Modul 3

Generalization, Underfitting, Overfitting

Data Science Program

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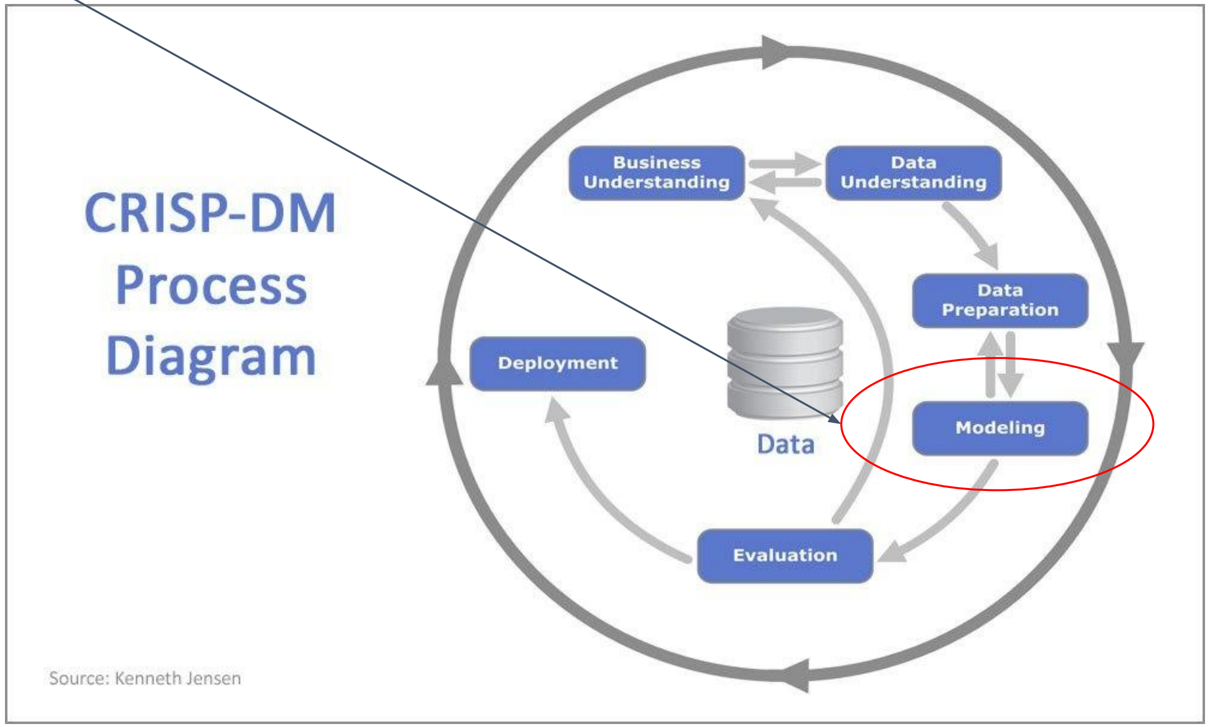
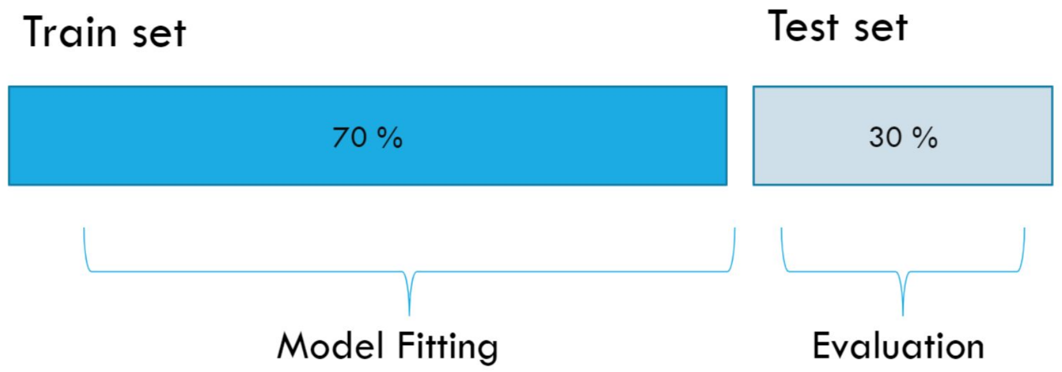
Outline

- What is Generalization ?
- What are Overfitting and Underfitting ?
- Model Complexity vs Performance
- Illustration of Generalization, Overfitting and Underfitting:
  - KNN
  - Decision Tree
- Generalization in Linear Model



What is Generalization ?

