Overfitting and Model Tuning

Overfitting and Model Tuning

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Reading Materials

- Max Kuhn. Chapter 4.

Prediction Problem

Given data of $X = [X_1, X_2, ..., X_d]$ and Y. Find the relation between X and Y.

Prediction Problem - Examples

- One Input Variable X

X	Y
13	4.0
6	3.5
14	3
10	3.9
7	2.7
12	3.8
1	1.5

How are X and Y related?

Prediction Problem - Examples

- Multiple Input Variables

X_1	X_2	...	X_{35}	Y
1	-1	...	2	Tree
2.1	0	...	6	Not a Tree
3	0	...	8	Tree

How are X and Y related?

Prediction Problem

- If Y is continous, we have a **regression** problem.
- If Y is categorical, we have a **classification** problem.
- If Y is binary, we have a **binary classification** problem.

Prediction Problem - Examples

- This is a regression problem since Y is continuous.

X	Y
13	4.0
6	3.5
14	3
10	3.9
7	2.7
12	3.8
1	1.5

Prediction Problem - Examples

- This is a binary classification Problem since $\underbrace{Y \text{ is binary}}$.

X_1	X_2	...	X_{35}	Y
1	-1	...	2	Tree
2.1	0	...	6	Not a Tree
3	0	...	8	Tree

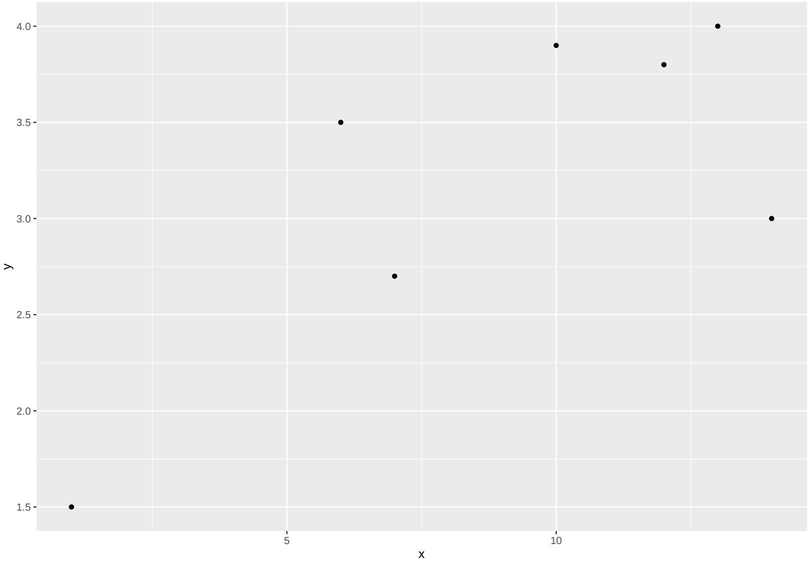
Overfitting

- Consider the data:

X	Y
13	4.0
6	3.5
14	3
10	3.9
7	2.7
12	3.8
1	1.5

- We will fit these data by polynomial model.
- In polynomial model, Y is a polynomial function of X.

Overfitting



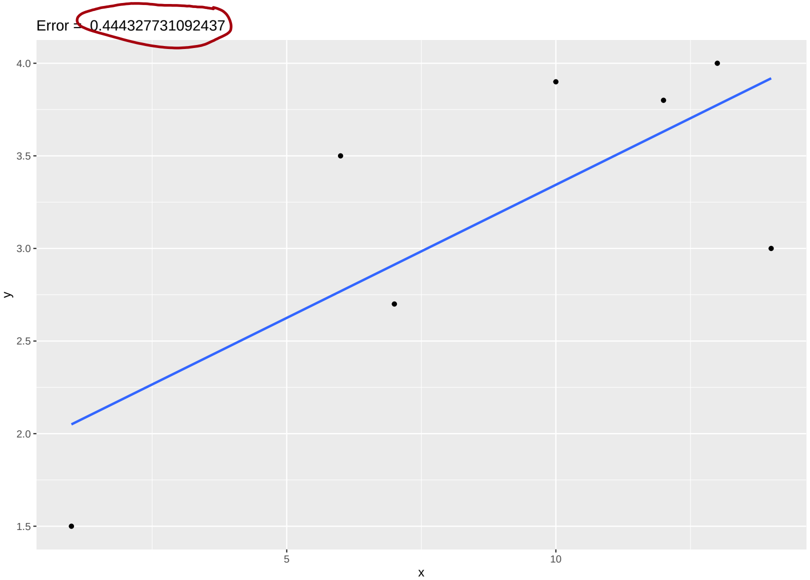
- We will fit these data by **polynomial model**.
- In polynomial model, Y is a polynomial function of X.

