Artificial Intelligence

CSC 665

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Machine Learning V

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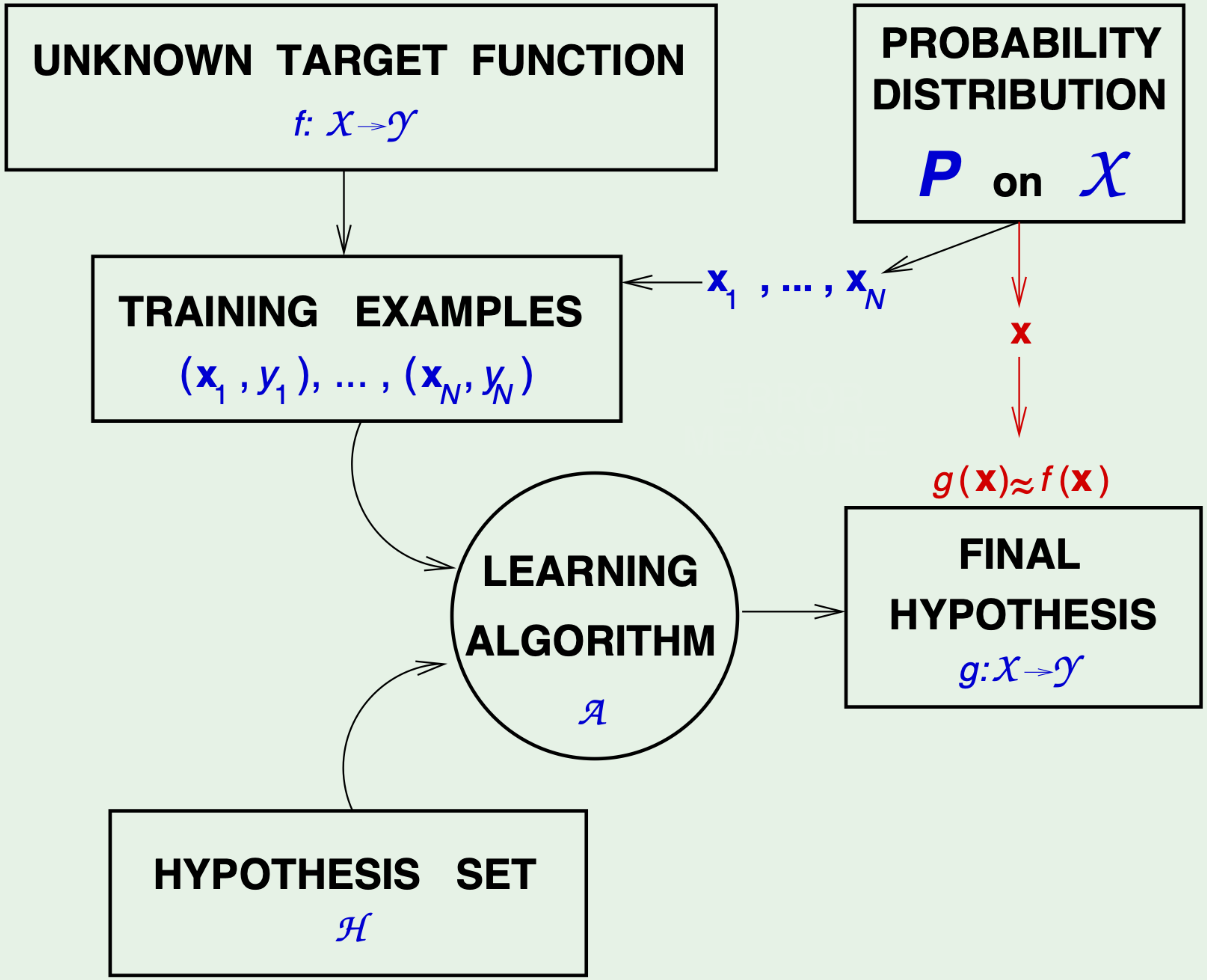
- **Search:** make decisions by looking ahead
- **Logic:** deduce new facts from existing facts
- **Constraints:** find a way to satisfy a given specification
- **Probability:** reason quantitatively about uncertainty
- **Learning:** make future predictions from past observations