- In supervised learning, we build model on a dataset (seen data) and then be able to make accurate predictions on new data (unseen data)
- Thus, we need to divide data into two set, training set and test set
- **Training set** is used to **fit** the **model** and from **test set** we can **infer** the ML algorithm **performance**
- When building any model, test data can’t get involved at all
- If a model is able to make accurate predictions on the unseen data, we say it is able to generalize from the training set to the test set



Why is Generalization ?

- We are interested in the accuracy of the prediction that we obtain when we apply our method to new unseen data
- In practice, We might try several different method
- No one method dominates all others over all possible data set
- We want to build an ML that is able to generalize as accurately as possible

Illustration : Predicting Customer Who will buy a boat

Age	Number of cars owned	Owns house	Number of children	Marital status	Owns a dog	Bought a boat
66	1	yes	2	widowed	no	yes
52	2	yes	3	married	no	yes
22	0	no	0	married	yes	no
25	1	no	1	single	no	no
44	0	no	2	divorced	yes	no
39	1	yes	2	married	yes	no
26	1	no	2	single	no	no
40	3	yes	1	married	yes	no
53	2	yes	2	divorced	no	yes
64	2	yes	3	divorced	no	no
58	2	yes	2	married	yes	yes
33	1	no	1	single	no	no

Goal :
- send promotional email to people who are likely to actually make a purchase

Let's build some rule:
- if the customer is older than 45, has less than 3 children and is not in divorce, then they want to buy a boat. (this result 100% accurate)
- and still so many rules you can find by looking at this dataset
- Which rule could generalize new unseen data ?

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What are Underfitting and Overfitting ?

Age	Number of cars owned	Owns house	Number of children	Marital status	Owns a dog	Bought a boat
66	1	yes	2	widowed	no	yes
52	2	yes	3	married	no	yes
22	0	no	0	married	yes	no
25	1	no	1	single	no	no
44	0	no	2	divorced	yes	no
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64	2	yes	3	divorced	no	no
58	2	yes	2	married	yes	yes
33	1	no	1	single	no	no

Underfitting :
- too simple
- “Everybody who owns a house buys a boat”

Overfitting:
- too complex
- “the customer older than 45, has less than 3 children and is not n divorce, then they want to buy a boat”

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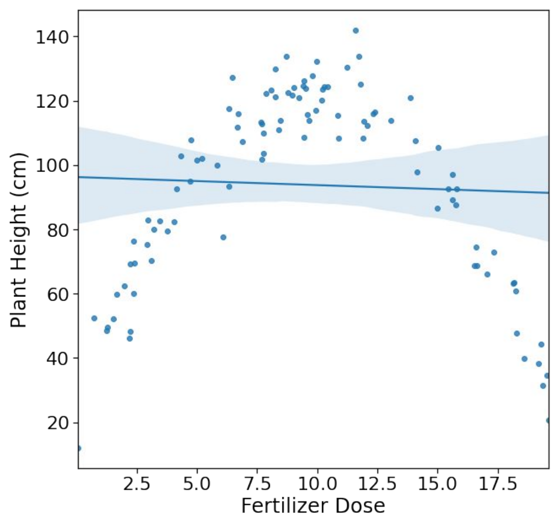
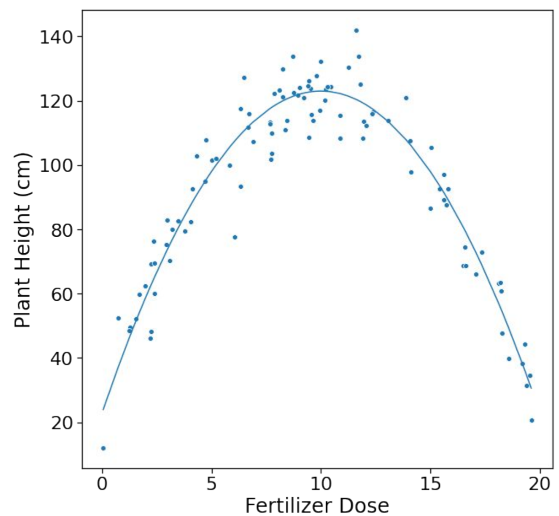
Capturing Underlying Data Trends