Overfitting - Polynomial Model

- In polynomial model, we need to specify the degree of the polynomial, n. Let try a few.
- If $n = 1$, we have a familiar **linear model**.
- **Question: Does increasing n resuls in a better model?**

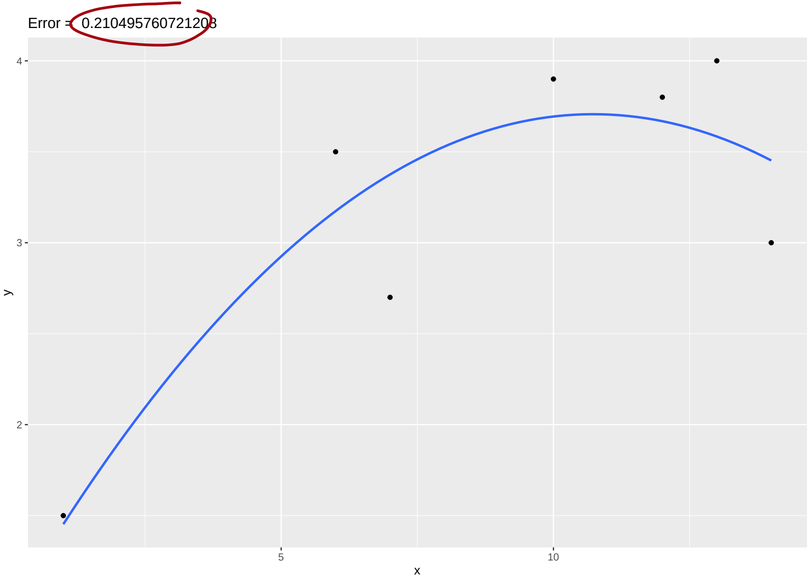
Overfitting - Polynomial Model

- $n = 1$.



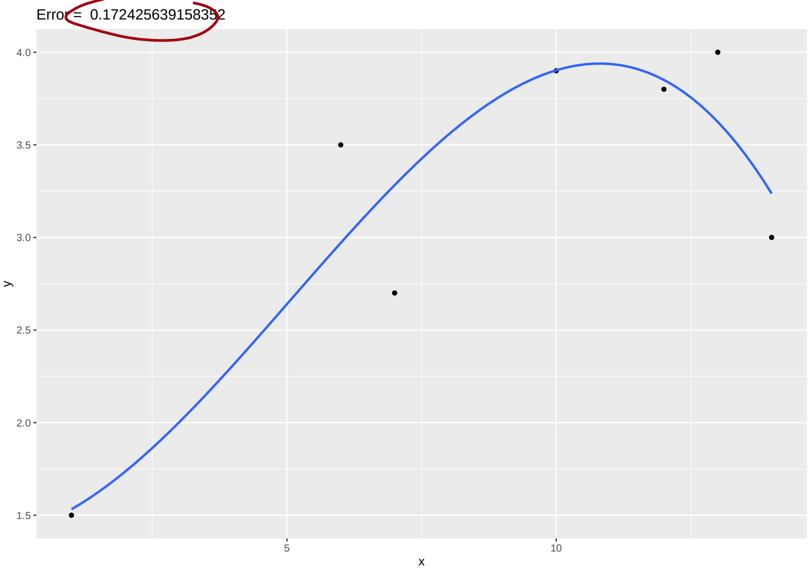
Overfitting - Polynomial Model

- $n = 2$.



