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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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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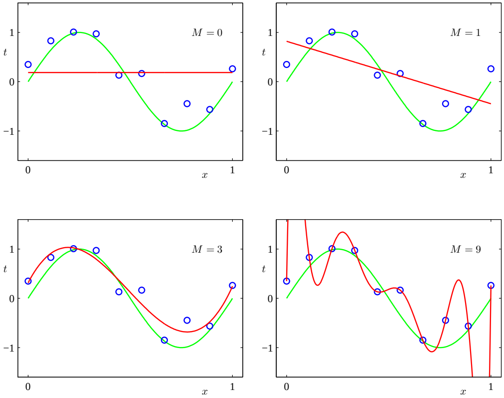

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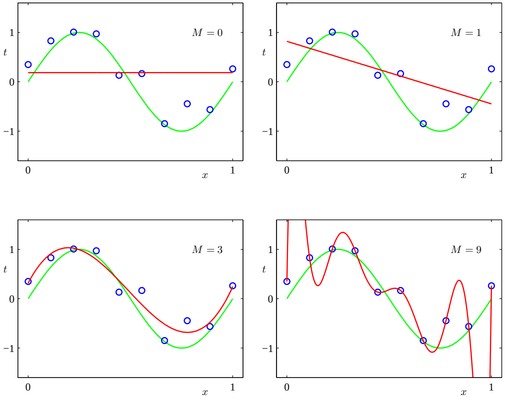

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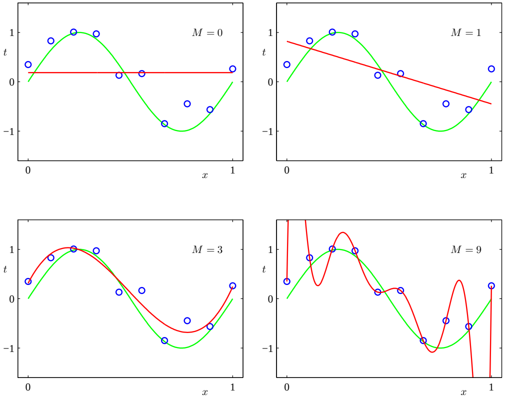

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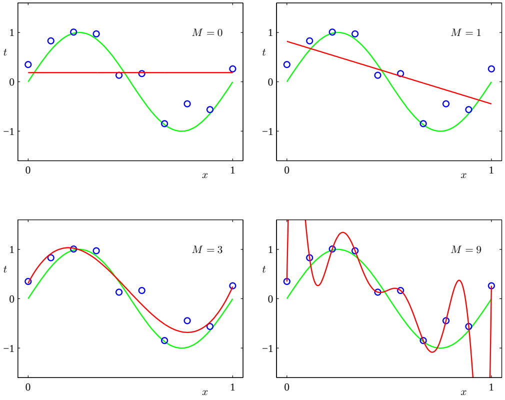

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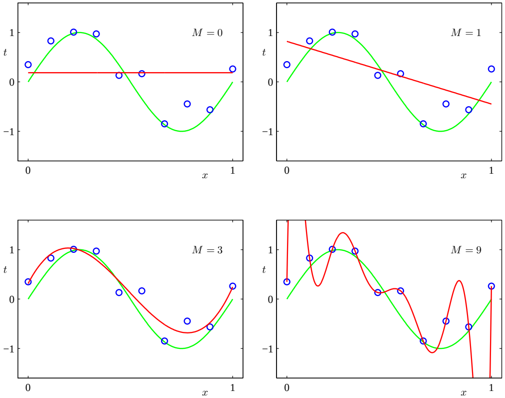

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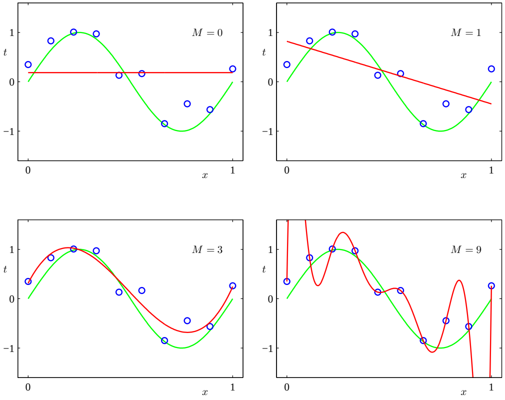

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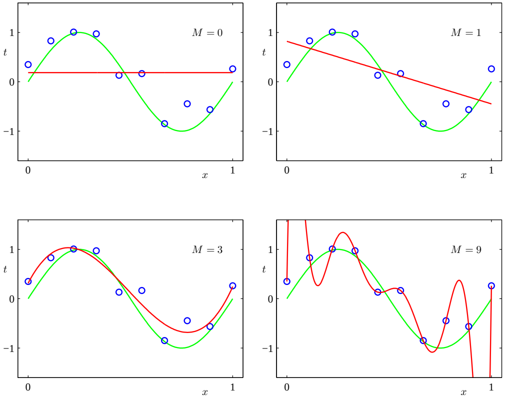

Discussion:

- 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.

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

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  - L_2-regularization (Ridge Regression)

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  - 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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- Issues: we have fewer data both for the learning and validation tasks (trade-off)

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- Polynomial Regression, Ridge Regression, and Lasso Regression
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This lecture:

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

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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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$\Rightarrow$ 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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In words, we can compute a probabilistic upper bound on the true risk.

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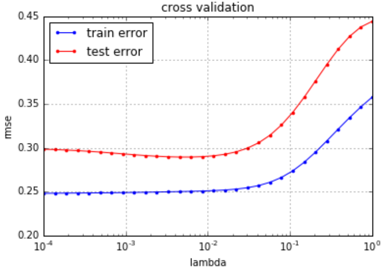

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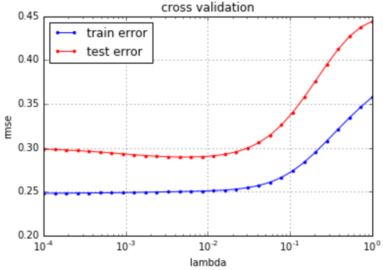

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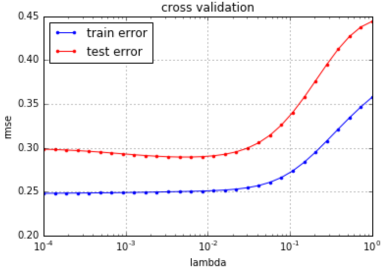

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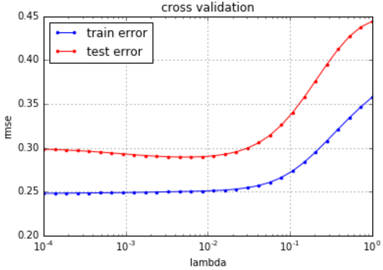

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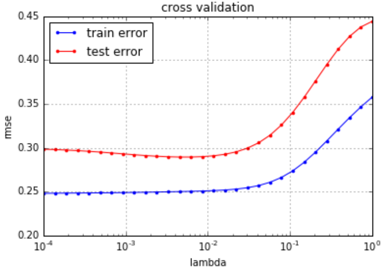

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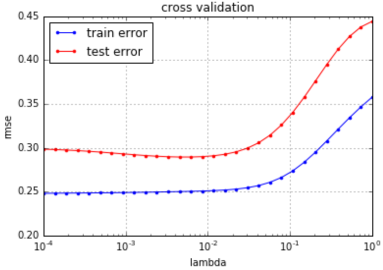

Issues: the existence of the generalization gap $|L_{S_{\text{test}}}(f_{S_{\text{train}},\lambda_k}) - L_{\mathcal{D}}(f_{S_{\text{train}},\lambda_k})|$!

