Bias-Variance Decomposition

Machine Learning- CS-433
1 Oct 2025
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(Slide credits: Martin Jaggi & Nicolas Flammarion)

EPFL

Last time

How can we judge if a given predictor is good?

How to select the best models of a family?

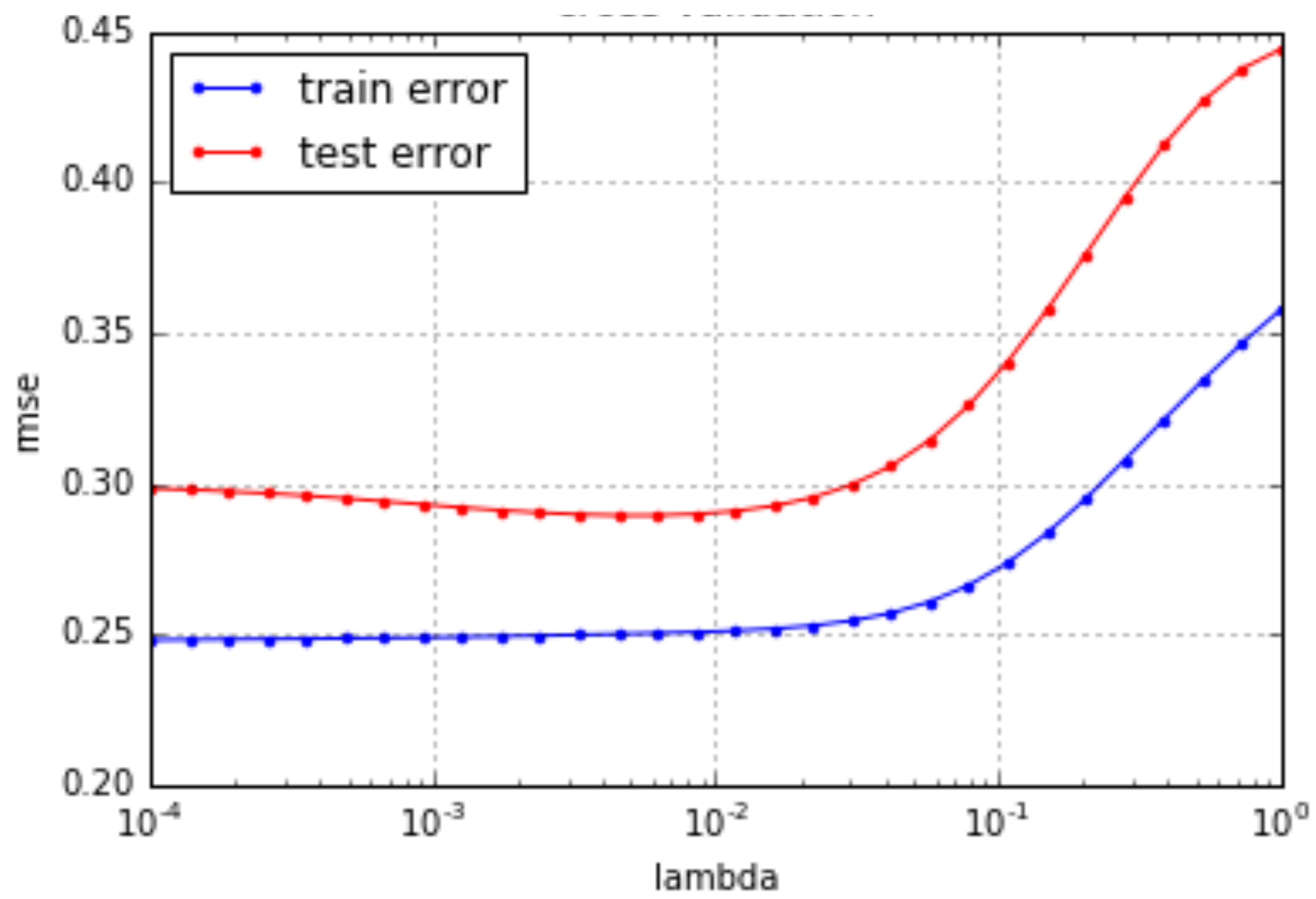
➡Bound the difference between the true and empirical risks

➡Split data into train and test sets (learn with the train and test on the test)

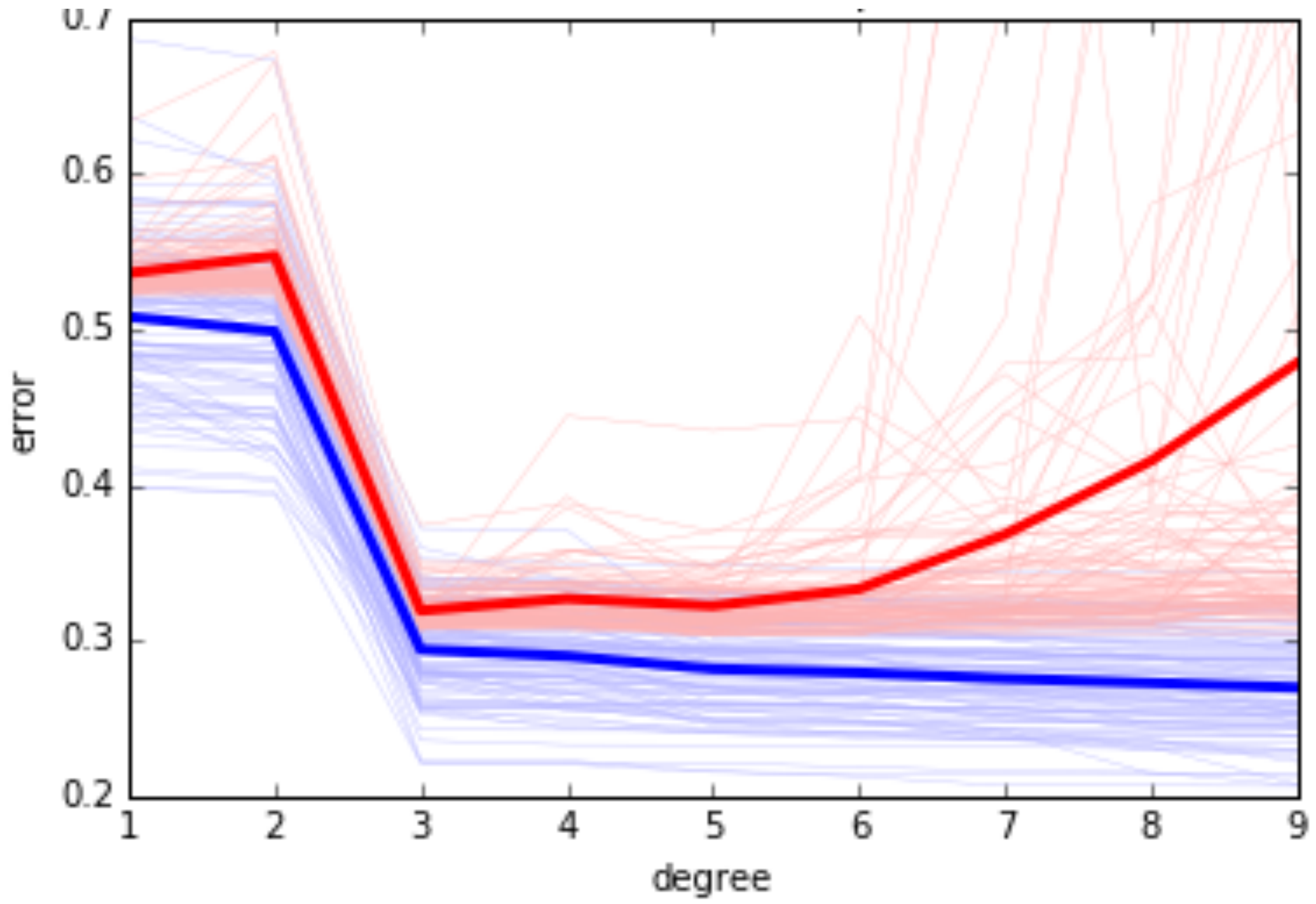
Motivation: Hyperparameter search (where hyperparameters often control model complexity)

But we haven’t investigated the role of the complexity of the class

Model selection curves

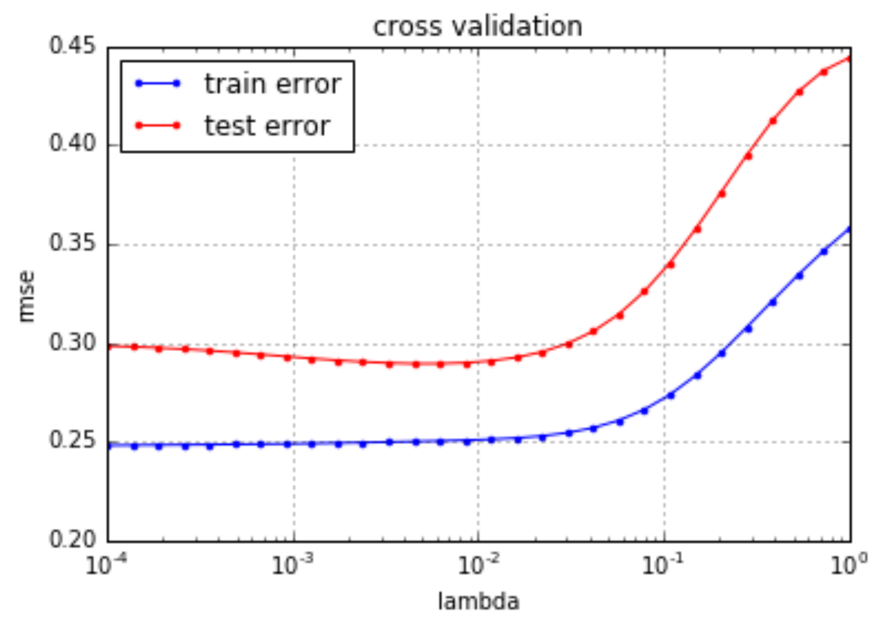


Ridge regression



Degree in case of a polynomial feature expansion

Today



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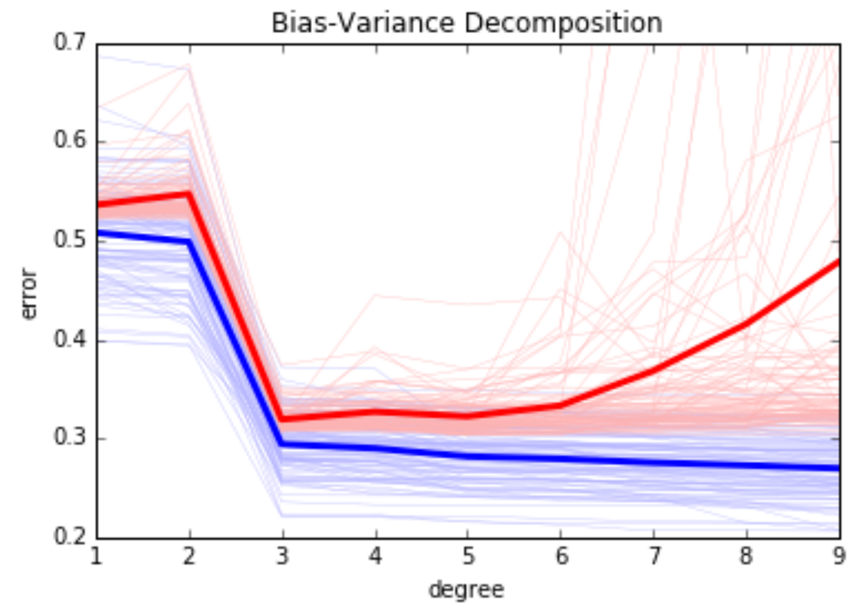


Polynomial feature expansion

How does the risk behave as a function of the complexity of the model class?