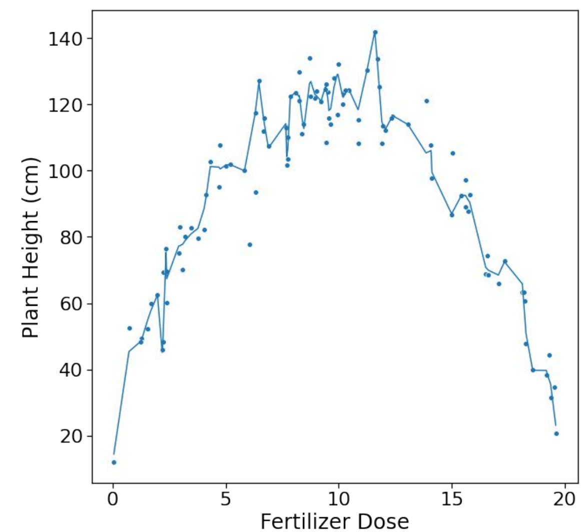
Which one is your preference?



Underfitting Model:
y = a + bx



Just Right:
y = a + bx + cx^2



Overfitting Model:
lowess regression

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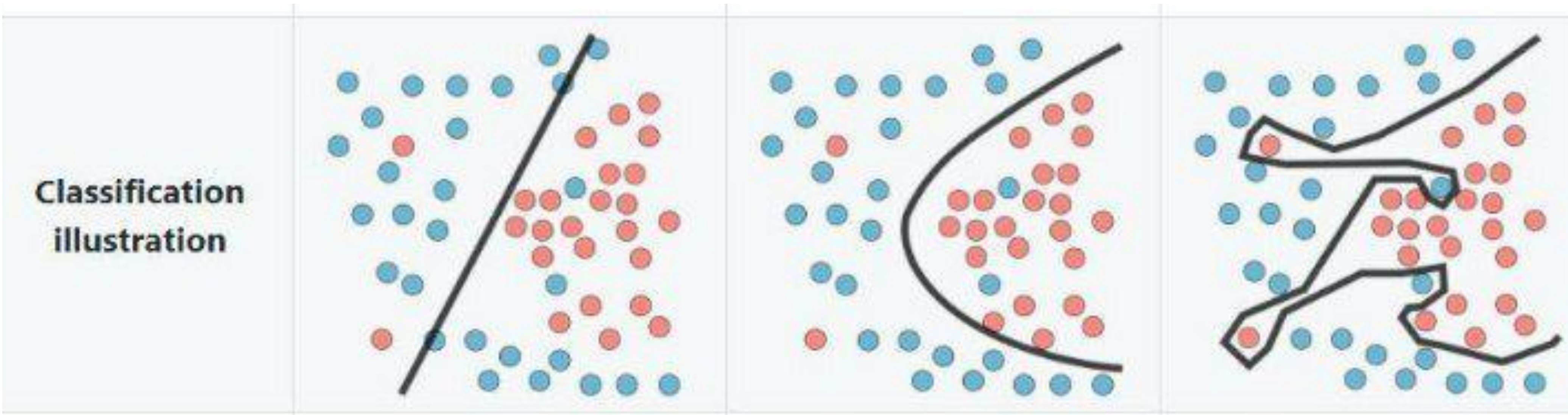
Capturing Underlying Data Trends