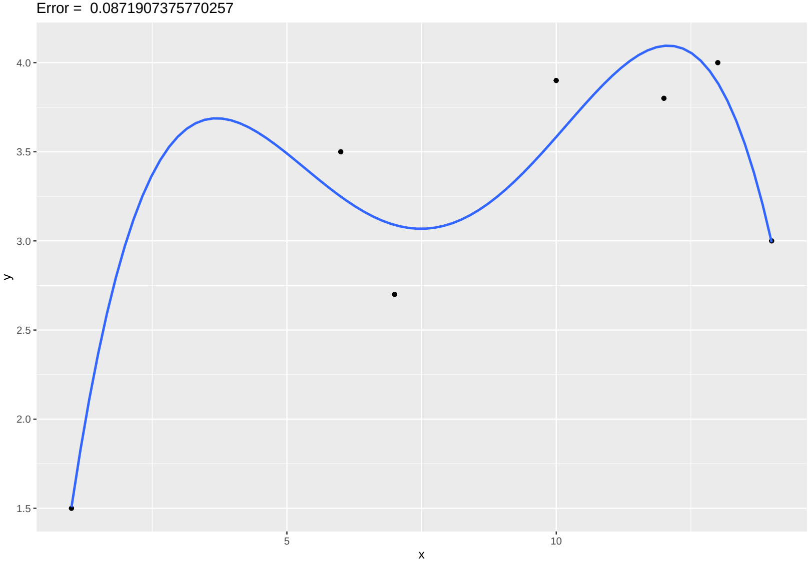
Overfitting - Polynomial Model

- $n = 3$.



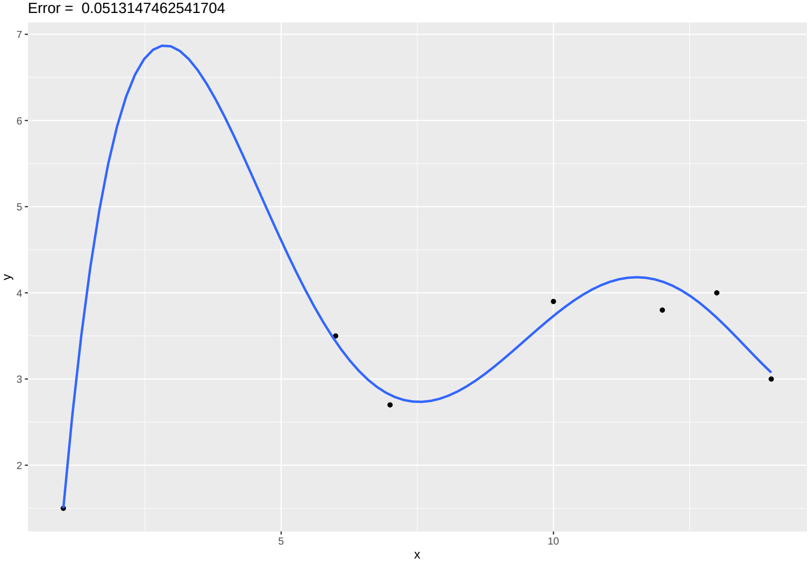
Overfitting - Polynomial Model

- $n = 4$.



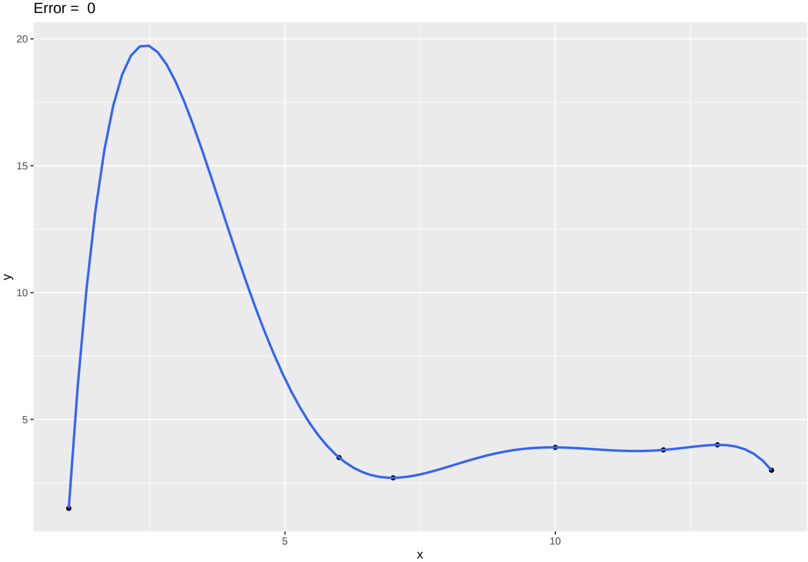
Overfitting - Polynomial Model

- $n = 5$.



