Lecture 4: Model Selection and Bias-Variance Decomposition

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WESTLAKE UNIVERSITY | SCHOOL OF ENGINEERING

Reading materials

- Chapter 3.2, Bishop, Pattern Recognition and Machine Learning
- Chapter 2, Stanford CS-229,
  `https://cs229.stanford.edu/notes2022fall/main_notes.pdf`
- Bias-Variance decomposition by Scott Fortmann-Roe:
  `http://scott.fortmann-roe.com/docs/BiasVariance.html`
- Double-descent phenomenon by Mikhail Belkin et al:
  `https://www.pnas.org/content/116/32/15849.short`

Reference

- EPFL, CS-433 Machine Learning, `https://github.com/epfml/ML_course`

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3 Bias-Variance Decomposition

4 Before Introducing Multilayer Perceptron: Logistic Regression

Definitions of under-fit and over-fit

Let's consider the polynomial regression problem (for a one-dimensional input x_n):

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y_n &\approx w_0 + w_1 x_n + w_2 x_n^2 + \ldots + w_M x_n^M \\
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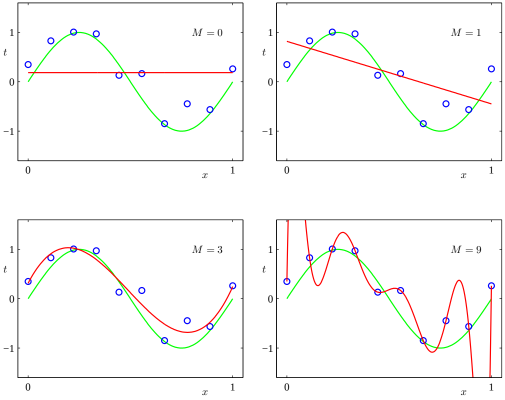

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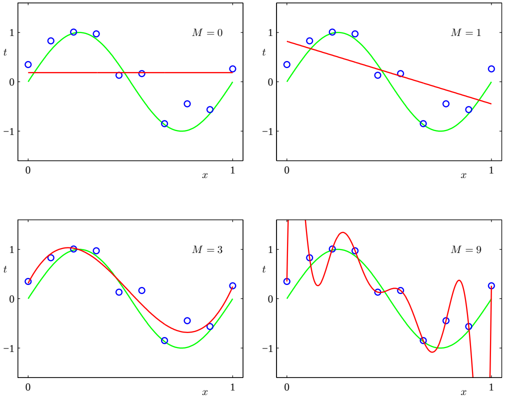

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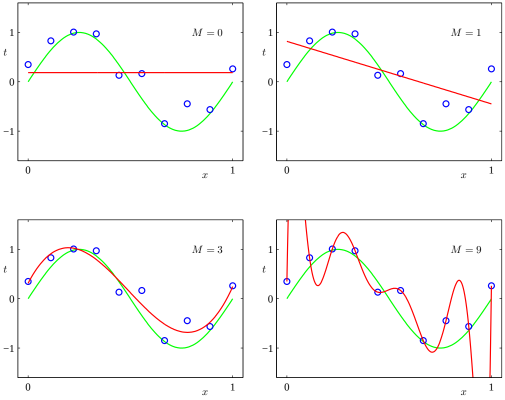

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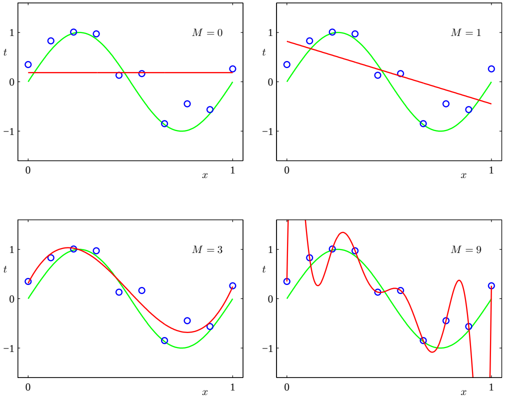

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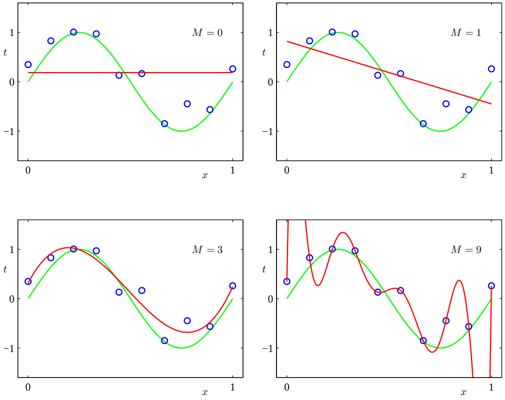

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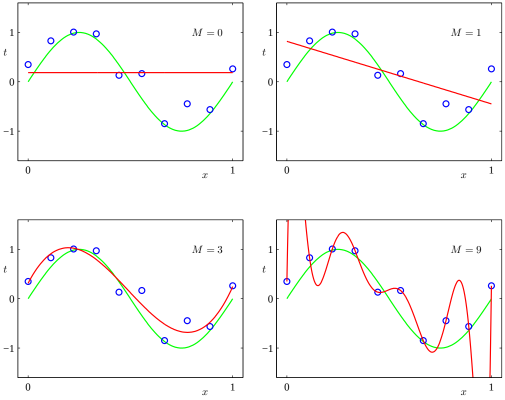

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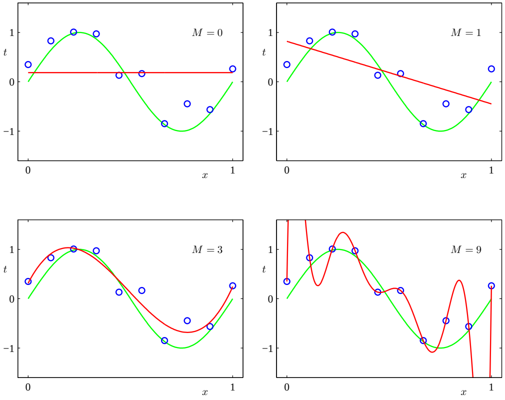

Discussion:

- Both of these phenomena (under-fit and over-fit) are undesirable.
- This discussion is made more difficult:
  - since all we have is data.
  - we do not know a priori what part is the underlying signal and what part is noise.

Regularization

Through regularization, we can penalize complex models and favor simpler ones:

$$\min_{\mathbf{w}} \quad \mathcal{L}(\mathbf{w}) + \Omega(\mathbf{w}) \tag{2}$$

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  - L_2-regularization (Ridge Regression)

$$\min_{\mathbf{w}} \quad \frac{1}{2N} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 \; + \; \lambda \, \|\mathbf{w}\|_2^2 \; , \tag{3}$$

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- Trade-off between under-fitting and over-fitting. In practice,
  - λ can control the model complexity.
  - The polynomial feature extension can enrich the complexity.

How do we trade-off the under-fitting and over-fitting?

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True Error, Empirical Error, and Training Error

- **True Error** (the **expected error** over all samples chosen according to $\mathcal{D}$):

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The reason that $L_S(f_S)$ might not be close $L_{\mathcal{D}}(f_S)$ is of course over-fitting.

Problem: validating the model on the same data subset we trained it on!

Splitting the data and Test Error

- **Fix:** Split the data into a *training* set S_{train} and a *test* set S_{test} (a.k.a. *validation* set):

$$S = S_{\text{train}} \bigcup S_{\text{test}} \tag{10}$$

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- Since S_{train} and S_{test} are independent, we hope that $L_{S_{\text{test}}}(f_{S_{\text{train}}}) \approx L_{\mathcal{D}}(f_{S_{\text{train}}})$
- Issues: we have fewer data both for the learning and validation tasks (trade-off)

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This lecture:

- Generalization Gap and Model Selection
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- Before Introducing Multilayer Perceptron: Logistic Regression

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- Classification
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Generalization gap: How far is the test from the true error?