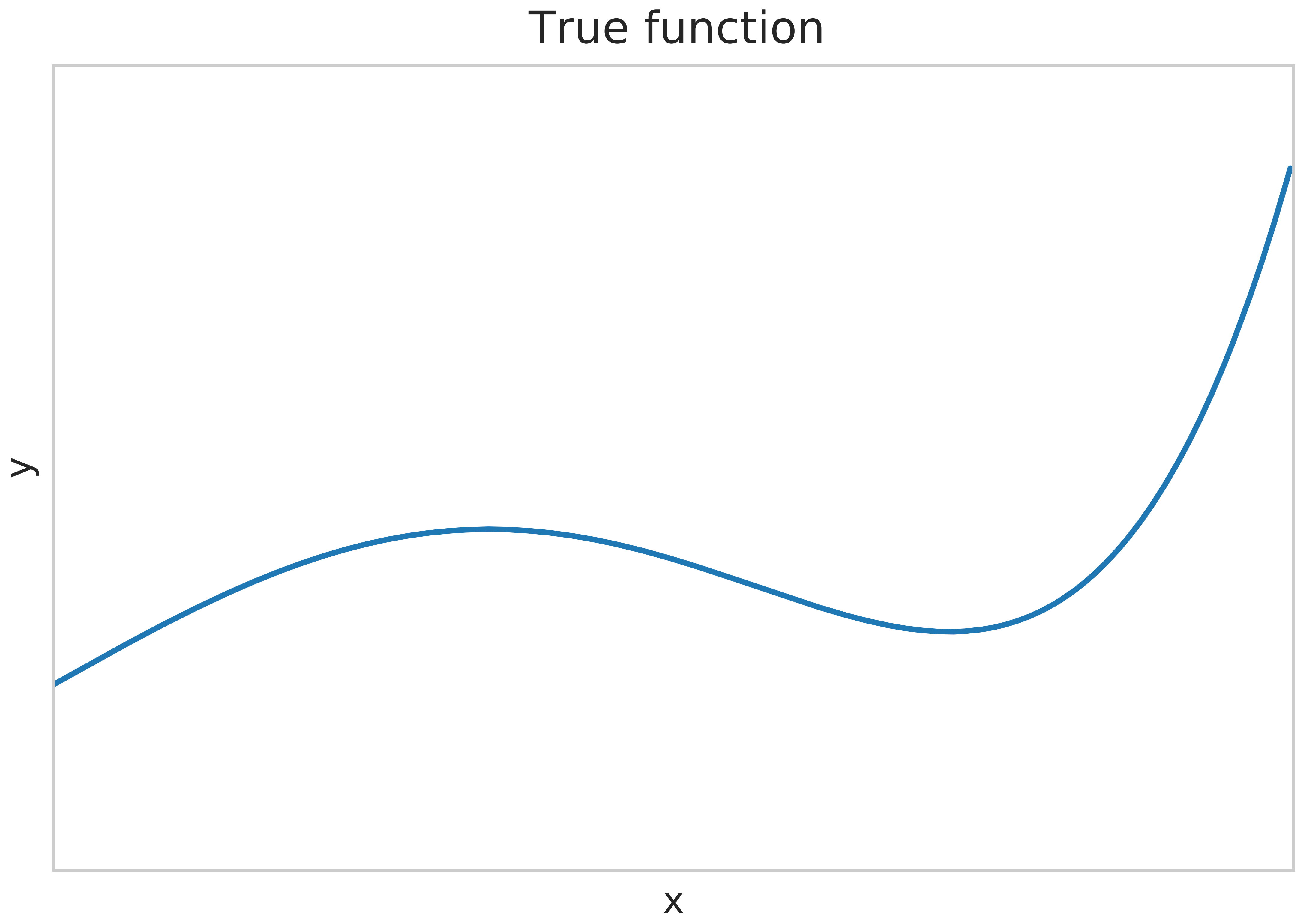
➡ ***Bias-Variance tradeoff***

It will help us to decide how complex and rich we should make our model

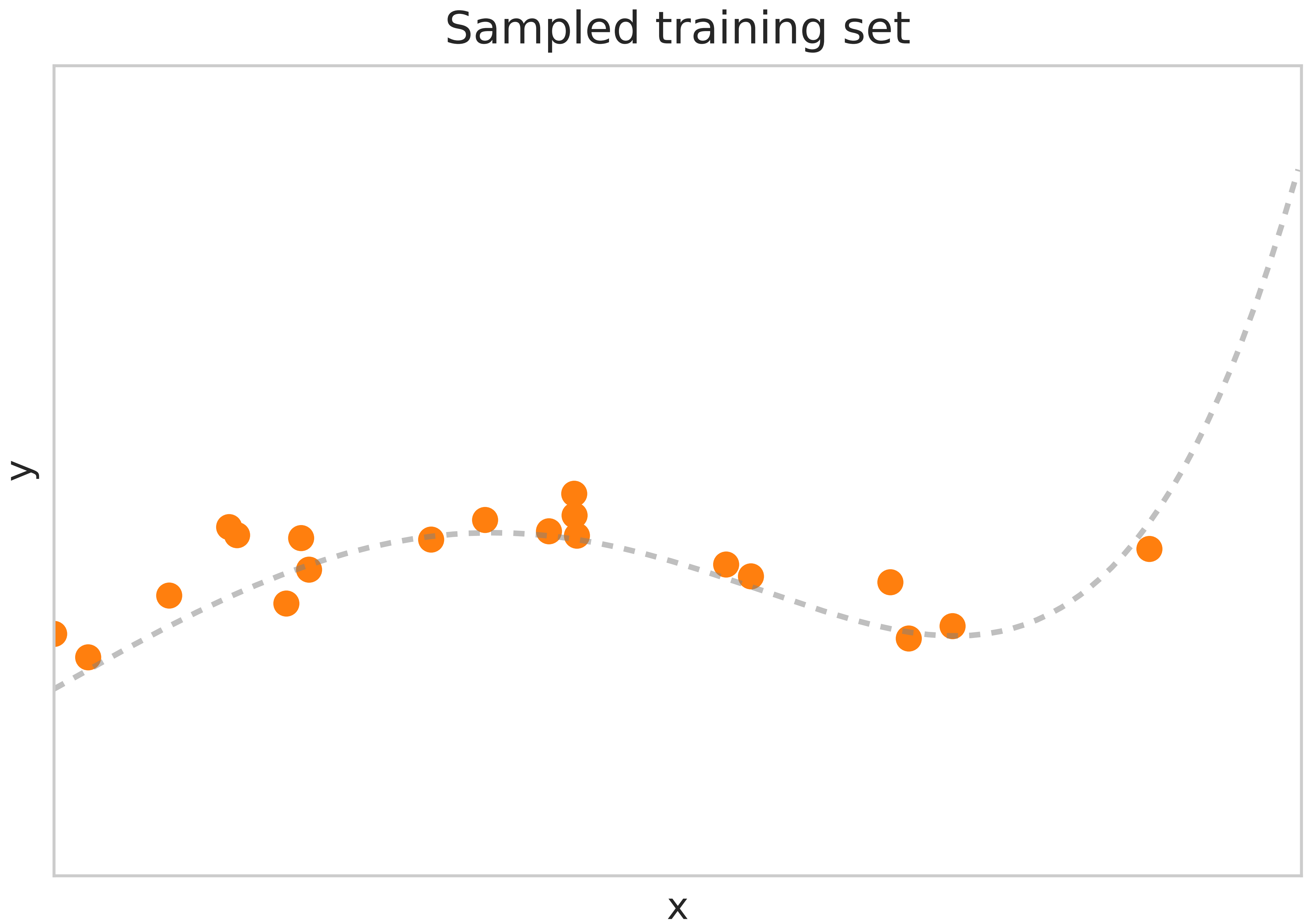
Before: quantitative

Now: ***qualitative***

A small experiment: 1D-regression



A small experiment: 1D-regression

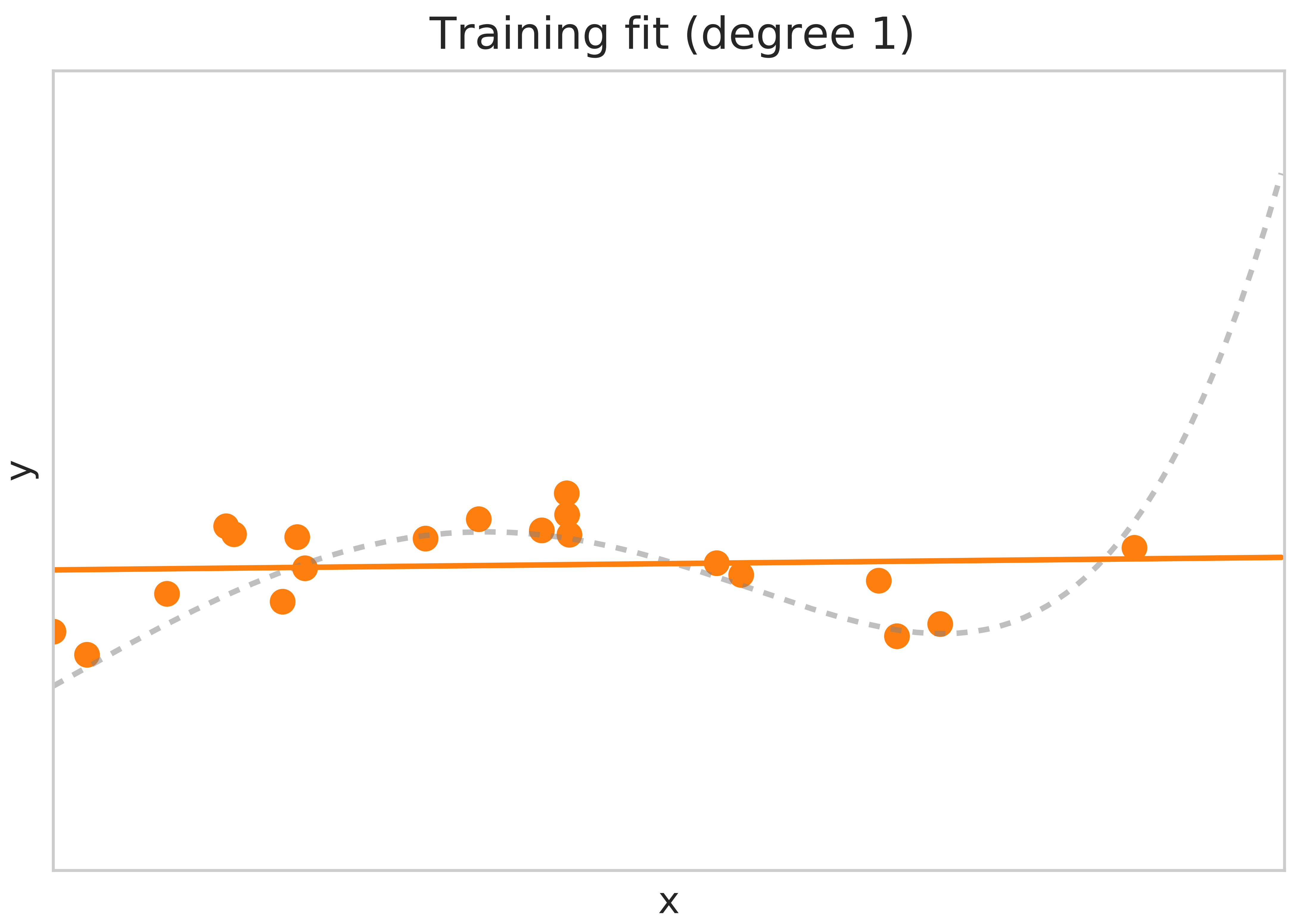


Linear regression using polynomial feature expansion $(x, x^2, x^3, \cdots, x^d)$

The maximum degree d measures the complexity of the class

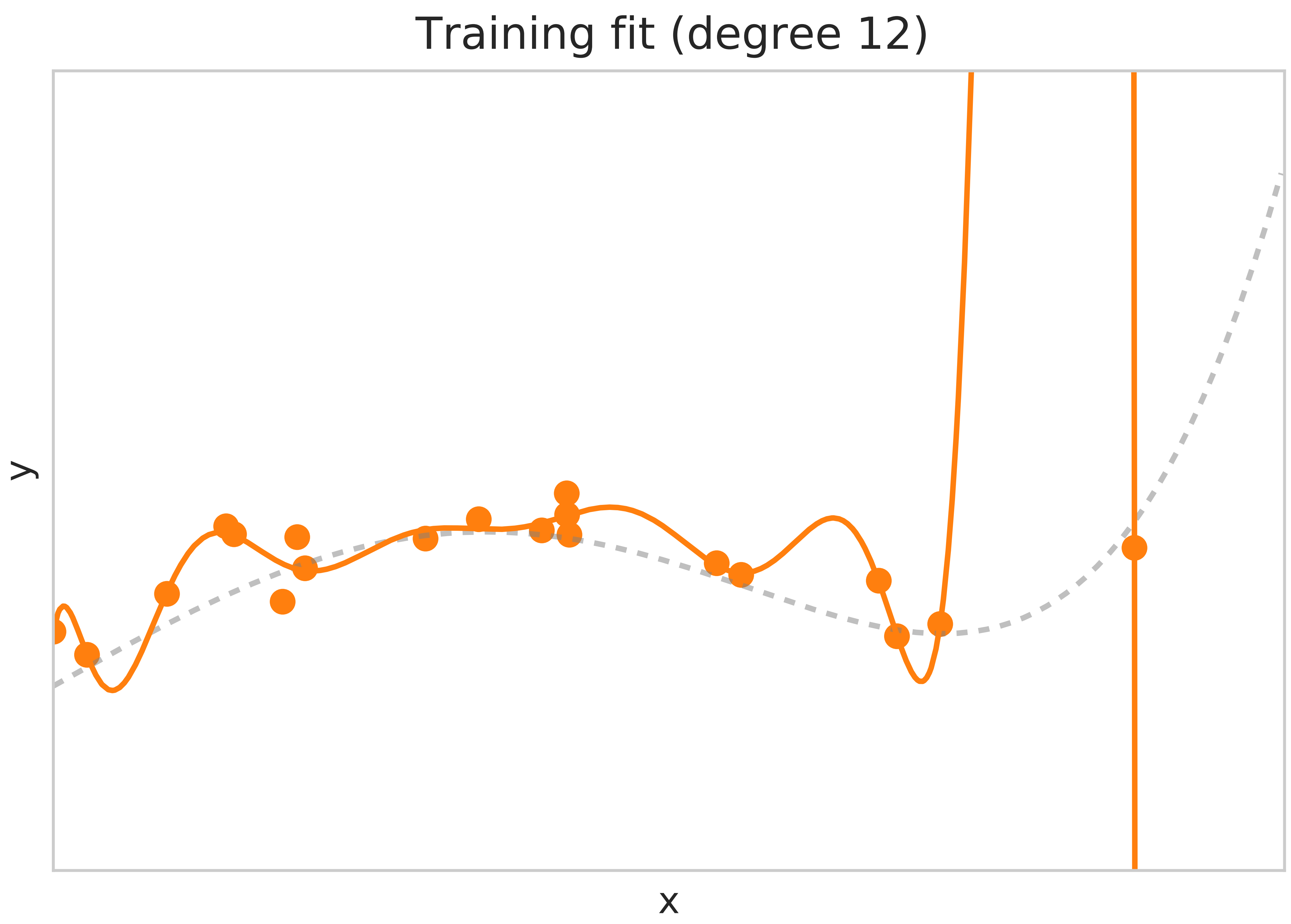
➡ How far should you go?

Simple model: bad fit



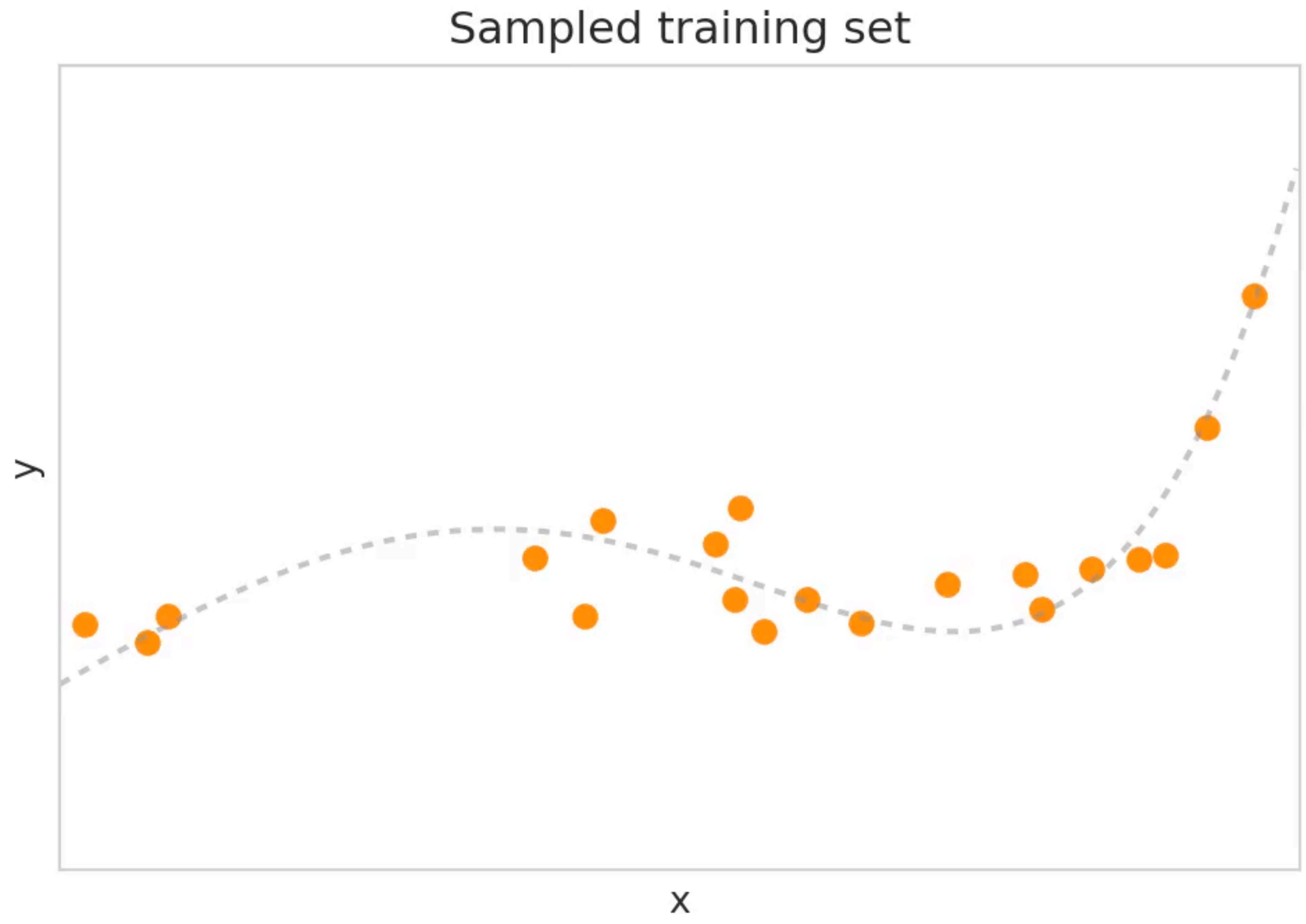
No linear function would be a good predictor. The model class is not rich enough

Complex model: good fit?



High degree polynomial will be a good fit. But?

But there is randomness in the data



We have observed one particular S_{train} but we could have observed several others!

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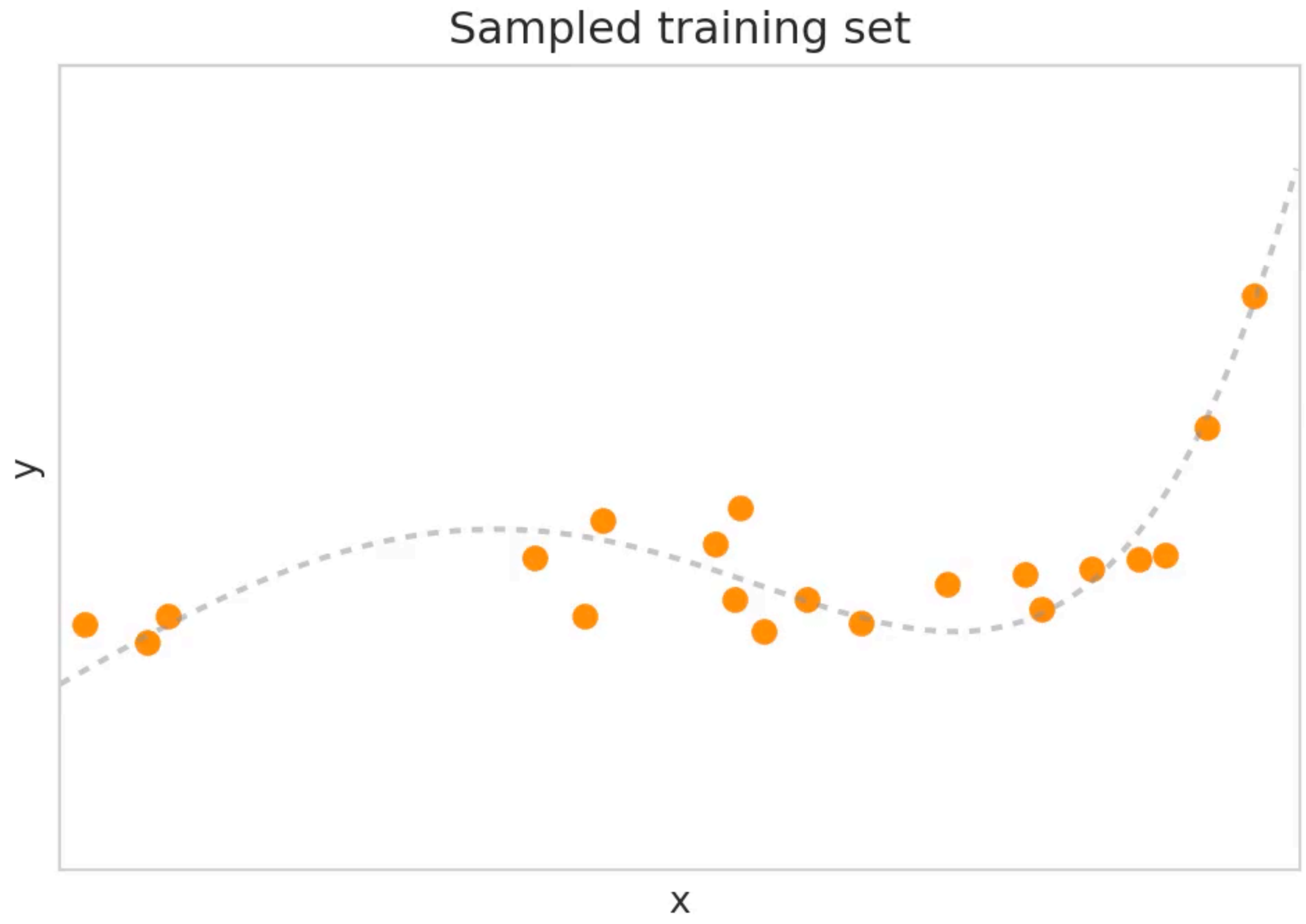

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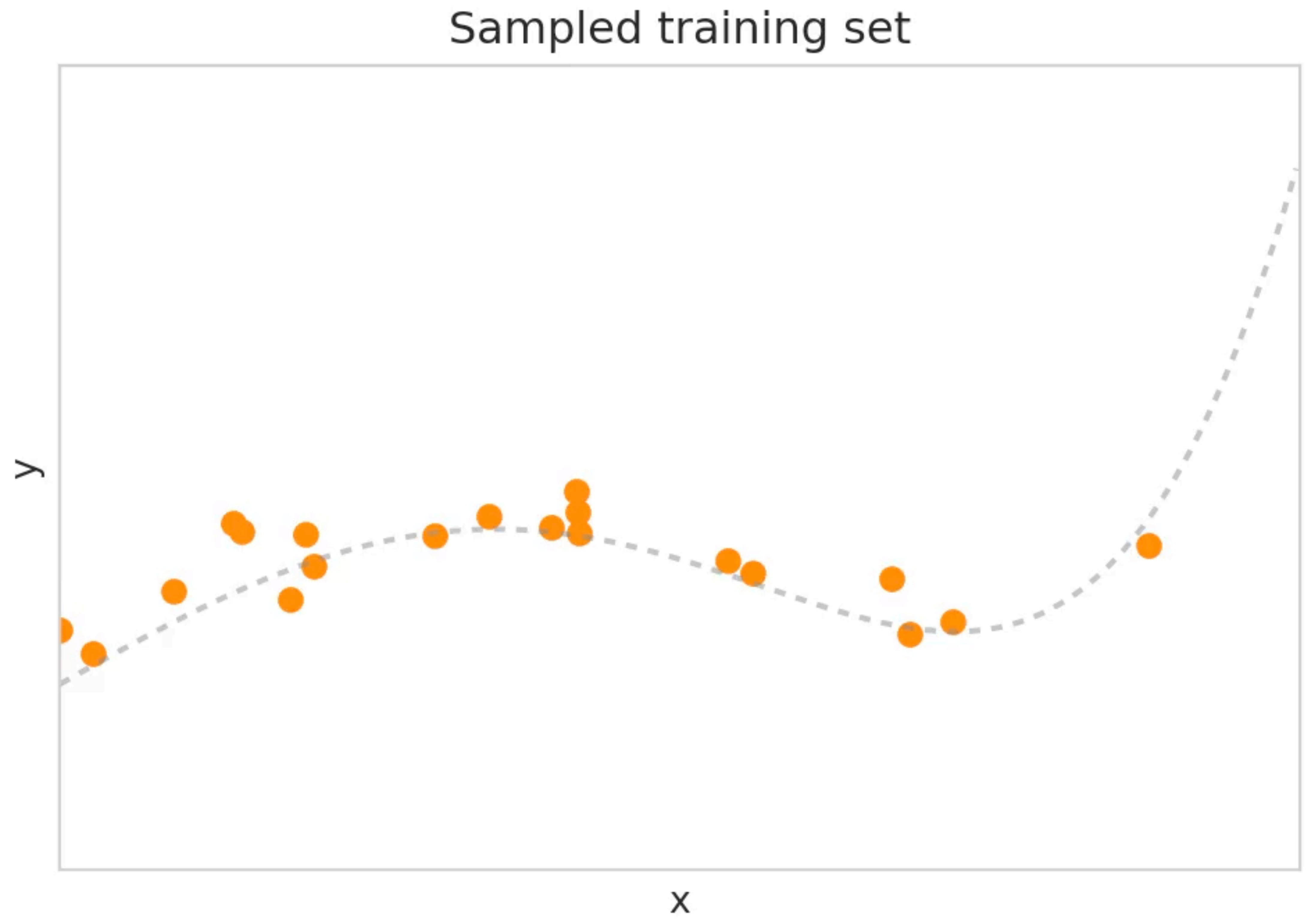

