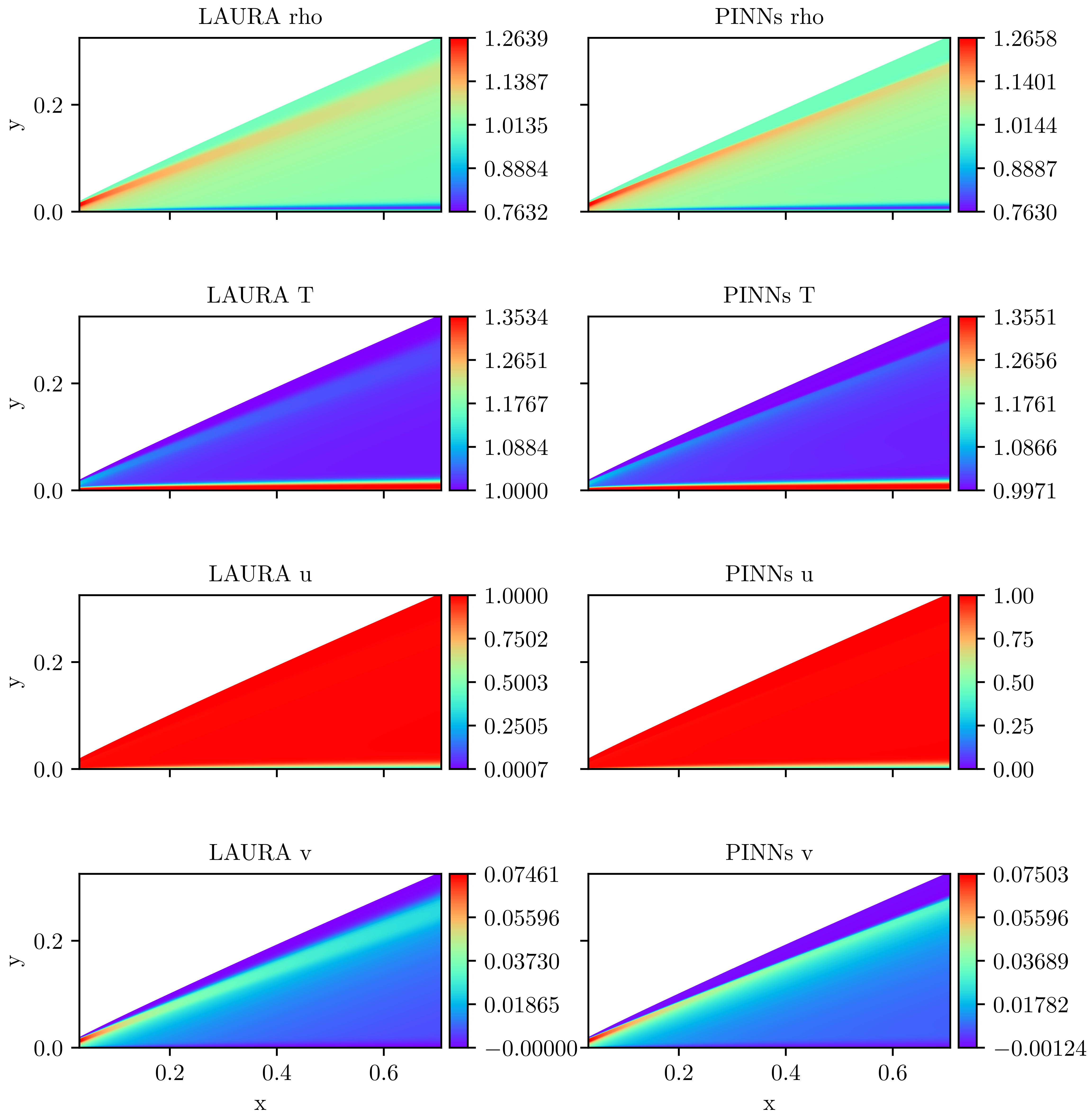
```python
def steady_navier_stokes_2d(coords, prim_vars):
    rho = prim_vars[:,0:1]
    T = prim_vars[:,1:2]
    u = prim_vars[:,2:3]
    v = prim_vars[:,3:]
    p = rho*T/(gamma*M_inf**2)

    mu = (s2 + T_inf) * tf.maximum(T,1.0)**1.5 / (s2 + T_inf*tf.maximum(T,1.0))
    k = mu / ((gamma-1) * M_inf**2 * Pr)

    rho_x, rho_y, T_x, T_y, u_x, u_y, v_x, v_y = gradients(prim_vars, coords)
    p_x, p_y = [dde.grad.jacobian(p, coords, j=j) for j in range(2)]

    tauxx = mu * ((4.0/3.0)*u_x - (2.0/3.0)*v_y)
    tauyy = mu * ((4.0/3.0)*v_y - (2.0/3.0)*u_x)
    tauxy = mu * (u_y + v_x)

    qx = -k * T_x
    qy = -k * T_y

    tauxx_x = dde.grad.jacobian(tauxx, coords, j=0)
    tauxy_x, tauxy_y = [dde.grad.jacobian(tauxy, coords, j=j) for j in range(2)]
    tauyy_y = dde.grad.jacobian(tauyy, coords, j=1)

    qx_x = dde.grad.jacobian(qx, coords, j=0)
    qy_y = dde.grad.jacobian(qy, coords, j=1)

    mass   = rho*(u_x + v_y) + u*rho_x + v*rho_y
    x_mtm  = rho*(u*u_x + v*u_y) + p_x - (tauxx_x + tauxy_y)/Re_inf
    y_mtm  = rho*(u*v_x + v*v_y) + p_y - (tauxy_x + tauyy_y)/Re_inf
    energy = (
        rho*(u*u*u_x + u*v*(v_x+u_y) + v*v*v_y) + gamma/(gamma-1.0)*(
            u*p_x + v*p_y - T*(u*rho_x + v*rho_y)/(gamma*M_inf**2)
        ) - (
            u*tauxx_x + tauxx*u_x + v*tauxy_x + tauxy*v_x +
            u*tauxy_y + tauxy*u_y + v*tauyy_y + tauyy*v_y -
            qx_x - qy_y
        ) / Re_inf
    )

    return [mass, x_mtm, y_mtm, energy]
```