- **True Error:**

$$L_{\mathcal{D}}(f) = \mathbb{E}_{(y,\mathbf{x})\sim\mathcal{D}}\left[\ell\left(y, f\left(\mathbf{x}\right)\right)\right]. \tag{12}$$

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In expectation, they are the same:

$$L_{\mathcal{D}}(f) = \mathbb{E}_{S_{\text{test}}\sim\mathcal{D}}\left[L_{S_{\text{test}}}(f)\right] , \tag{15}$$

where the expectation is over the samples of the test set.

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Given a model f and a test set $S_{test} \sim \mathcal{D}$ i.i.d. (not used to learn f) and a loss $\ell(\cdot,\cdot) \in [a,b]$:

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⇒ The more data points we have, the more confident we are that the empirical loss we measure is close to the true loss.

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$$\Pr\left[\underbrace{L_{\mathcal{D}}(f)}_{\text{not computable}} \geq \underbrace{L_{S_{\text{test}}}(f)}_{\text{computable}} + \underbrace{\sqrt{\frac{(b-a)^2 \ln(2/\delta)}{2\,|S_{\text{test}}|}}}_{\text{deviation}}\right] \leq \delta\,. \tag{17}$$

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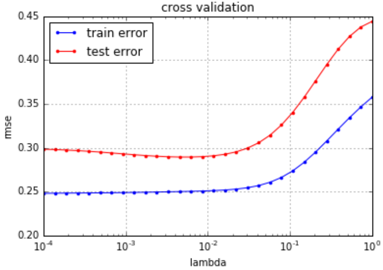

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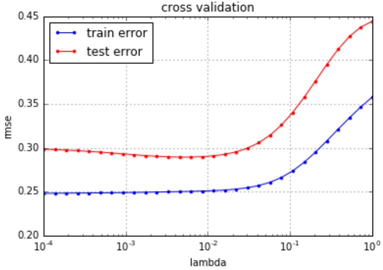

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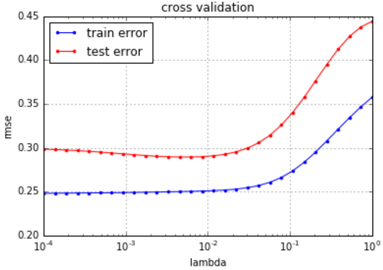

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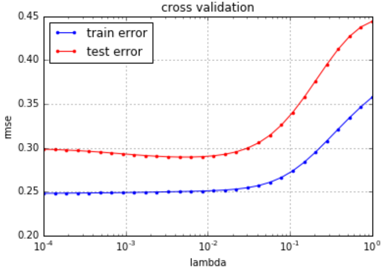

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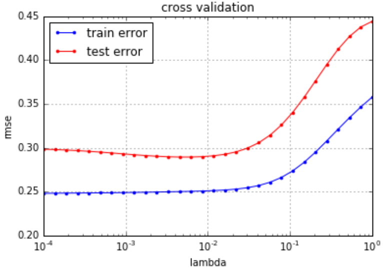

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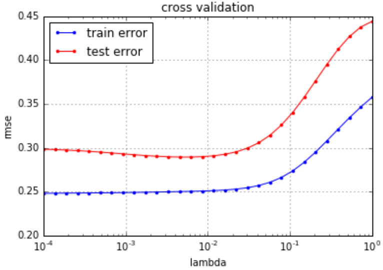

Issues: the existence of the generalization gap $|L_{S_{\text{test}}}(f_{S_{\text{train}},\lambda_k}) - L_{\mathcal{D}}(f_{S_{\text{train}},\lambda_k})|$!

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We can bound the maximum deviation for all K candidates, by

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$\Rightarrow$ So we can test many different models without incurring a large penalty.

- $k^\star = \arg\min_k L_{\mathcal{D}}(f_k)$, i.e., $f_{k^\star}$ denotes the function with the smallest true risk.
- $\hat{k} = \arg\min_k L_{S_{\text{test}}}(f_k)$, i.e., $f_{\hat{k}}$ denotes the function with the smallest empirical risk.

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If we choose the "best" function according to the empirical risk,
then its true risk is not too far away from the true risk of the optimal choice.

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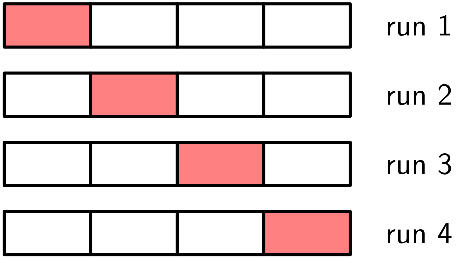

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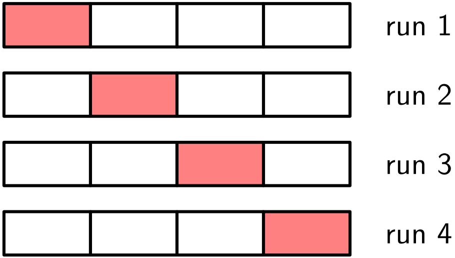

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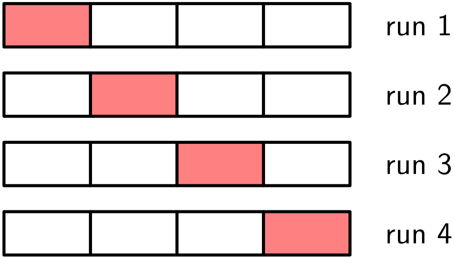

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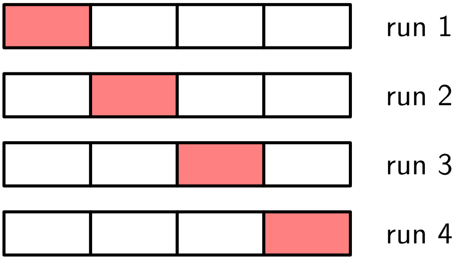

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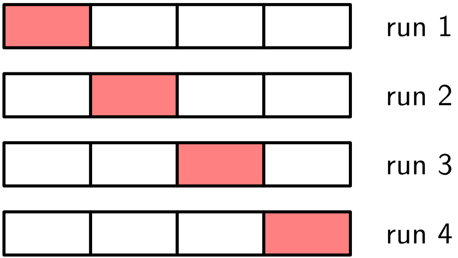

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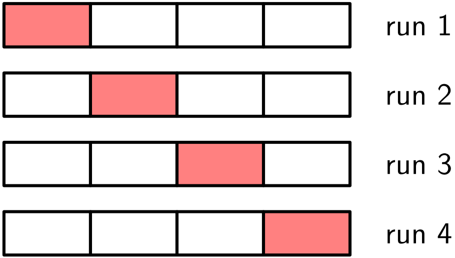

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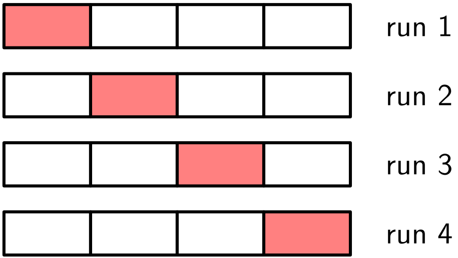

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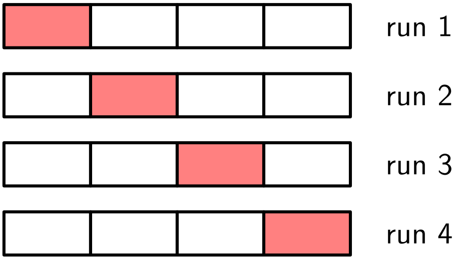

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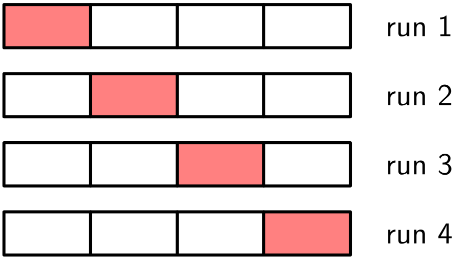

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- Cross-validation returns an unbiased estimate of the generalization error and its variance.