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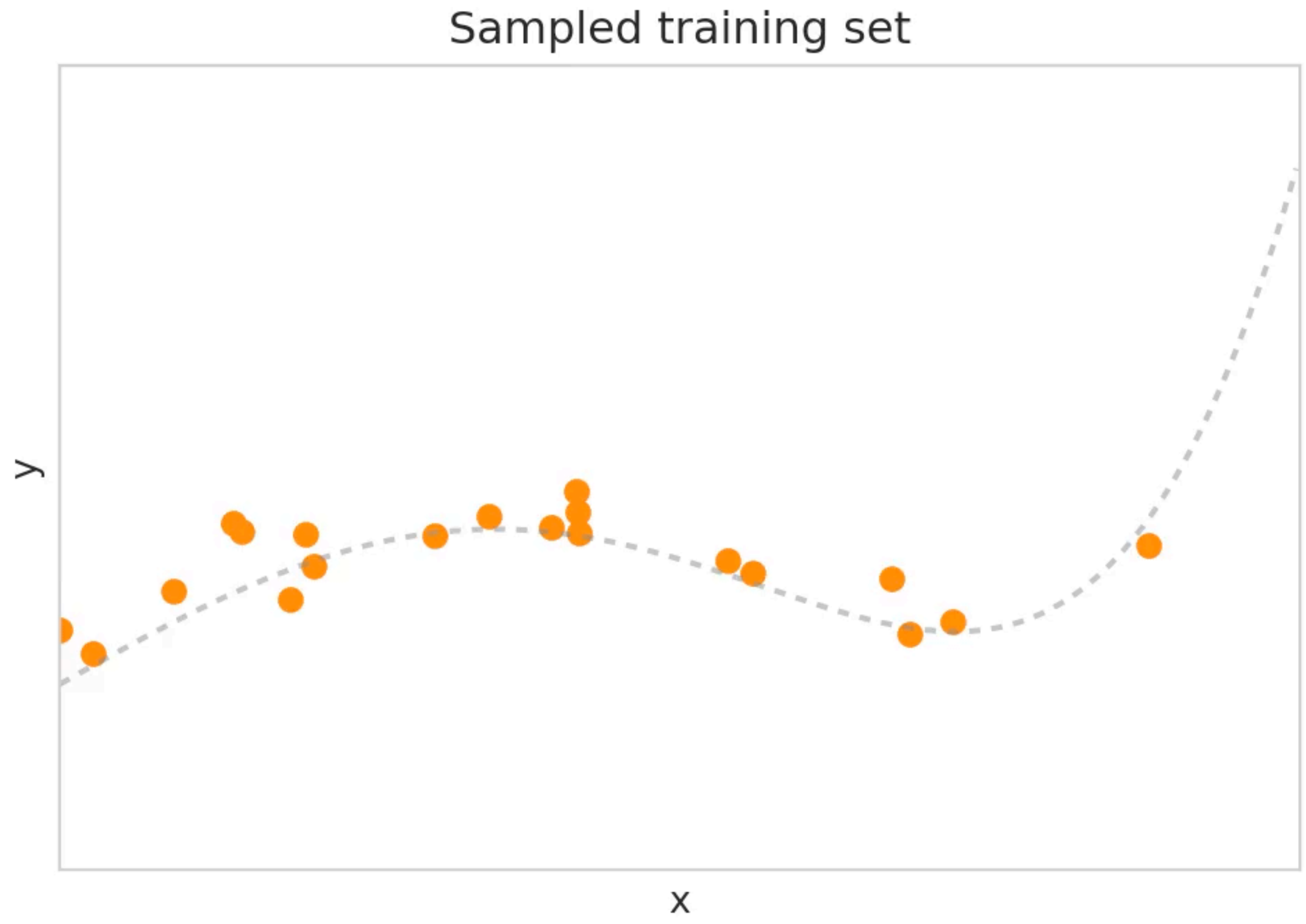

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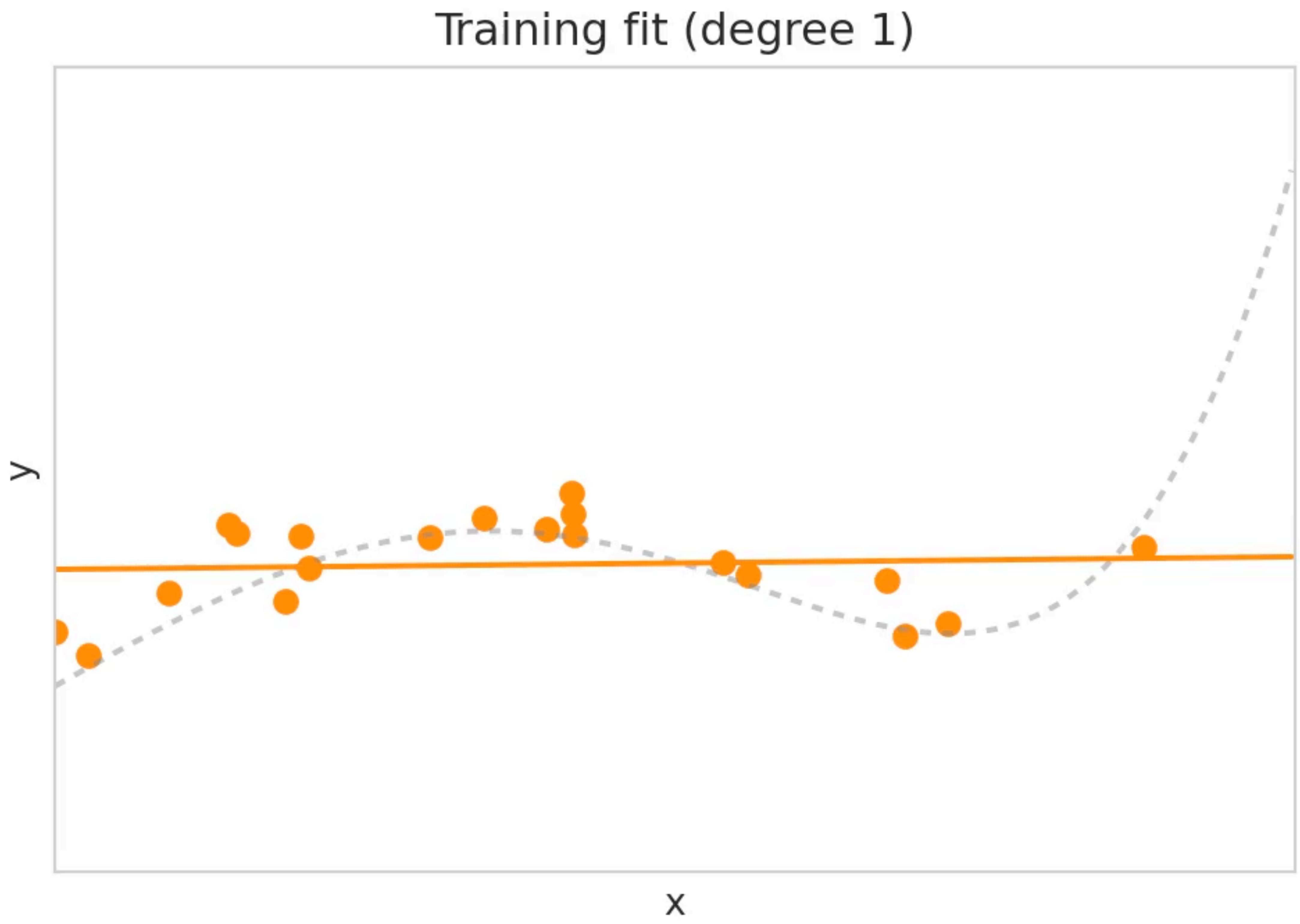
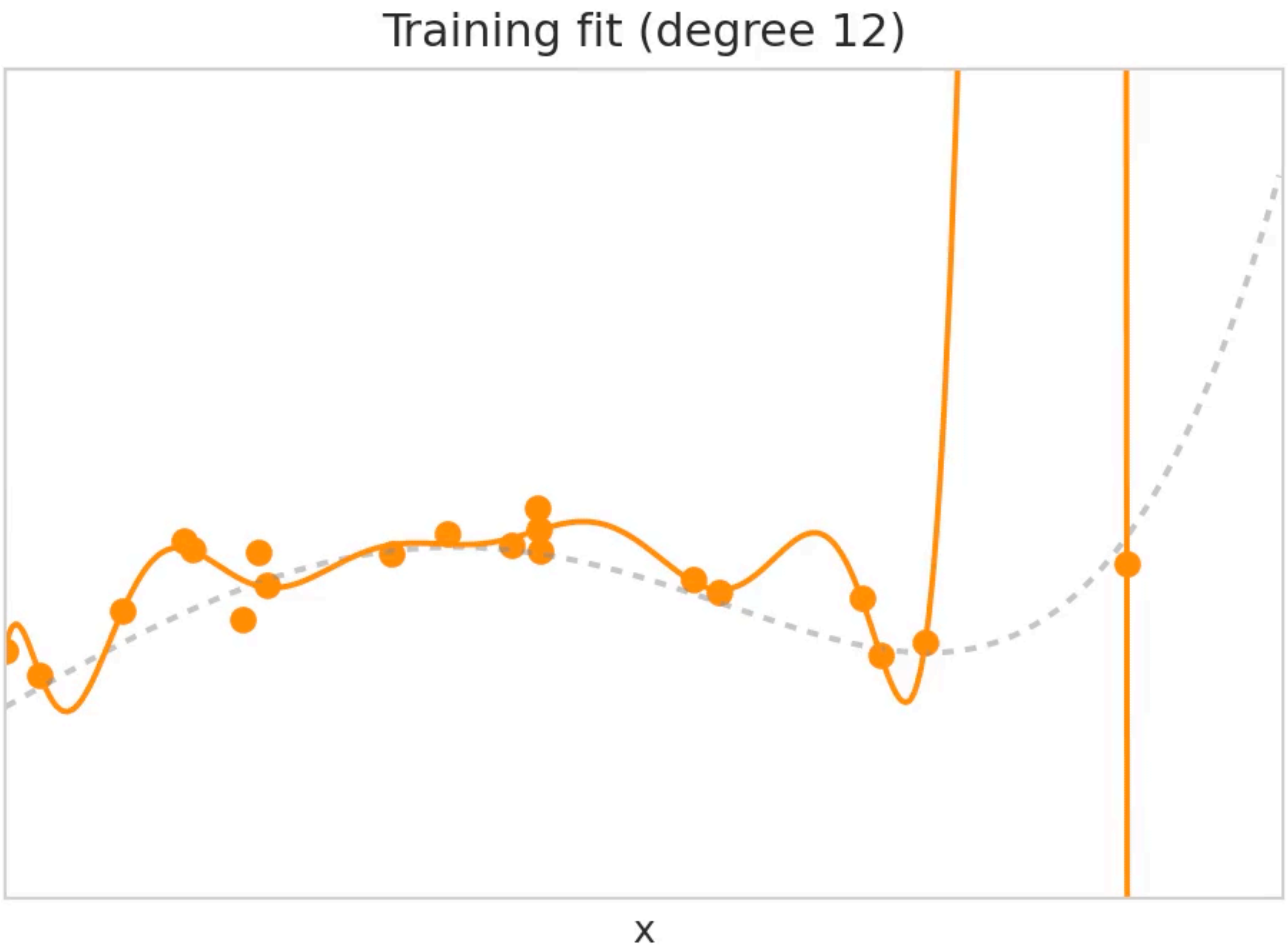


Moving a single observation will cause only a small shift in the position of the line

Underfitting



Changing one of the observations may change the prediction considerably

Overfitting

Simple models are less sensitive

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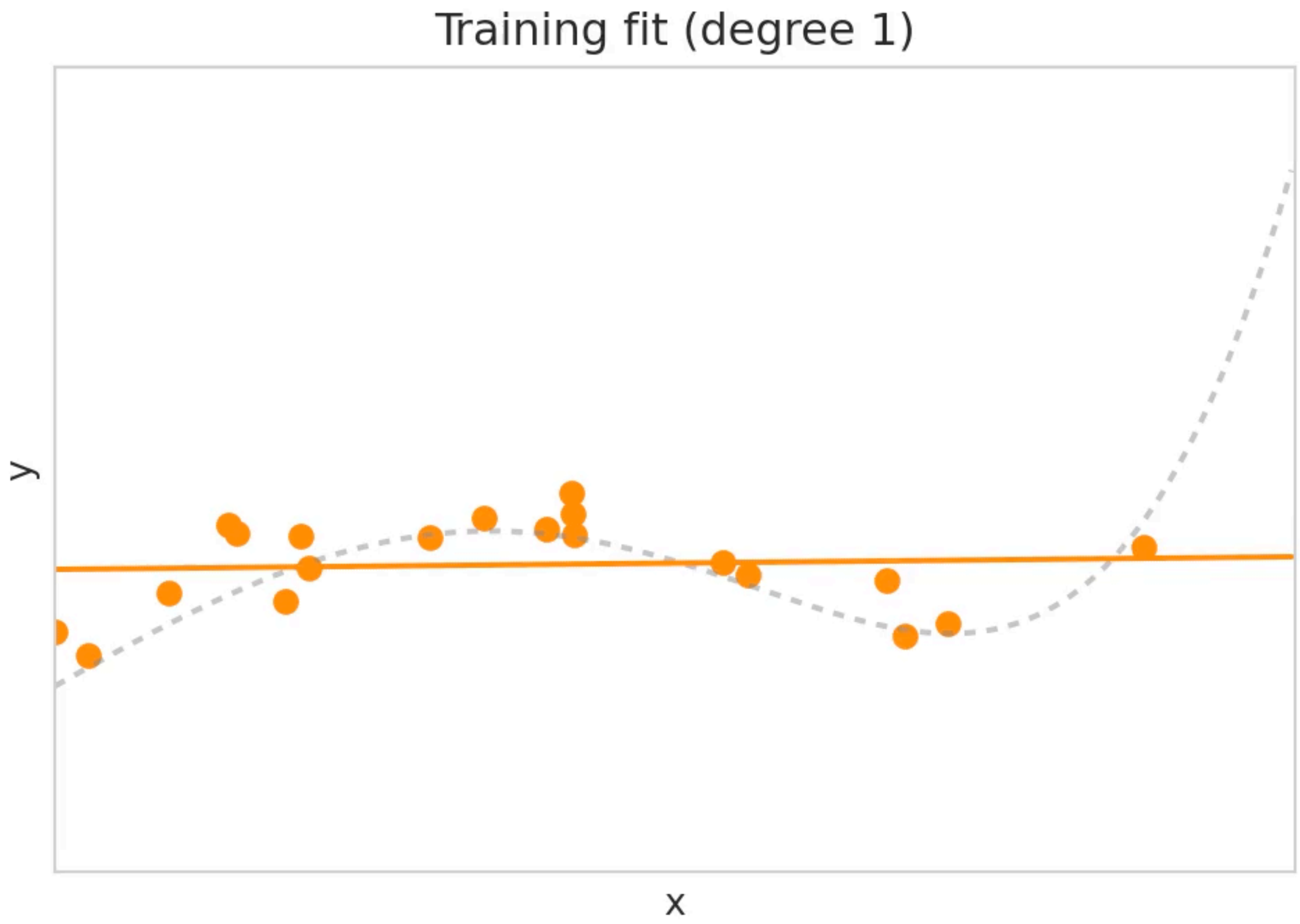