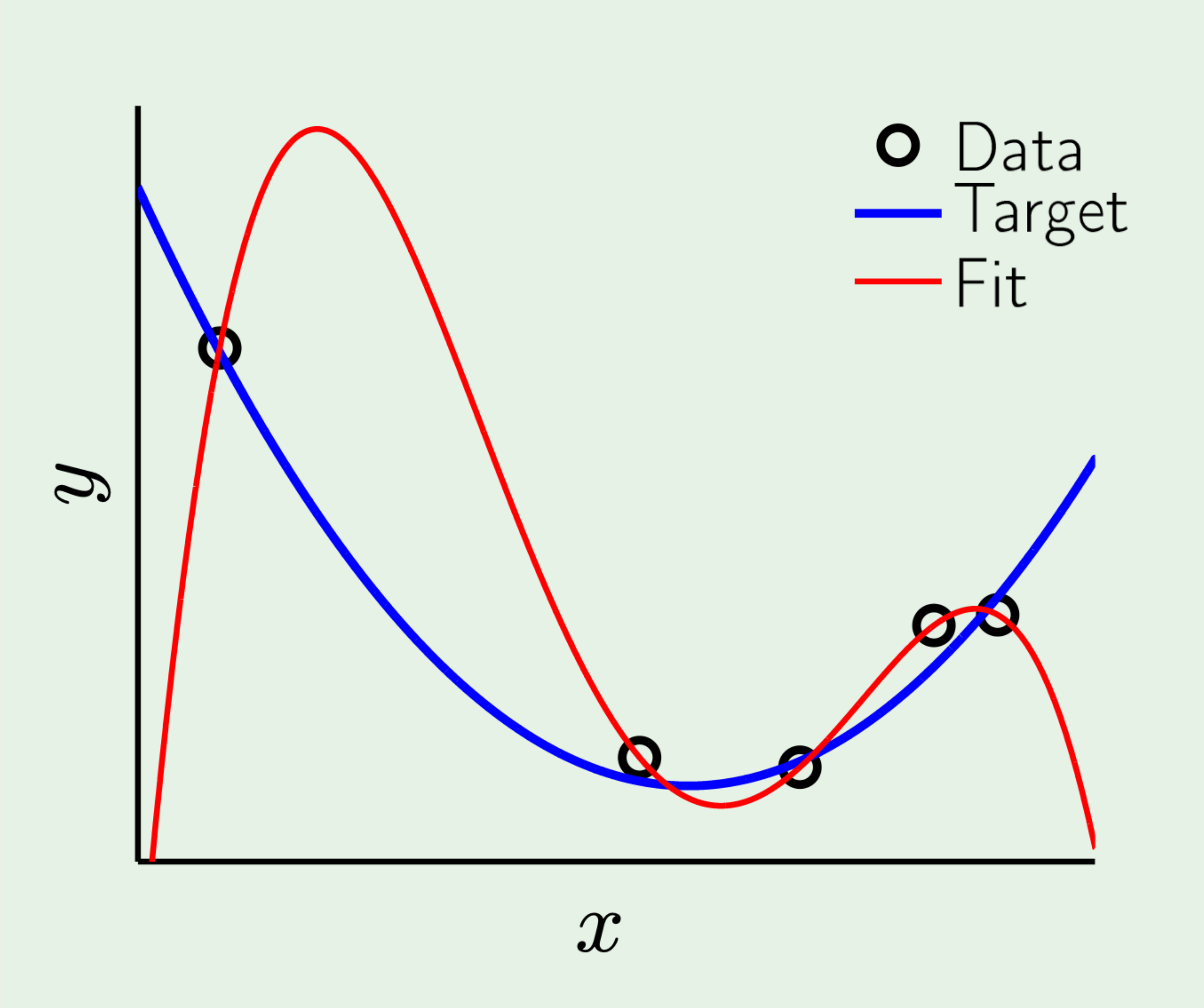


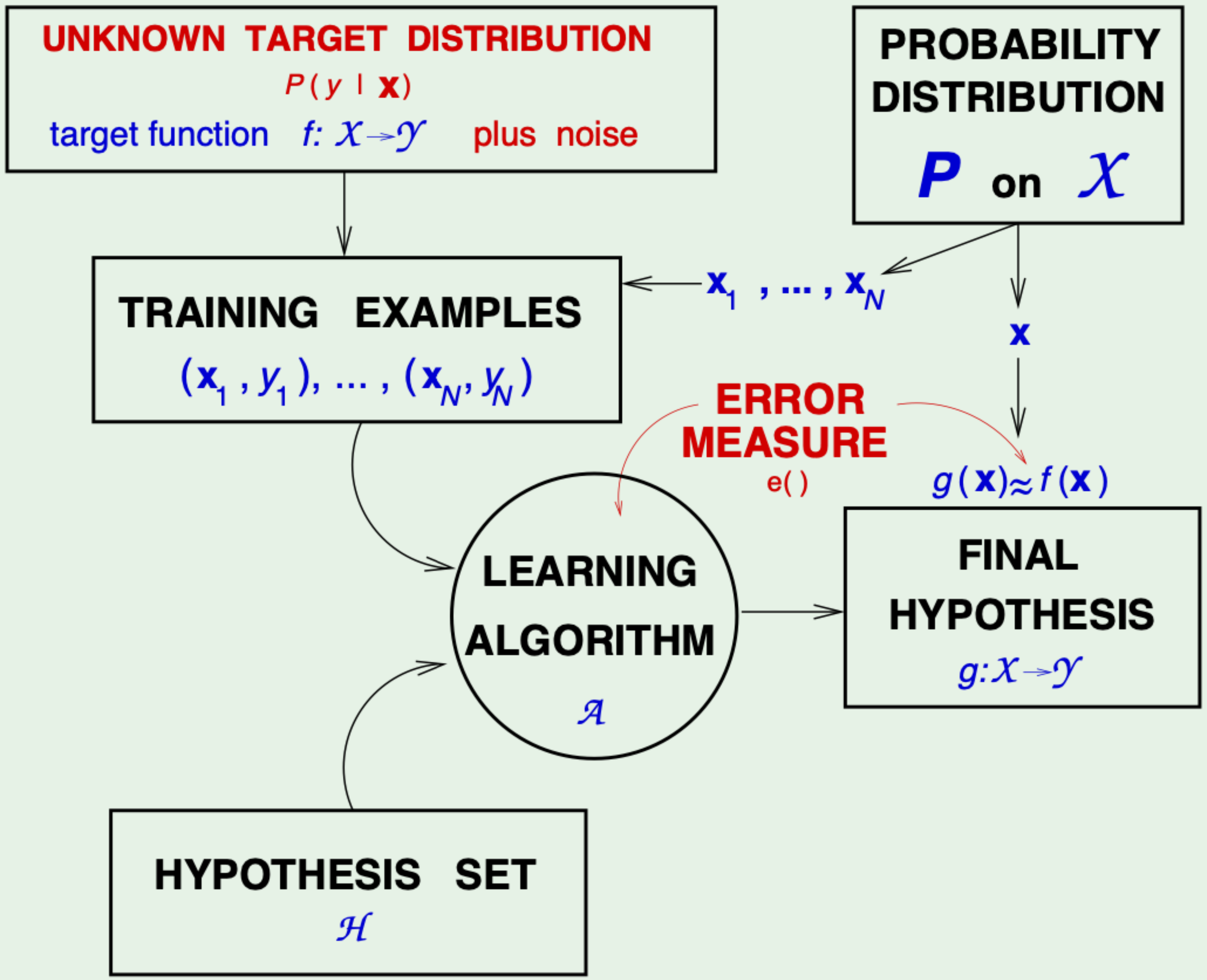
UNKNOWN TARGET FUNCTION
$f: \mathcal{X} \to \mathcal{Y}$
PROBABILITY DISTRIBUTION
P on $\mathcal{X}$
$\mathbf{x}_1, \ldots, \mathbf{x}_N$
$\mathbf{x}$
TRAINING EXAMPLES
$(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)$
$g(\mathbf{x}) \approx f(\mathbf{x})$
LEARNING ALGORITHM
$\mathcal{A}$
FINAL HYPOTHESIS
$g: \mathcal{X} \to \mathcal{Y}$
HYPOTHESIS SET
$\mathcal{H}$

Overfitting

Overfitting by example

- In practice, datasets often contains **noise**
- $y = f(x) + \varepsilon \quad (\varepsilon \sim P_{\text{noise}})$
- On the right:
  - f is a 2nd degree polynomial
  - $\varepsilon \sim \mathcal{N}(0, \sigma^2)$ for small σ
- Since the training dataset only contains 5 points, a 4th degree polynomial **fits perfectly**
- I.e. $C_{\text{train}} = 0$ but C_{test} will be **large**
- Our hypothesis failed to generalize because ***it fits the noise***

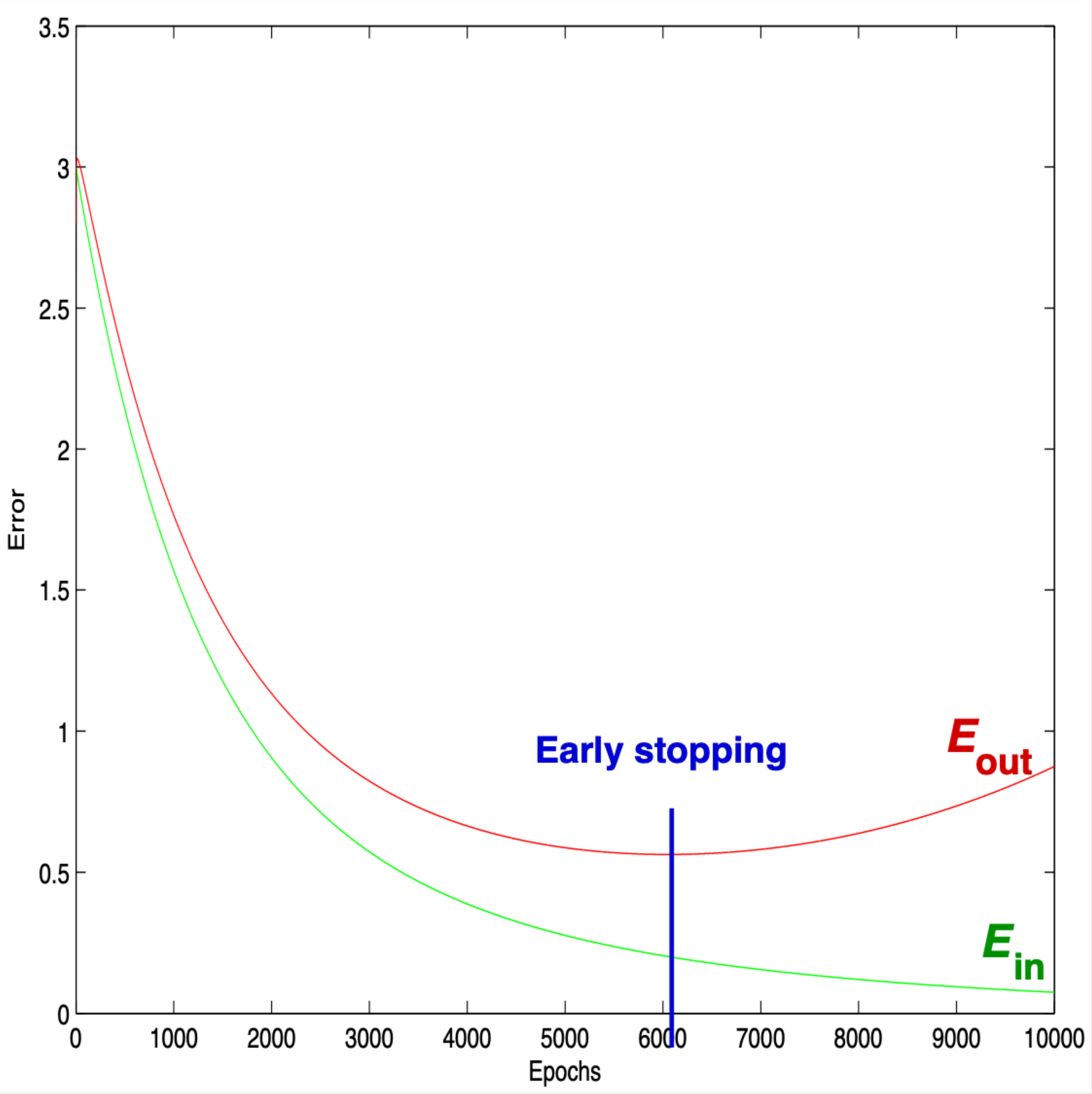




UNKNOWN TARGET DISTRIBUTION
P (y | x)
target function f: X → Y plus noise
PROBABILITY DISTRIBUTION
P on X
TRAINING EXAMPLES
(x1 , y1), ... , (xN, yN)
x1 , ... , xN
x
ERROR MEASURE
e( )
g (x) ≈ f (x)
LEARNING ALGORITHM
A
FINAL HYPOTHESIS
g: X → Y
HYPOTHESIS SET
H