Underfitting Model | Just Right | Overfitting Model

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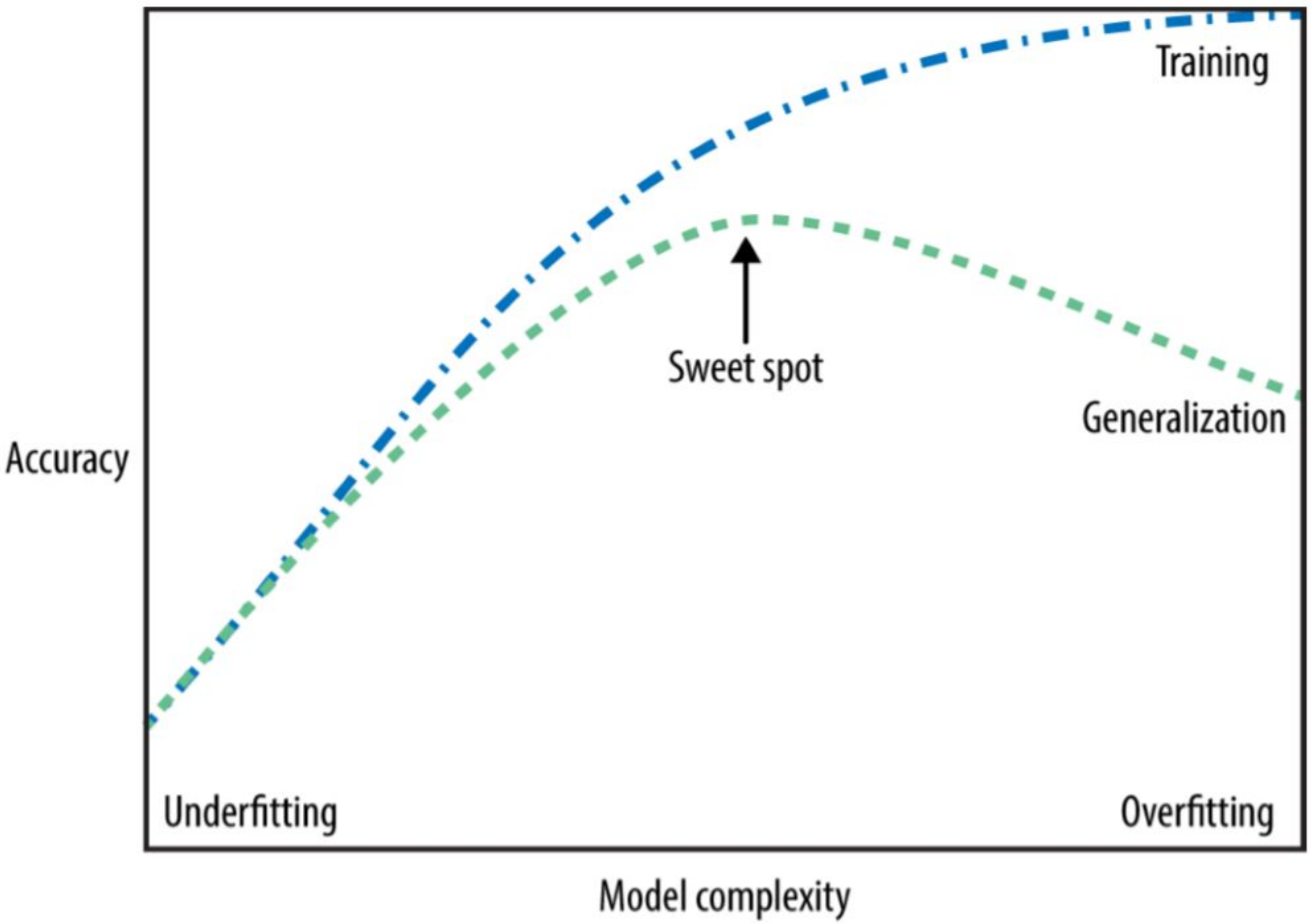
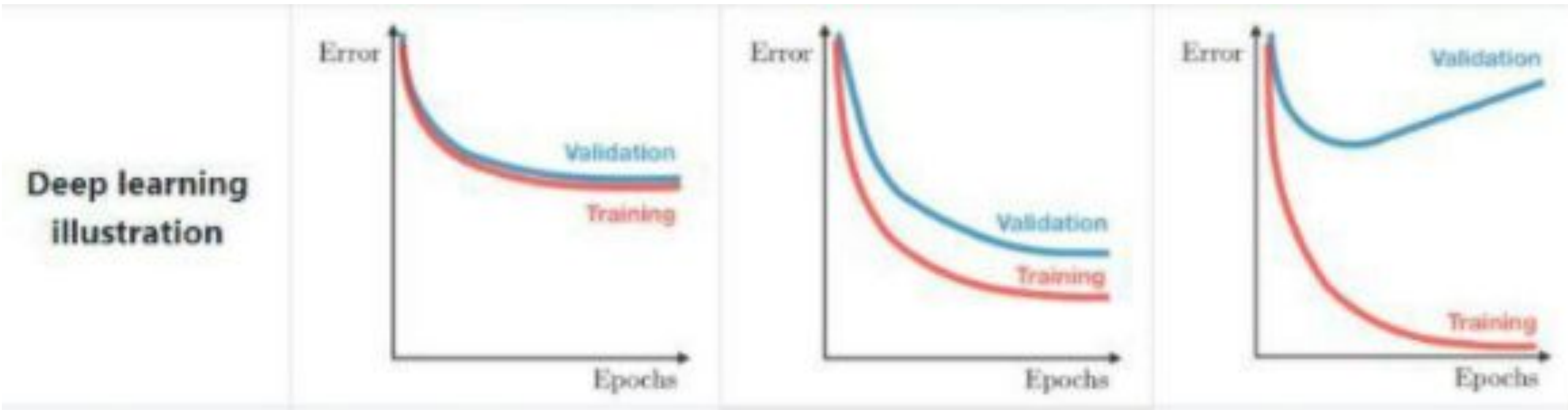
Model Complexity vs Model Performance