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

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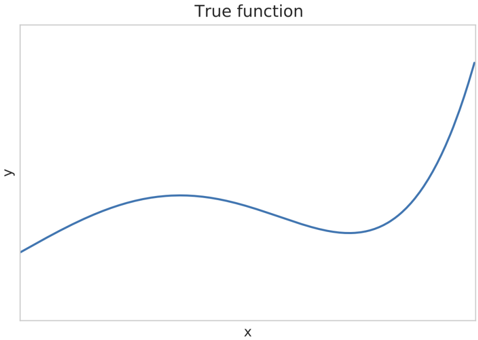

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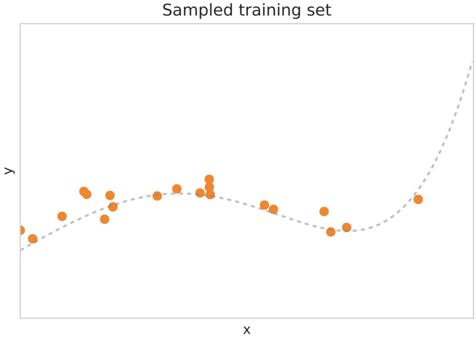

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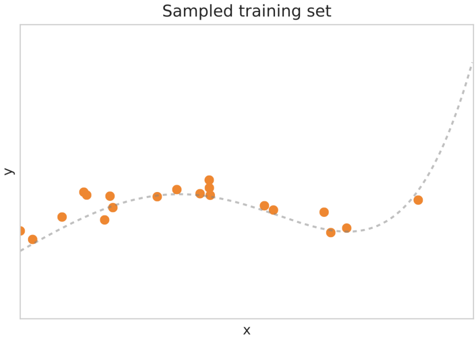

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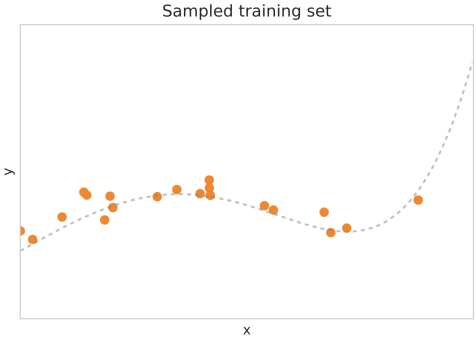

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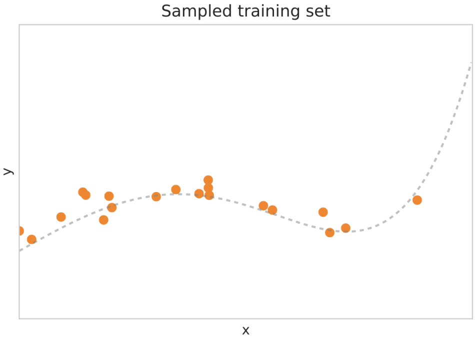

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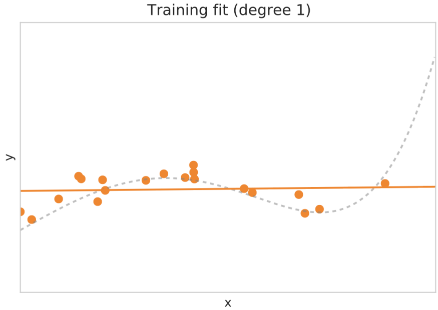

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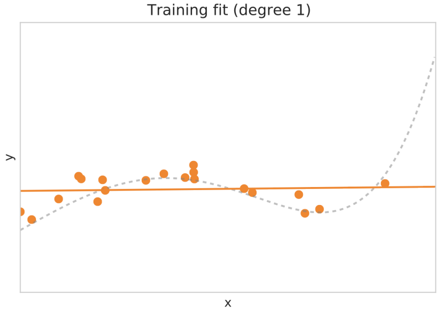

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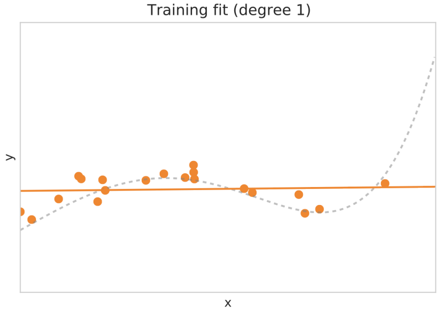

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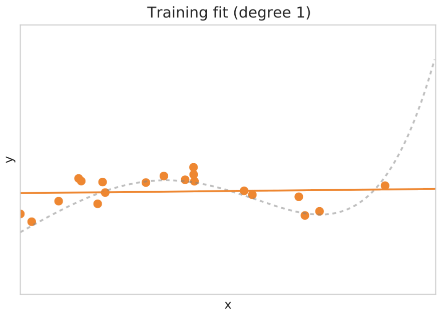

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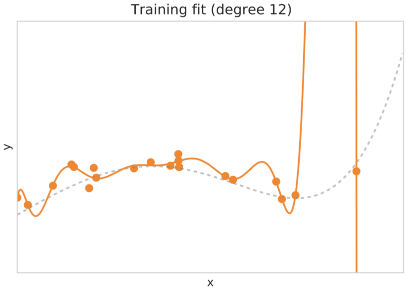

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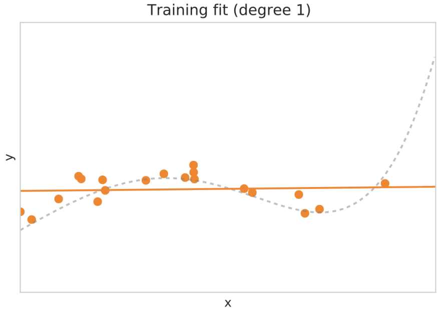

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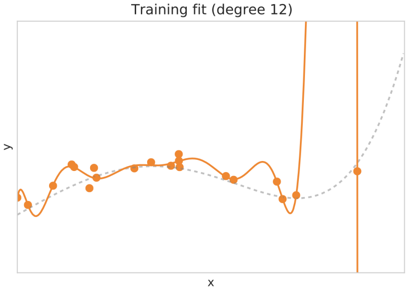

- We can find a model that fits the data well

Motivation example: 1D-regression

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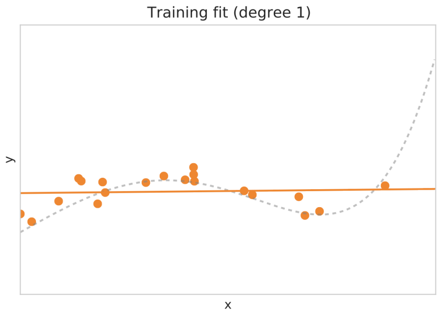
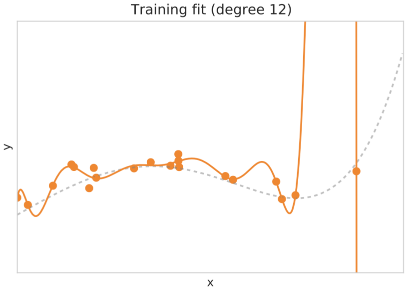


- No linear function would be a good predictor.
- The model is not rich/expressive enough.

If we consider a high-degree polynomial:



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- Is it a good predictor?

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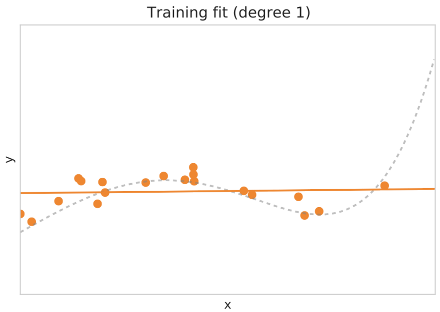

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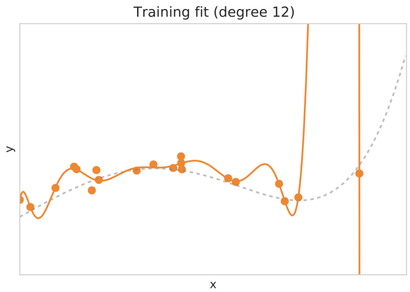
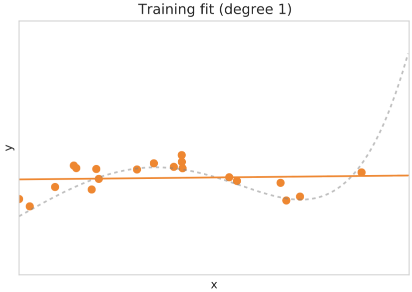
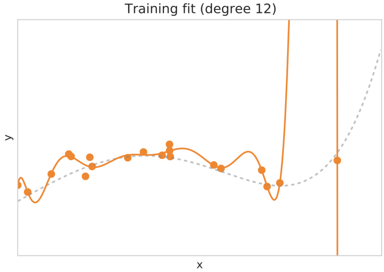


- We can find a model that fits the data well
- Is it a good predictor?
- No: Large generalization error

Motivation example: 1D-regression

Simple models are less sensitive.