Another example

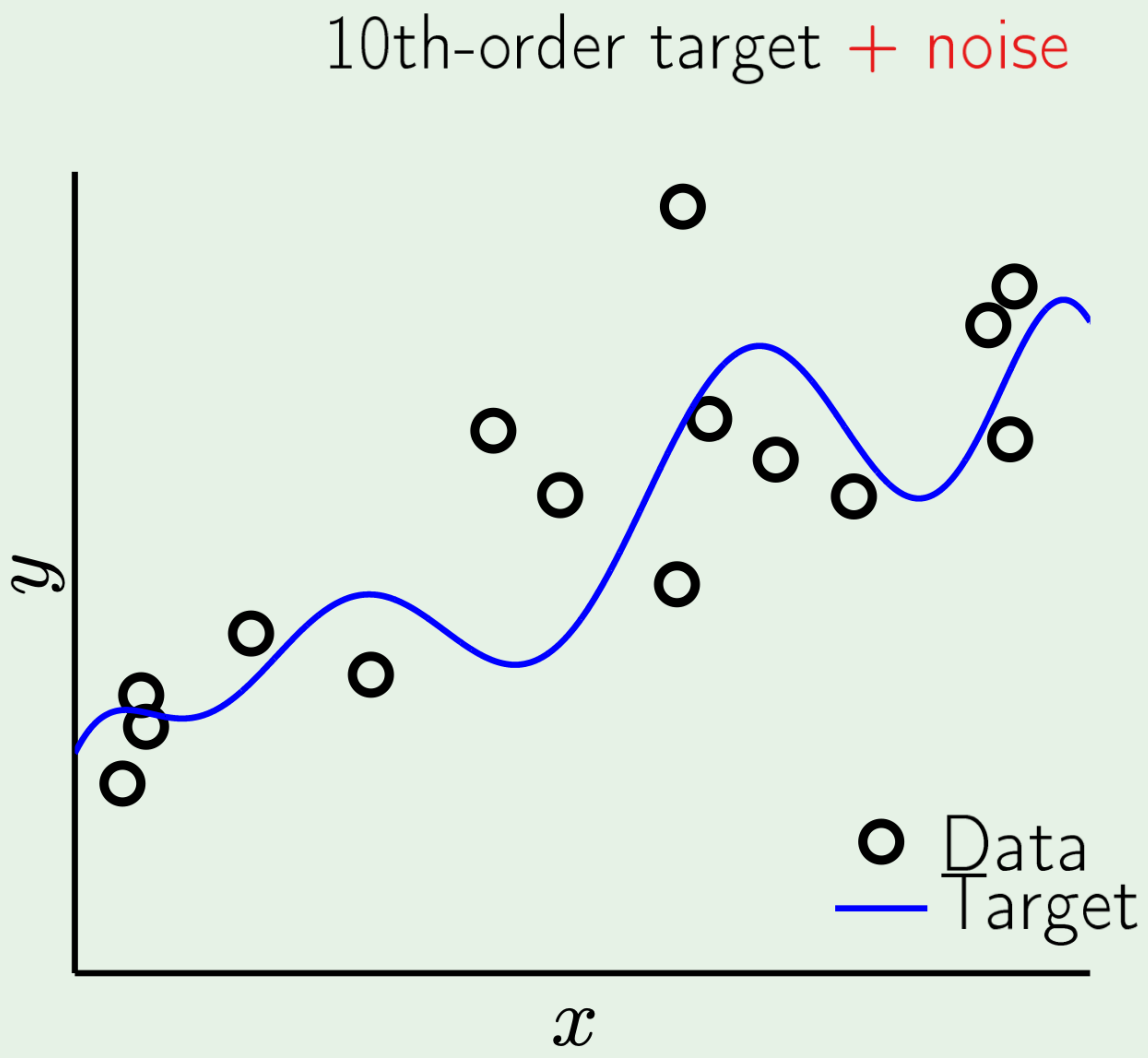
- Consider training a neural network by stochastic gradient descent
- An **epoch** is a pass through the entire training dataset
- After each epoch, measure error/loss/cost of current hypothesis on both training dataset (E_{in}) and held-out test set (E_{out})
- Before blue line: **fitting**
- After blue line: **overfitting**
- (In many modern deep learning models this figure is incomplete due to "double descent")



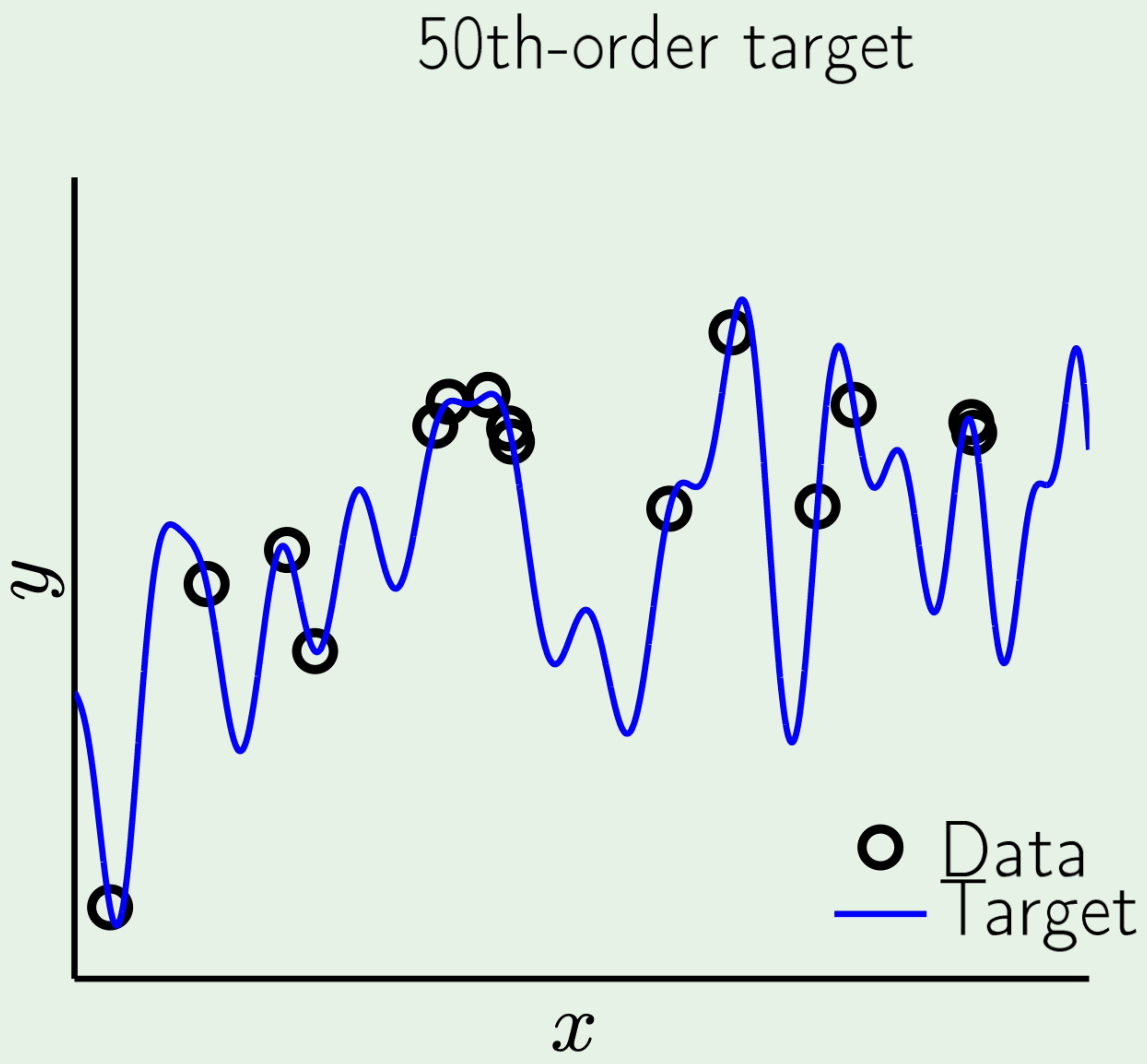
A simple definition

- Overfitting happens when you have **low training cost, but high test cost**
- Overfitting means your hypothesis **fails to generalize** to new unseen examples
- Overfitting happens because you have fit the data more than is warranted — you are **fitting the noise**