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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.

$$\Pr\left[L_{\mathcal{D}}(f_{\hat{k}}) \geq L_{\mathcal{D}}(f_{k^\star}) + \sqrt{\frac{(b-a)^2 \ln(2K/\delta)}{2\,|S_{\text{test}}|}}\right] \leq \delta \tag{20}$$

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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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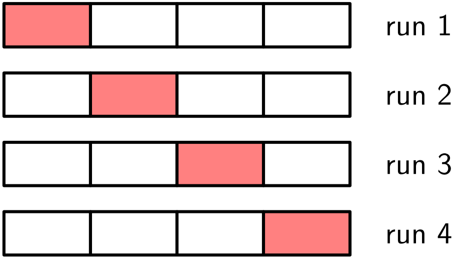

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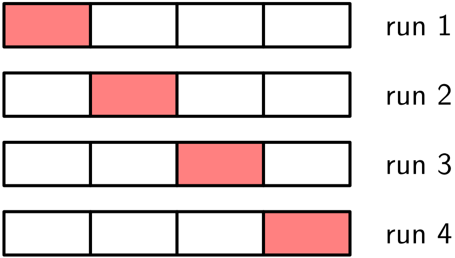

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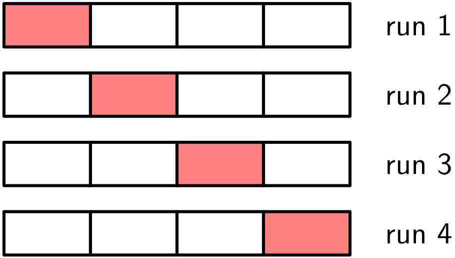

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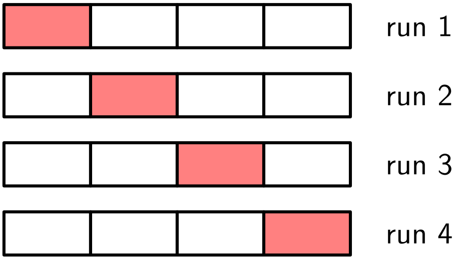

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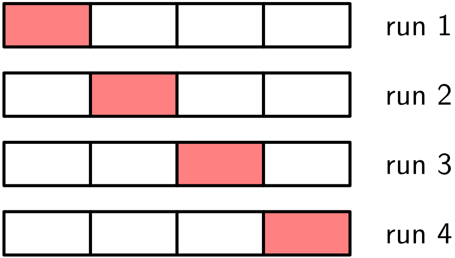

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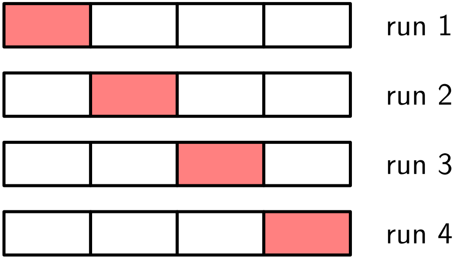

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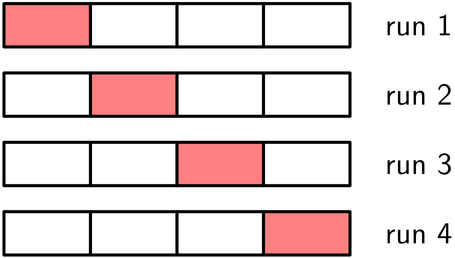

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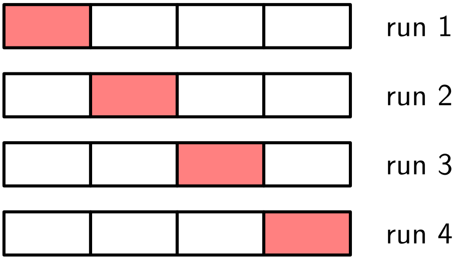

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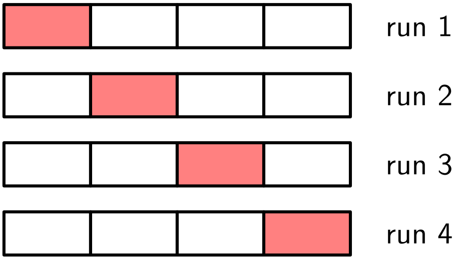

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- It will help us to decide how complex and rich we should make our model

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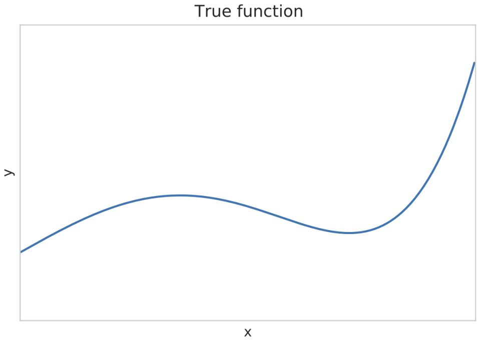

We have a true underlying function in blue we would like to recover.

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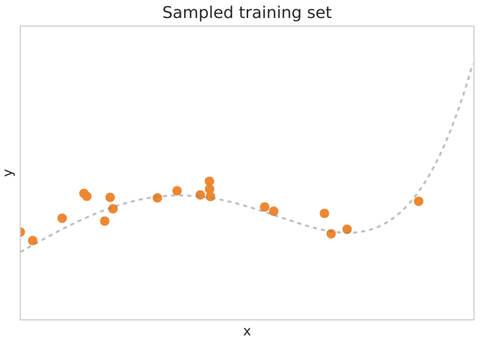

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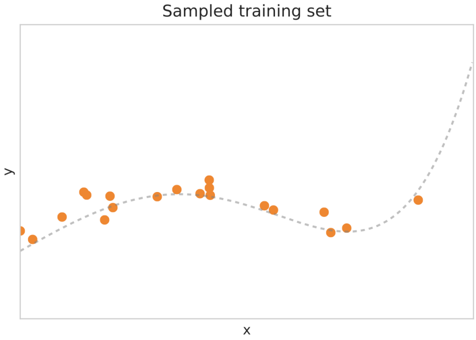

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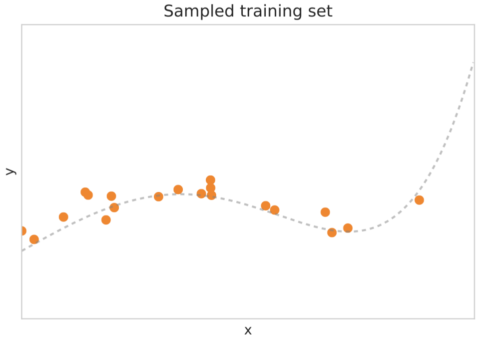

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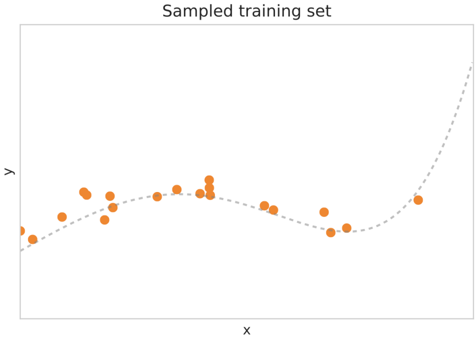

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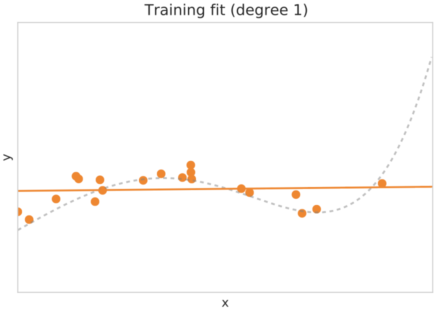

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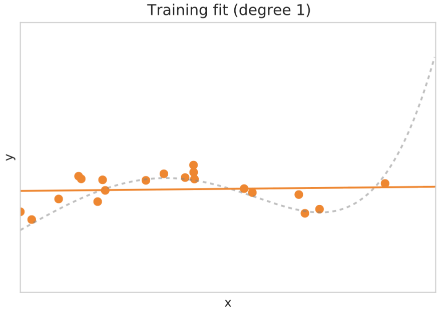

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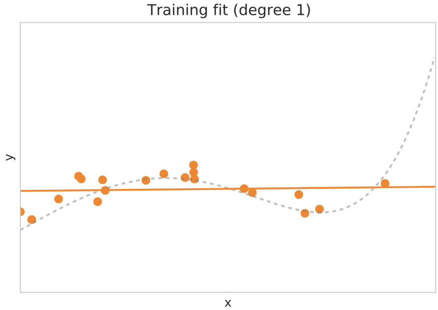

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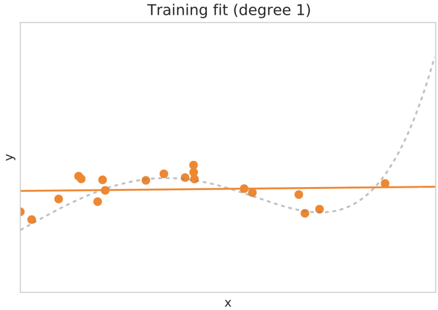

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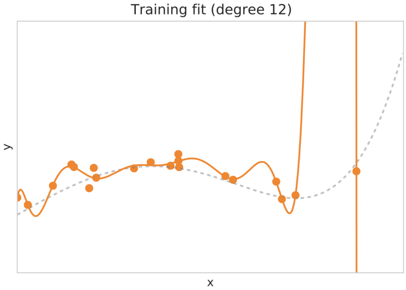