Comparison with LAURA for flat plate

- Freestream conditions

M_∞	Re_∞	T_∞ [K]	T_{wall} [K]	γ	C [K]	Pr
3.0	5.0×10^4	300.0	300.0	1.4	110.33	0.72

- Network architecture and training
  - Dense feed-forward network, 6 hidden layers with 32 nodes
  - Layer-wise adaptive activation function
  - 50,000 Adam iterations with learning rate of 0.001
  - Further converged with L-BFGS algorithm
- LAURA results
  - 81x227 node grid
  - Mesh adaptation to resolve shock



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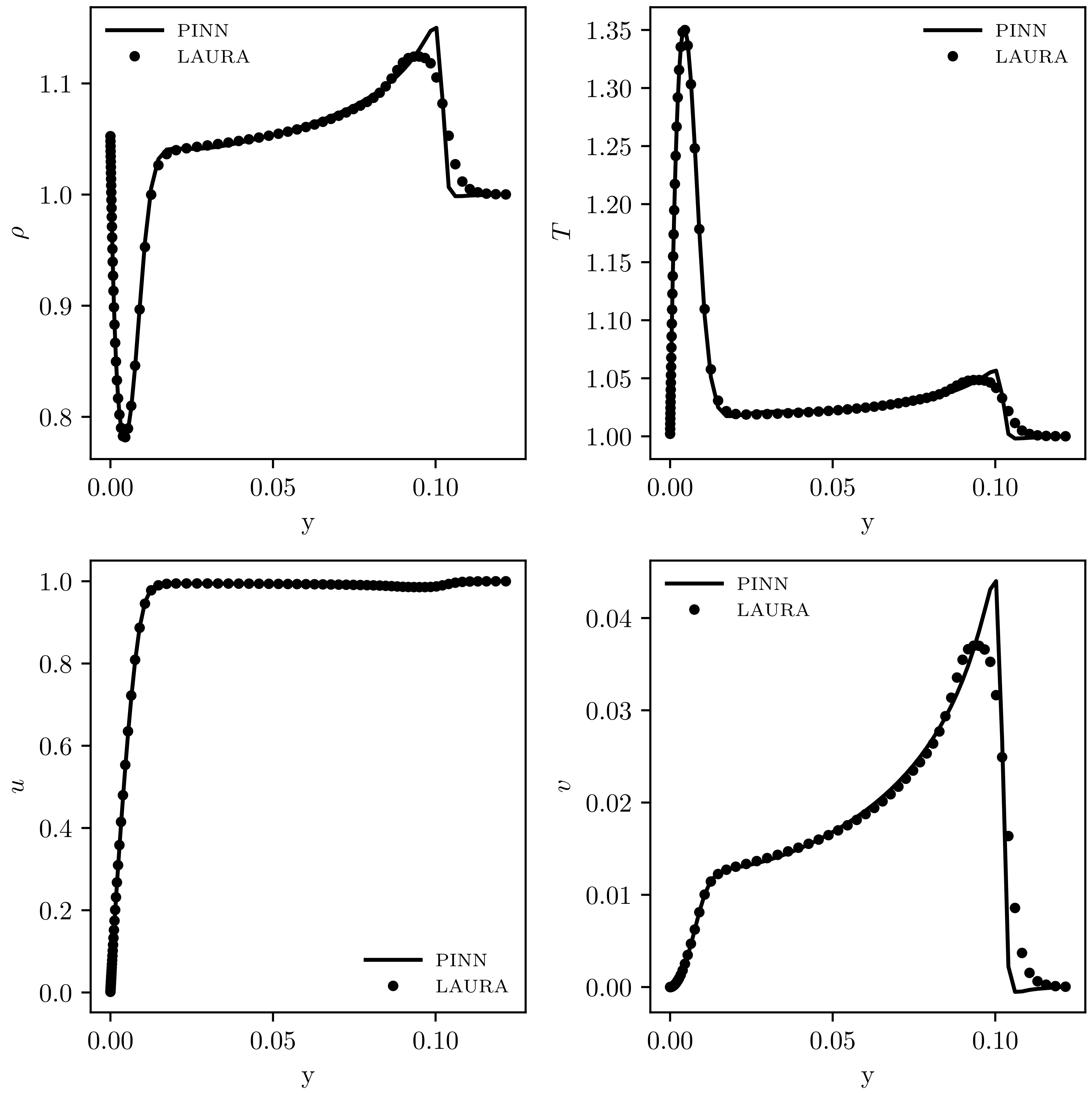

Wall-normal slice at $x \approx 0.25$

- Boundary and shock layers well resolved with PINN
- Heat flux computed along the entire wall (continuous function) by taking gradient of temperature solution network
- Does not require gradient approximation/interpolation as with CFD solution