Case study

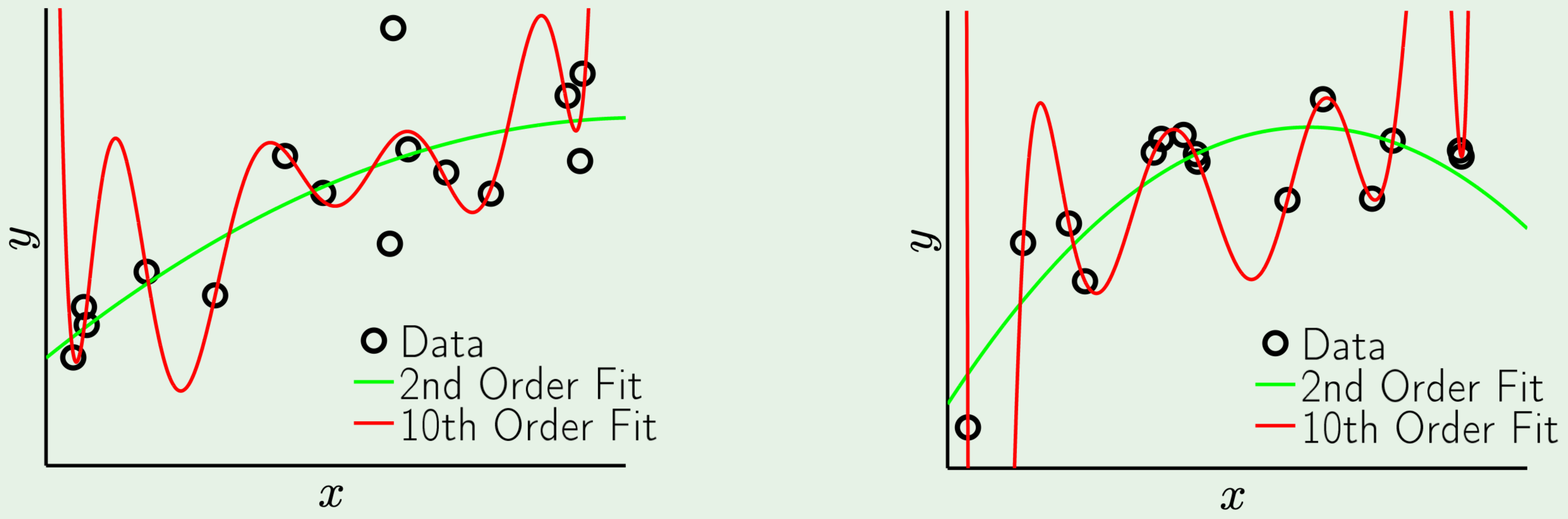


10th-order target + noise
y
x
Data
Target

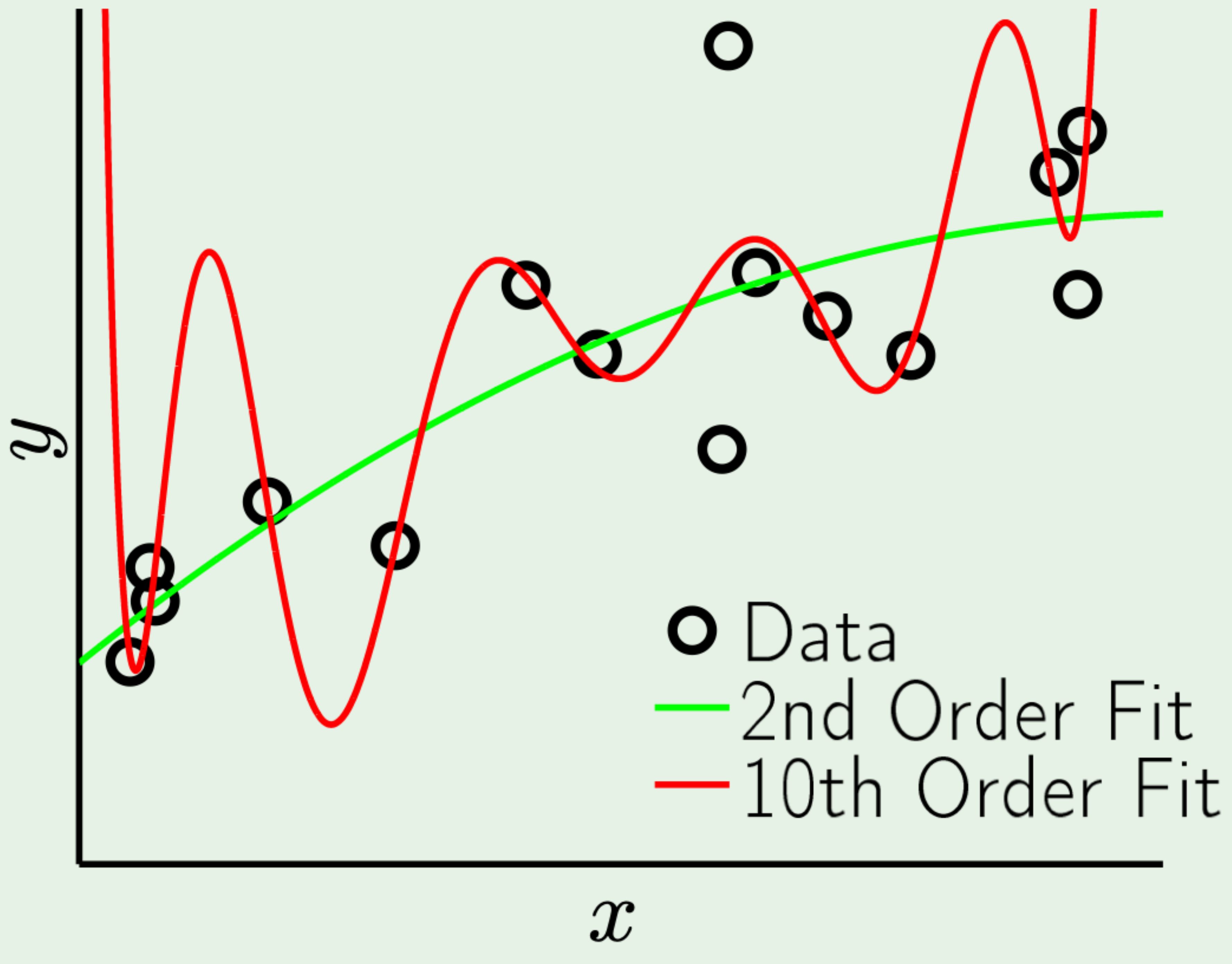


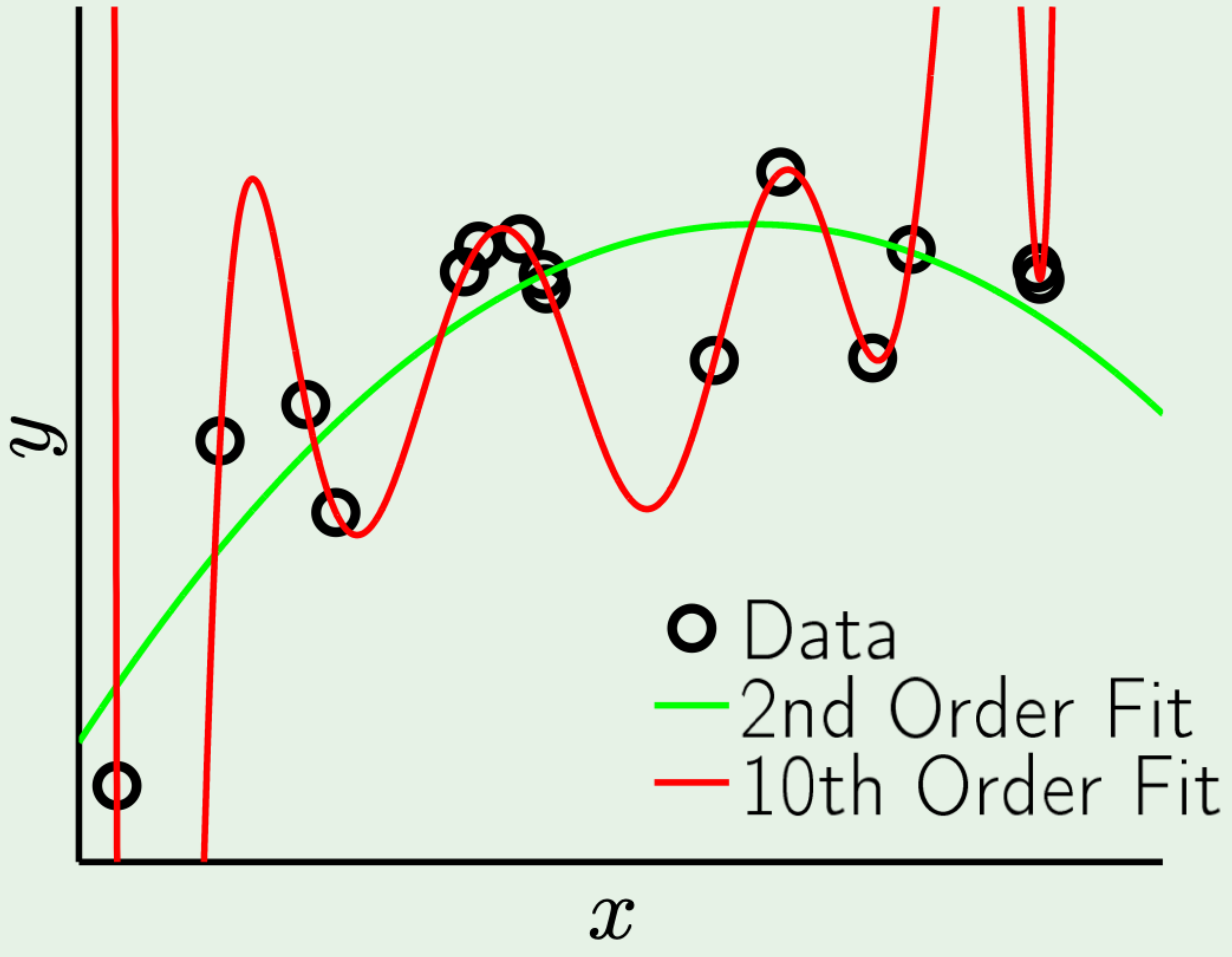
50th-order target
y
x
Data
Target

Two fits for each target



Two fits for each target





Noisy low-order target

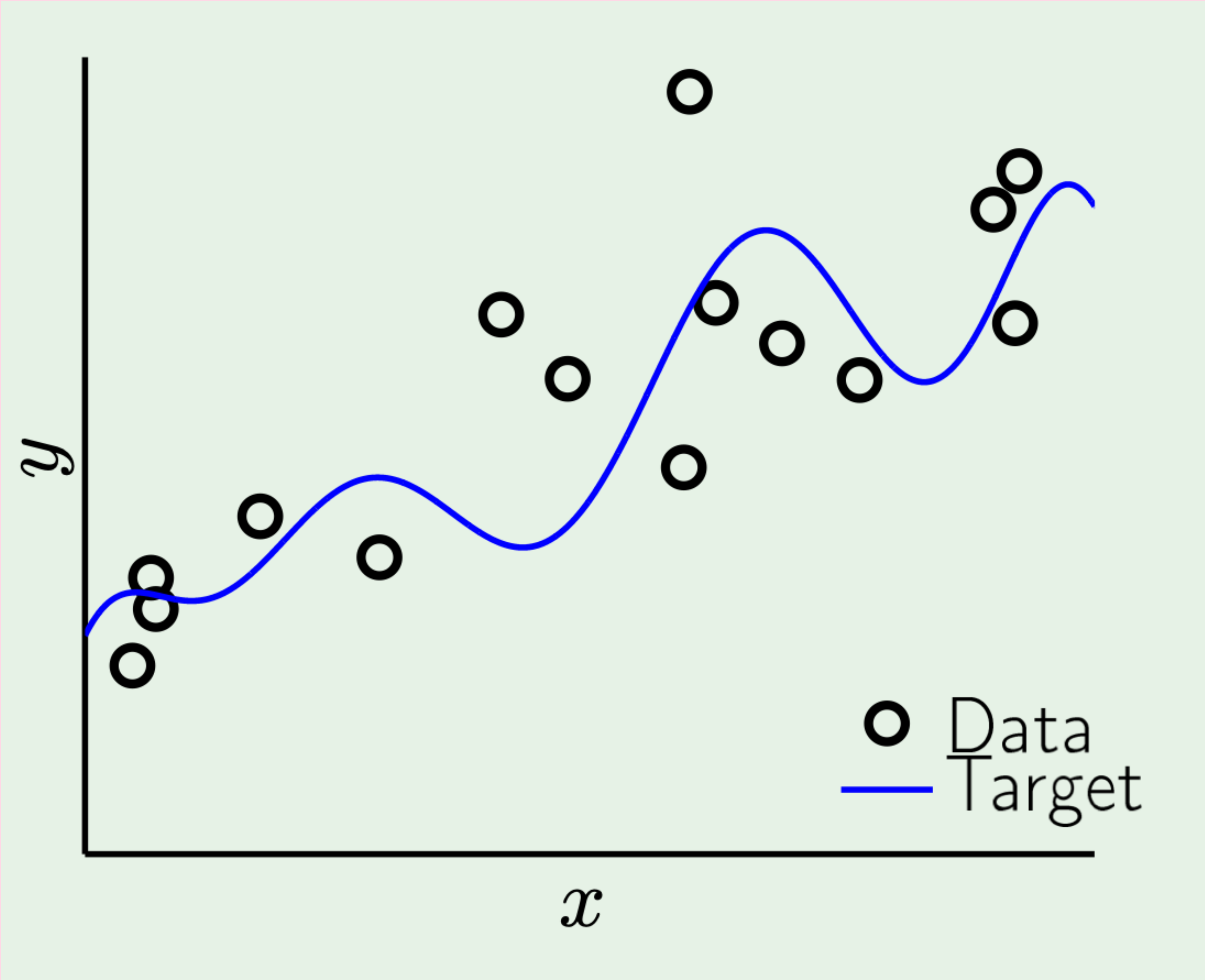
	2nd Order	10th Order
E_{in}	0.050	0.034
E_{out}	0.127	**9.00**

Noiseless high-order target

	2nd Order	10th Order
E_{in}	0.029	10^{-5}
E_{out}	0.120	**7680**

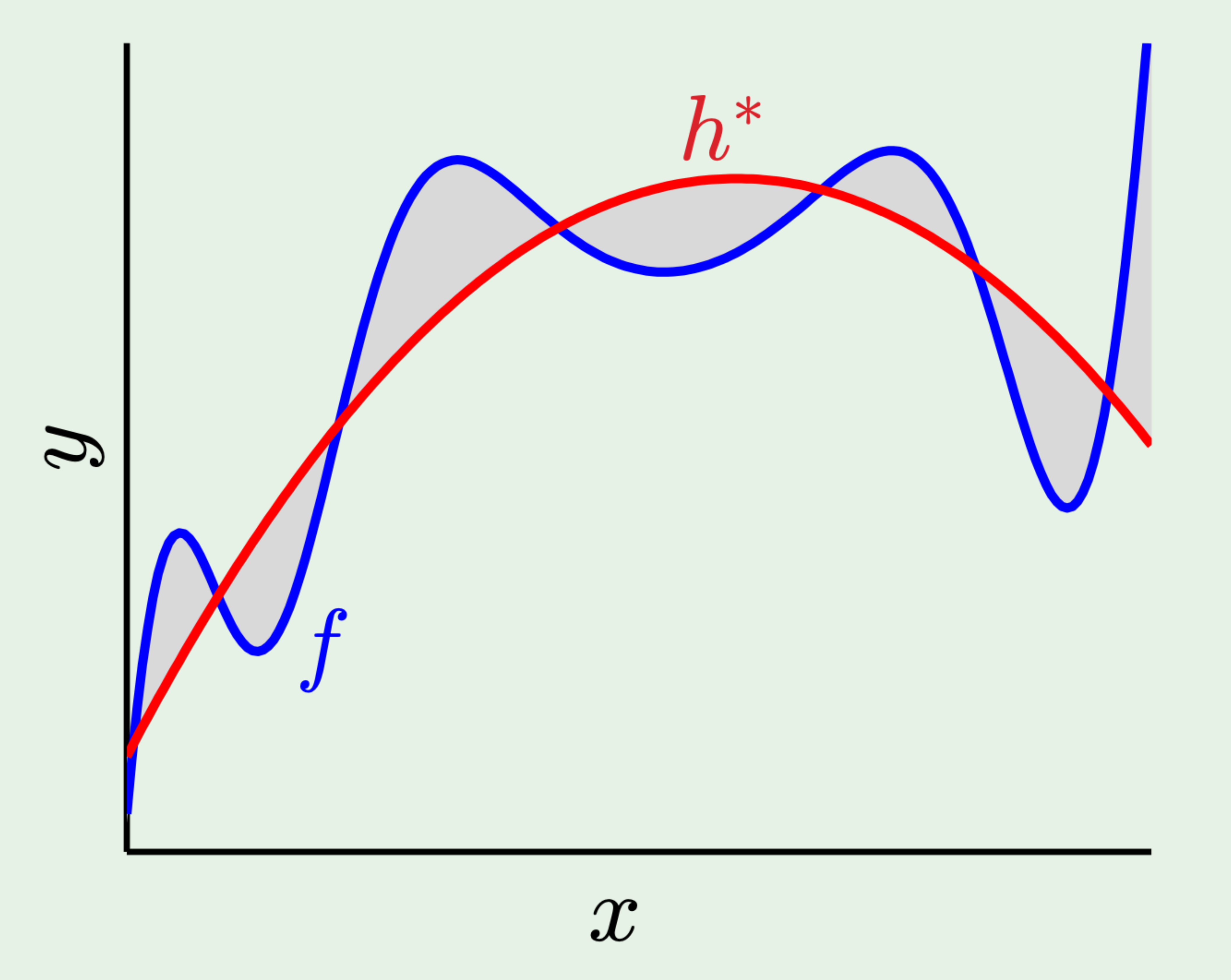
Stochastic noise

- Stochastic noise is often modeled as an additive random variable: $y = f(x) + \varepsilon$
- Fitting stochastic noise is bad, because it pulls your hypothesis away from the target f
- The best estimate of $f(x) + \varepsilon$ is $f(x)$



Deterministic noise

- Deterministic noise is the part of f that $\mathscr{H}$ cannot capture: $f(x) - h^{\star}(x)$
- $h^{\star}$ is the best hypothesis from $\mathscr{H}$, assuming "infinite data"
- But an $h \in \mathscr{H}$ learned from any finite dataset may be very far from $h^{\star}$
- How far depends on the dataset
- Hence, "noise"