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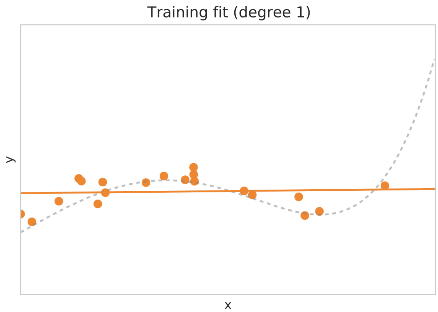

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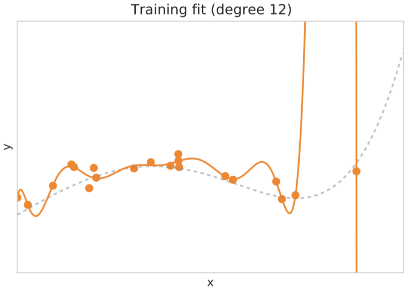

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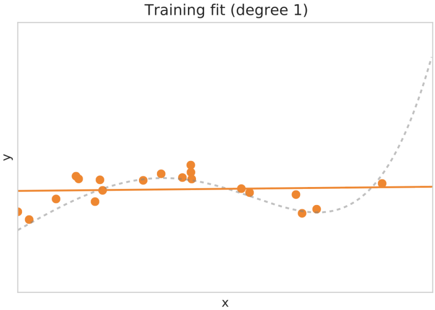

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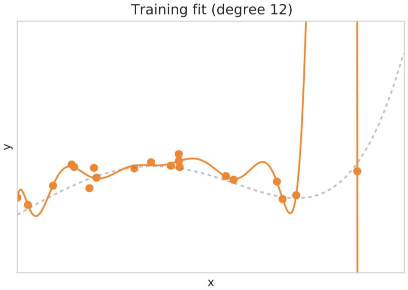
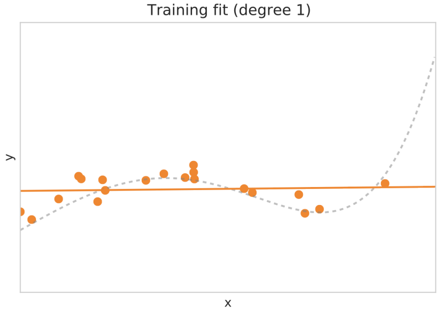


- We can find a model that fits the data well
- Is it a good predictor?

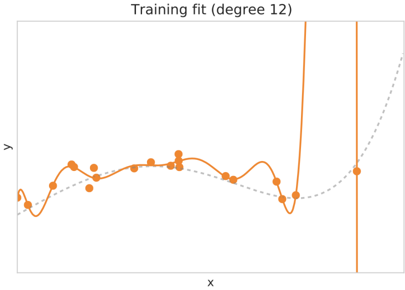
Motivation example: 1D-regression

If we restrict ourselves to simple models:



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

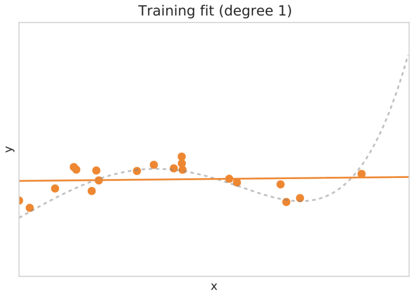
If we consider a high-degree polynomial:

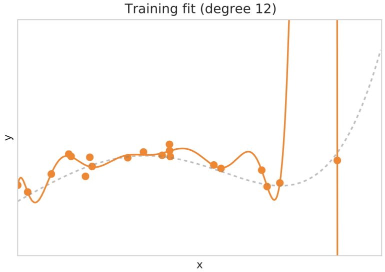


- We can find a model that fits the data well
- Is it a good predictor?
- No: Large generalization error

Motivation example: 1D-regression

Simple models are less sensitive.





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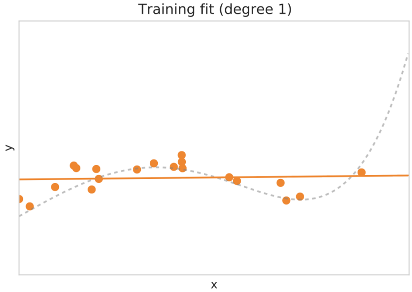

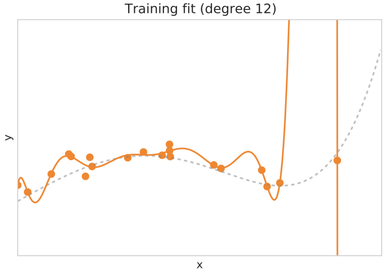

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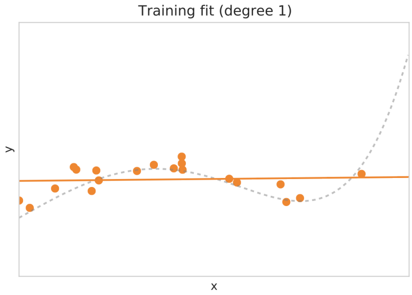

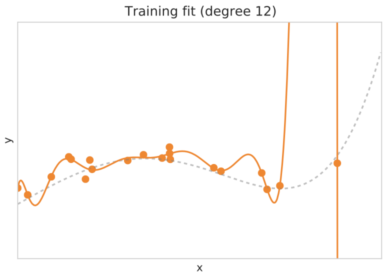

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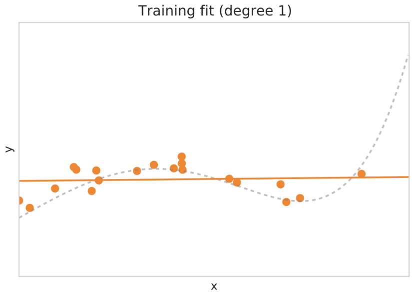

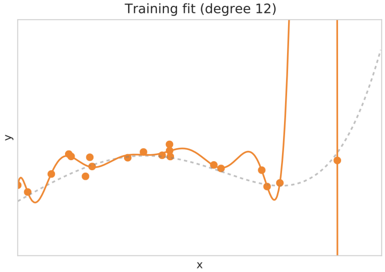

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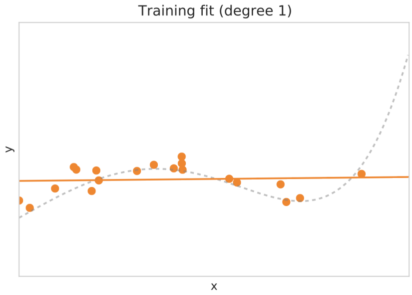

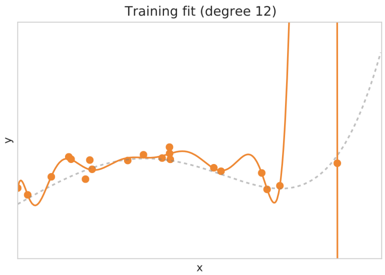

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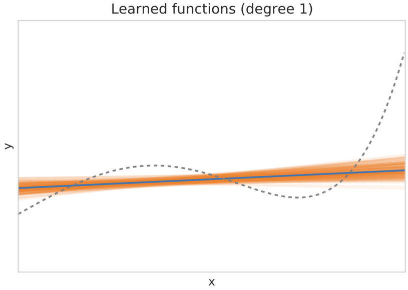
Simple models have large biases but low variance.