- High Training Set Error and High Validation Set Error ->
  - High Bias (Underfitting)
- Low Training Set Error and High Validation Set Error ->
  - High Variance (Overfitting)
- There is a sweet spot in between that will yield the best generalization performance. This is the model we want to find.
- Data has strong relation to model complexity : If more data means more variation, More variation in data allow you to train more complex model without overfitting



Overfitting and Underfitting in Deep Learning



Overfitting and Underfitting Recap

OVERFITTING

- Too complex
- Fits the training data too well
- Good performance in training set but bad at test set
- High variance, low bias

Solutions:

✔ Reduce number of features

✔ Increase training samples

UNDERFITTING

- Too Simple
- Doesn't capture underlying data trend
- Bad performance both at training set and test set
- High bias, low variance

Solutions:

✔ Train more complex model

✔ Obtain more features

A good model has slightly lower training error than test error

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Underfitting and Overfitting in KNN

Analyze data bankloan.csv

- Apply KNN Classifier
  - target : default
  - features : employ, debtinc, creddebt, othdebt
- Using different k (1,3,5,...100) : Apply scaling and Validate the model using accuracy in 20% testing data and 80% training data
- compare accuracies obtained from training data and testing data

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Model Complexity in Decision Tree

Analyze data bankloan.csv

- Apply Decision Tree Classifier
  - target : default
  - features : employ, debtinc, creddebt, othdebt
- Using different maximum depth of the tree (1,2,3,...25) : Validate the model using accuracy in 20% testing data and 80% training data
- compare accuracies obtained from training data and testing data
- you may try another hyperparameter such as minimum samples split, minimum samples leaf, etc.

Generalization in Linear Model

- Too many feature used in linear models makes model more complex and may leads to overfitting
- We can either use :
  - reduce the effect/magnitude of certain features (Ridge)
  - make zero effect/magnitude for certain features (Lasso)
- Ridge or Lasso can be used as a solution to multicollinearity
- Which one to use ?
  - as the simplest way, you can directly check the performance on test data

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Ridge (L2 Regularization)

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + ... + \beta_k X_k + \varepsilon$$

Reduce the magnitude close to zero

Formula :

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}\beta_j^2 = \mathrm{RSS} + \lambda\sum_{j=1}^{p}\beta_j^2$$

Hyperparameter Properties

1. Alpha : typically used {....1000,100,10,1,0.1,0.01,0.0001,...}
2. Increasing alpha
   a. forces coefficients to move more toward zero but never zero
   b. reduce model complexity

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Lasso (L1 Regularization)

$$\boxed{Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_k X_k + \varepsilon}$$

Reduce some of the magnitude to zero

Formula :

$$\sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 + \lambda \sum_{j=1}^{p} |\beta_j| = \mathrm{RSS} + \lambda \sum_{j=1}^{p} |\beta_j|$$

Hyperparameter Properties

1. Alpha : typically used {....1000,100,10,1,0.1,0.01,0.0001,...}
2. increasing alpha
   a. less feature used because of zero magnitude
   b. reduce model complexity
   c. getting easier to interpret

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Model Complexity in Ridge

Analyze data boston dataset from sklearn

- Apply Decision Tree Classifier
  - target : target (house price)
  - features : CRIM, ZN, INDUS, CHAS, NOX, RM, AGE, DIS, RAD, TAX, PTRATIO, B, LSTAT, MEDV
- Using different alpha (100000, 10000, 1000, 100, 10, 1, 0.1, 0.001) : Validate the model using mse in 20% testing data and 80% training data
- compare mse obtained from training data and testing data

Model Complexity in Lasso

Analyze data boston dataset from sklearn

- Apply Decision Tree Classifier
  - target : target (house price)
  - features : CRIM, ZN, INDUS, CHAS, NOX, RM, AGE, DIS, RAD, TAX, PTRATIO, B, LSTAT, MEDV
- Using different alpha (100000, 10000, 1000, 100, 10, 1, 0.1, 0.001) : Validate the model using mse in 20% testing data and 80% training data
- compare mse obtained from training data and testing data