Overfitting - Polynomial Model

- $n = 6$.



Overfitting - Polynomial Model

- **Question**: What are the errors when $n > 6$?

Overfitting - Polynomial Model

- **Question**: What are the errors when $n > 6$?
- **Answer**: The errors are all zeros. (There are actually many solutions for each degree greater than 6.)

Overfitting - Polynomial Model

- **Question**: What is the best model?

Overfitting - Polynomial Model

- **Question**: What is the best model?
- **Answer**: We do not know. We need a validation dataset to validate the models.

Overfitting - Polynomial Model

- The errors we have seen are called **training errors**

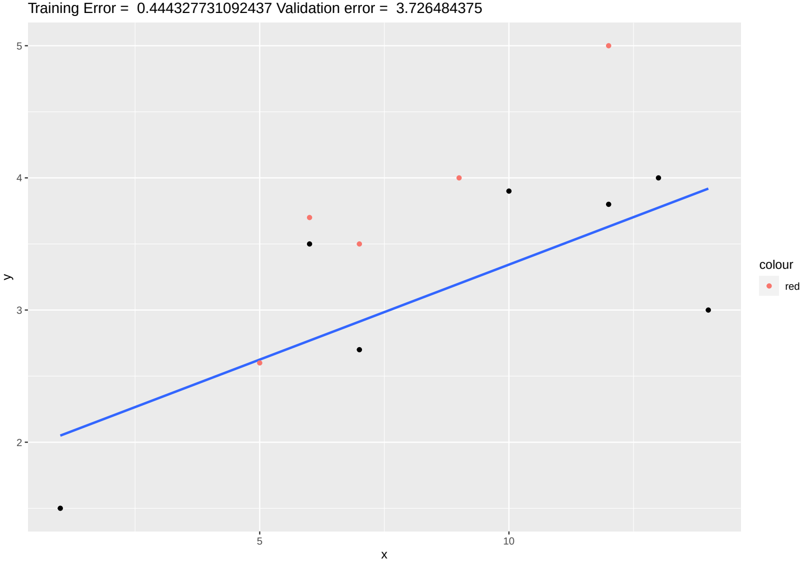
Overfitting - Polynomial Model

- Let's validate these models with a validation dataset
- Validation Data

X	Y
5	2.6
7	3.5
9	4.0
6	3.7
12	5.0

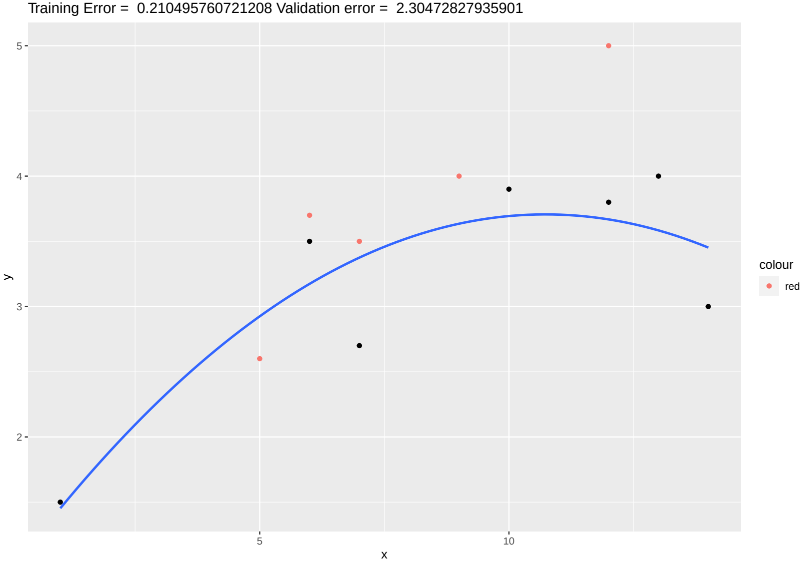
Overfitting - Polynomial Model

- $n = 1$.