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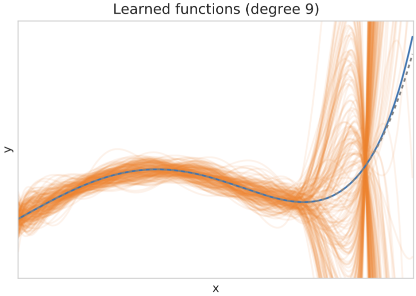

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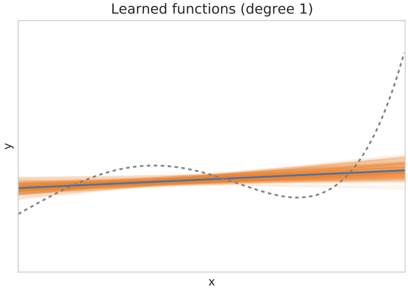

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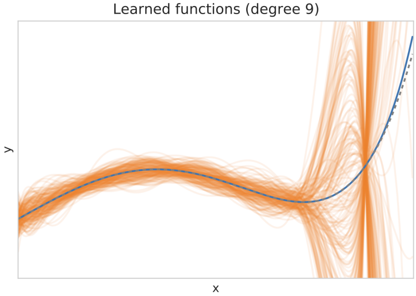

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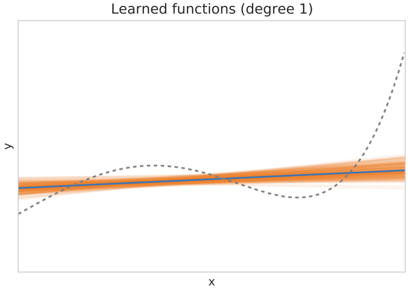

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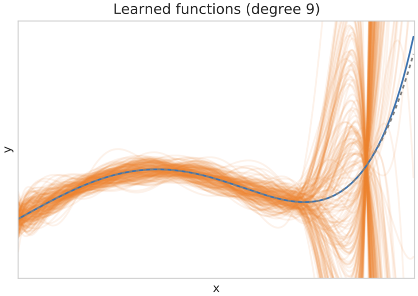

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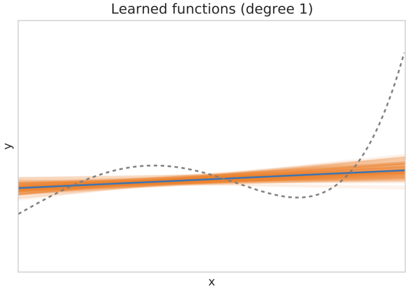

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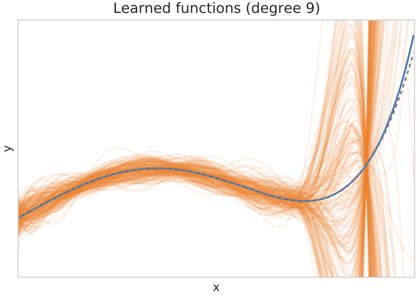

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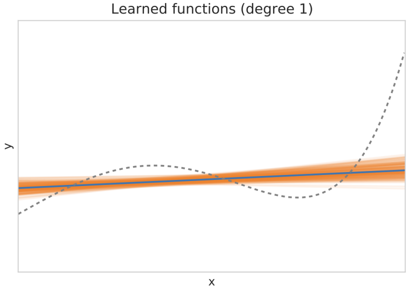

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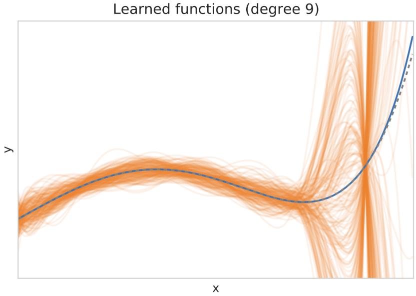

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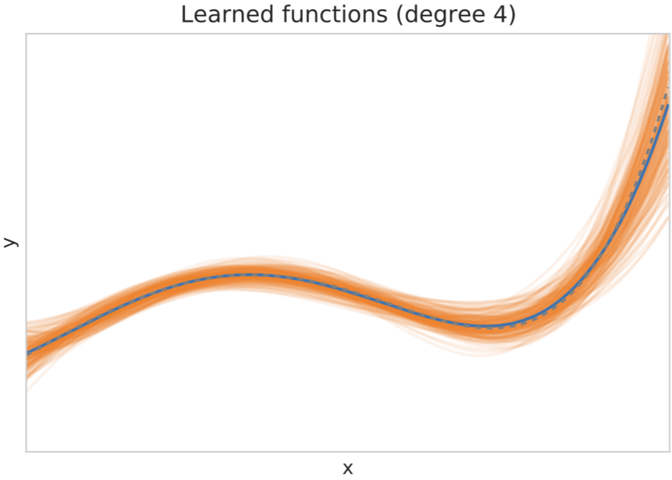

Data model

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

$$\boxed{y} = \boxed{f}(\boxed{x}) + \boxed{\epsilon} \tag{21}$$

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Error decomposition

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Training data $S_{\text{train}} \sim \mathcal{D}$ i.i.d.	$\rightarrow$	Algorithm $\mathcal{A}$

Error decomposition

Training data		Algorithm		Prediction
$S_{\text{train}} \sim \mathcal{D}$ i.i.d.	$\rightarrow$	$\mathcal{A}$	$\rightarrow$	$f_{S_{\text{train}}} = \mathcal{A}(S_{\text{train}})$

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$$\mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[(y - f_S(\mathbf{x}))^2\right] \tag{22}$$

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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

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

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$$= \mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[\qquad\qquad\qquad\qquad\qquad\right] \tag{30}$$

$$\tag{31}$$

$$\tag{33}$$

We can further decompose $\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[(f(\mathbf{x}_0) - f_{S_{\text{train}}}(\mathbf{x}_0))^2\right]$ into two terms:

$$\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[(f(\mathbf{x}_0) - f_{S_{\text{train}}}(\mathbf{x}_0))^2\right] \tag{28}$$

$$= \mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[(f(\mathbf{x}_0) - \mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right] + \mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right] - f_{S_{\text{train}}}(\mathbf{x}_0))^2\right] \tag{29}$$

$$= \mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[\left(f(\mathbf{x}_0) - \mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right]\right)^2 \qquad\qquad \right] \tag{30}$$

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We can further decompose $\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[(f(\mathbf{x}_0)-f_{S_{\text{train}}}(\mathbf{x}_0))^2\right]$ into two terms:

$$
\begin{aligned}
&\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[(f(\mathbf{x}_0)-f_{S_{\text{train}}}(\mathbf{x}_0))^2\right] && (28)\\
&=\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[(f(\mathbf{x}_0)-\mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right]+\mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right]-f_{S_{\text{train}}}(\mathbf{x}_0))^{2}\right] && (29)\\
&=\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[\left(f(\mathbf{x}_0)-\mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right]\right)^2+\left(\mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right]-f_{S_{\text{train}}}(\mathbf{x}_0)\right)^2\right] && (30)\\
& && (31)
\end{aligned}
$$

$$(33)$$

We can further decompose $\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[(f(\mathbf{x}_0)-f_{S_{\text{train}}}(\mathbf{x}_0))^2\right]$ into two terms:

$$
\begin{aligned}
&\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[(f(\mathbf{x}_0)-f_{S_{\text{train}}}(\mathbf{x}_0))^2\right] && (28)\\
&=\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[(f(\mathbf{x}_0)-\mathbb{E}_{S_{\text{train'}}}[f_{S_{\text{train'}}}(\mathbf{x}_0)]+\mathbb{E}_{S_{\text{train'}}}[f_{S_{\text{train'}}}(\mathbf{x}_0)]-f_{S_{\text{train}}}(\mathbf{x}_0))^2\right] && (29)\\
&=\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[\left(f(\mathbf{x}_0)-\mathbb{E}_{S_{\text{train'}}}[f_{S_{\text{train'}}}(\mathbf{x}_0)]\right)^2+\left(\mathbb{E}_{S_{\text{train'}}}[f_{S_{\text{train'}}}(\mathbf{x}_0)]-f_{S_{\text{train}}}(\mathbf{x}_0)\right)^2\right] && (30)\\
&\quad\underbrace{+\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[2\left((f(\mathbf{x}_0)-\mathbb{E}_{S_{\text{train'}}}[f_{S_{\text{train'}}}(\mathbf{x}_0)]\right)\left(\mathbb{E}_{S_{\text{train'}}}[f_{S_{\text{train'}}}(\mathbf{x}_0)]-f_{S_{\text{train}}}(\mathbf{x}_0)\right))\right]}_{0} && (31)\\
& && (33)
\end{aligned}
$$

We can further decompose $\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[(f(\mathbf{x}_0) - f_{S_{\text{train}}}(\mathbf{x}_0))^2\right]$ into two terms:

$$
\begin{aligned}
&\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[(f(\mathbf{x}_0) - f_{S_{\text{train}}}(\mathbf{x}_0))^2\right] && (28)\\
&= \mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[(f(\mathbf{x}_0) - \mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right] + \mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right] - f_{S_{\text{train}}}(\mathbf{x}_0))^2\right] && (29)\\
&= \mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[\left(f(\mathbf{x}_0) - \mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right]\right)^2 + \left(\mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right] - f_{S_{\text{train}}}(\mathbf{x}_0)\right)^2\right] && (30)\\
&\qquad \underbrace{+\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[2\left(\left(f(\mathbf{x}_0) - \mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right]\right)\left(\mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right] - f_{S_{\text{train}}}(\mathbf{x}_0)\right)\right)\right]}_{0} && (31)\\
&= \underbrace{\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[\left(f(\mathbf{x}_0) - \mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right]\right)^2\right]}_{\text{bias}} && (32)\\
& && (33)
\end{aligned}
$$