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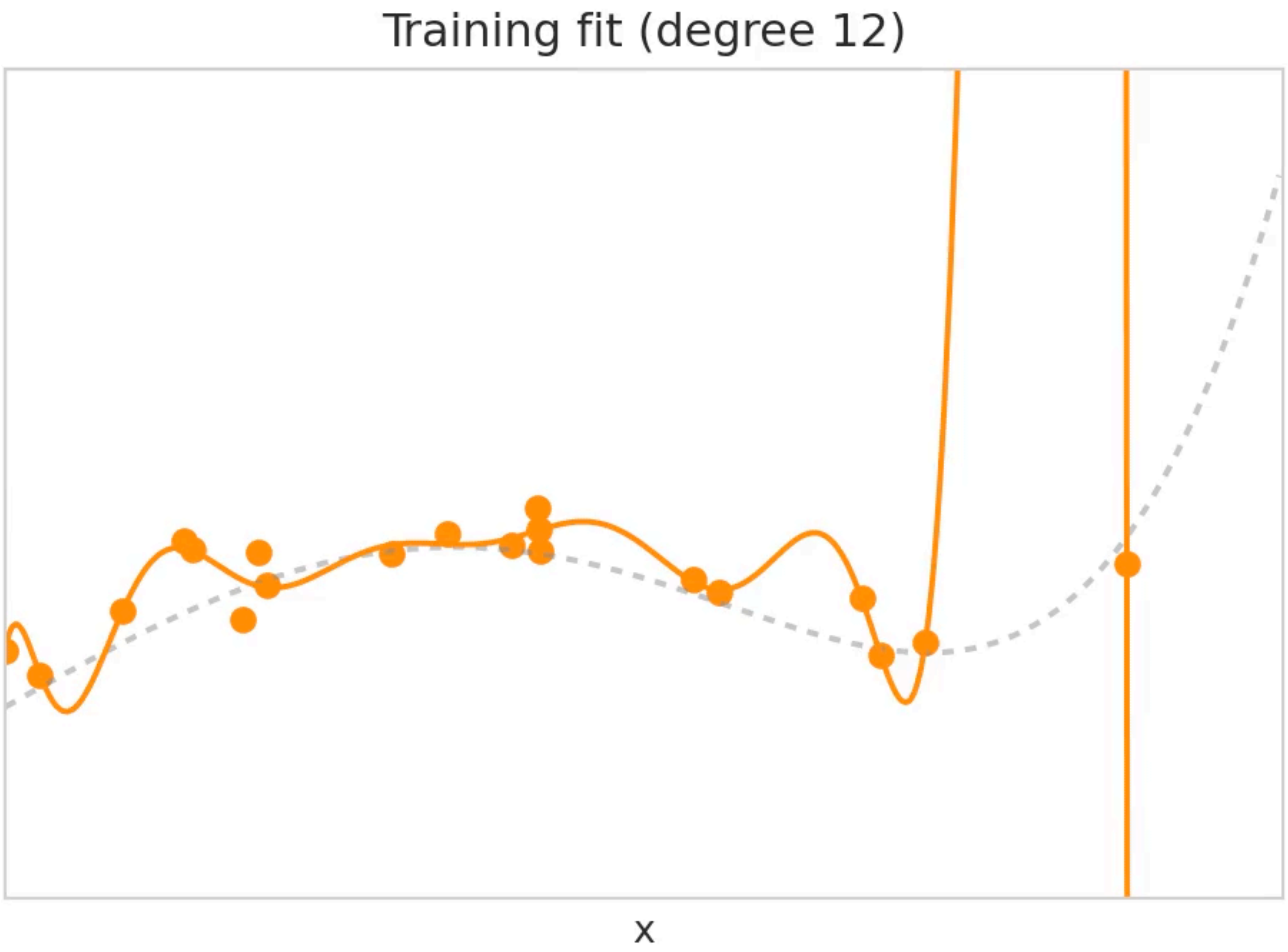

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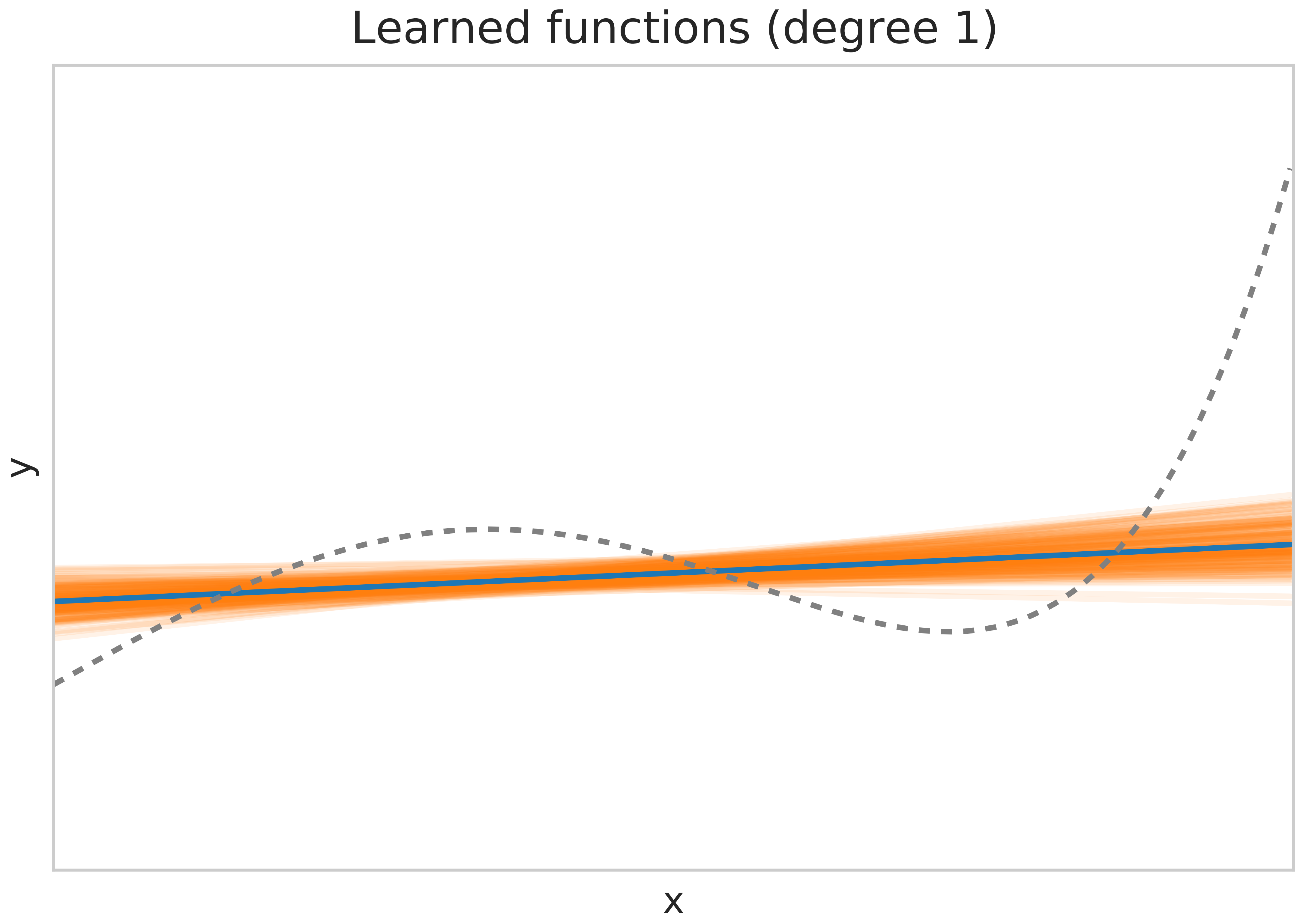
Overfitting

Simple models are less sensitive

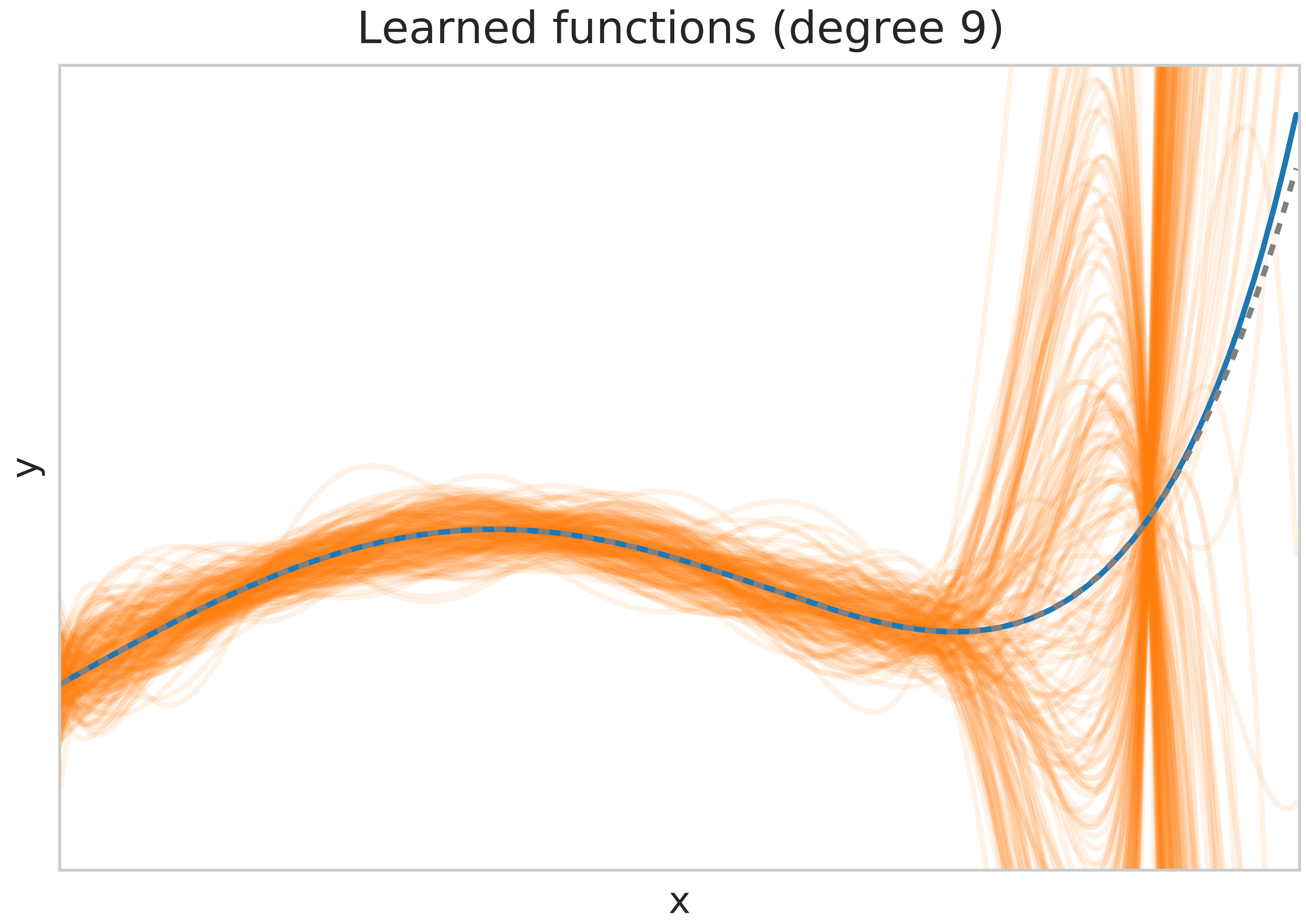
Simple models have large bias but low variance



The average of the predictions f_S does not fit the data well: **large bias**

The variance of the predictions f_S as a function of S is small: **small variance**

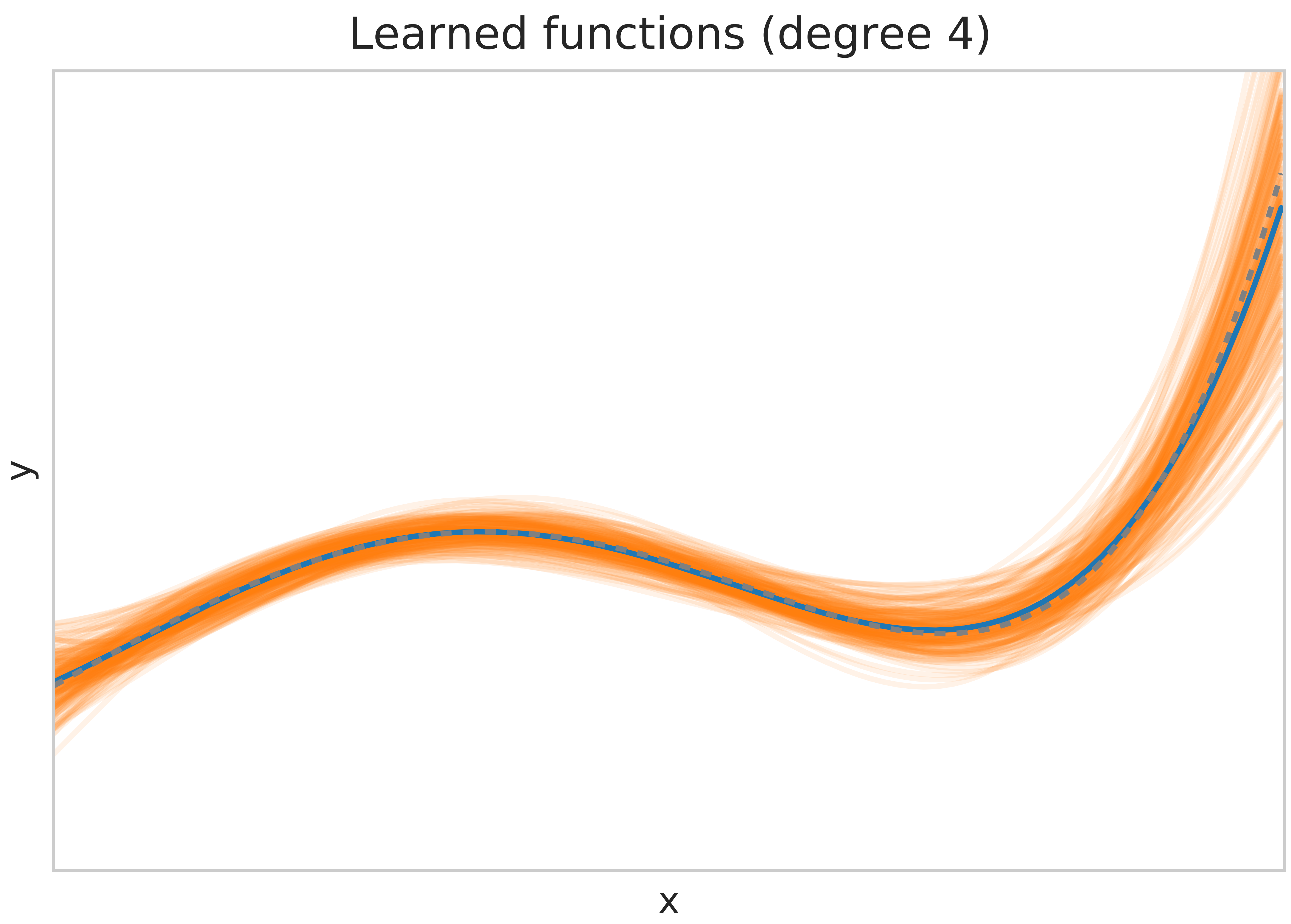
Complex models have low bias but high variance



The average of the predictions f_S fits the data well: **small bias**

The variance of the predictions f_S as a function of S is large: **large variance**

We need to balance bias & variance correctly



Data model: output perturbed by some noise

Output

True model perturbed by some noise

Joint distribution $(x, y) \sim \mathcal{D}$

$$y = f(x) + \varepsilon$$

True model

f arbitrary and unknown function

The model is generally **not realizable**,

i.e., f is not in our model class

Input

$x \sim \mathcal{D}_x$

(fixed but unknown)

Noise

$\varepsilon \sim \mathcal{D}_\varepsilon$ i.i.d.,

independent of x

$\mathbb{E}[\varepsilon] = 0$

We consider the square loss and will provide a decomposition of the true error

Error Decomposition

$S = \{(x_n, y_n)\}_{n=1}^{N} \sim \mathcal{D}$ i.i.d. $\qquad \mathcal{A} \qquad f_S = \mathcal{A}(S)$

We are interested in how the ***expected error*** of f_S:

$$\mathbb{E}_{(x,y)\sim\mathcal{D}}[(y - f_S(x))^2]$$

behaves as a ***function of the train set*** S and model class complexity

Error Decomposition

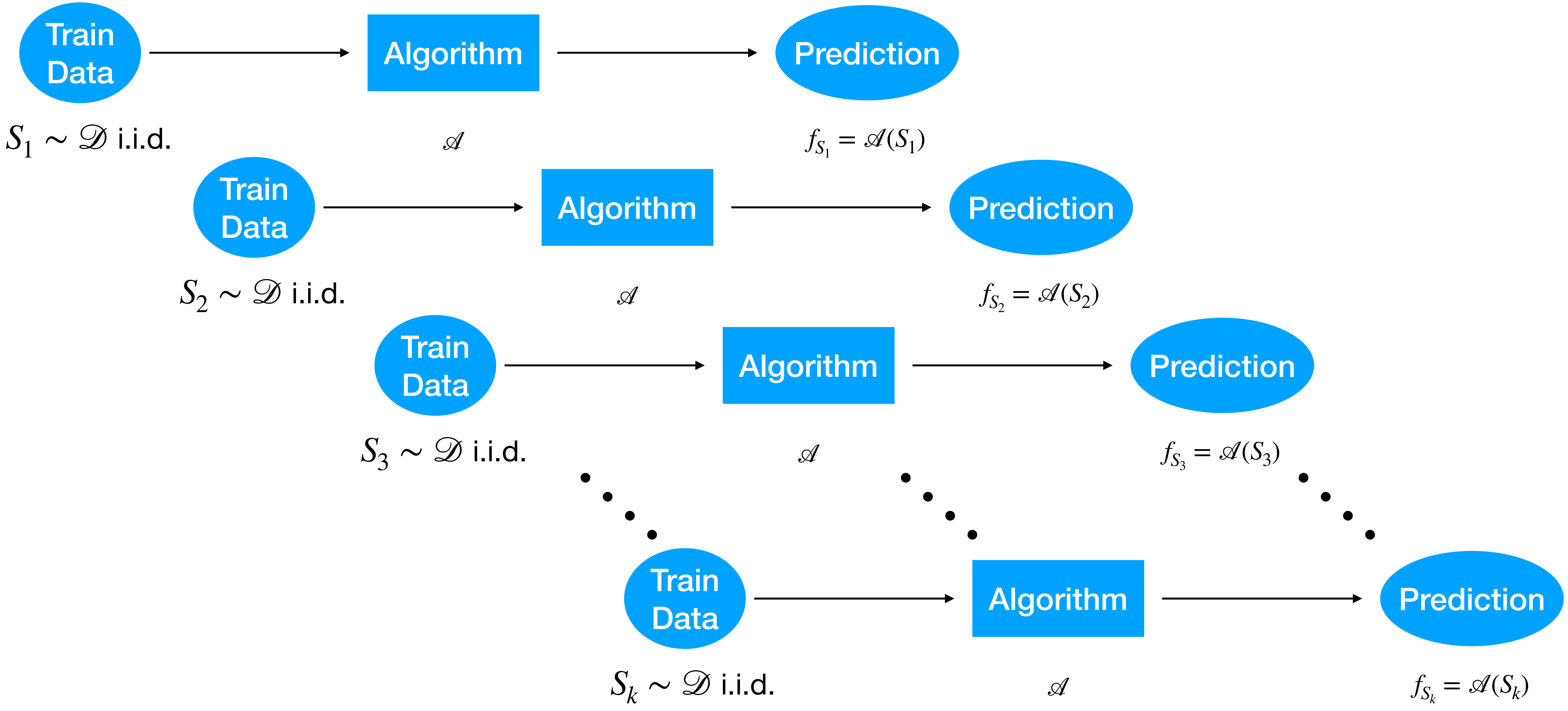
$S = \{(x_n, y_n)\}_{n=1}^{N} \sim \mathscr{D}$ i.i.d. $\qquad \mathscr{A} \qquad f_S = \mathscr{A}(S)$