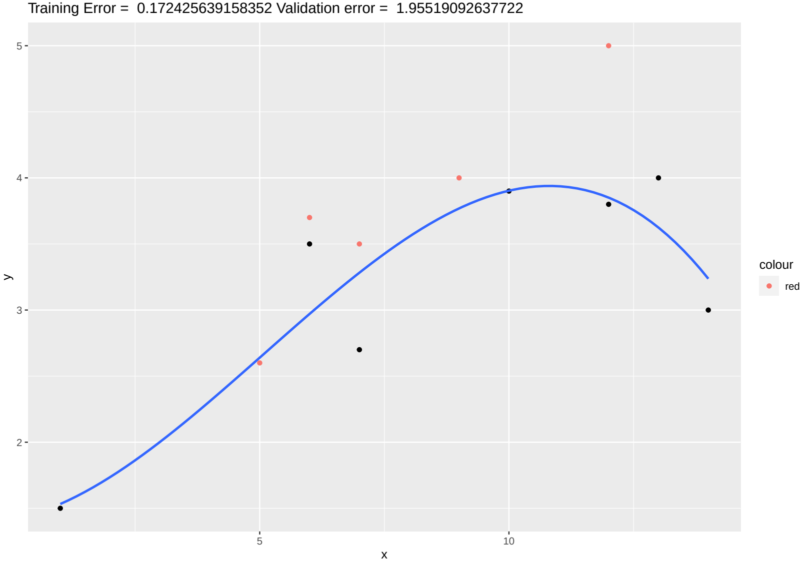
Overfitting - Polynomial Model

- $n = 2$.



Overfitting - Polynomial Model

- $n = 3$.



Overfitting - Polynomial Model

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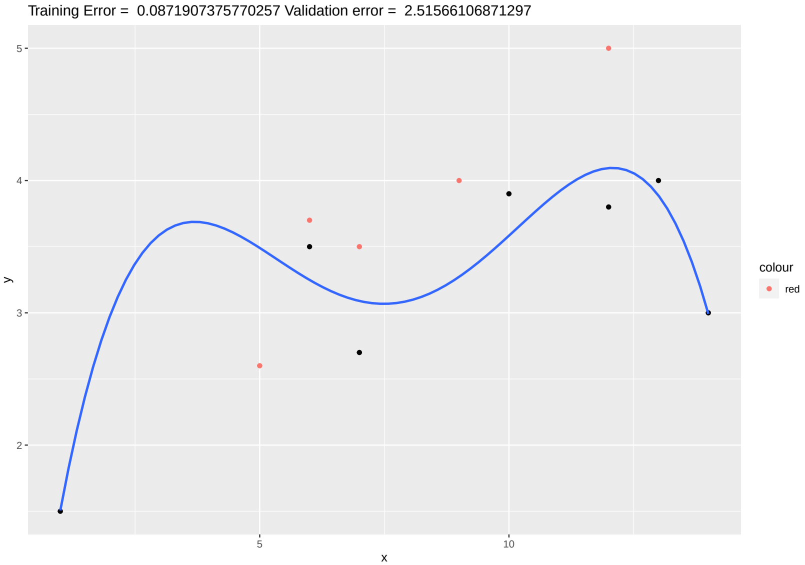
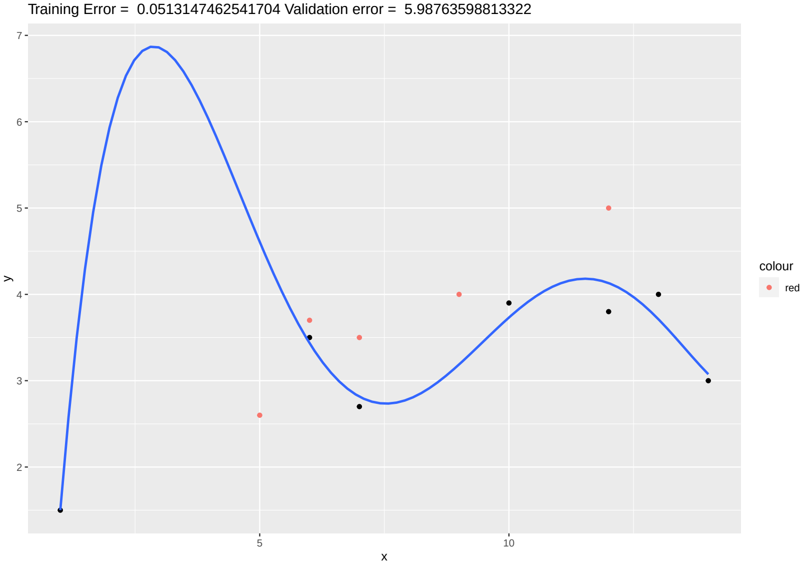