We can further decompose $\mathbb{E}_{S_{\text{train}} \sim \mathcal{D}} \left[(f(\mathbf{x}_0) - f_{S_{\text{train}}}(\mathbf{x}_0))^2 \right]$ into two terms:

$$
\begin{aligned}
&\mathbb{E}_{S_{\text{train}} \sim \mathcal{D}} \left[(f(\mathbf{x}_0) - f_{S_{\text{train}}}(\mathbf{x}_0))^2 \right] && (28)\\
&= \mathbb{E}_{S_{\text{train}} \sim \mathcal{D}} \left[(f(\mathbf{x}_0) - \mathbb{E}_{S_{\text{train'}}} \left[f_{S_{\text{train'}}}(\mathbf{x}_0) \right] + \mathbb{E}_{S_{\text{train'}}} \left[f_{S_{\text{train'}}}(\mathbf{x}_0) \right] - f_{S_{\text{train}}}(\mathbf{x}_0))^2 \right] && (29)\\
&= \mathbb{E}_{S_{\text{train}} \sim \mathcal{D}} \left[\left(f(\mathbf{x}_0) - \mathbb{E}_{S_{\text{train'}}} \left[f_{S_{\text{train'}}}(\mathbf{x}_0) \right]\right)^2 + \left(\mathbb{E}_{S_{\text{train'}}} \left[f_{S_{\text{train'}}}(\mathbf{x}_0) \right] - f_{S_{\text{train}}}(\mathbf{x}_0)\right)^2 \right] && (30)\\
&\quad \underbrace{+ \mathbb{E}_{S_{\text{train}} \sim \mathcal{D}} \left[2 \left(\left(f(\mathbf{x}_0) - \mathbb{E}_{S_{\text{train'}}} \left[f_{S_{\text{train'}}}(\mathbf{x}_0) \right]\right) \left(\mathbb{E}_{S_{\text{train'}}} \left[f_{S_{\text{train'}}}(\mathbf{x}_0) \right] - f_{S_{\text{train}}}(\mathbf{x}_0) \right) \right) \right]}_{0} && (31)\\
&= \underbrace{\mathbb{E}_{S_{\text{train}} \sim \mathcal{D}} \left[\left(f(\mathbf{x}_0) - \mathbb{E}_{S_{\text{train'}}} \left[f_{S_{\text{train'}}}(\mathbf{x}_0) \right]\right)^2 \right]}_{\text{bias}} && (32)\\
&\quad + \underbrace{\mathbb{E}_{S_{\text{train}} \sim \mathcal{D}} \left[\left(\mathbb{E}_{S_{\text{train'}}} \left[f_{S_{\text{train'}}}(\mathbf{x}_0) \right] - f_{S_{\text{train}}}(\mathbf{x}_0)\right)^2 \right]}_{\text{variance}} && (33)
\end{aligned}
$$

Bias-Variance Decomposition

$$
\begin{aligned}
\mathbb{E}_{S_{\text{train}} \sim \mathcal{D}, \boldsymbol{\epsilon} \sim \mathcal{D}_{\boldsymbol{\epsilon}}} \left[(f(\mathbf{x}_0) - f_{S_{\text{train}}}(\mathbf{x}_0))^2 \right] &= \mathrm{Var}_{\boldsymbol{\epsilon} \sim \mathcal{D}_{\boldsymbol{\epsilon}}}[\boldsymbol{\epsilon}] && \text{(noise variance)} \\
&+ (f(\mathbf{x}_0) - \mathbb{E}_{S_{\text{train'}}}[f_{S_{\text{train'}}}(\mathbf{x}_0)])^2 && \text{(Bias)} \\
&+ \mathbb{E}_{S_{\text{train}} \sim \mathcal{D}} \left[(\mathbb{E}_{S_{\text{train'}}}[f_{S_{\text{train'}}}(\mathbf{x}_0)] - f_{S_{\text{train}}}(\mathbf{x}_0))^2 \right], && \text{(Variance)}
\end{aligned}
$$

Bias-Variance Decomposition

$$\begin{aligned}
\mathbb{E}_{S_{\text{train}}\sim\mathcal{D},\boldsymbol{\epsilon}\sim\mathcal{D}_{\boldsymbol{\epsilon}}}\left[(f(\mathbf{x}_0)-f_{S_{\text{train}}}(\mathbf{x}_0))^2\right] &= \mathsf{Var}_{\boldsymbol{\epsilon}\sim\mathcal{D}_{\boldsymbol{\epsilon}}}[\boldsymbol{\epsilon}] && \text{(noise variance)}\\
&+ (f(\mathbf{x}_0)-\mathbb{E}_{S_{\text{train'}}}[f_{S_{\text{train'}}}(\mathbf{x}_0)])^2 && \text{(Bias)}\\
&+ \mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[(\mathbb{E}_{S_{\text{train'}}}[f_{S_{\text{train'}}}(\mathbf{x}_0)]-f_{S_{\text{train}}}(\mathbf{x}_0))^2\right], && \text{(Variance)}
\end{aligned}$$

which always lowers bound the true error.

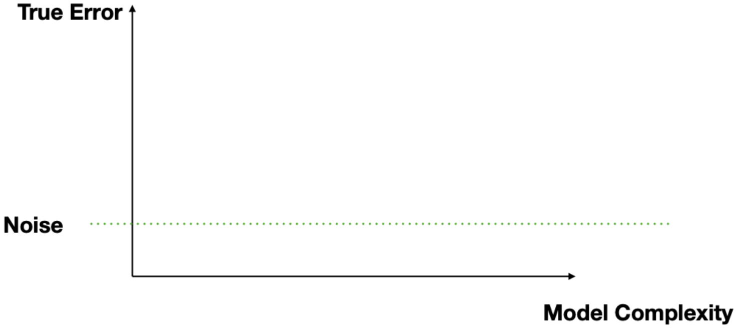
Bias-Variance Decomposition

$$
\begin{aligned}
\mathbb{E}_{S_{\text{train}}\sim\mathcal{D},\epsilon\sim\mathcal{D}_\epsilon}\left[\left(f(\mathbf{x}_0)-f_{S_{\text{train}}}(\mathbf{x}_0)\right)^2\right] &= \text{Var}_{\epsilon\sim\mathcal{D}_\epsilon}[\epsilon] && \text{(noise variance)}\\
&+\left(f(\mathbf{x}_0)-\mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right]\right)^2 && \text{(Bias)}\\
&+\mathbb{E}_{S_{\text{train}}\sim\mathcal{D}}\left[\left(\mathbb{E}_{S_{\text{train'}}}\left[f_{S_{\text{train'}}}(\mathbf{x}_0)\right]-f_{S_{\text{train}}}(\mathbf{x}_0)\right)^2\right], && \text{(Variance)}
\end{aligned}
$$

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 $\text{Var}_{\epsilon \sim \mathcal{D}_\epsilon}[\epsilon]$—a strict lower bound on what error we can achieve



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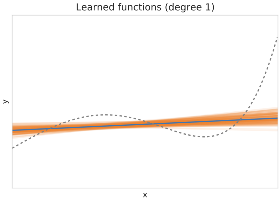
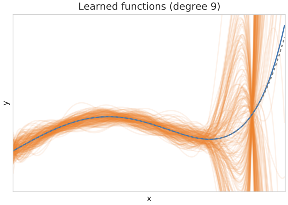
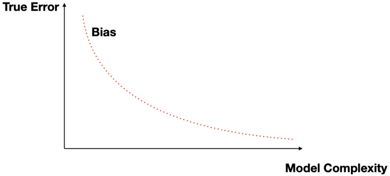
Component 1: Noise $\text{Var}_{\epsilon \sim \mathcal{D}_\epsilon}[\epsilon]$—a strict lower bound on what error we can achieve

- 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

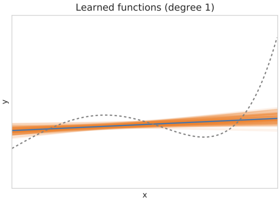
Component 2: Bias $\left(f(\mathbf{x}_0) - \mathbb{E}_{S_{\text{train}}}\left[f_{S_{\text{train}}}(\mathbf{x}_0)\right]\right)^2$

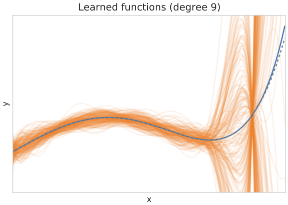


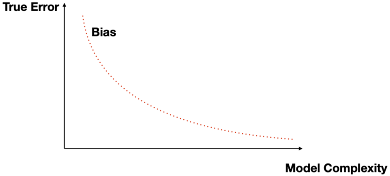




Component 2: Bias $\left(f(\mathbf{x}_0) - \mathbb{E}_{S_{\text{train}'}}\left[f_{S_{\text{train}'}}(\mathbf{x}_0)\right]\right)^2$

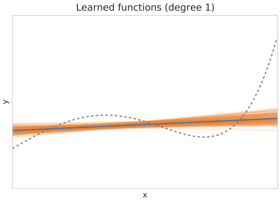


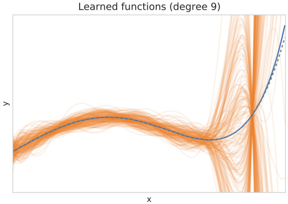


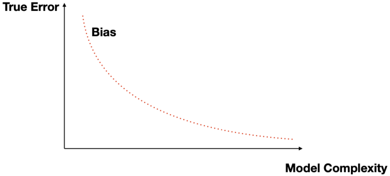


- It measures how far off in general the models' predictions are from the correct value.