The decomposition will hold true at ***every single point*** x. Therefore, to simplify, we consider the expected error of f_S for a fixed element x_0:

$$L(f_S) = \mathbb{E}_{\varepsilon \sim \mathscr{D}_\varepsilon}[(f(x_0) + \varepsilon - f_S(x_0))^2]$$

This is a random variable. The randomness comes for the train set S

We run the experiment many times



We are interested in the ***average*** and the ***variance*** of the ***predictions*** $(f_{S_1}, \cdots, f_{S_k})$ over these multiple runs

A decomposition in three terms

We are interested in the expectation of the true risk over the training set S

$$\mathbb{E}_{S \sim \mathcal{D}}[L(f_S)] = \mathbb{E}_{S \sim \mathcal{D}}\left[\mathbb{E}_{\varepsilon \sim \mathcal{D}_\varepsilon}[(f(x_0) + \varepsilon - f_S(x_0))^2]\right]$$
$$= \mathbb{E}_{S \sim \mathcal{D}, \varepsilon \sim \mathcal{D}_\varepsilon}[(f(x_0) + \varepsilon - f_S(x_0))^2]$$

We will decompose this quantity in ***three non-negative terms*** and will interpret each of these terms

First we expand the square:

$$\mathbb{E}_{S\sim\mathcal{D},\,\varepsilon\sim\mathcal{D}_\varepsilon}[(f(x_0)+\varepsilon-f_S(x_0))^2] = \mathbb{E}_{\varepsilon\sim\mathcal{D}_\varepsilon}[\varepsilon^2]$$
$$+2\mathbb{E}_{S\sim\mathcal{D},\,\varepsilon\sim\mathcal{D}_\varepsilon}[\varepsilon(f(x_0)-f_S(x_0))]$$
$$+\mathbb{E}_{S\sim\mathcal{D}}[(f(x_0)-f_S(x_0))^2]$$

Using that $\mathbb{E}_{\varepsilon\sim\mathcal{D}_\varepsilon}[\varepsilon]=0$ and $\varepsilon \perp\!\!\!\perp S$:

- $\mathbb{E}_{\varepsilon\sim\mathcal{D}_\varepsilon}[\varepsilon^2] = \mathsf{Var}_{\varepsilon\sim\mathcal{D}_\varepsilon}[\varepsilon]$
- $\mathbb{E}_{S\sim\mathcal{D},\,\varepsilon\sim\mathcal{D}_\varepsilon}[\varepsilon(f(x_0)-f_S(x_0))] = \mathbb{E}_{\varepsilon\sim\mathcal{D}_\varepsilon}[\varepsilon]\cdot\mathbb{E}_{S\sim\mathcal{D}}[f(x_0)-f_S(x_0)] = 0$

Therefore

$$\boxed{\mathbb{E}_{S\sim\mathcal{D},\,\varepsilon\sim\mathcal{D}_\varepsilon}[(f(x_0)+\varepsilon-f_S(x_0))^2] = \mathsf{Var}_{\varepsilon\sim\mathcal{D}_\varepsilon}[\varepsilon] + \mathbb{E}_{S\sim\mathcal{D}}[(f(x_0)-f_S(x_0))^2]}$$

Trick: we add and subtract the constant term $\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]$, where S' is a second training set independent from S

$$\mathbb{E}_{S\sim\mathscr{D}}[(f(x_0)-f_S(x_0))^2] = \mathbb{E}_{S\sim\mathscr{D}}\left[(f(x_0)-\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]+\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]-f_S(x_0))^2\right]$$

$$= \mathbb{E}_{S\sim\mathscr{D}}\Big[(f(x_0)-\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)])^2+(\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]-f_S(x_0))^2$$

$$+2(f(x_0)-\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)])(\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]-f_S(x_0))\Big]$$

Cross-term:

$$\mathbb{E}_{S\sim\mathscr{D}}\Big[\big(f(x_0)-\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]\big)\cdot\big(\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]-f_S(x_0)\big)\Big]$$

$$= \big(f(x_0)-\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]\big)\cdot\mathbb{E}_{S\sim\mathscr{D}}\big[(\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]-f_S(x_0))\big]$$

$$= \big(f(x_0)-\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]\big)\cdot\big(\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]-\mathbb{E}_{S\sim\mathscr{D}}[f_S(x_0)]\big) = 0.$$

$$\boxed{\mathbb{E}_{S\sim\mathscr{D}}[(f(x_0)-f_S(x_0))^2] = (f(x_0)-\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)])^2+\mathbb{E}_{S\sim\mathscr{D}}[(\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]-f_S(x_0))^2]}$$

Bias-Variance Decomposition

We obtain the following decomposition into three positive terms:

$$\mathbb{E}_{S\sim\mathscr{D},\,\varepsilon\sim\mathscr{D}_\varepsilon}[(f(x_0)+\varepsilon-f_S(x_0))^2] \quad = \quad \mathrm{Var}_{\varepsilon\sim\mathscr{D}_\varepsilon}[\varepsilon] \longleftarrow \textbf{Noise variance}$$

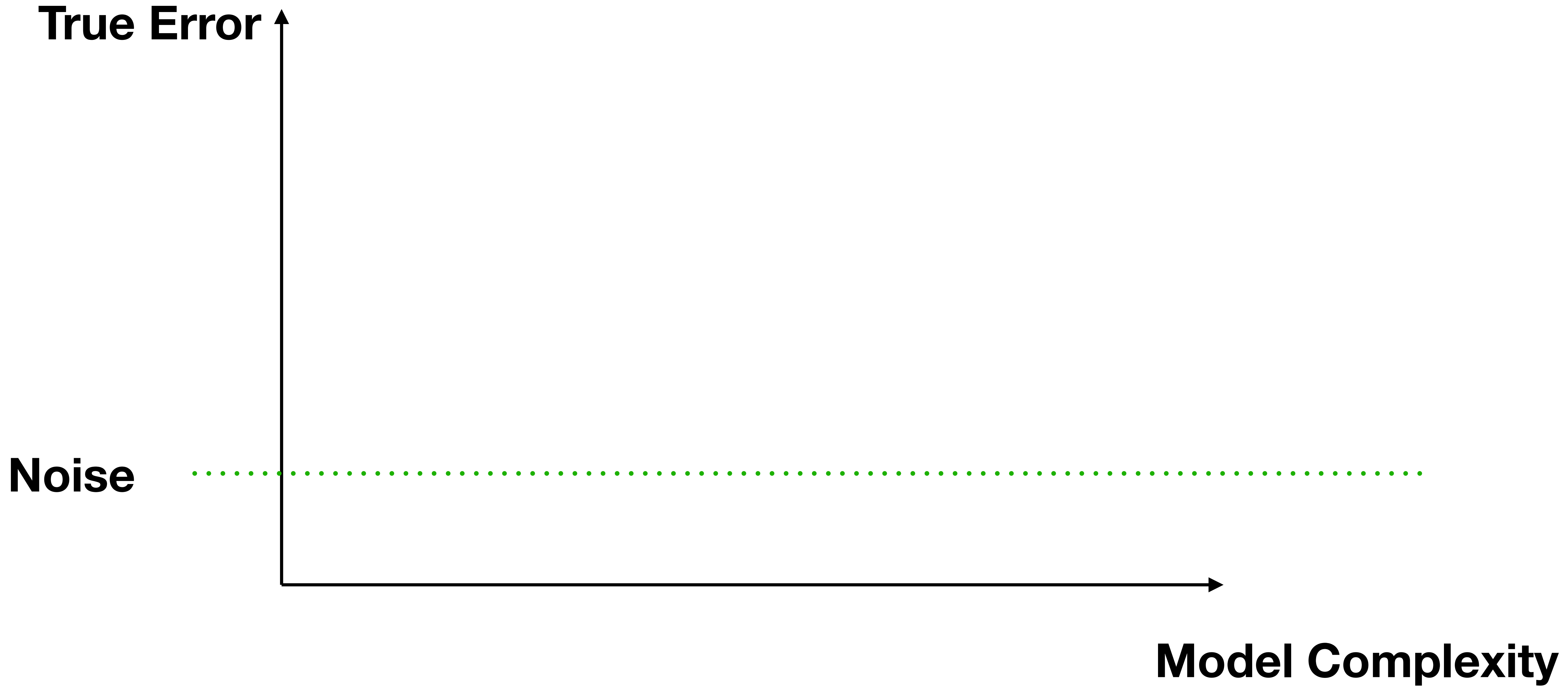
$$\textbf{Bias} \longrightarrow \quad + \quad (f(x_0)-\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)])^2$$

$$\textbf{Variance} \longrightarrow \quad + \quad \mathbb{E}_{S\sim\mathscr{D}}\left[(f_S(x_0)-\mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)])^2\right]$$

each of which always provides a lower bound of the true error

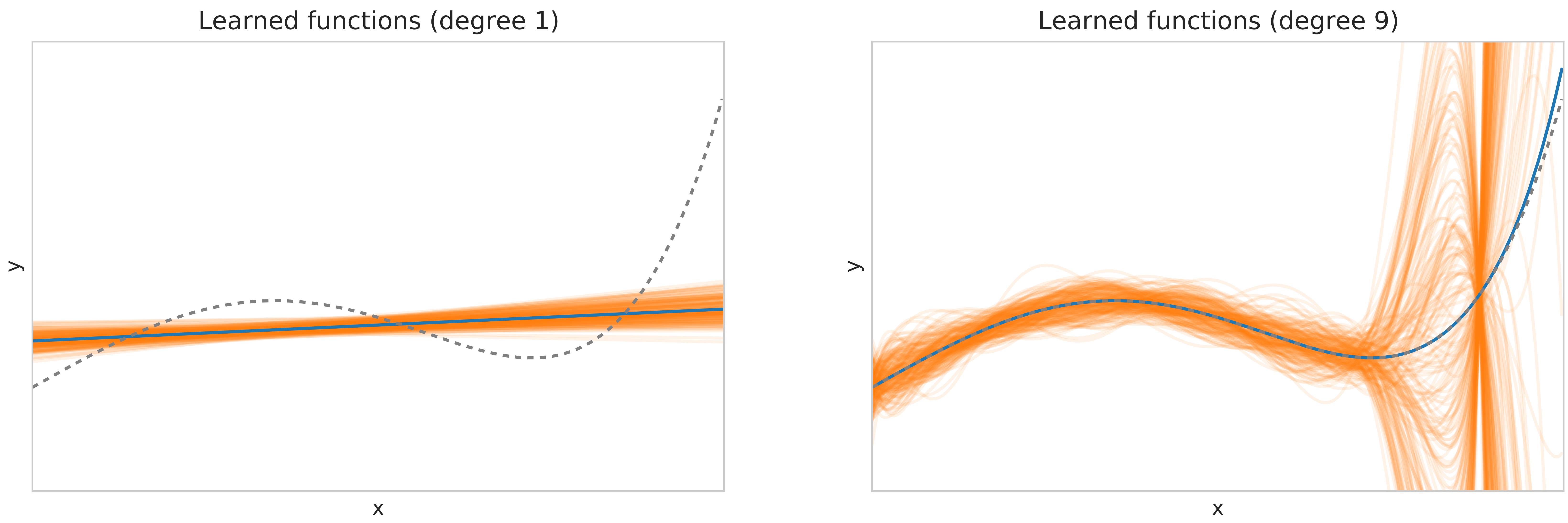
➡ To minimize the true error, we must choose a method that achieves **low bias and low variance** simultaneously

Noise: a strict lower bound on the achievable error



- It is not possible to go below the noise level
- Even if we know the true model f, we still suffer from the noise: $L(f) = \mathbb{E}[\varepsilon^2]$
- It is not possible to predict the noise from the data since they are independent

Bias: $(f(x_0) - \mathbb{E}_{S\sim\mathscr{D}}[f_S(x_0)])^2$



- Squared of the difference between the actual value $f(x_0)$ and the expected prediction
- It measures how far off in general the models' predictions are from the correct value
- If model **complexity** is **low**, **bias** is typically **high**
- If model **complexity** is **high**, **bias** is typically **low**

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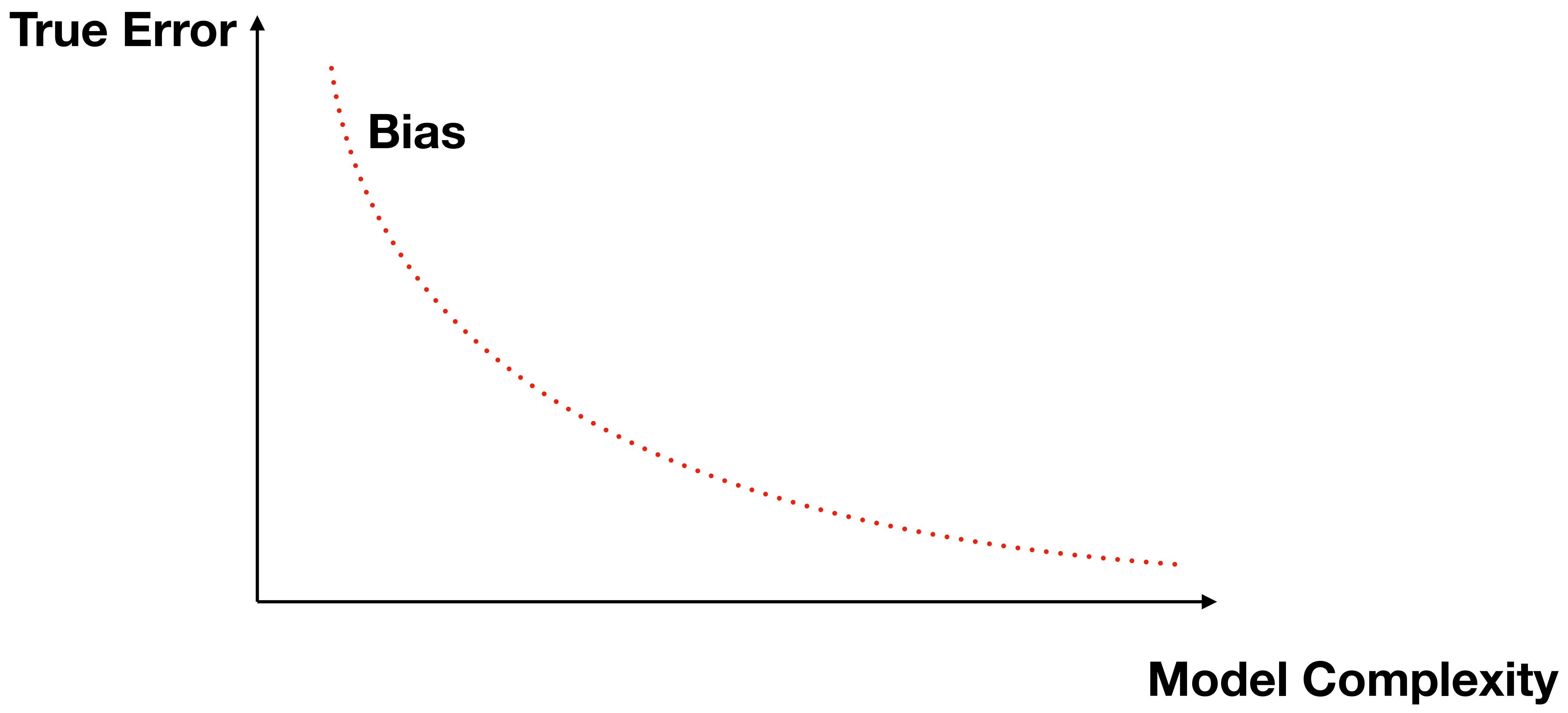

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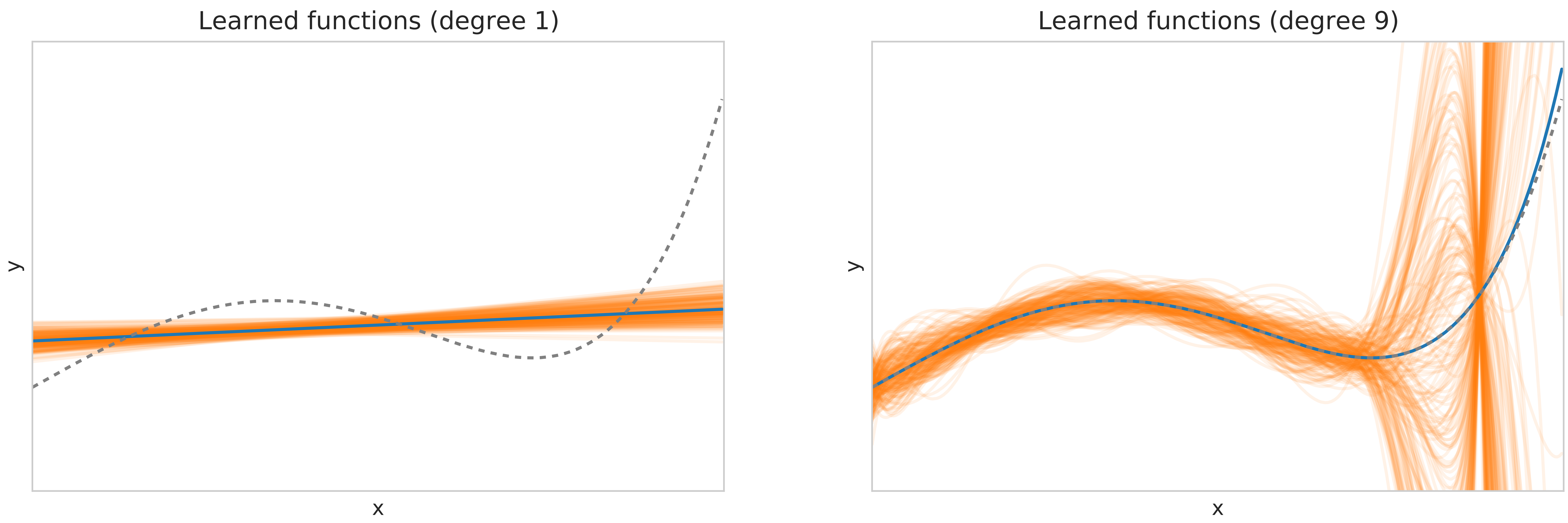
Variance: $\mathbb{E}_{S\sim\mathscr{D}}\left[\left(f_S(x_0) - \mathbb{E}_{S'\sim\mathscr{D}}[f_{S'}(x_0)]\right)^2\right]$