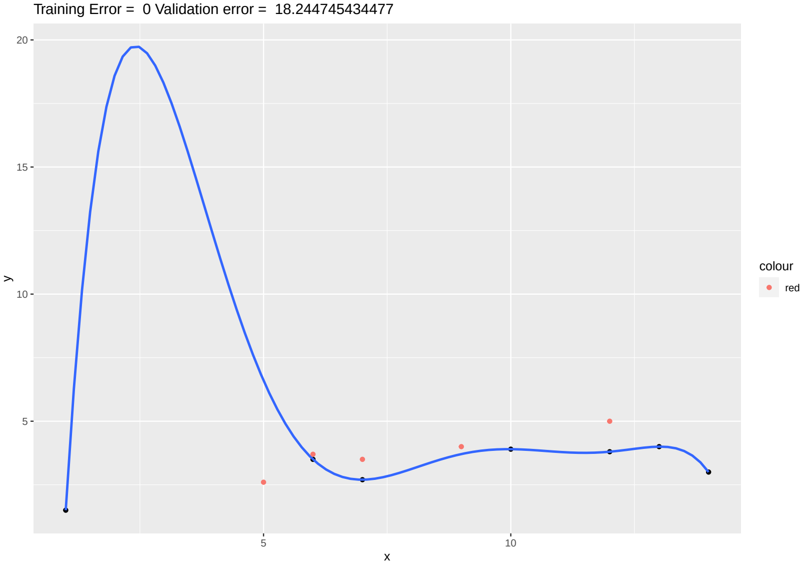
Overfitting - Polynomial Model

- $n = 5$.



Overfitting - Polynomial Model

- $n = 6$.



Overfitting - Polynomial Model

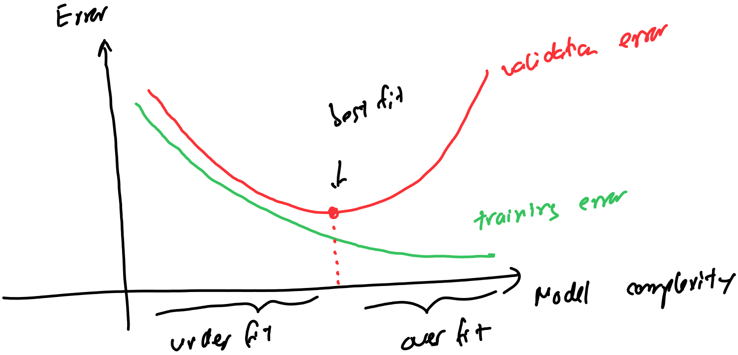
- Training Error vs. Validation Error

	Training Error	Validation Error
$n = 1$	0.4443277	3.726484
$n = 2$	0.2104958	2.304728
$n = 3$	0.1724256	**1.955191 (Best!)**
$n = 4$	0.08719074	2.515661
$n = 5$	0.05131475	5.987636
$n = 6$	0	18.24475