Preventing overfitting

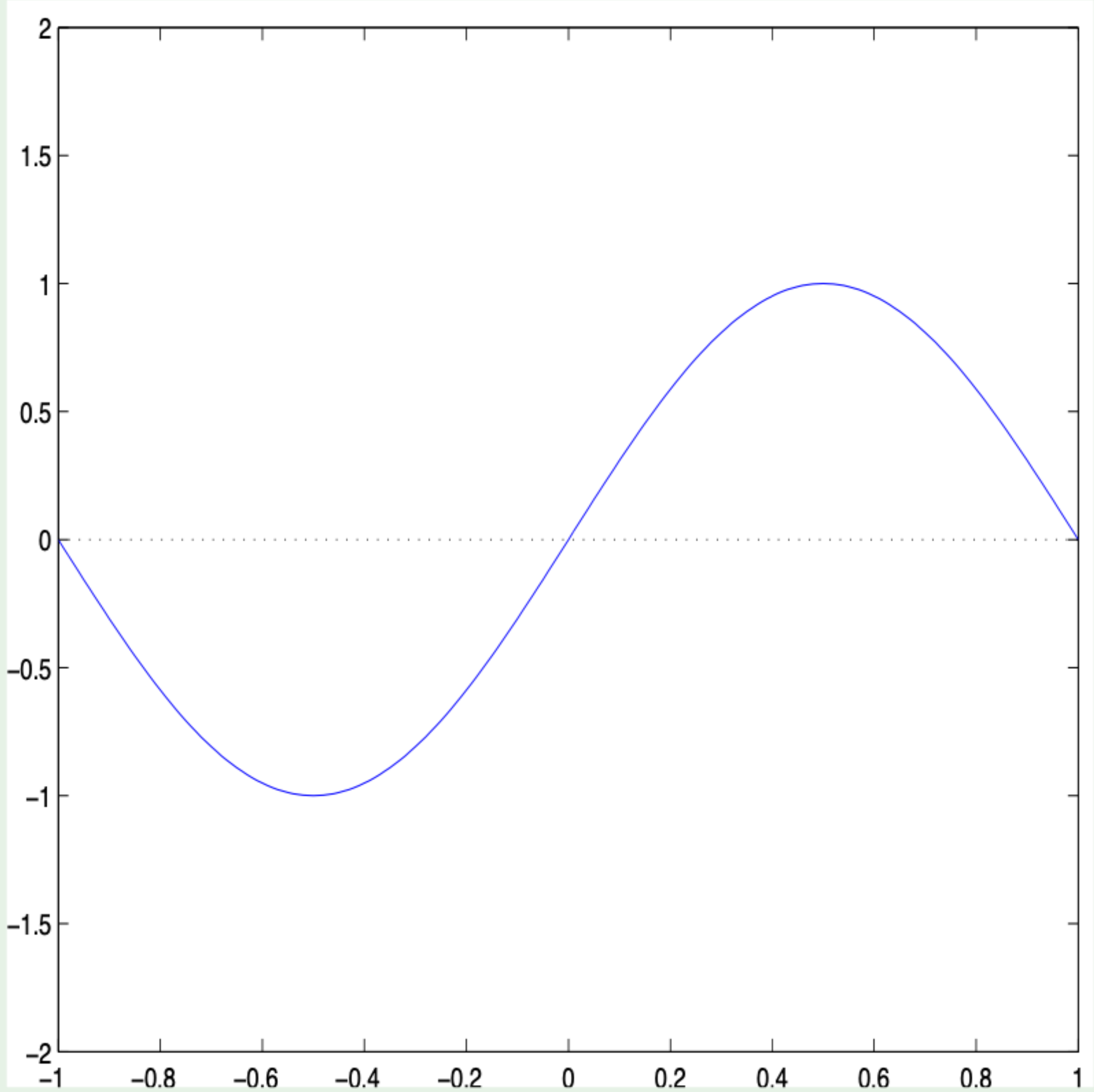
- **Regularization:** deliberately restrict the complexity of your chosen *h* so that you reduce its ability to fit noise. “Putting on the brakes.”
- **Validation:** use a held-out dataset to directly estimate the thing you care about, which is the error rate on unseen examples. “Checking the bottom line.”

Regularization

Example: sine target

f

$f : [-1,1] \to \mathbb{R} \qquad f(x) = \sin(\pi x)$



Only two training examples! $\quad N = 2$

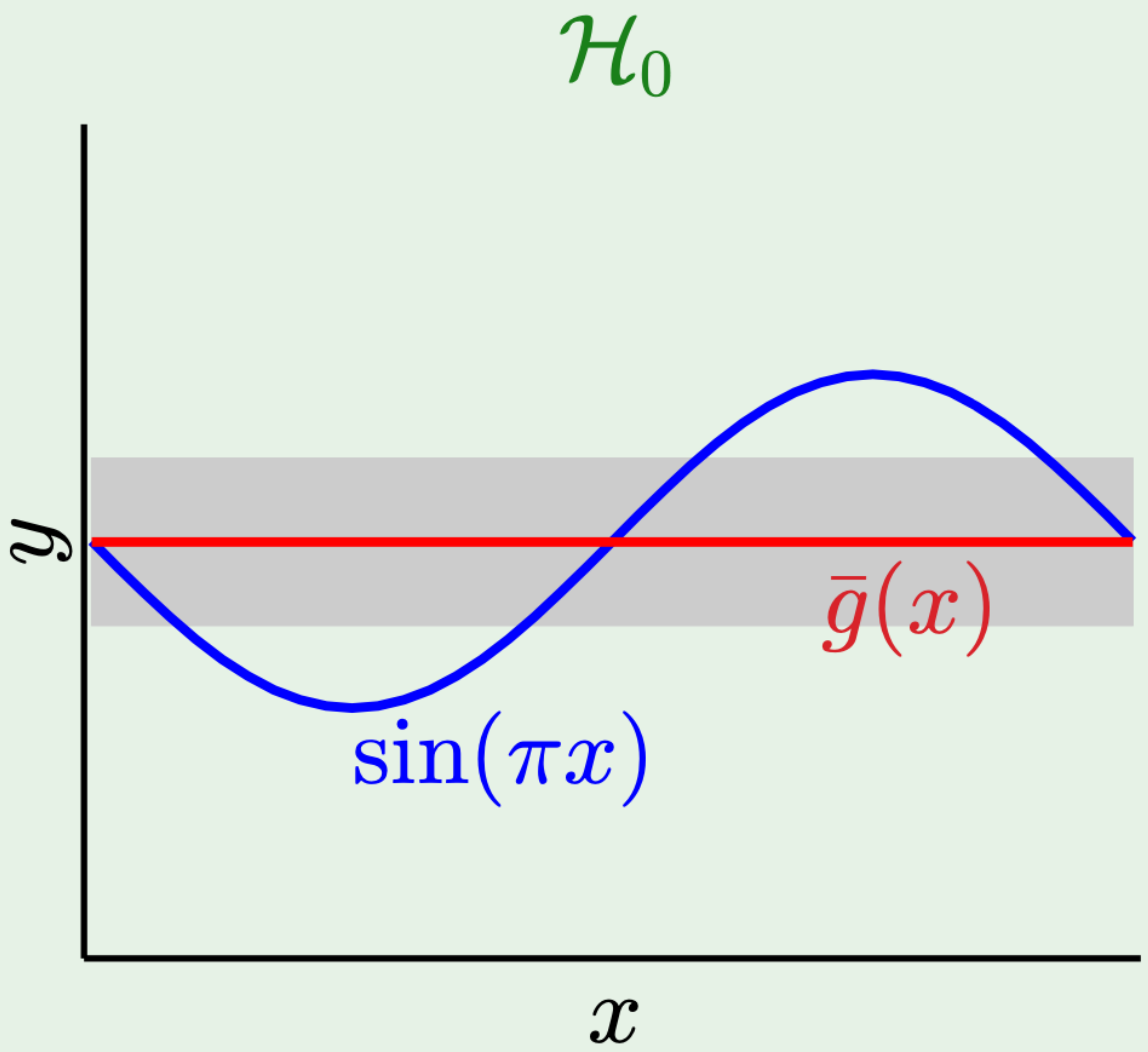
Two models used for learning:

$$\mathcal{H}_0: \quad h(x) = b$$

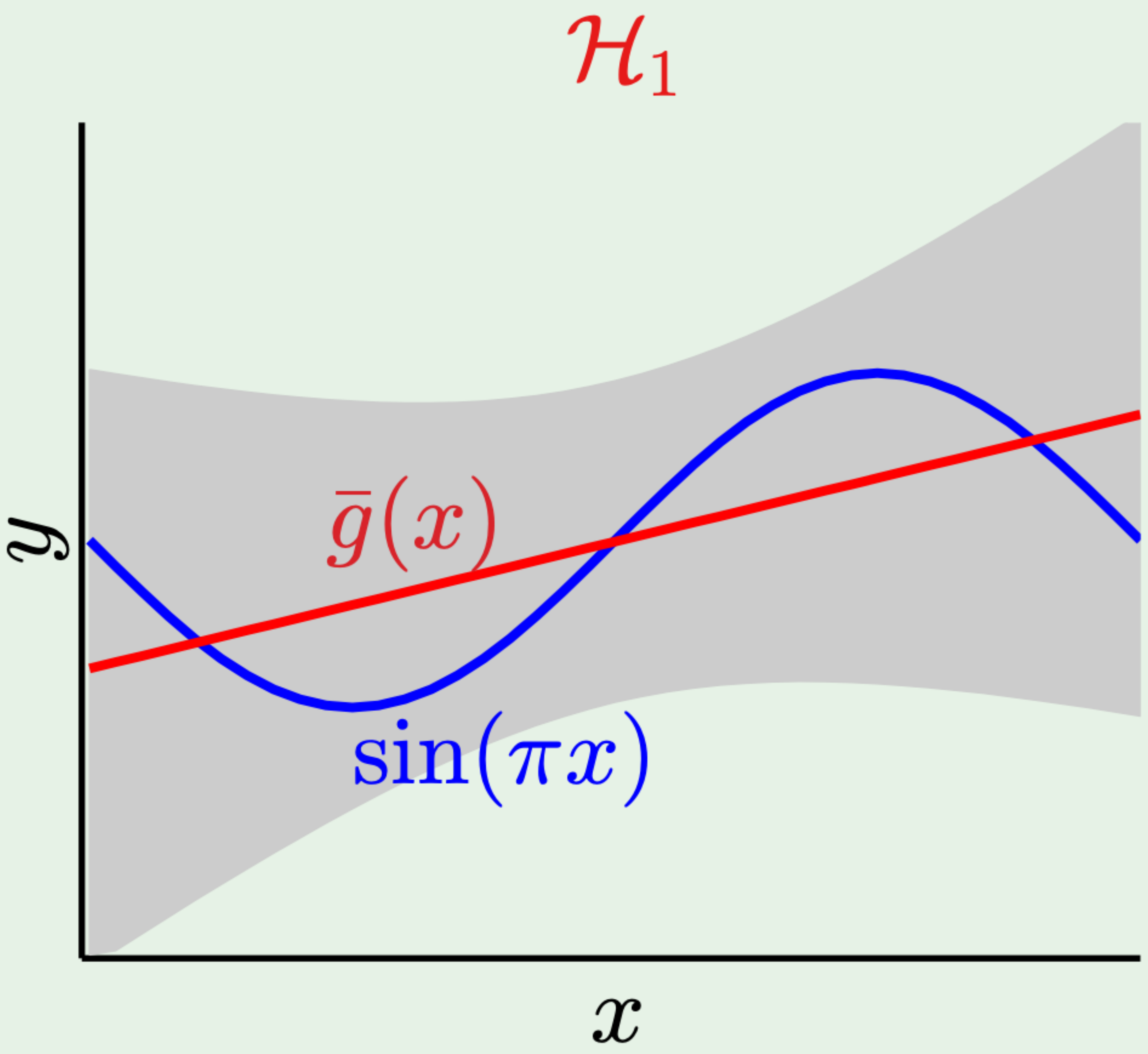
$$\mathcal{H}_1: \quad h(x) = ax + b$$

Which is better, $\mathcal{H}_0$ or $\mathcal{H}_1$?

and the winner is . . .