- Variance of the prediction function
- It measures the variability of predictions at a given point across different training set realizations
- If we consider complex models, small variations in the training set can lead to significant changes in the predictions

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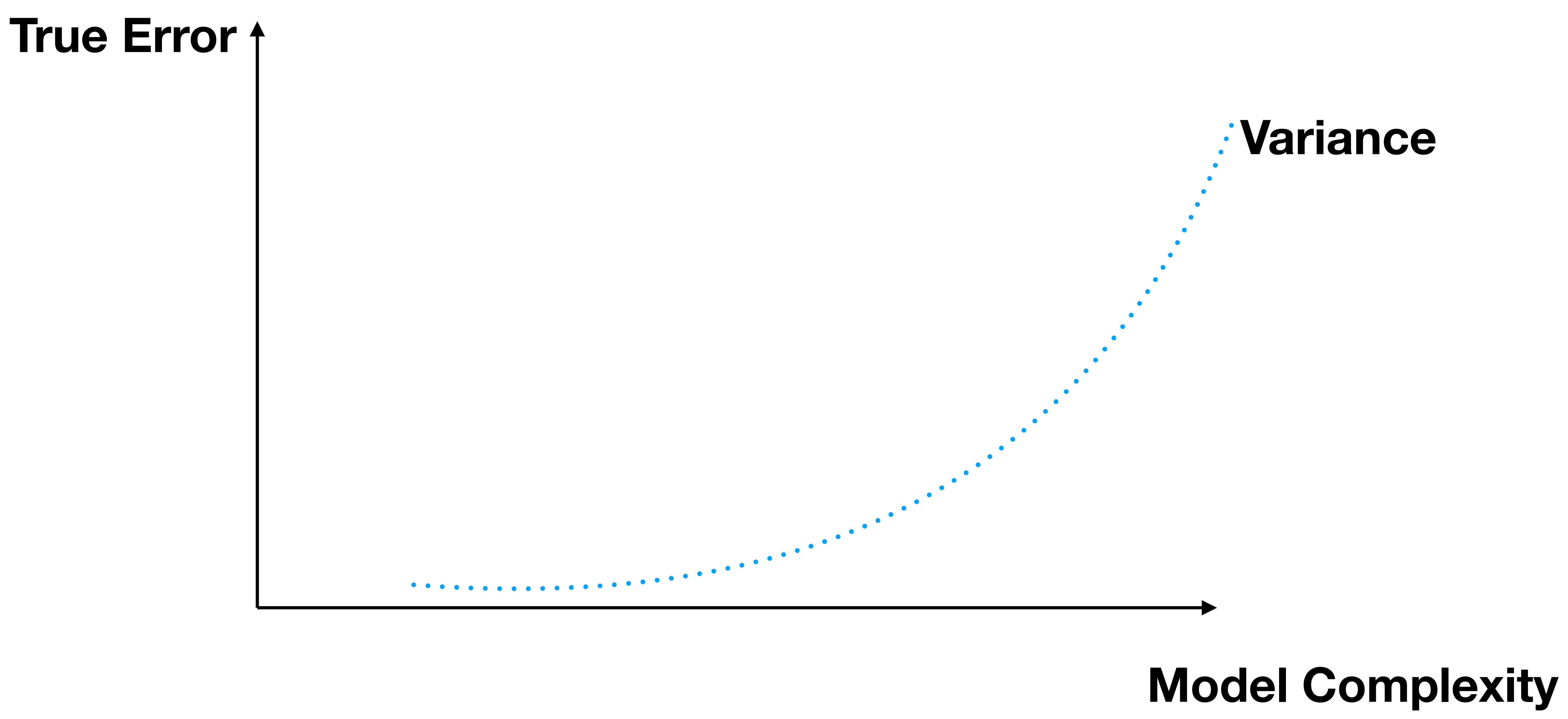

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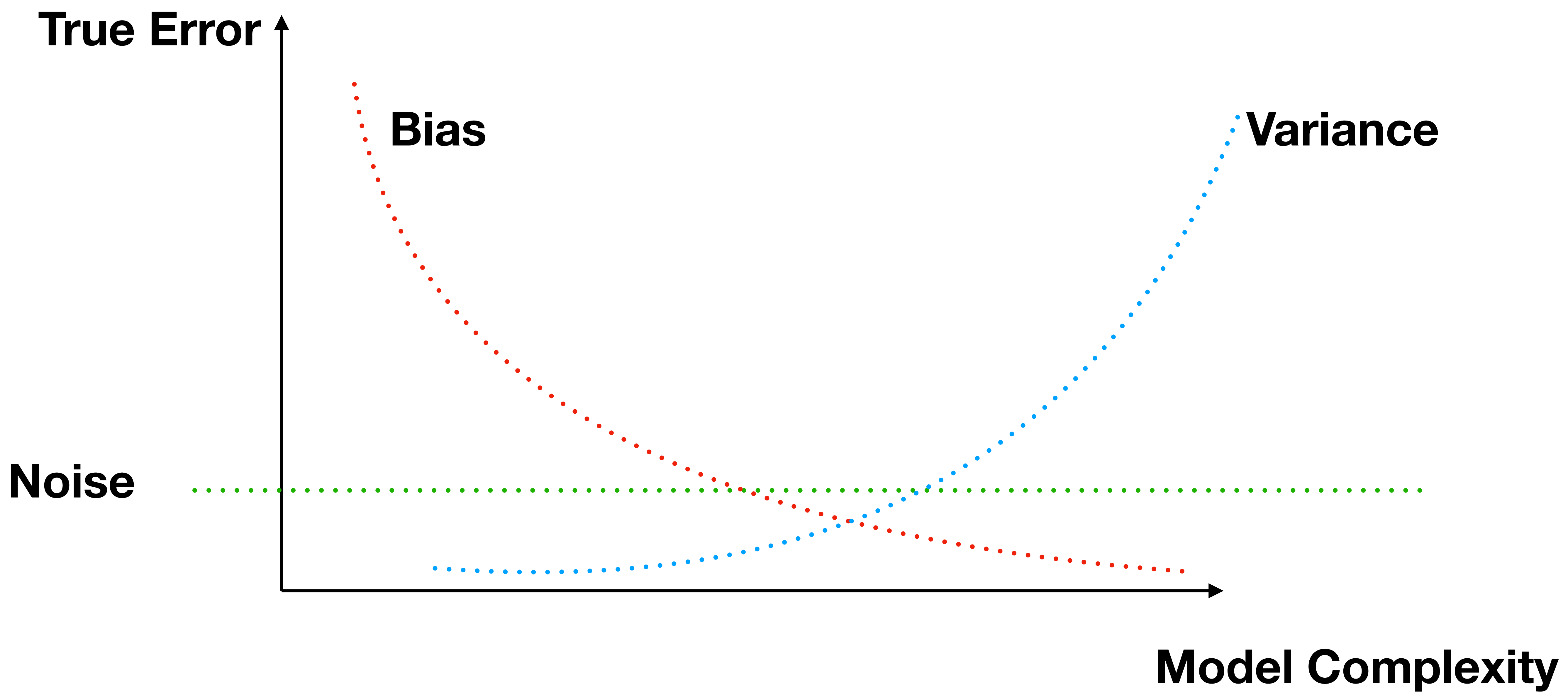
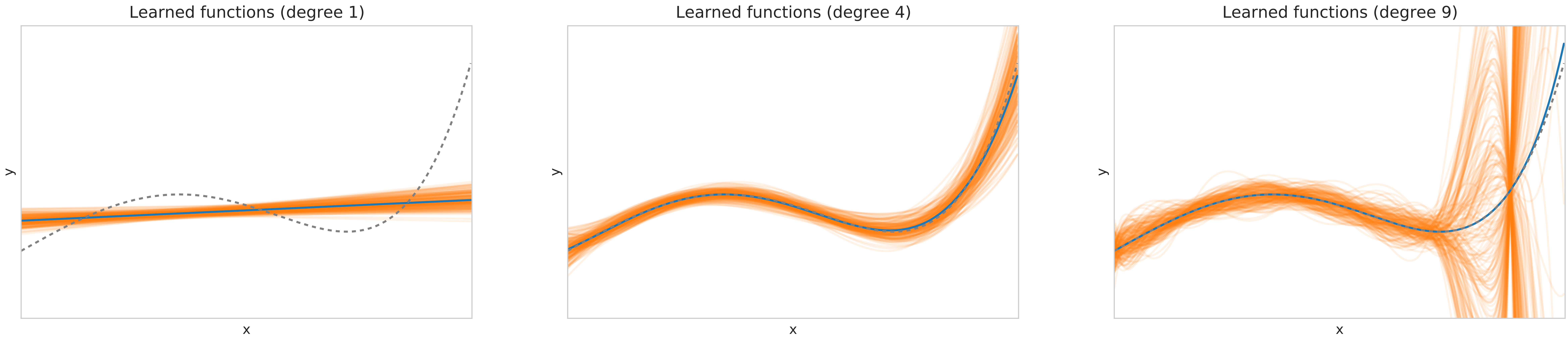
Bias Variance tradeoff and U-shape curve



- If model complexity is too low, approximation will be poor (underfitting)
- If model complexity is too high, it may cause issues with variance (overfitting)

➡ This phenomenon is known as the bias-variance tradeoff

Challenge: Identify a method that ensures both low variance and low bias



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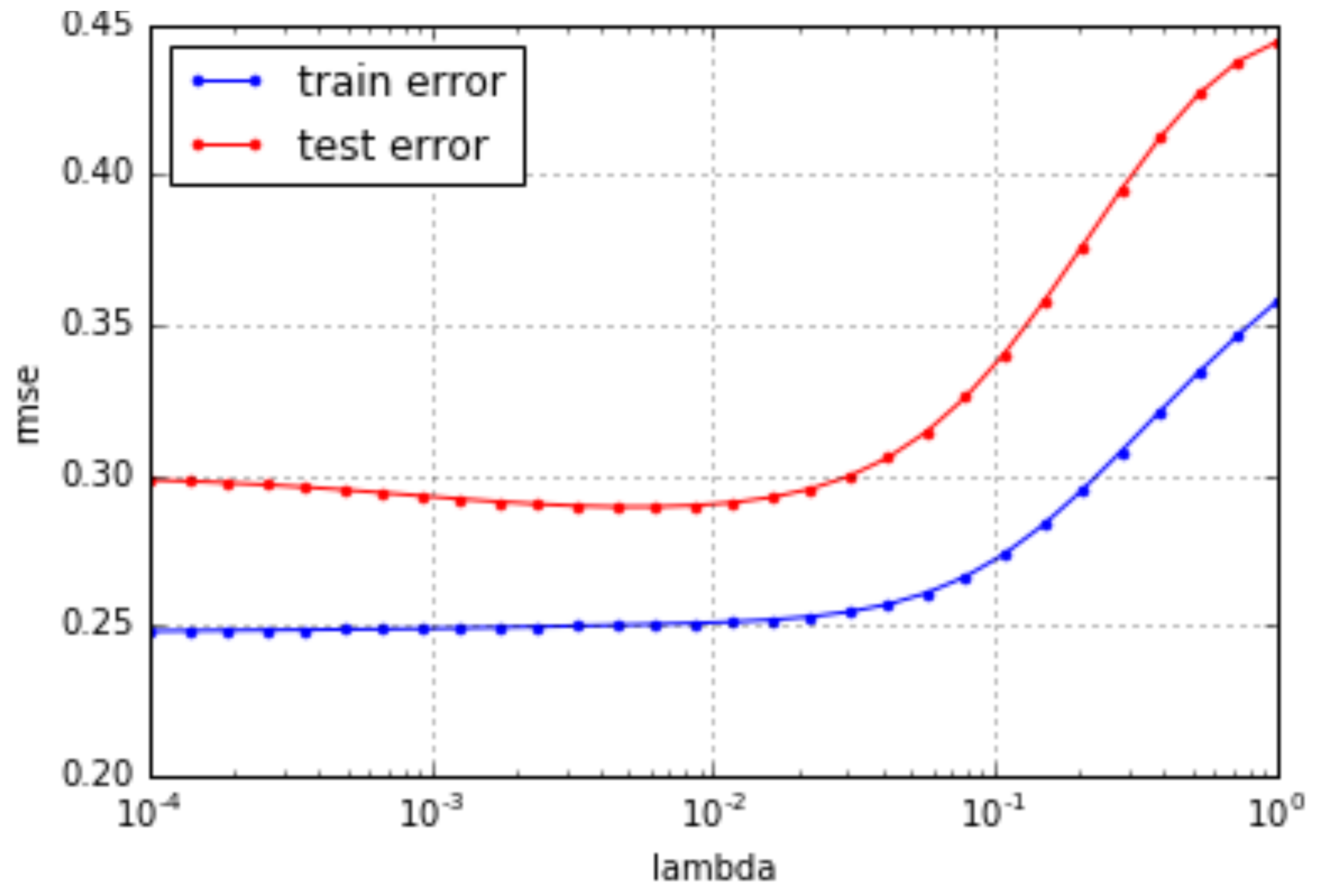
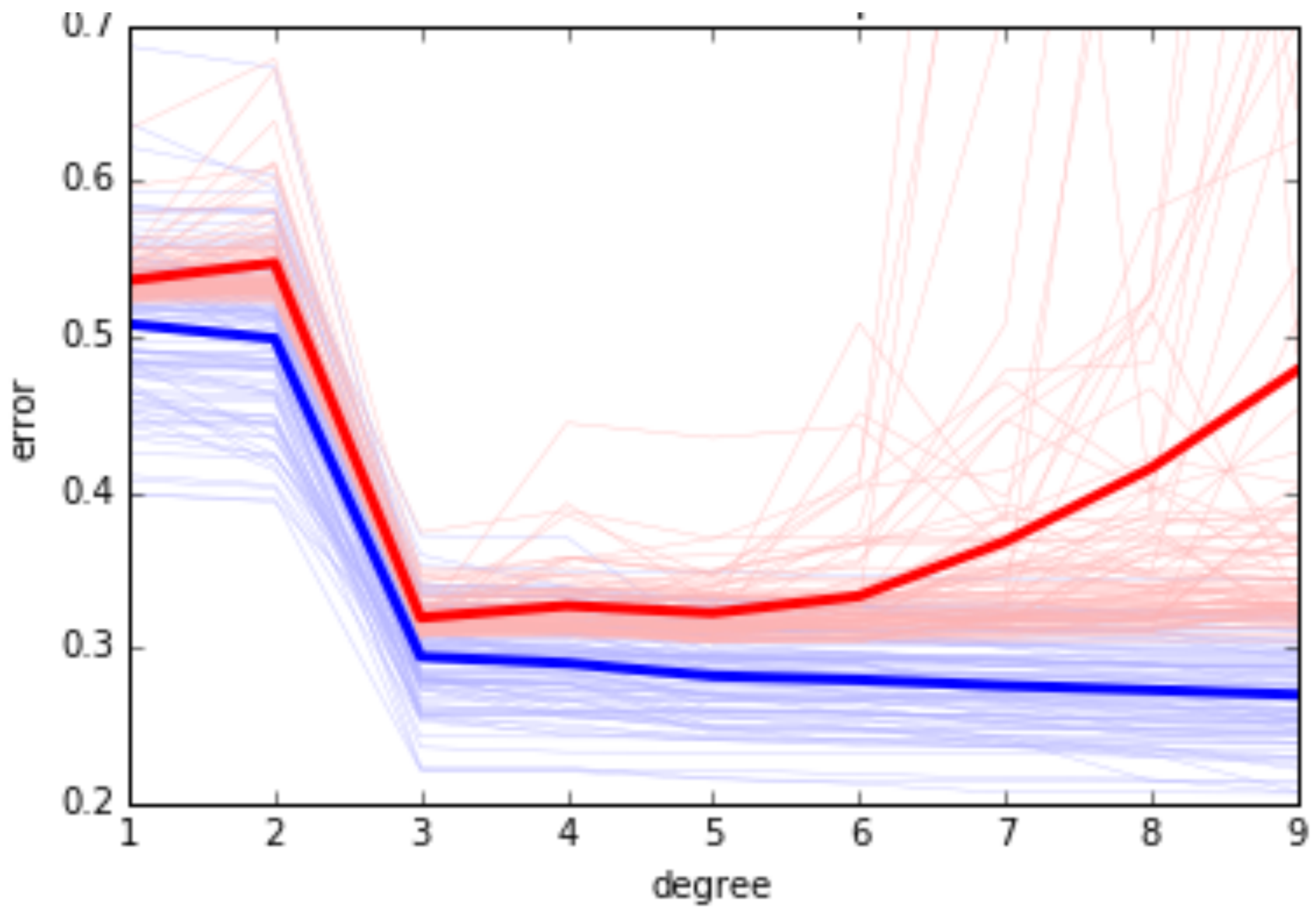