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







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

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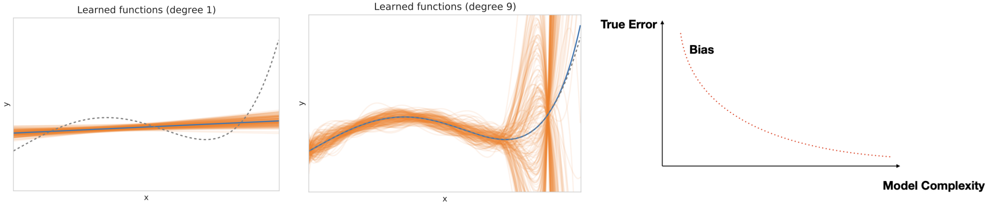
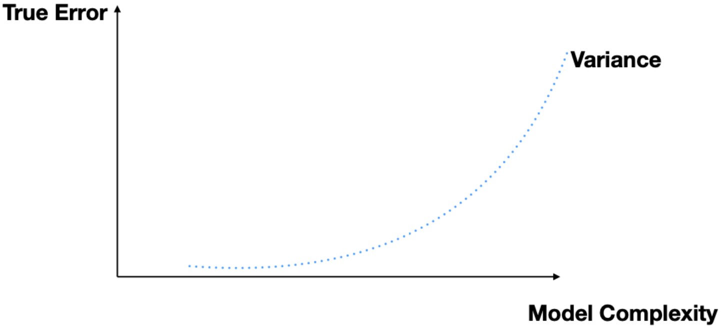
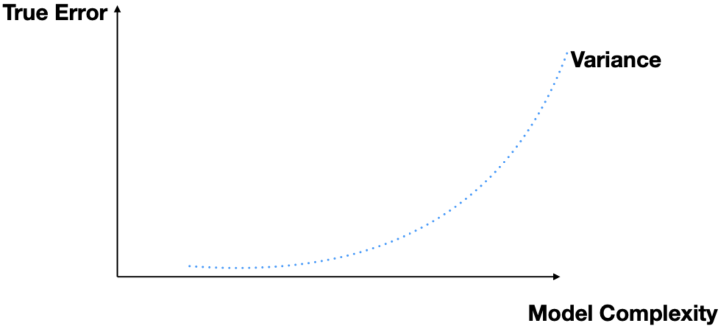


- It measures how far off in general the models' predictions are from the correct value.
- If complexity is small, then high bias.
- If complexity is high, then low bias.

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



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



- Variance of the prediction function.

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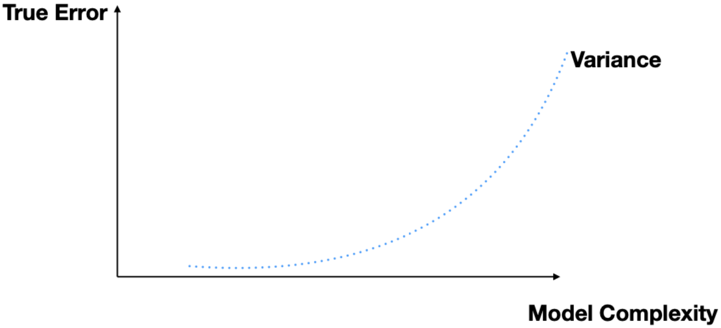

- Variance of the prediction function.
- It is how much the predictions for a given point vary between different realizations of the training set.

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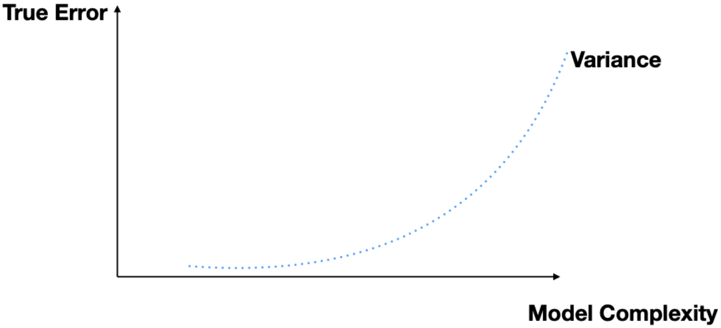
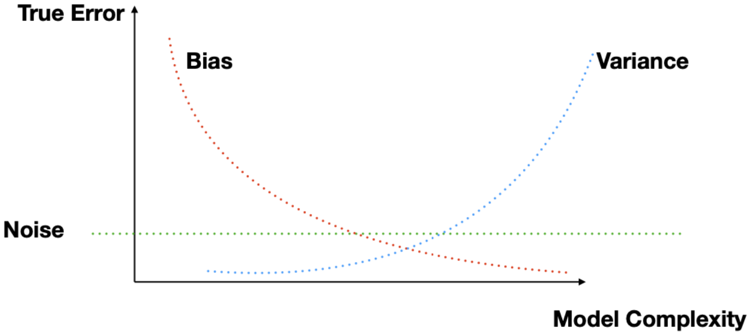
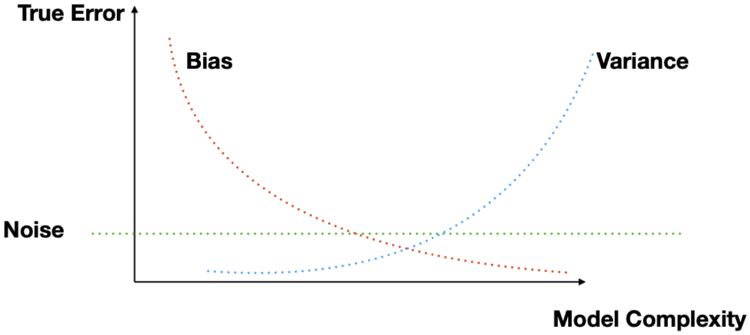


- Variance of the prediction function.
- It is how much the predictions for a given point vary between different realizations of the training set.
- If we consider complicated models, then small variations in the training set can result in large changes in the prediction.

Bias Variance tradeoff and U-shape curve

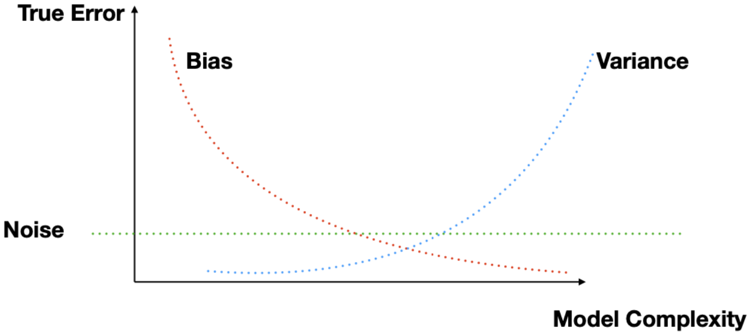


Bias Variance tradeoff and U-shape curve

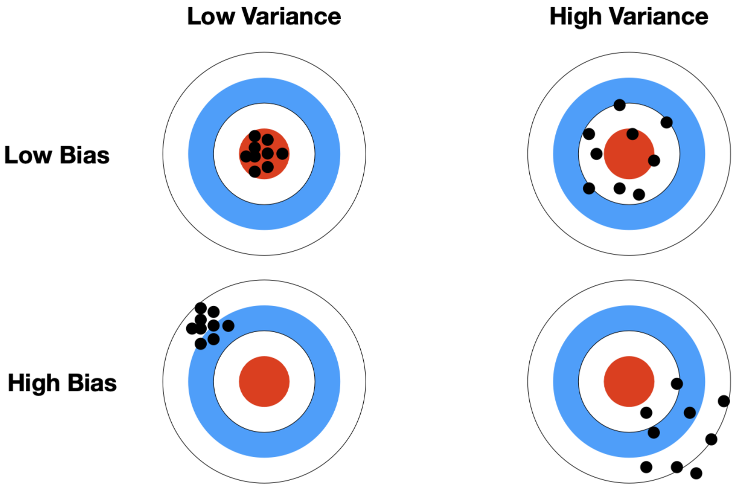


- If the complexity is too low, you cannot approximate well (under-fitting)