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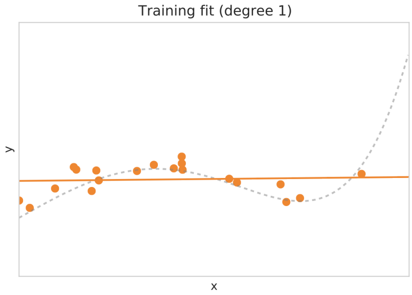

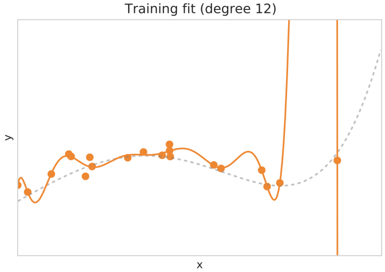

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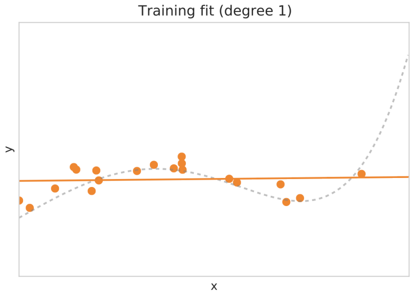

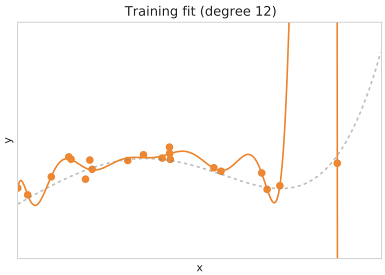

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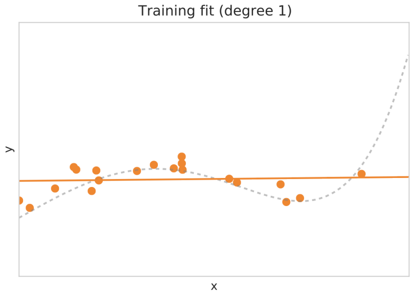

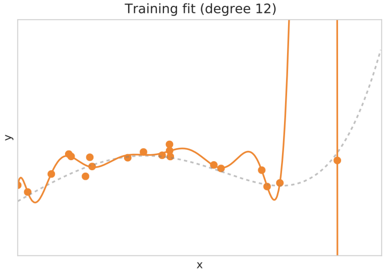

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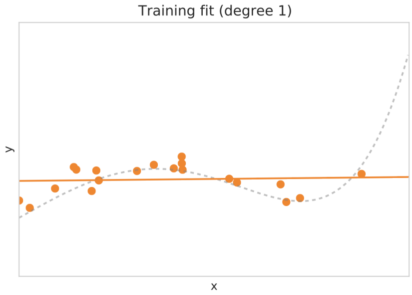

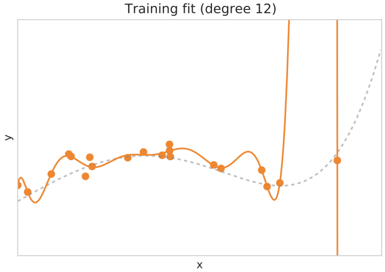

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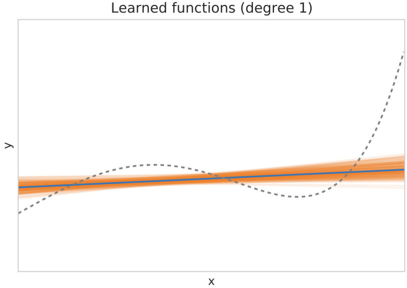
Simple models have large biases but low variance.



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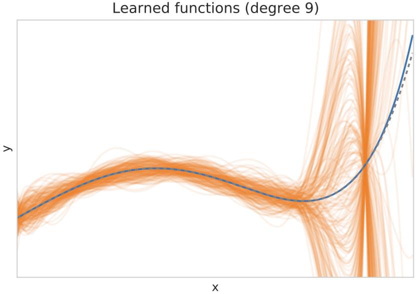

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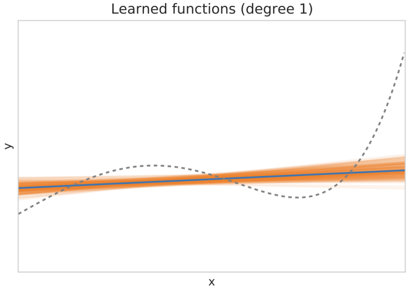

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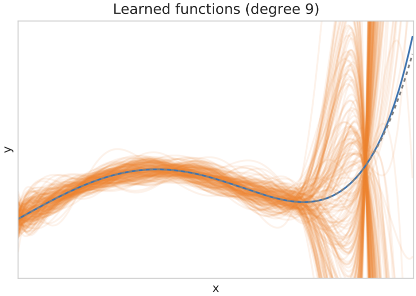

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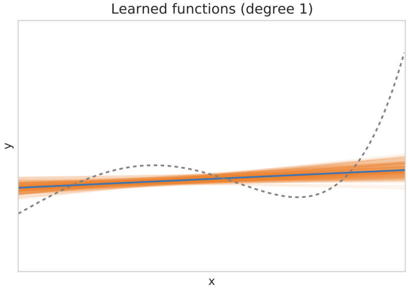

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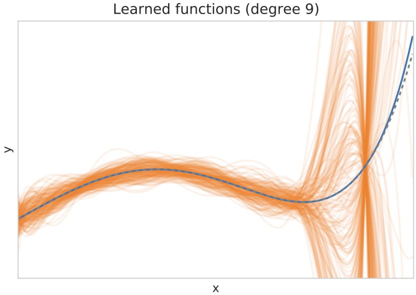

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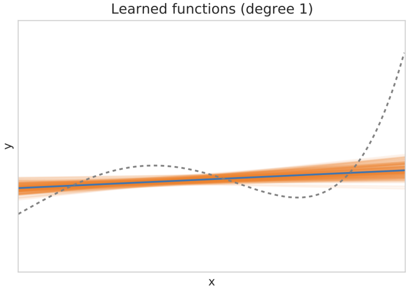

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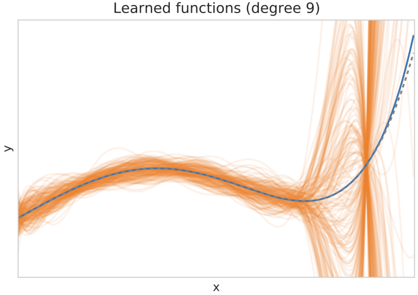

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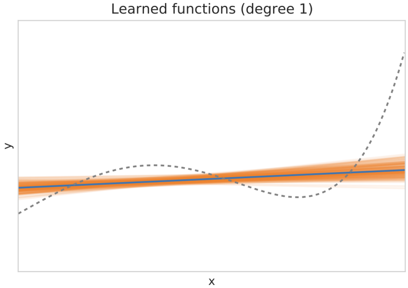

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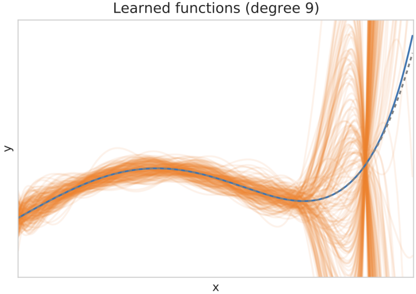