Ridge regression



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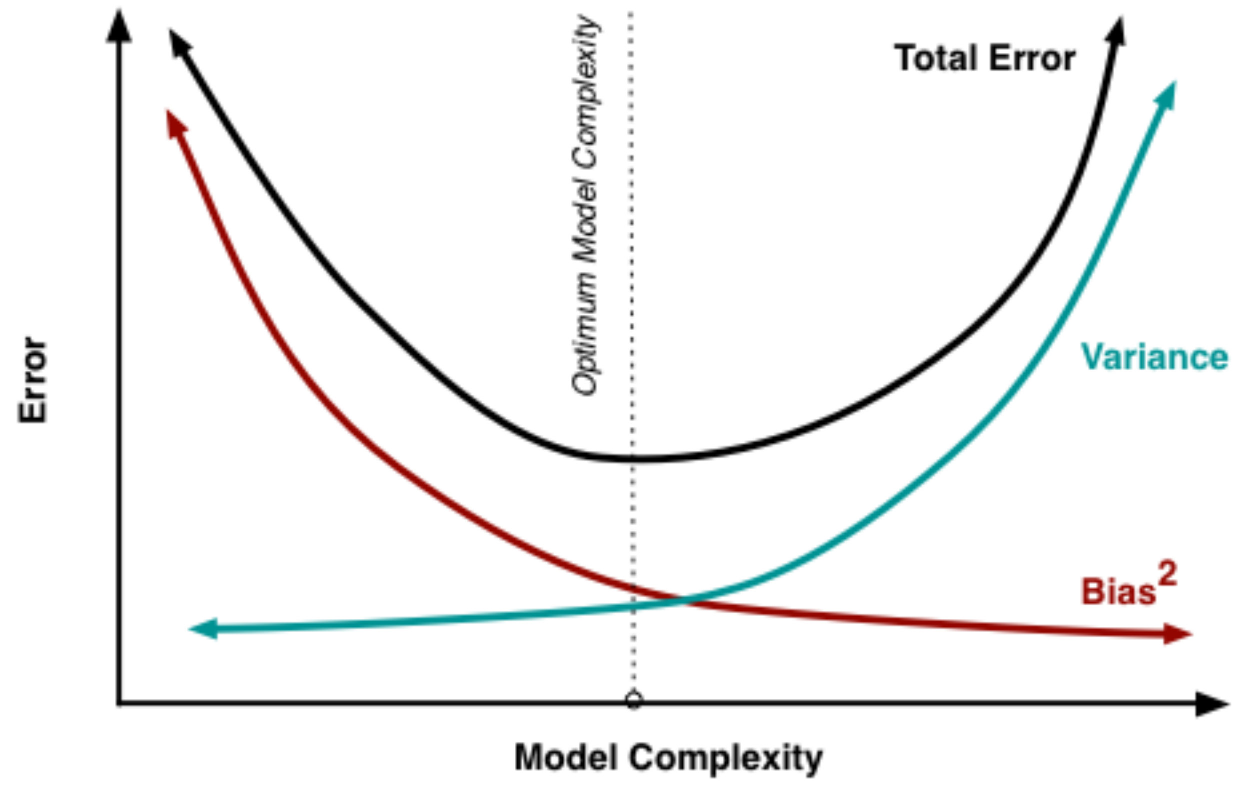
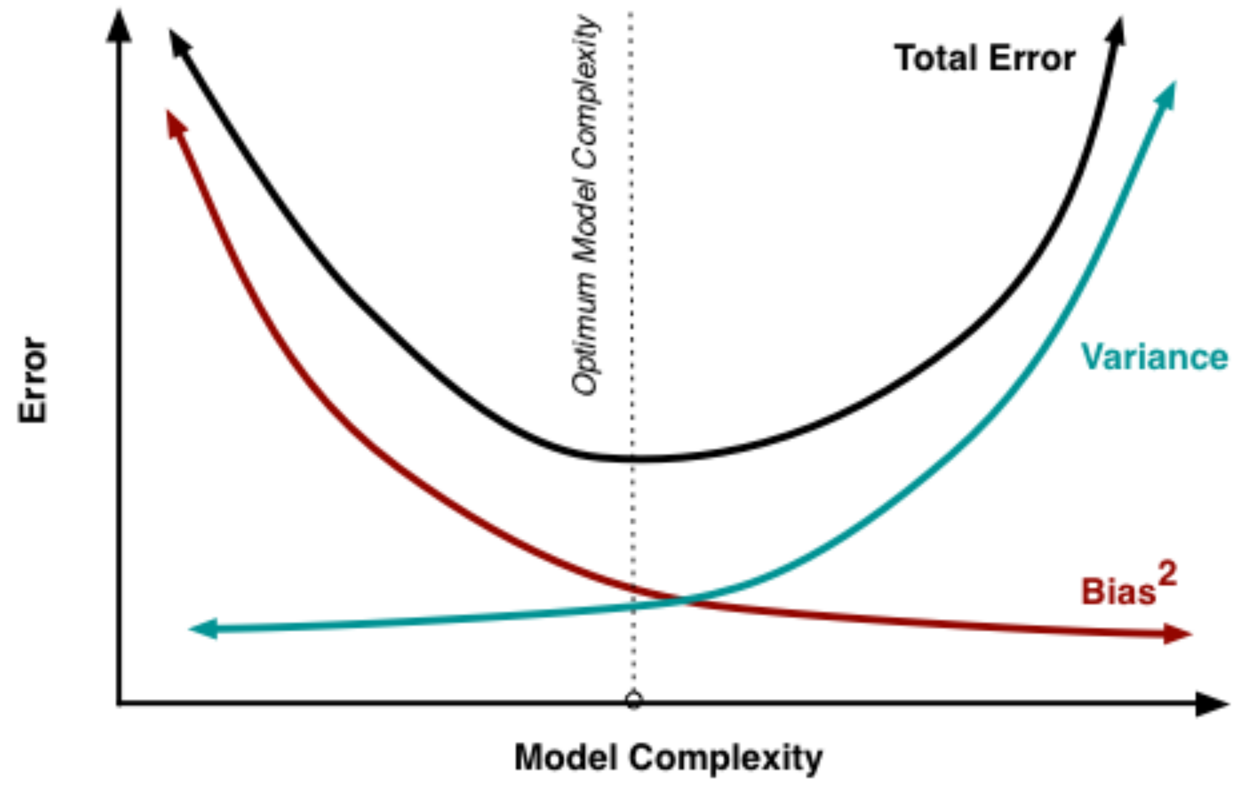
In practice…



Total Error
Optimum Model Complexity
Variance
Error
Bias2
Model Complexity

In practice…



Don't know bias!

If model is trained only once per complexity level: don't have variance!

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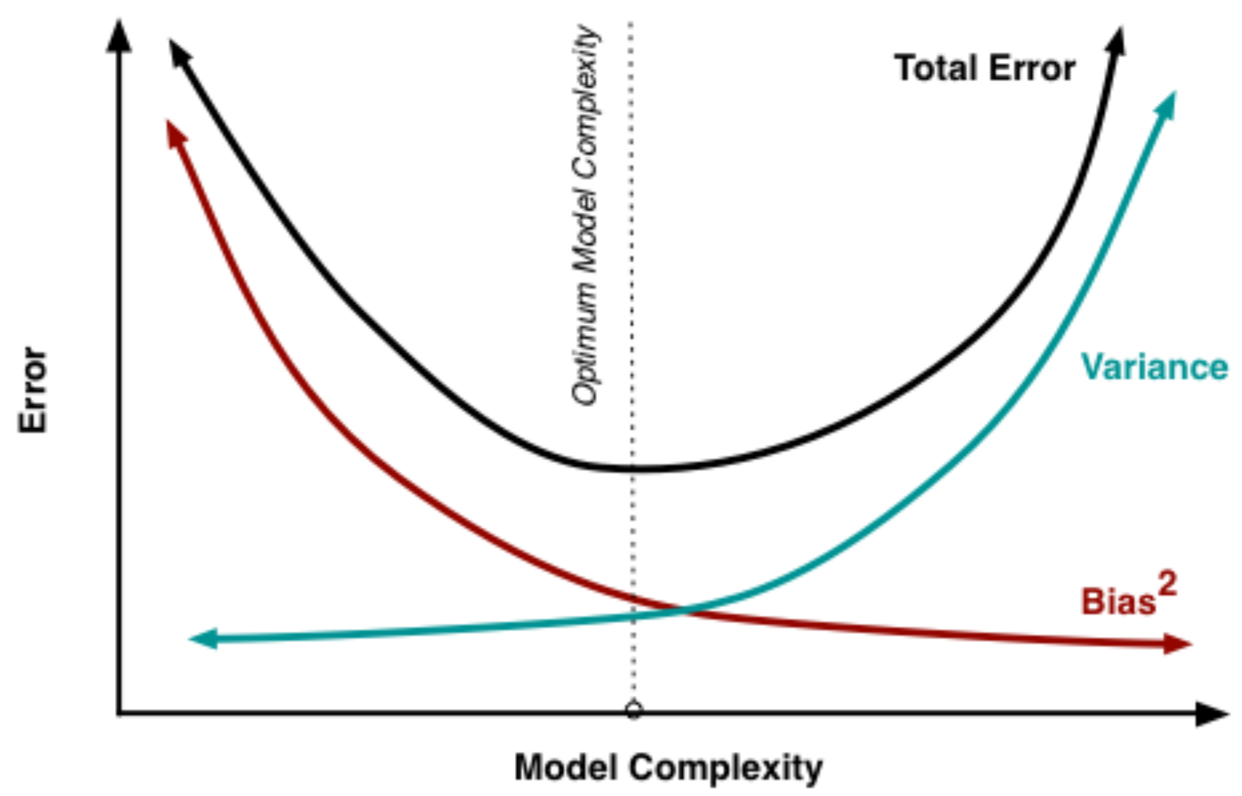

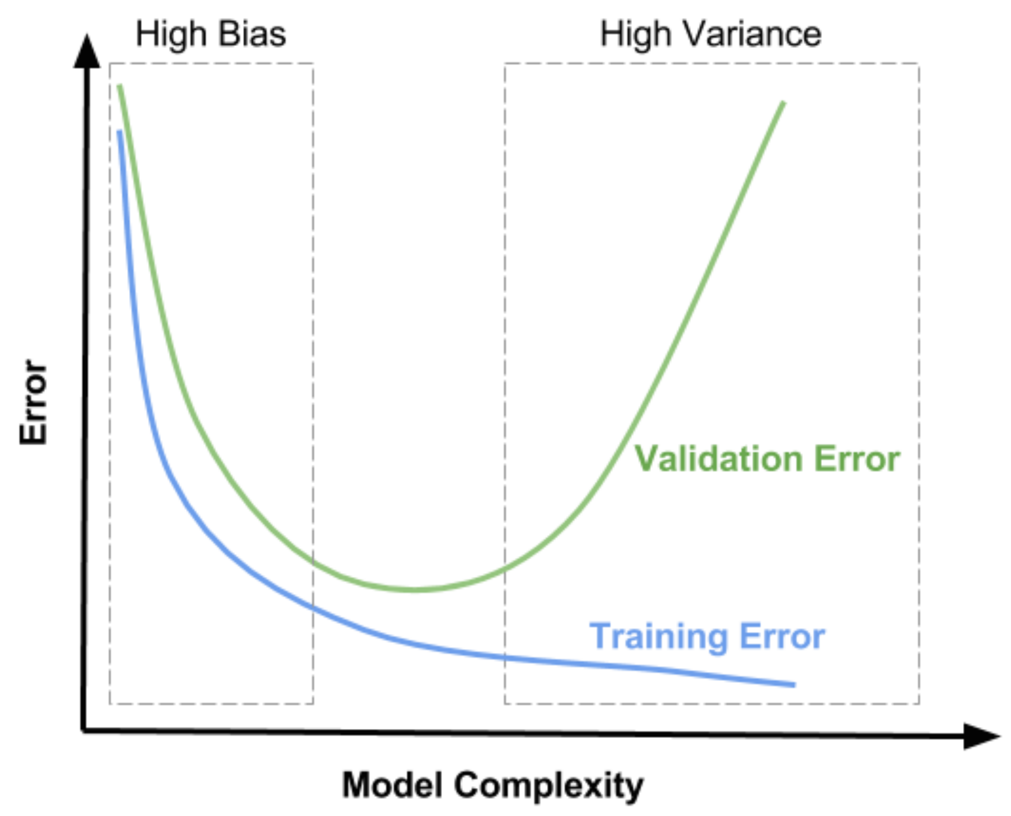

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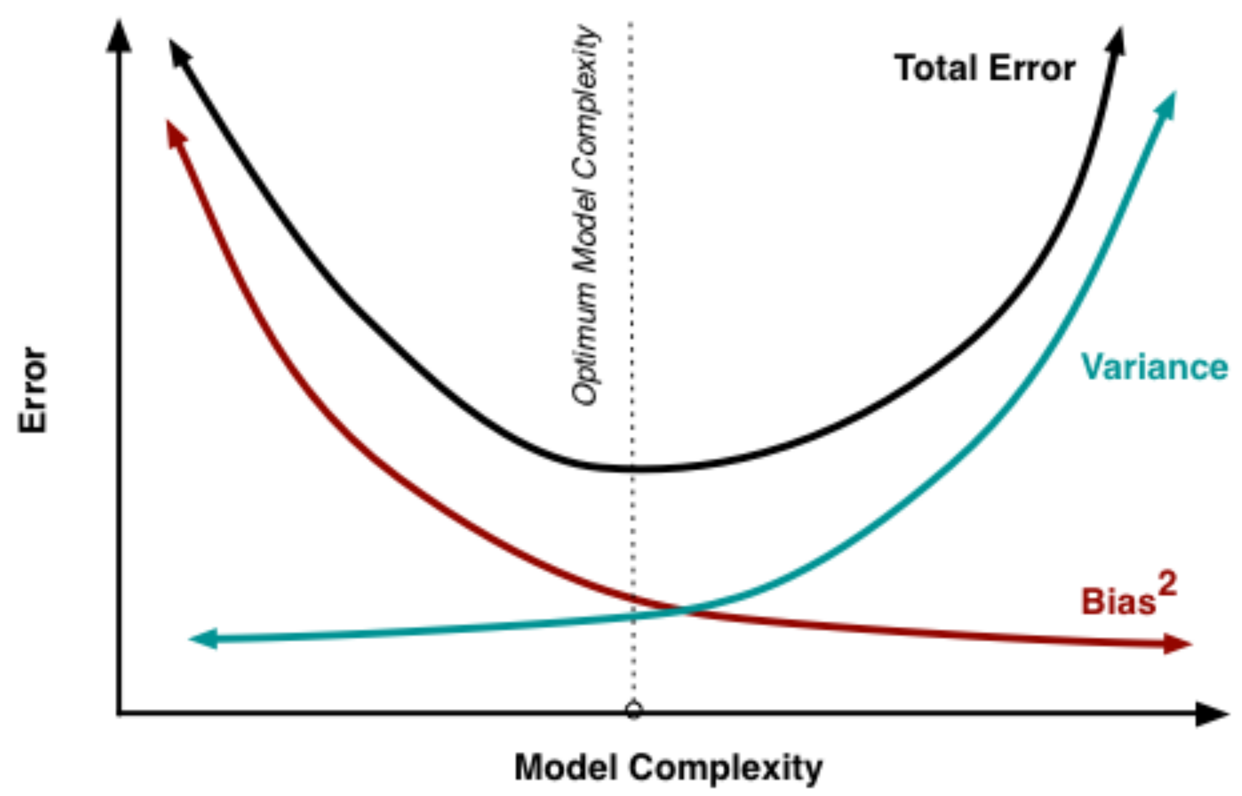

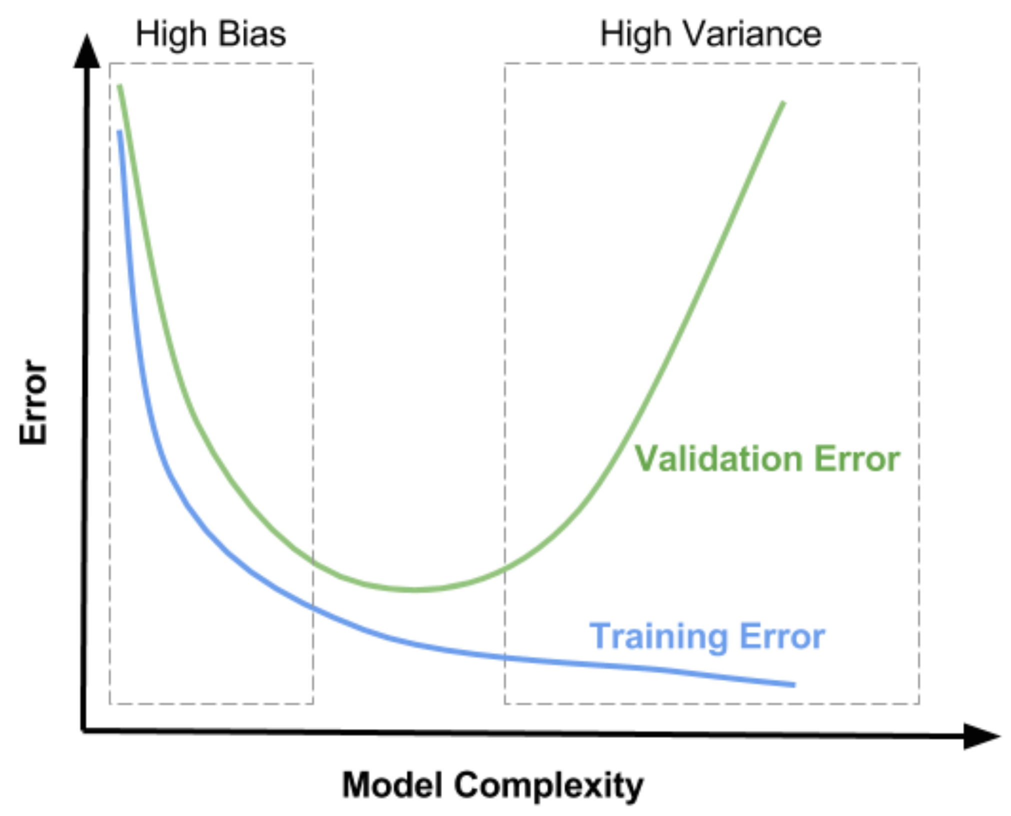

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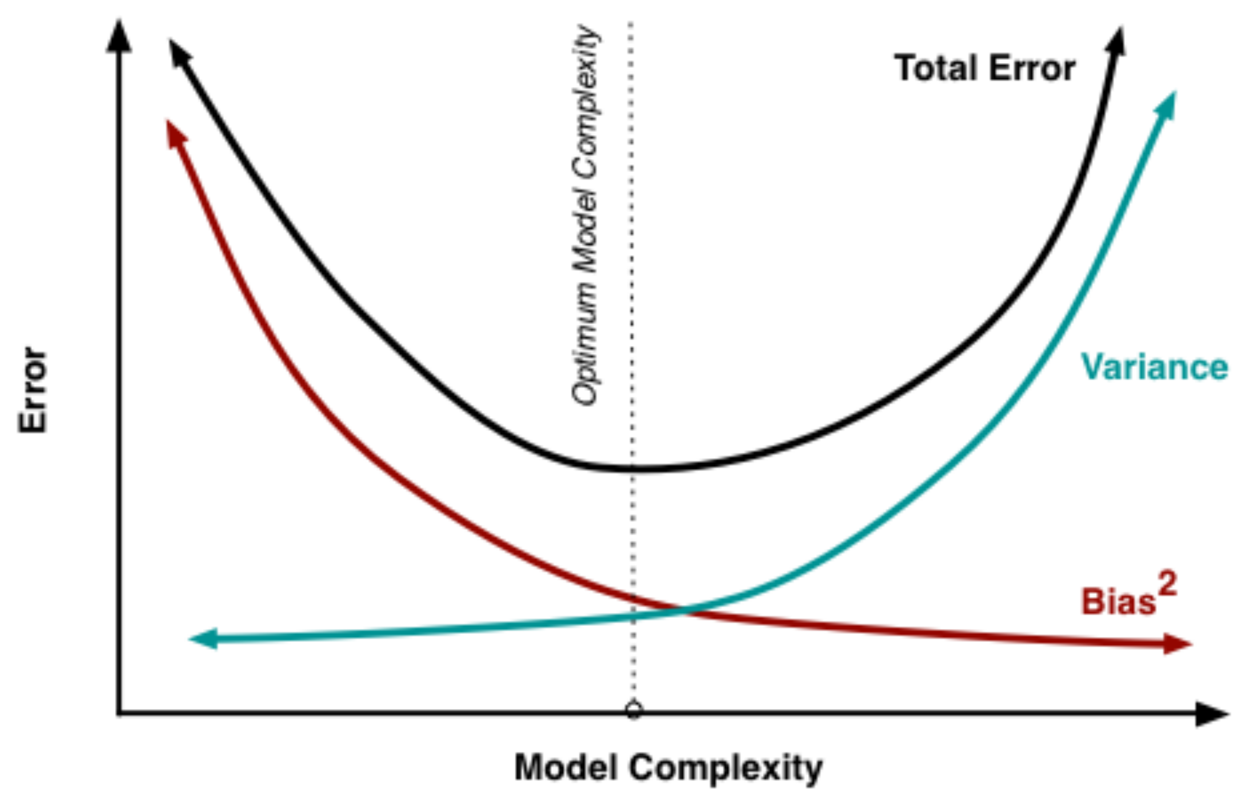
Can't draw curve before sweeping over hyperparameter values!