the model underfits the data

best fit

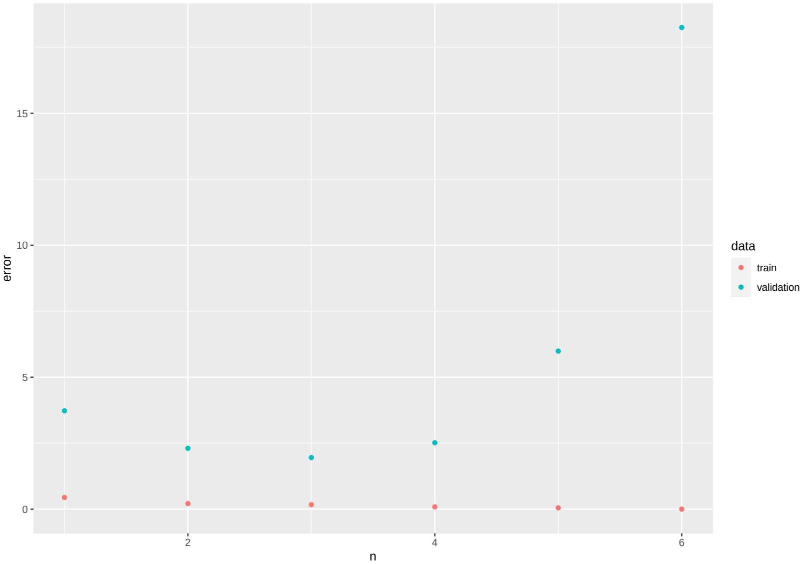
the model overfits



Error
validation error
best fit
training error
Model complexity
under fit
over fit

Overfitting - Polynomial Model

- Training Error vs. Validation Error

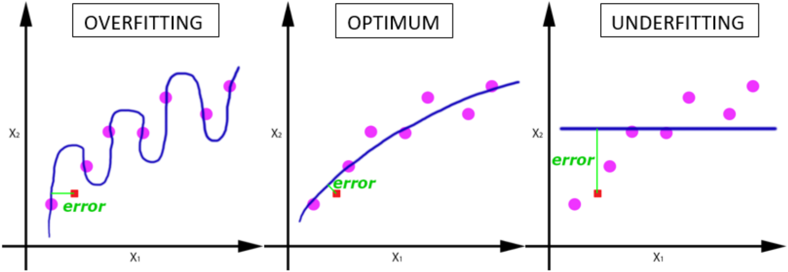


Overfitting - Polynomial Model

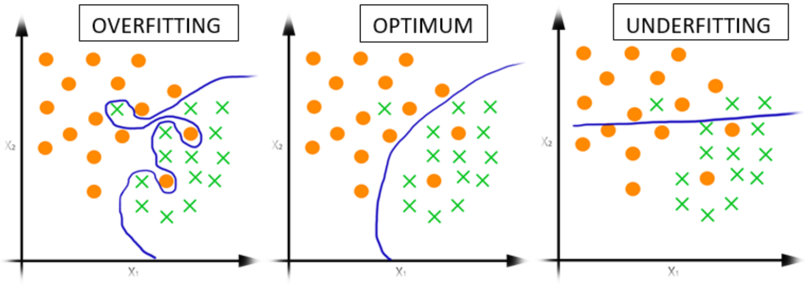
- As the degree n increases, the training errors decrease
- Model 6 ($n = 6$) is the best (perfect) in training but the worst in validation.
- The best model is the model with the best (lowest) error in **validation data**.

Overfitting - Polynomial Model ## - Model 4, 5 and 6 are **overfitted** - Model 1 and 2 are **underfitted** - Model 3 is the best model.

Overfitting in Regression



Overfitting in Classification



Model Complexity/Capacity

- In polynomial models, the larger n, the more complex/capable the model.
- Model complexity can be measured by the number of parameters/unknown of the model.

$\boxed{\text{A Model}}$:

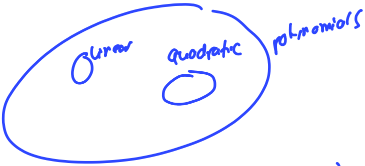
linear model : $y = ax + b$ → parameters : a, b

Quadratic model : $y = ax^2 + bx + c$ → para : a, b, c

$\underbrace{\text{polynomial model}}_{\text{a family of models}}$: $y = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x + a_0$

→ para : $a_n, a_{n-1}, \ldots, a_1, a_0$

hyper-parameter : n



A family of models has hyper-parameter | turns parameter

Model Complexity/Capacity

- Linear model:

$$y = ax + b$$

- **Question**: How many unknowns/parameters in linear model?