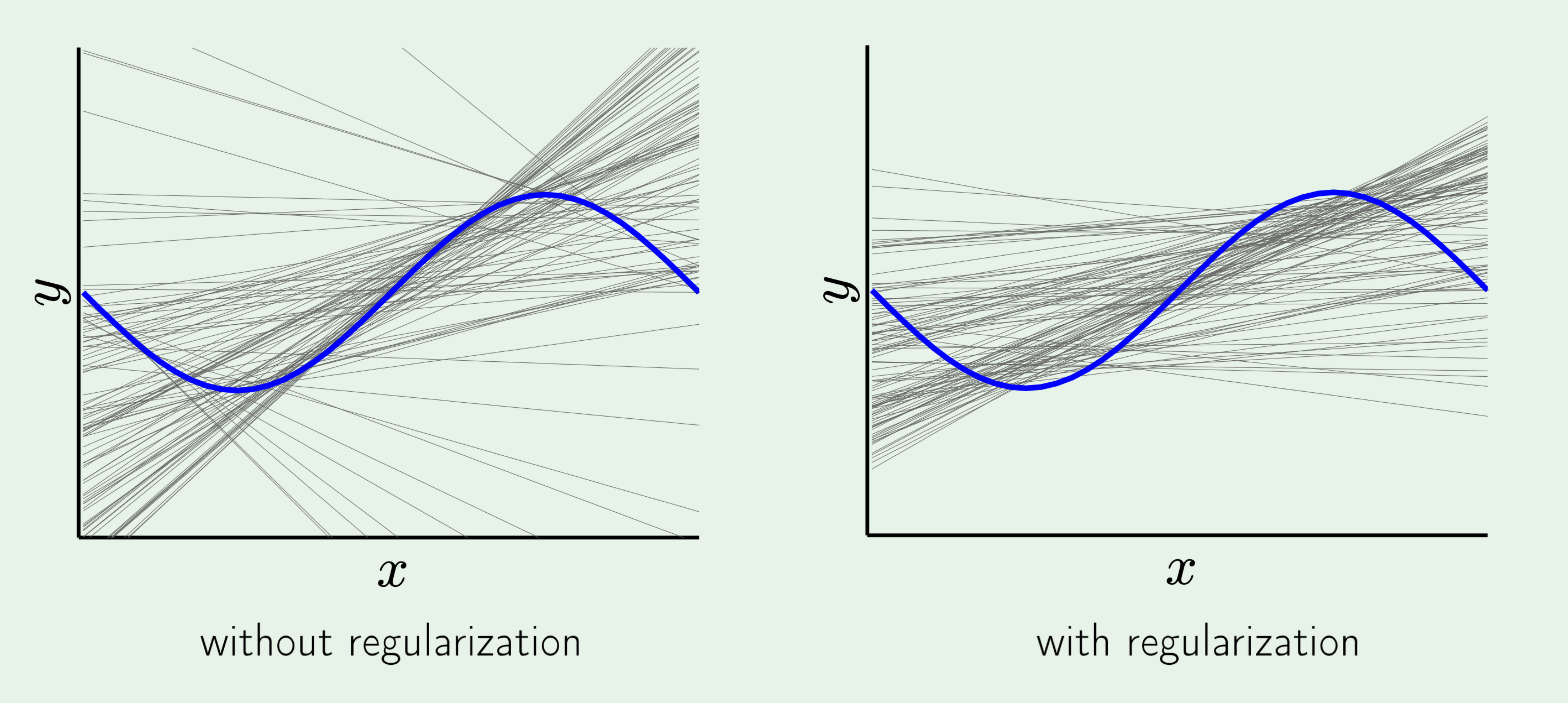


bias $=$ **0.50** var $=$ **0.25**

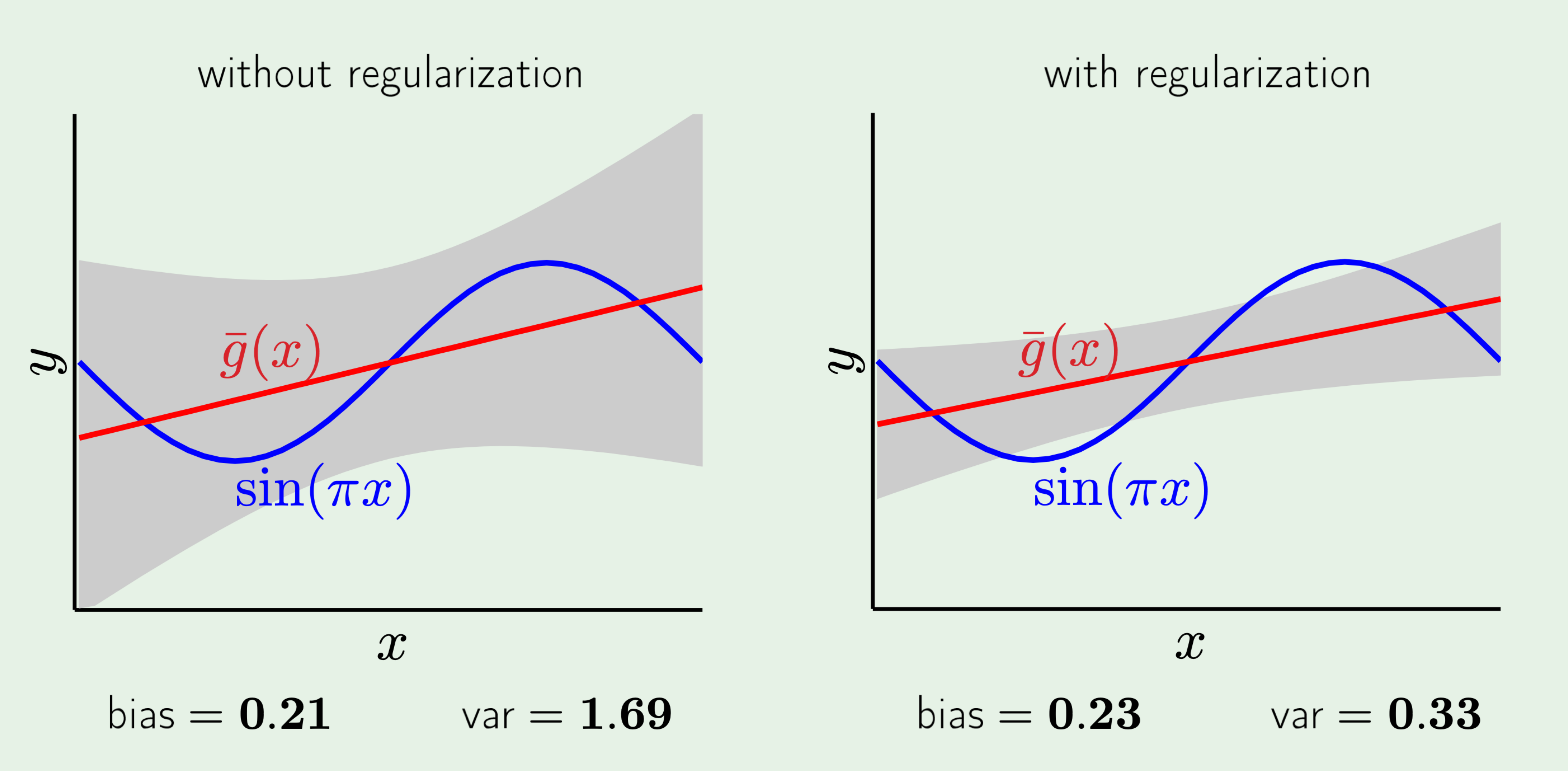


bias $=$ **0.21** var $=$ **1.69**

The sales pitch



The sales pitch

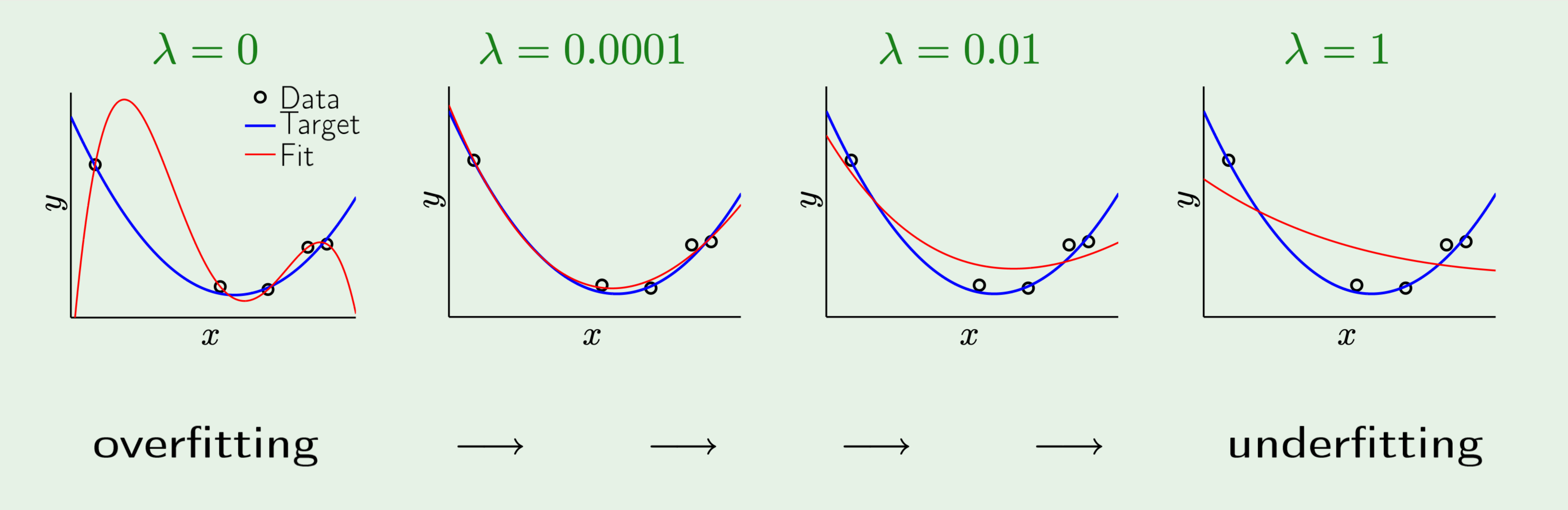


Preventing overfitting

- $\mathscr{H}_0$ can be thought of as a constrained version of $\mathscr{H}_1$ in which $w = 0$ in $h(x) = wx + b$
- This is a hard constraint on the model parameters
- Soft constraint: consider all hypotheses $wx + b$ such that $w^2 \leq A$ for some budget hyperparameter A
- w can be nonzero, but not too big
- Equivalently, minimize an augmented cost function $C(h) = \sum_{i=1}^{n} (h(x_i) - y_i)^2 + \lambda w^2$

Controlling the degree of fitting

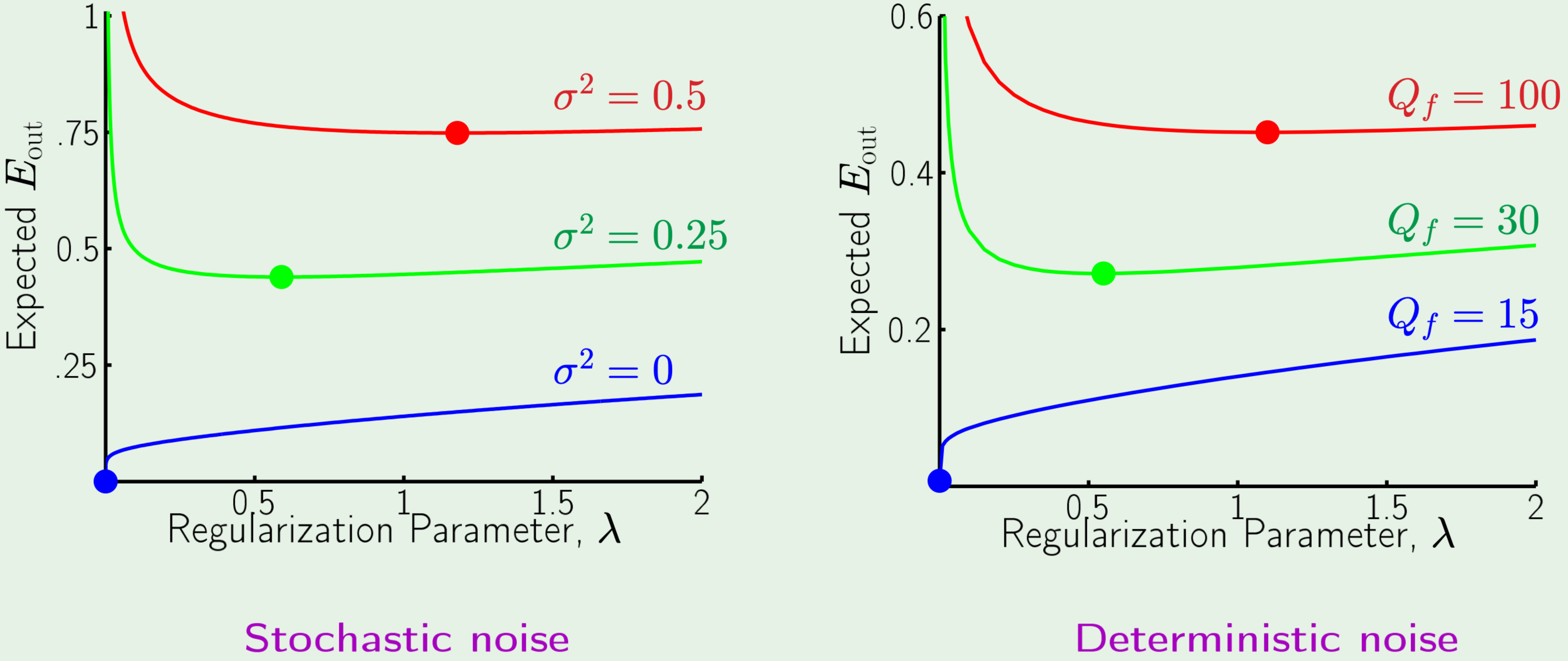
- λ is a regularization hyperparameter that controls the tradeoff between minimizing training error and using "reasonable" weights
- Large λ corresponds to small A



The regularizer, generalized

- More generally, if there are many weight parameters (as in a d degree polynomial regression model), $C(h) = \sum_{i=1}^{n} (h(x_i) - y_i)^2 + \lambda \sum_{j=1}^{d} w_j^2$
- This is called ℓ_2 regularization, because $\sum_{j=1}^{d} w_d^2 = \|w\|^2$ is the squared ℓ_2 norm of the weight vector

More noise requires more regularization



Early stopping is regularization

- The more SGD updates you make, the more opportunity the parameters have to become very large
- Early stopping is one way to prevent this growth in model complexity
- How do you know when to stop? Validation!