In practice...



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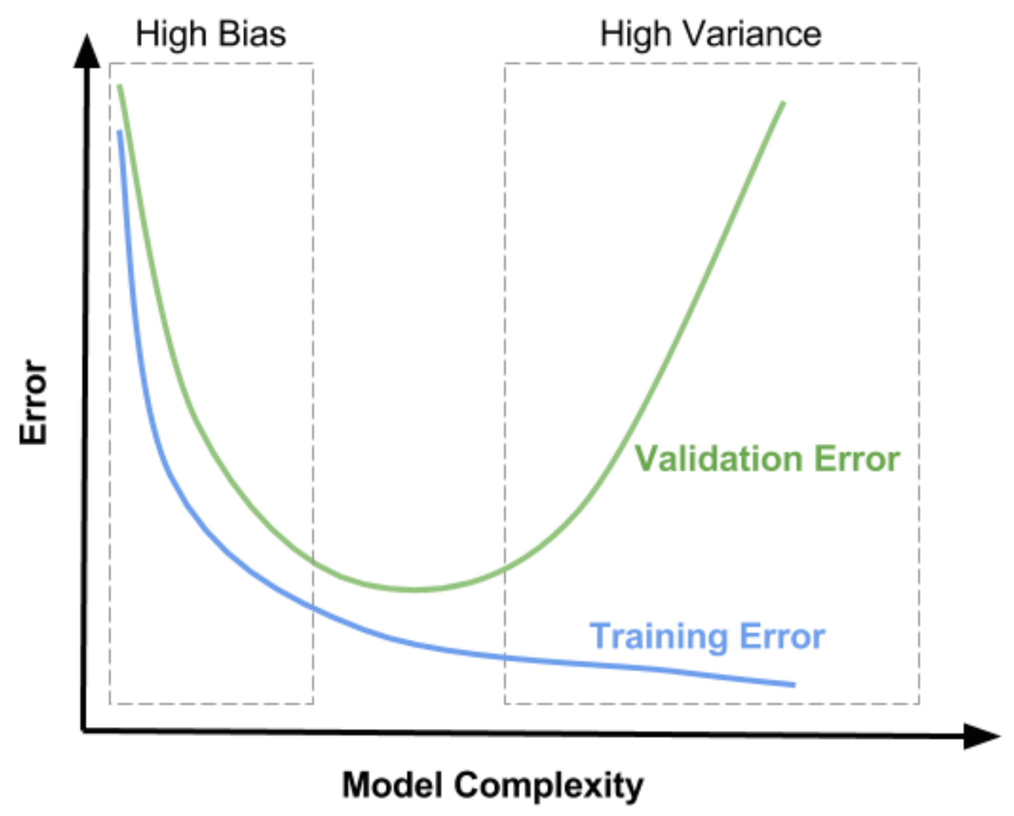

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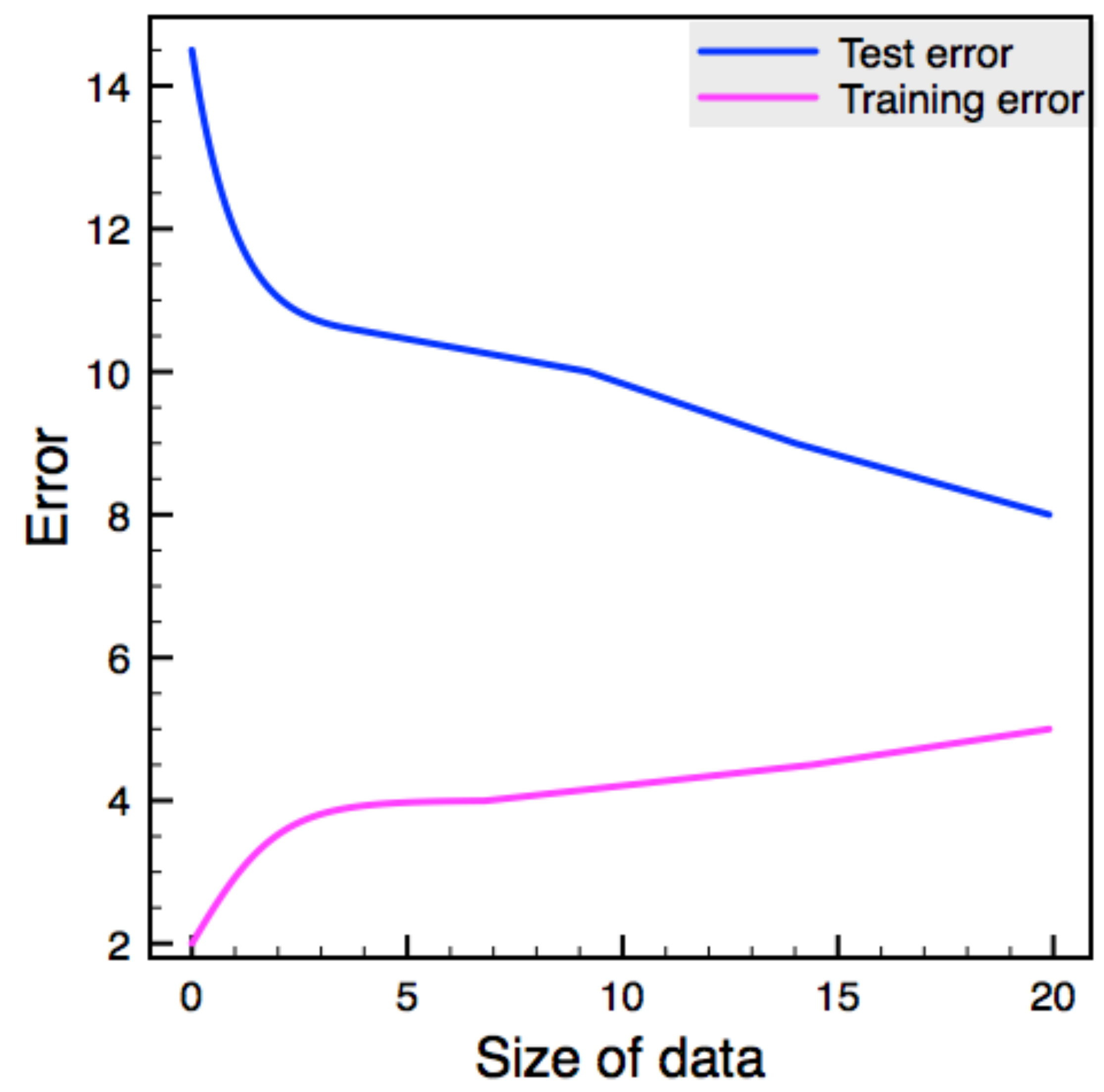
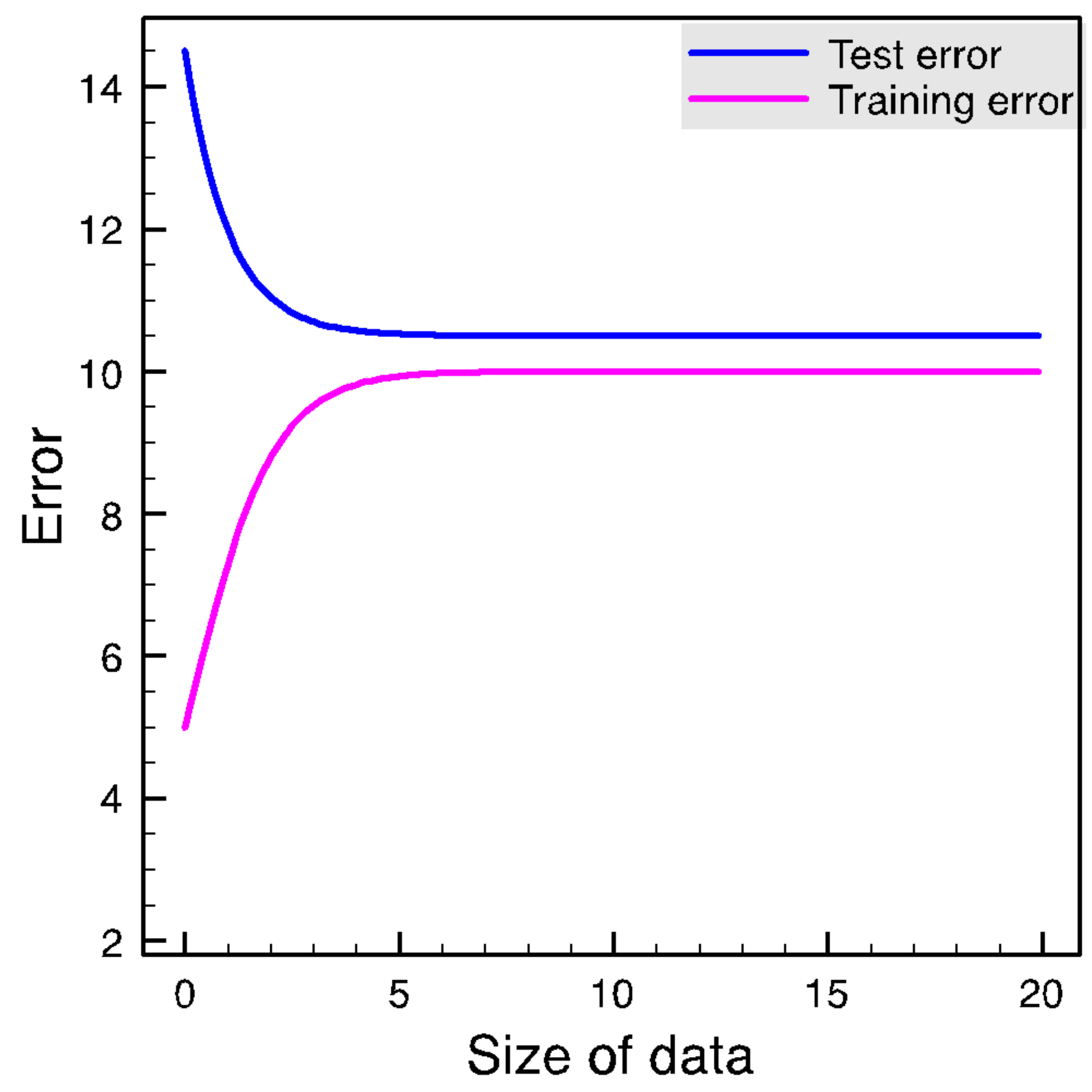
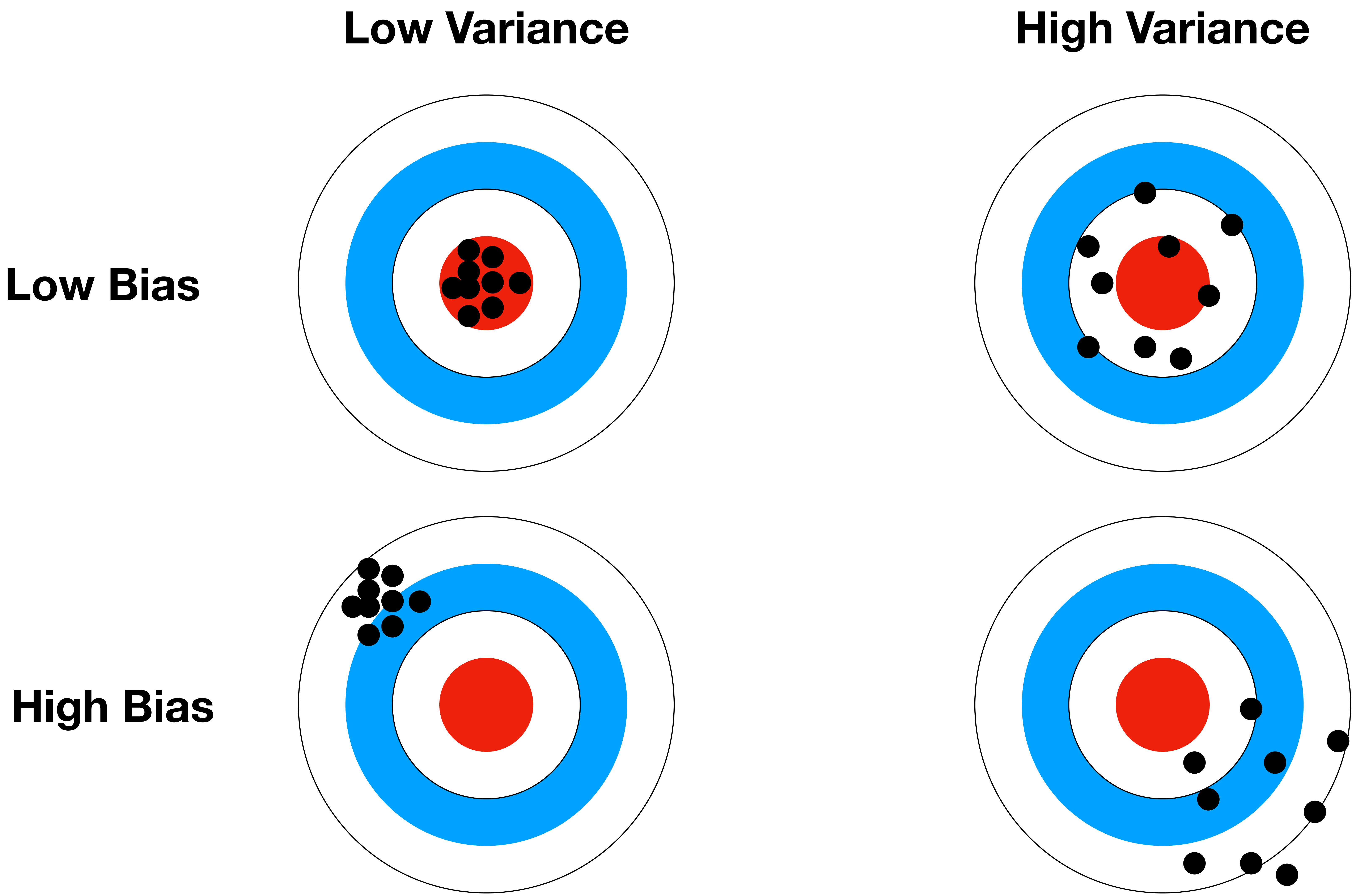


Draw learning curve! (esp. easy w/ SGD)

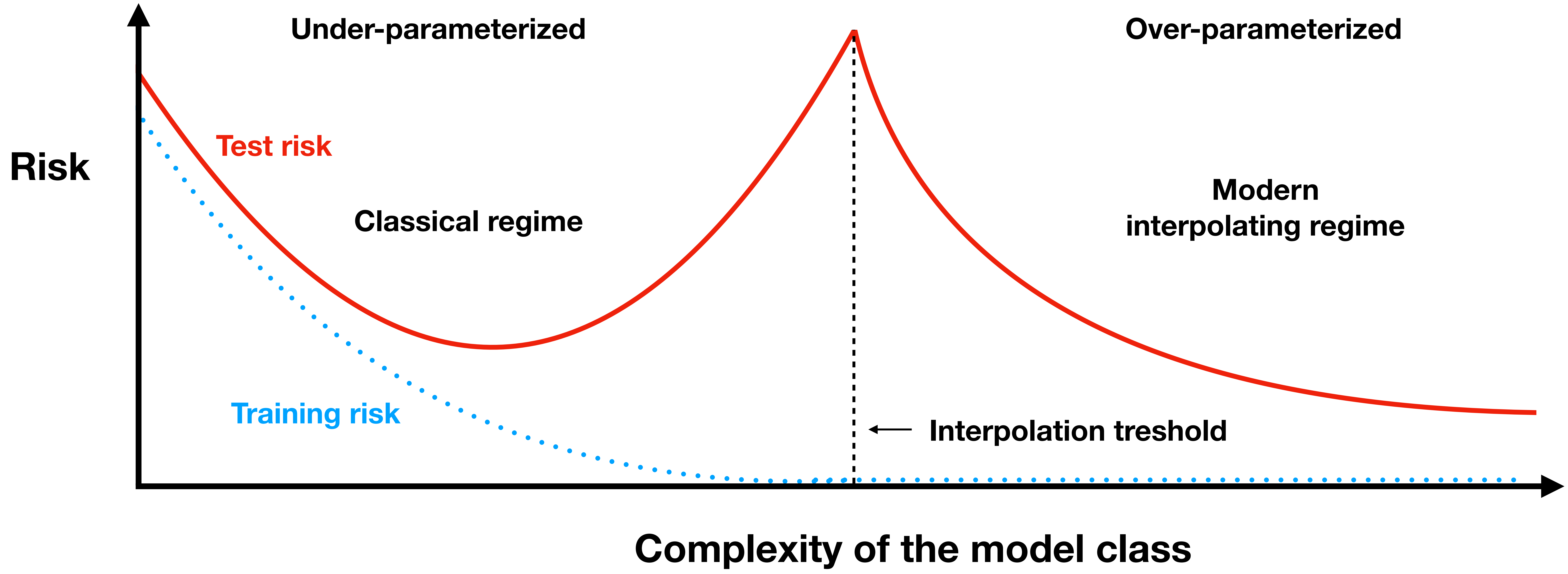


Conclusion



But this depends on the algorithm!

Double descent curve



Reconciling modern machine-learning practice and the classical bias–variance trade-off

Mikhail Belkin, Daniel Hsu, Siyuan Ma, and Soumik Mandal, PNAS, 2019