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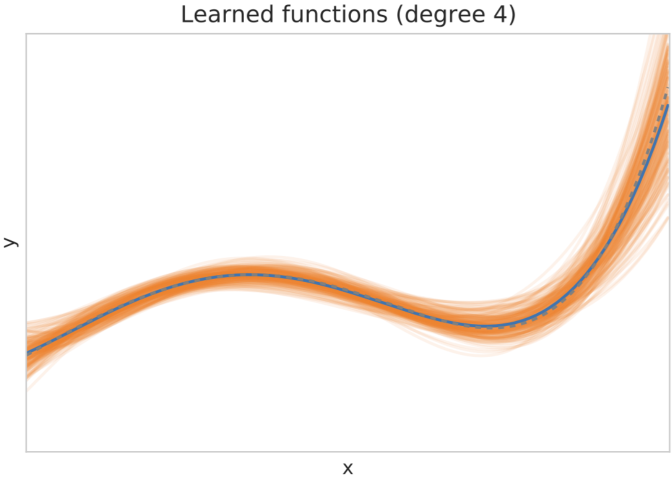

Data model

We assume that the data forms a joint distribution $(\mathbf{x}, y) \sim \mathcal{D}$, and is generated as

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- **Noise:** $\boldsymbol{\epsilon} \in \mathcal{D}_{\boldsymbol{\epsilon}}$ i.i.d., independent of $\mathbf{x}$ and $\mathbb{E}[\boldsymbol{\epsilon}] = 0$

Error decomposition

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Error decomposition

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- The decomposition will be true for every single point $\mathbf{x}$.
- To simplify, we consider the expected error of f_S for a fixed element $\mathbf{x}_0$:

$$L(f_{S_{\text{train}}}) = \mathbb{E}_{\epsilon\sim\mathcal{D}_\epsilon}\left[(f(\mathbf{x}_0) + \epsilon - f_{S_{\text{train}}}(\mathbf{x}_0))^2\right] \tag{23}$$

A decomposition in three terms

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

$$\mathbb{E}_{S_{\text{train}} \in \mathcal{D}} \left[L(f_{S_{\text{train}}}) \right] \tag{24}$$

(25)

(26)

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Using that $\mathbb{E}_{\boldsymbol{\epsilon} \in \mathcal{D}_{\boldsymbol{\epsilon}}} \left[\boldsymbol{\epsilon} \right] = 0$ and $\boldsymbol{\epsilon}$ is independent from S_{train}:

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Therefore

$$\mathbb{E}_{S_{\text{train}} \in \mathcal{D}} \left[L(f_{S_{\text{train}}}) \right] = \underbrace{\text{Var}_{\boldsymbol{\epsilon} \in \mathcal{D}_{\boldsymbol{\epsilon}}}[\boldsymbol{\epsilon}]}_{\text{noise variance}} + \mathbb{E}_{S_{\text{train}} \sim \mathcal{D}} \left[(f(\mathbf{x}_0) - f_{S_{\text{train}}}(\mathbf{x}_0))^2 \right] \tag{27}$$

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$$\underbrace{+\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[2\left(\left(f(\mathbf{x}_0)-\mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right]\right)\left(\mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right]-f_{S_{\text{train}}}(\mathbf{x}_0)\right)\right)\right]}_{0} \tag{31}$$

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\end{aligned}$$

Bias-Variance Decomposition

$$
\begin{aligned}
\mathbb{E}_{S_{\text{train}} \in \mathcal{D}}\left[L(f_{S_{\text{train}}})\right] &= \mathsf{Var}_{\boldsymbol{\epsilon} \sim \mathcal{D}_{\boldsymbol{\epsilon}}}[\boldsymbol{\epsilon}] && \text{(noise variance)} \\
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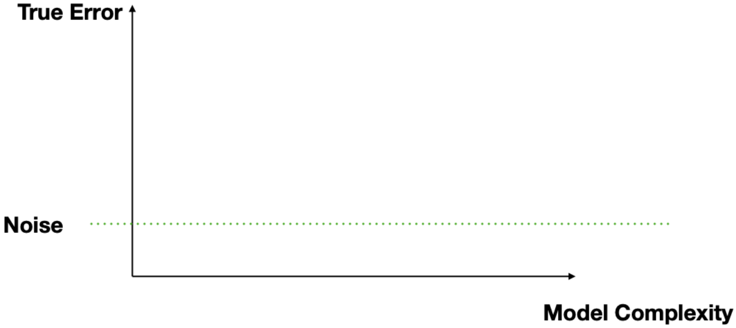
which always lowers bound the true error.

$\Rightarrow$ In order to minimize the true error, we need to select a method that **simultaneously achieves low bias and low variance**.

Component 1: Noise $\mathrm{Var}_{\epsilon \sim \mathcal{D}_\epsilon}[\epsilon]$—a strict lower bound on what error we can achieve



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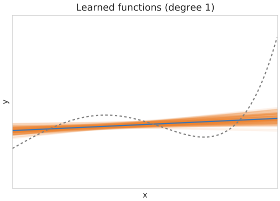
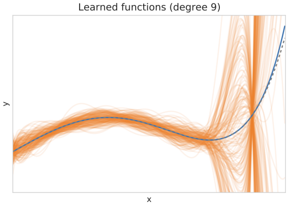
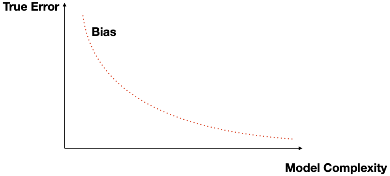
- It is not possible to go below the noise level
- Even if we know the true model f, we still suffer from $L(f) = \mathbb{E}\left[\epsilon^2\right]$
- It is not possible to predict the noise from the data since they are independent

Component 2: Bias $\left(f(\mathbf{x}_0) - \mathbb{E}_{S_{\text{train}'}}\left[f_{S_{\text{train}'}}(\mathbf{x}_0)\right]\right)^2$







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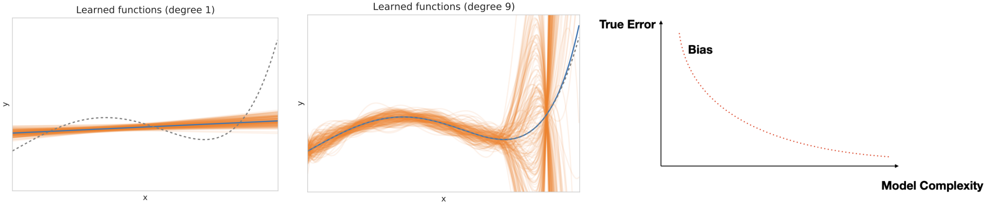

- It measures how far off in general the models' predictions are from the correct value.

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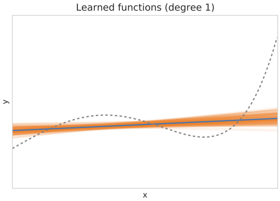

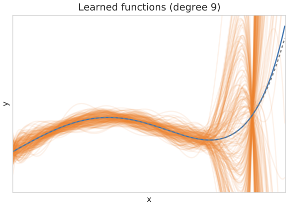

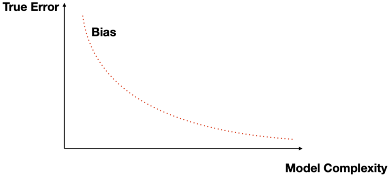

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- If complexity is small, then high bias.

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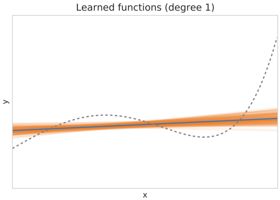
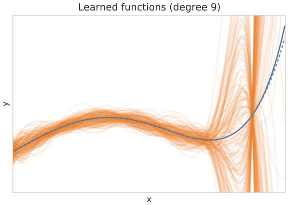
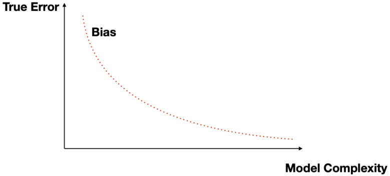
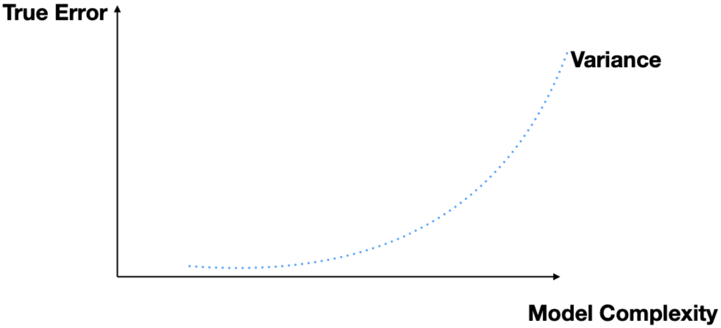






- It measures how far off in general the models' predictions are from the correct value.
- If complexity is small, then high bias.
- If complexity is high, then low bias.