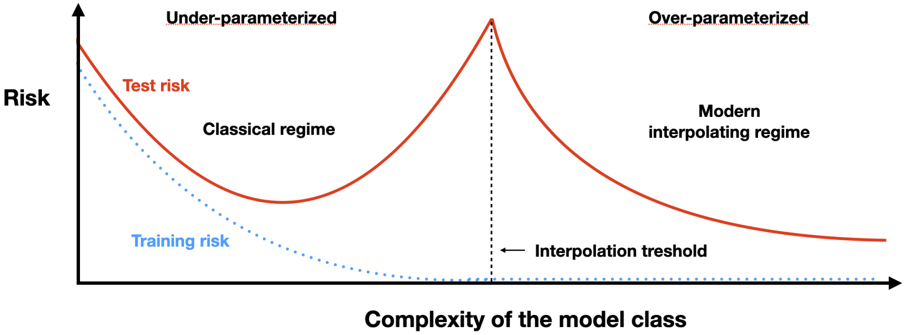
Bias Variance tradeoff and U-shape curve



- 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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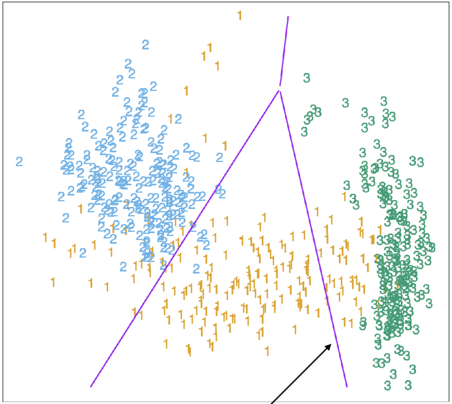
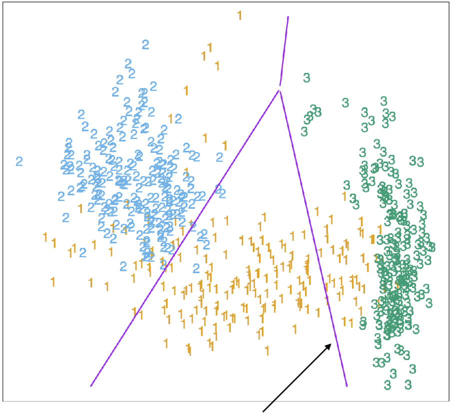


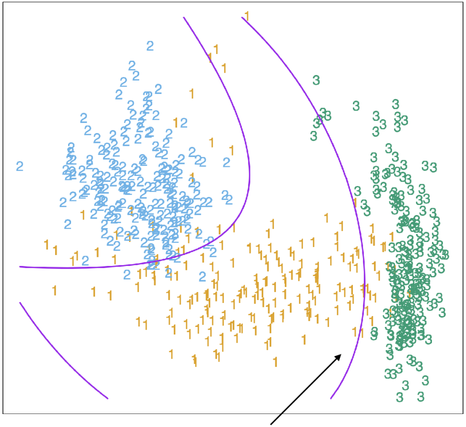
Linear Decision boundary

Classifier

A classifier $f : \mathcal{X} \to \mathcal{Y}$ divides the input space into a collection of regions belonging to each class.



Linear Decision boundary



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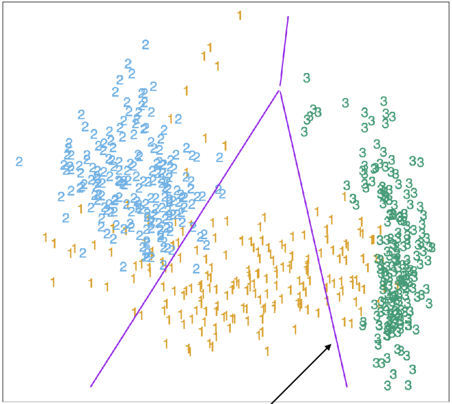

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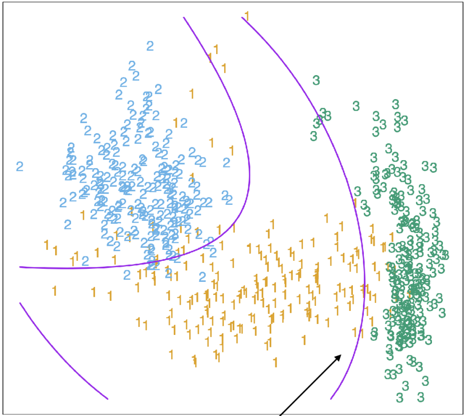


Nonlinear Decision boundary

The boundaries of these regions are called decision boundaries.

Classification: a special case of regression?

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

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

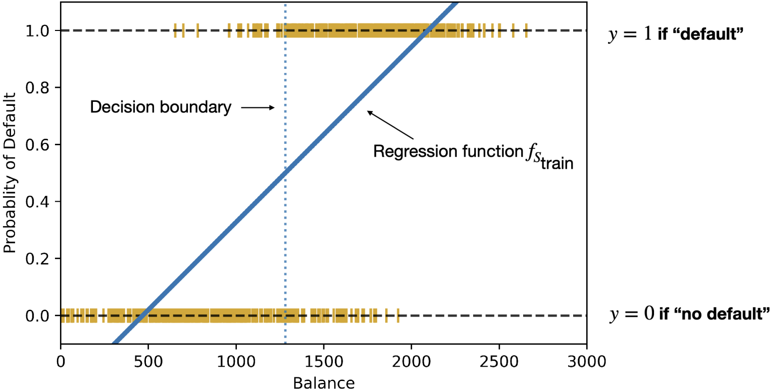
Classification: a special case of regression?

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

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

Could we use previously seen regression methods to solve it?

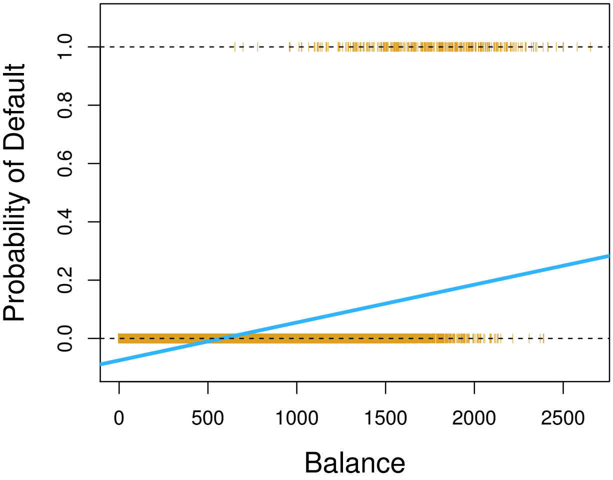
Is it a good idea to use some regression methods?