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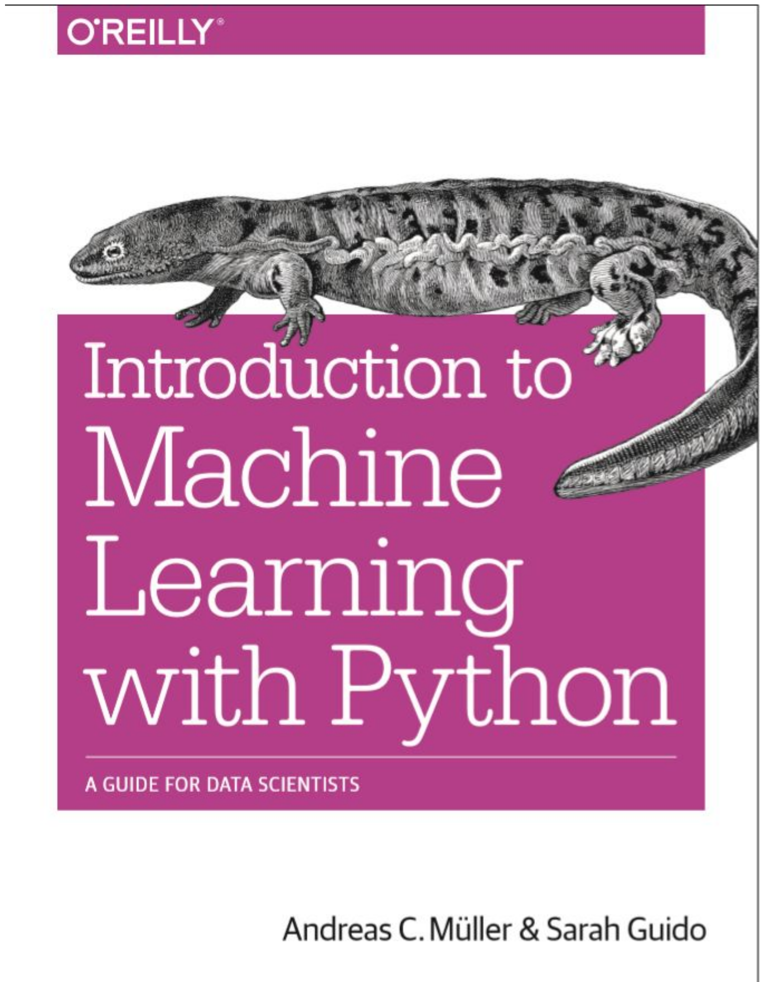
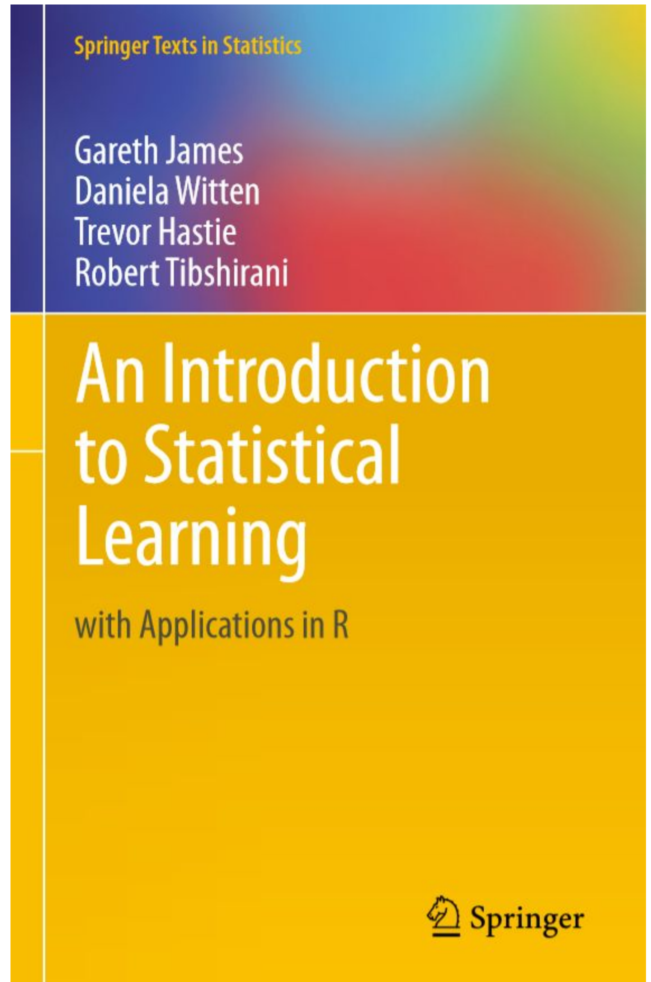
References





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