Component 3: Variance $\mathbb{E}_{S_{\text{train}} \sim \mathcal{D}} \left[\left(\mathbb{E}_{S_{\text{train'}}} [f_{S_{\text{train'}}}(\mathbf{x}_0)] - f_{S_{\text{train}}}(\mathbf{x}_0) \right)^2 \right]$



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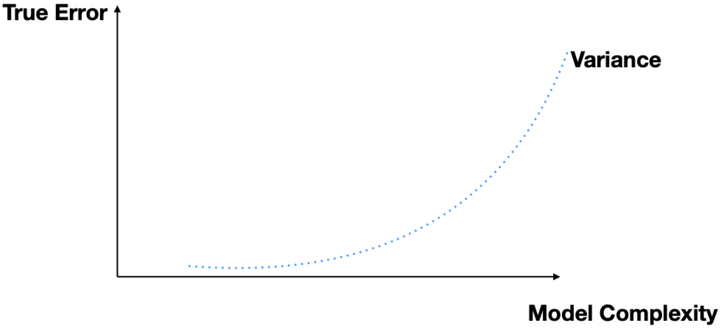

- Variance of the prediction function.

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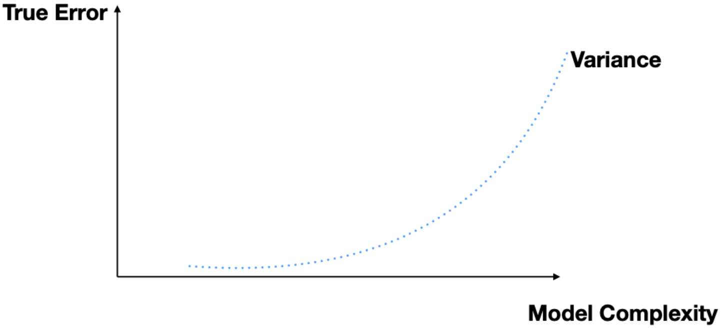

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- It is how much the predictions for a given point vary between different realizations of the training set.

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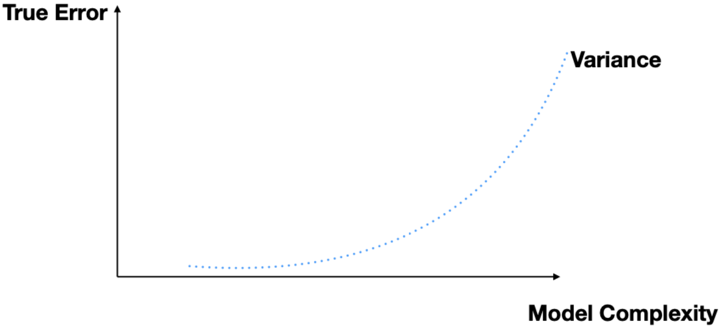
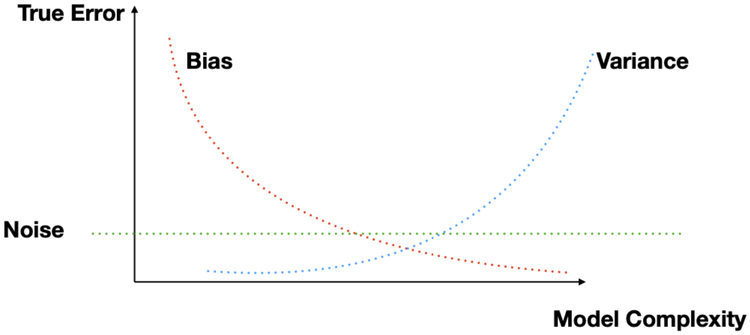


- Variance of the prediction function.
- It is how much the predictions for a given point vary between different realizations of the training set.
- If we consider complicated models, then small variations in the training set can result in large changes in the prediction.

Bias Variance tradeoff and U-shape curve



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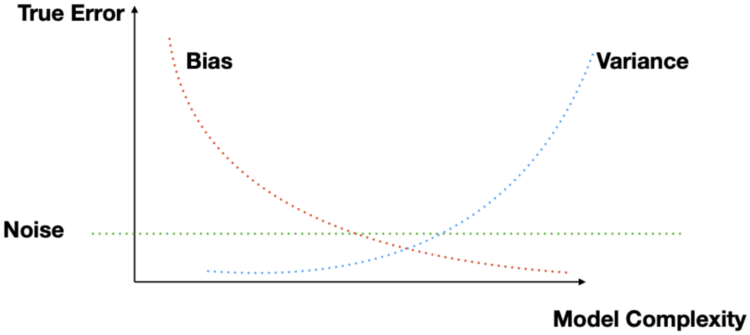

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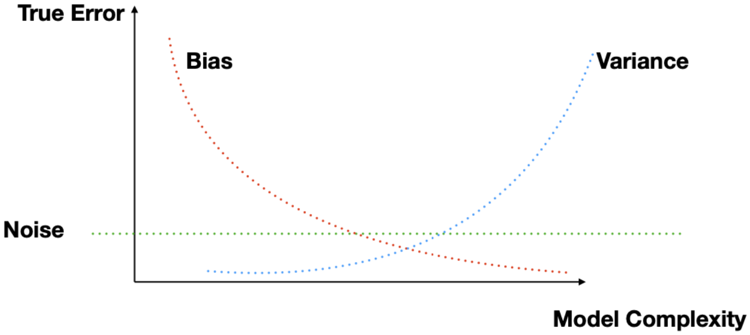
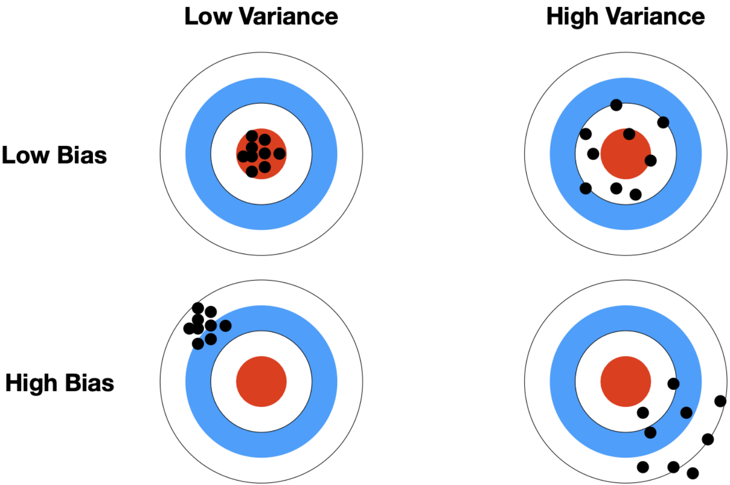
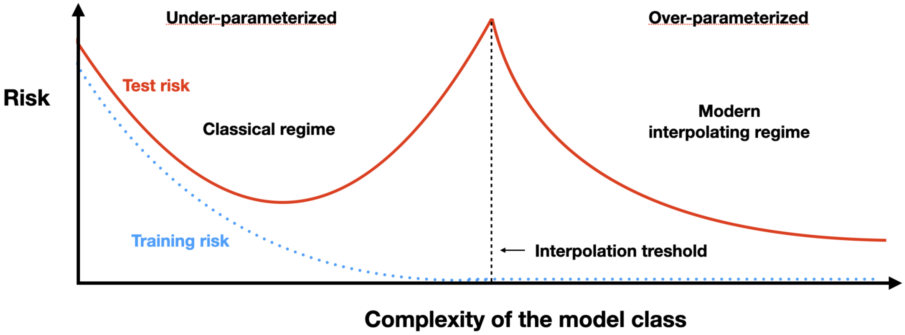


- If the complexity is too low, you cannot approximate well (under-fitting)
- If the complexity is too large, you have a problem with the variance (over-fitting)