We label the output as probability for sake of interpretation

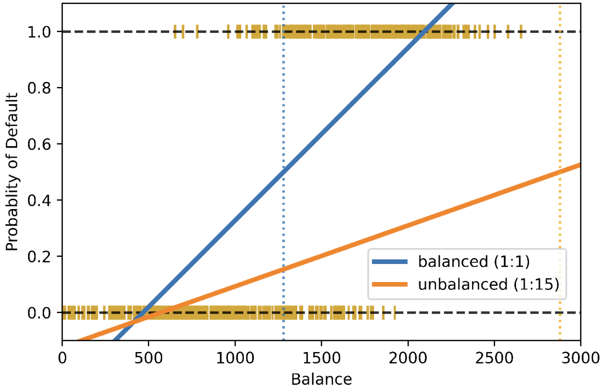
Classification is not just a special form of regression

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



Classification is not just a special form of regression

- Sensitivity to unbalanced data



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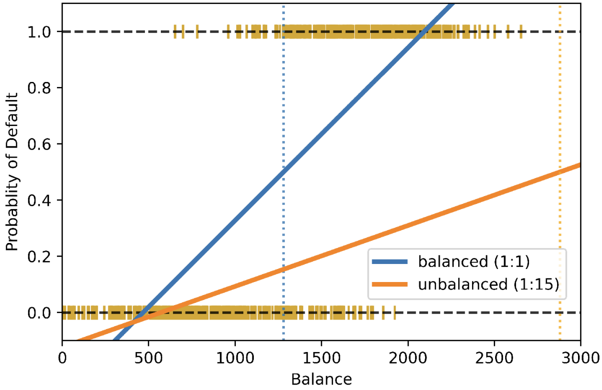
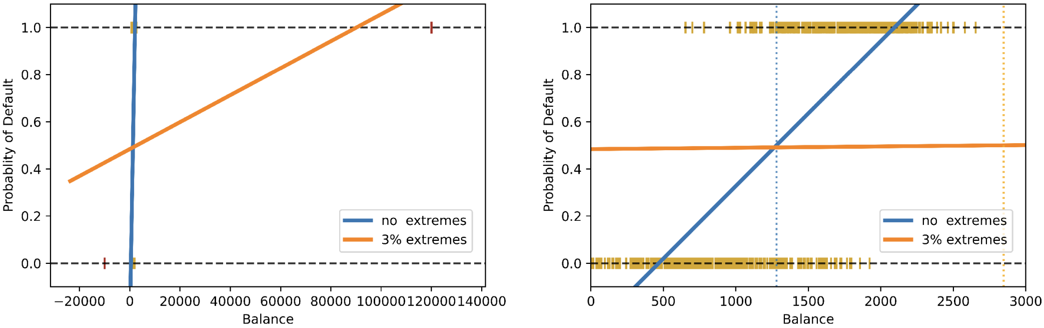


The position of the line depends crucially on how many points are in each class.

Classification is not just a special form of regression

- Sensitivity to extreme values:



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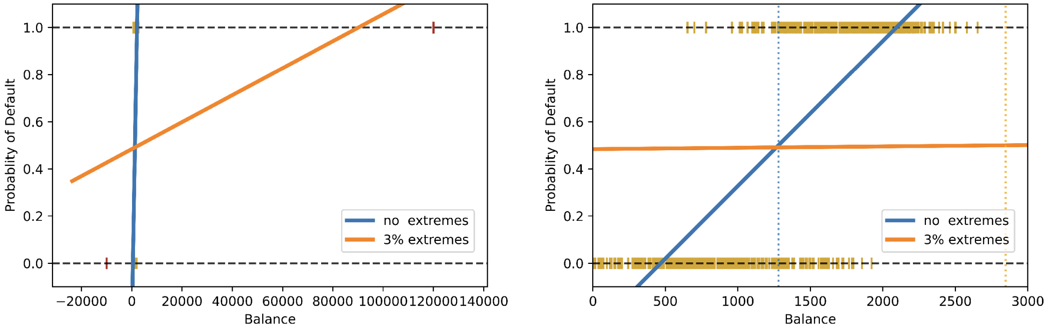

The position of the line depends crucially on where the points lie.

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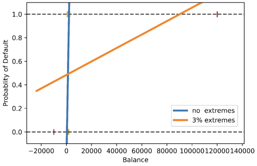

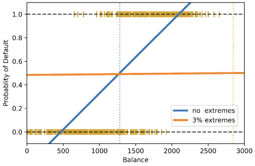

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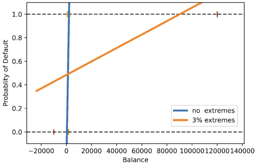

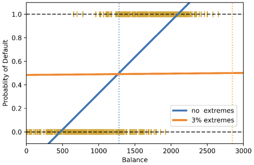

Solution: Transforming the predictions that take values in $(-\infty, \infty)$ into $[0, 1]$.

The logistic function

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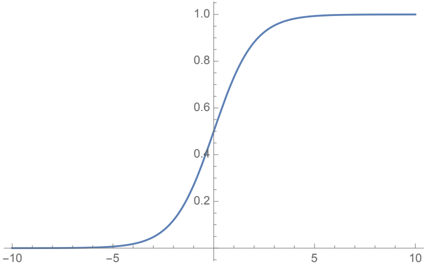

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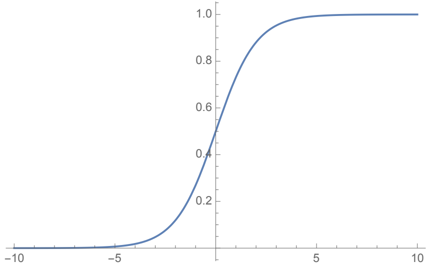

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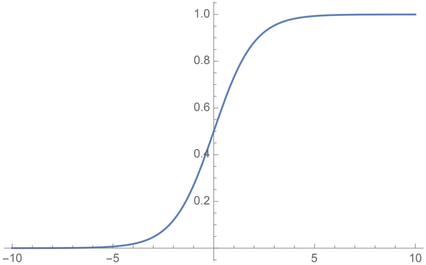

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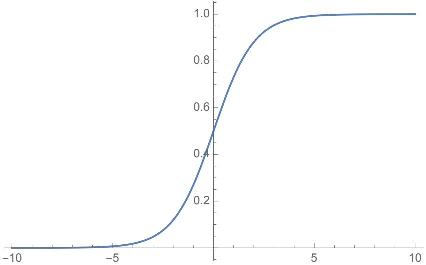

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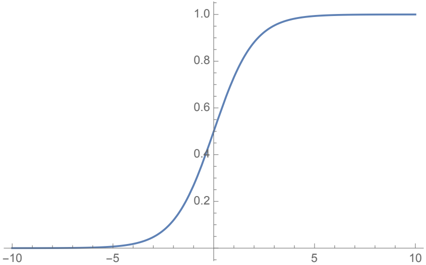

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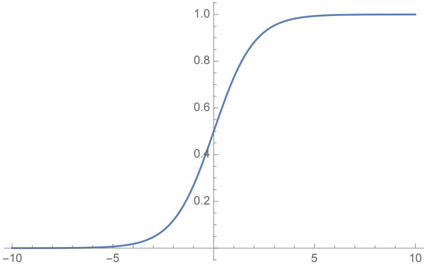

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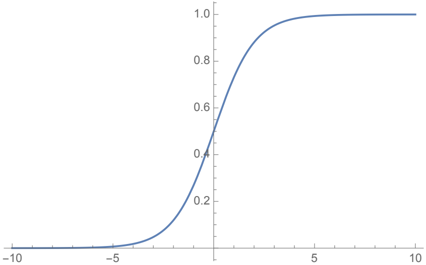

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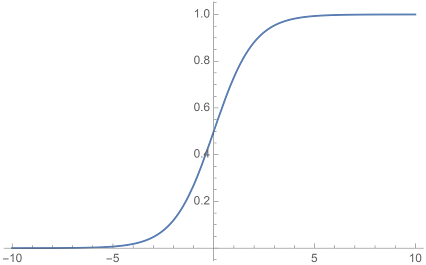

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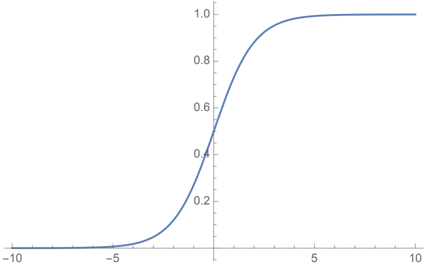

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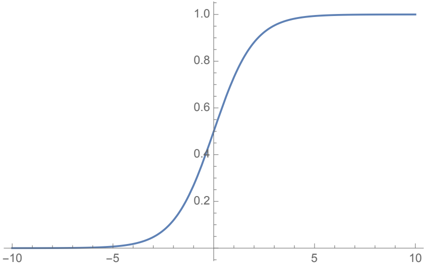

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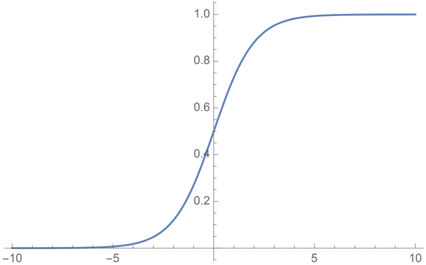

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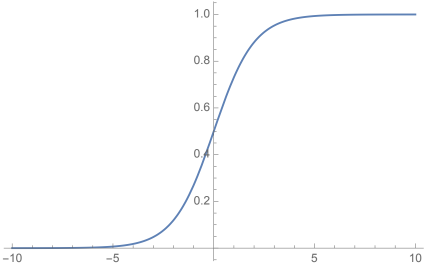

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As a result,

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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
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- Back-Propagation
- Introduction to Deep Learning Optimization