Model Complexity/Capacity

- Linear model ($n = 1$):

$$y = ax + b$$

- **Question**: How many unknowns/parameters in linear model?
- **Answer**: Two unknowns/paramters: a and b

Model Complexity/Capacity

- Quadratic model ($n = 2$):

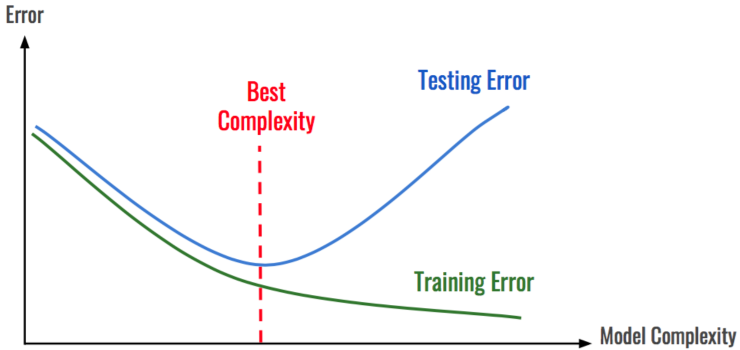
$$y = ax^2 + bx + c$$

- Three unknowns: a, b, and c.
- Quadratic model has **more unknowns/parameters** then linear model. Thus, quadratic model is **more complex** than linear model

Model Complexity/Capacity

- The mode complex the model, the easier it becomes overfitted!

Model Complexity/Capacity



Model Tuning

- We just "tuned" the the parameter n.
- The parameter n is called **tuning parameter**, or **hyperparameter**

Model Tuning

- Model tuning is the process of finding the **best** values for the tuning parameters of the model
- This is done through **trying out** many values for the tuning parameters then select the best values.

Model Training

- Model training is the process of finding the unknown/parameters of the model
- **Example**: Training linear model $y = ax + b$ is to find a and b that best fit the data

Model Training vs. Model Tuning

- Model training finds the **parameters**
- Model tuning finds **hyperparameters**

Model vs. Family of Models

- The polynomial model is a **family** of models.
- Linear model is just **one** model
- A family of models has “tuning parameters”.
- A single model, say, linear model, does not have tuning parameter
- Some model has multiple tuning parameters.

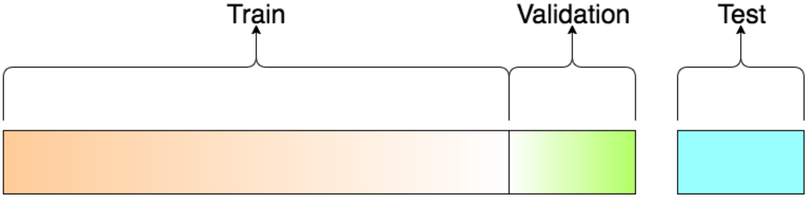
Data Splitting

- We need validation data for model tuning.
- **Question**: How can one of obtain validation data?

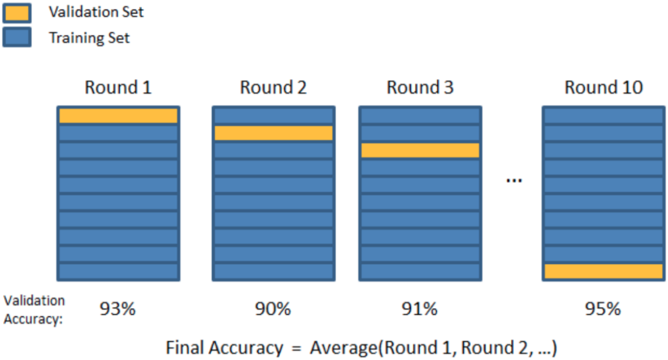
Data Splitting

- We need validation data for model tuning.
- **Question**: How can one of obtain validation data?
- **Answer**: We do not use the entire data to train models. We use a portion of it for training and save data for validation and testing.

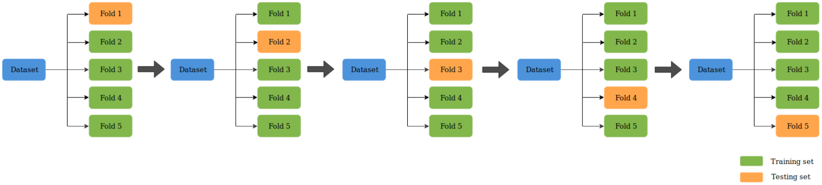
Data Splitting: Train-Validation-Test



k-folds Cross Validation



k-folds Cross Validation



k-folds Cross Validation and test