Low Variance
High Variance
Low Bias
High Bias

Double descent curve in Deep Learning



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Classifier

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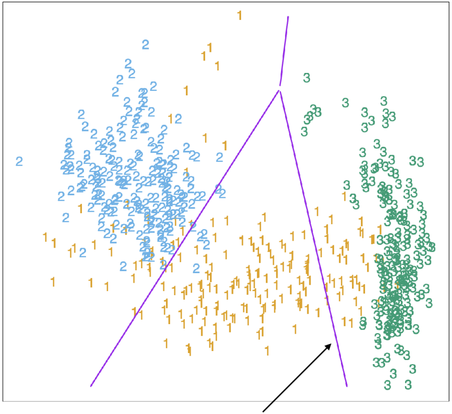

Linear Decision boundary

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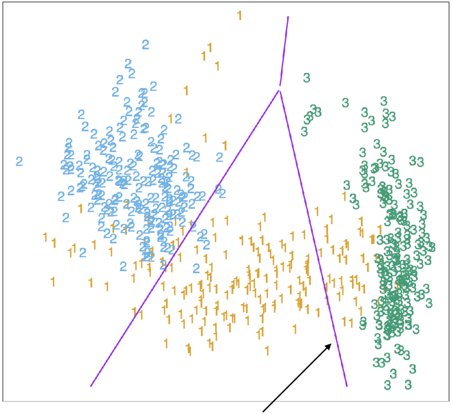

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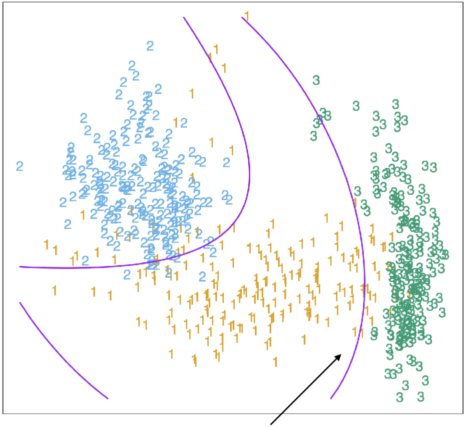

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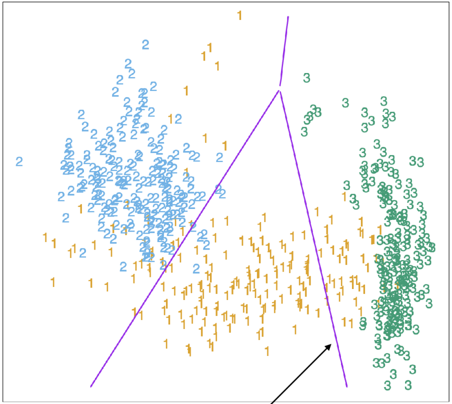

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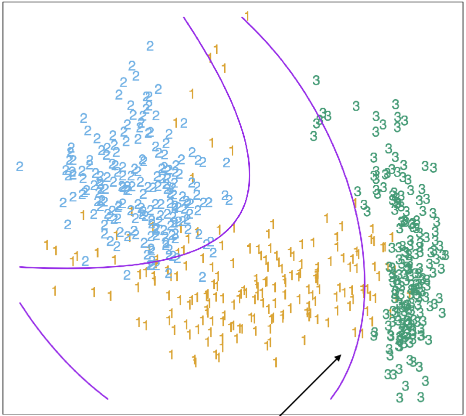

Nonlinear Decision boundary

The boundaries of these regions are called decision boundaries.

Classification: a special case of regression?

Classification is a **regression problem** with discrete labels:

$$(\mathbf{x}, y) \in \mathcal{X} \times \{0, 1\} \subset \mathcal{X} \times \mathbb{R} \tag{34}$$

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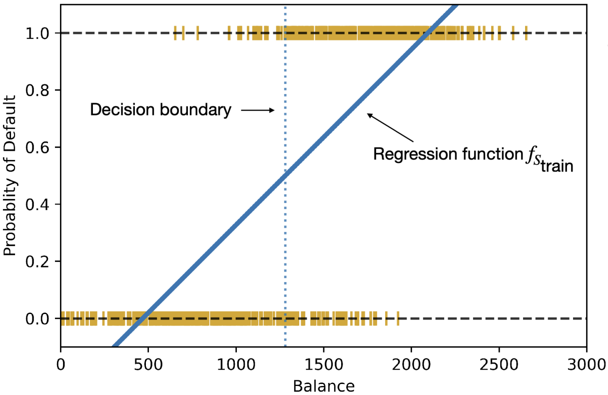
Classification is a **regression problem** with discrete labels:

$$(\mathbf{x}, y) \in \mathcal{X} \times \{0, 1\} \subset \mathcal{X} \times \mathbb{R} \tag{34}$$

Could we use previously seen regression methods to solve it?

Is it a good idea to use some regression methods?



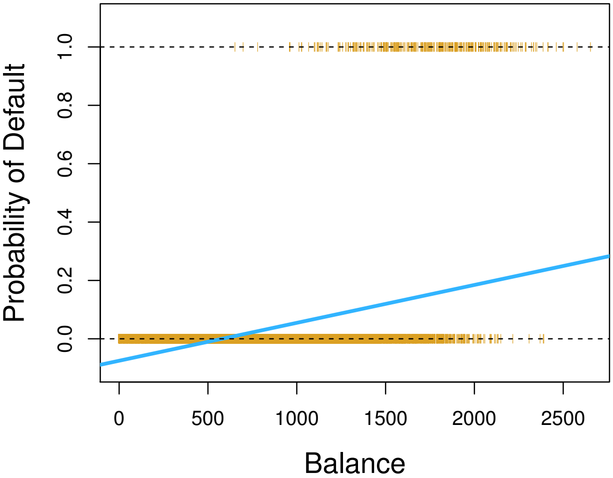
$y = 1$ **if "default"**

$y = 0$ **if "no default"**

We label the output as probability for sake of interpretation

Classification is not just a special form of regression

- The predicted values are not probabilities (not in $[0, 1]$)



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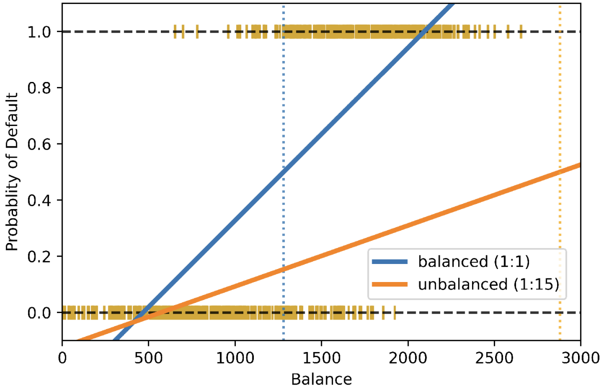

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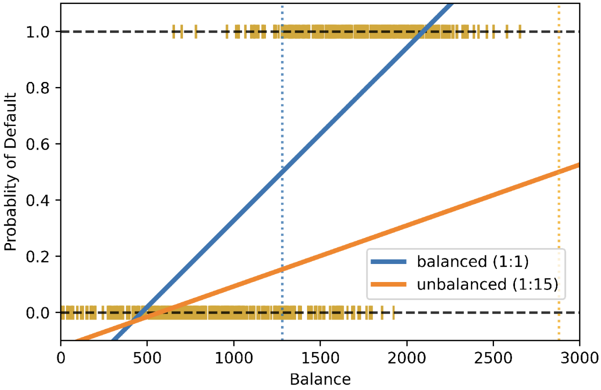

The position of the line depends crucially on how many points are in each class.

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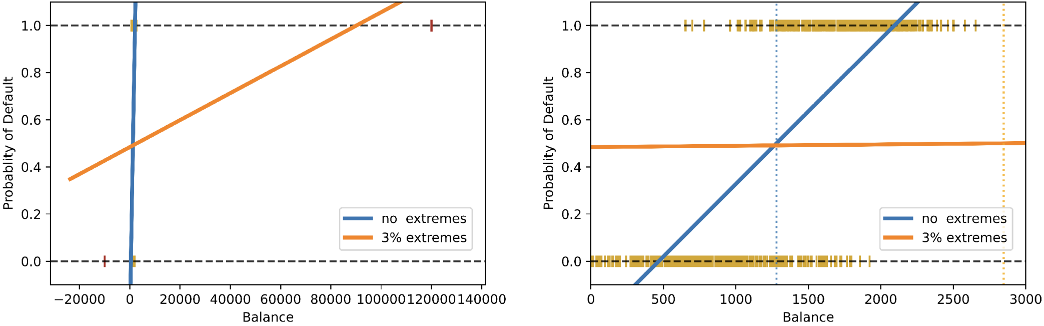

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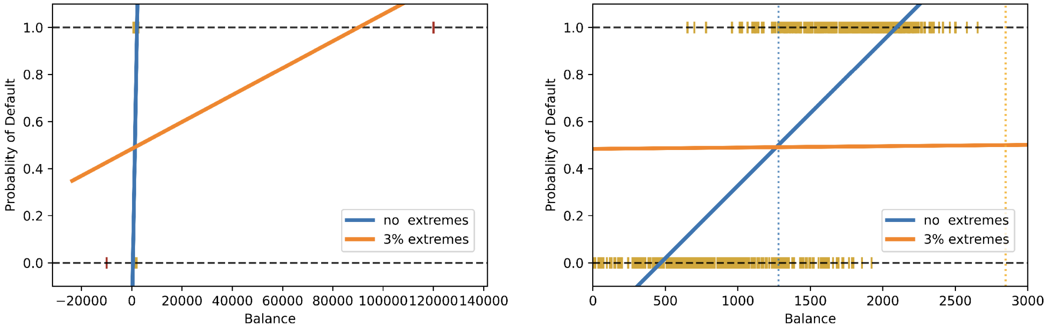

The position of the line depends crucially on where the points lie.

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Table of Contents

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- Generalization Gap
- Model Selection
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3 Bias-Variance Decomposition

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- Classification
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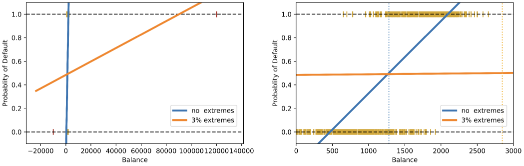

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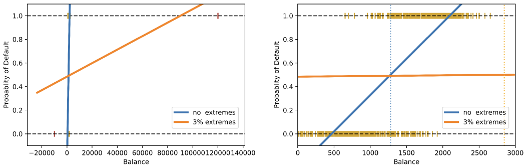

Solution: Transforming the predictions that take values in $(-\infty, \infty)$ into $[0, 1]$.

The logistic function

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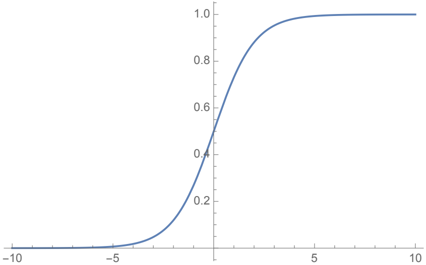

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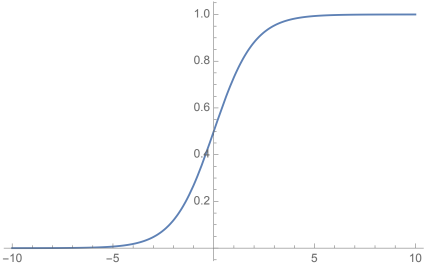

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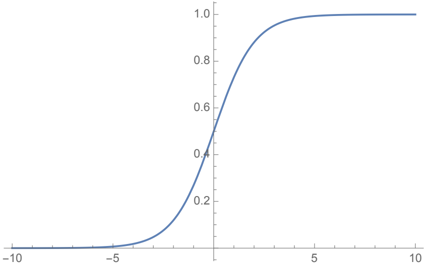

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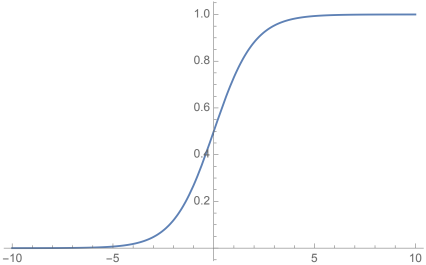

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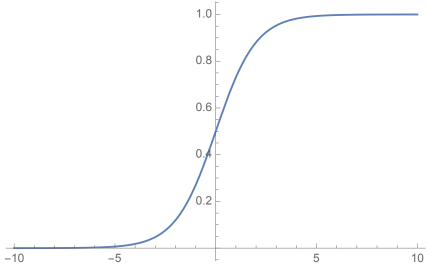

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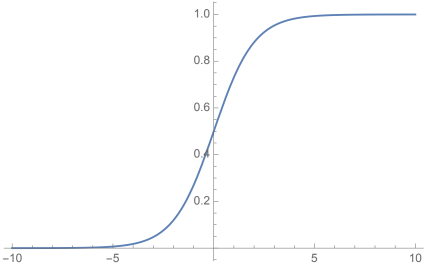

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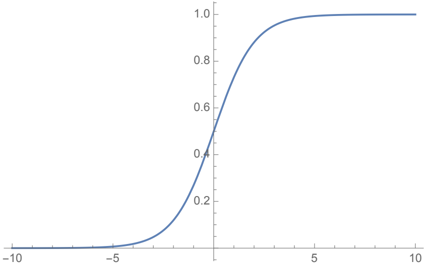

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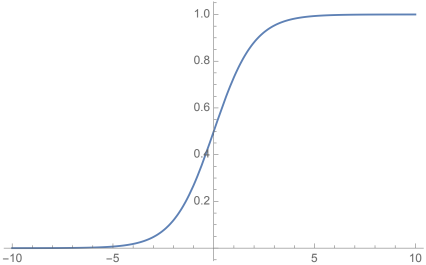

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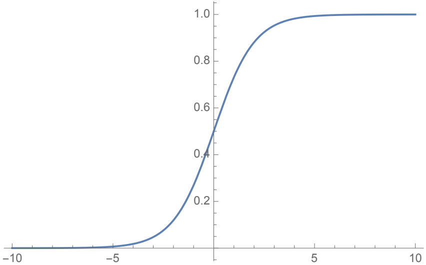

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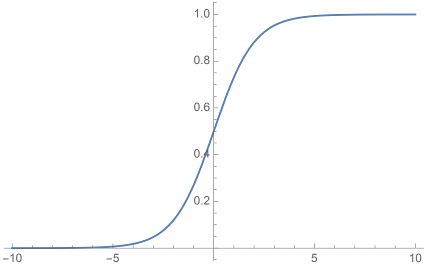

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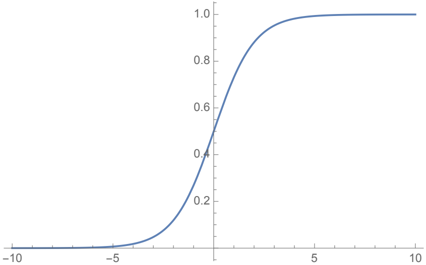

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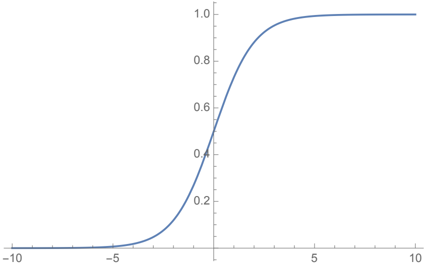

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Assume a training set S_{train}, consisting of i.i.d. samples $\{\mathbf{x}_n, y_n\}_{n=1}^{N}$ (fixed but unknown $\mathcal{D}$).

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Assume a training set S_{train}, consisting of i.i.d. samples $\{\mathbf{x}_n, y_n\}_{n=1}^N$ (fixed but unknown $\mathcal{D}$).

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As a result,

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Gradient of the negative log likelihood

Recall that

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$\Rightarrow$ It has no closed-form solution to $\nabla \mathcal{L}(\mathbf{w}) = 0$.

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Next lecture:

- Exponential Families and Generalized Linear Models
- Multi-Layer Perceptron
- Back-Propagation
- Introduction to Deep Learning Optimization (if time permits)