Introduction to Machine Learning

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Recommended Textbook

- An Introduction to Statistical Learning with Application in R (or in Python)
  - Book website
  - Online course videos
  - Notes from a book club from the R4DS online learning community
- Elements of Statistical Learning
  - Book website
  - Recommended for advanced students

Computer programming

- **R** – we will use R mostly in this class
  Download R, and install
  Download RStudio, and install
- **Python** – strongly recommended
  - Download and install Anaconda
  - Get started with Anaconda
  - Jupyter Notebooks is recommended environment (like RStudio)

Learning Resources

- Data
  - Most commonly used public data sets
  - Textbook data (James, et al.): install R package `ISLR`
  - UCI Machine Learning Repository
  - Kaggle
  - KDD Nuggets
- Lectures and other tutorials
  - Videos of textbook (ISLR)
  - DataCamp
  - Coursera
- Your AI friends
  - ChatGPT, Claude AI
  - many more...
- Course website
  - a publicly available site
  - Canvas (for assignment and other work)

You should take this course if...

- You are passionate about AI and data science
- You know that data are assets for businesses and you like exploring data
- You want to pursue this career
- You want to pursue advanced degrees in data science and AI

An article on who should purse a master's degree in BA.

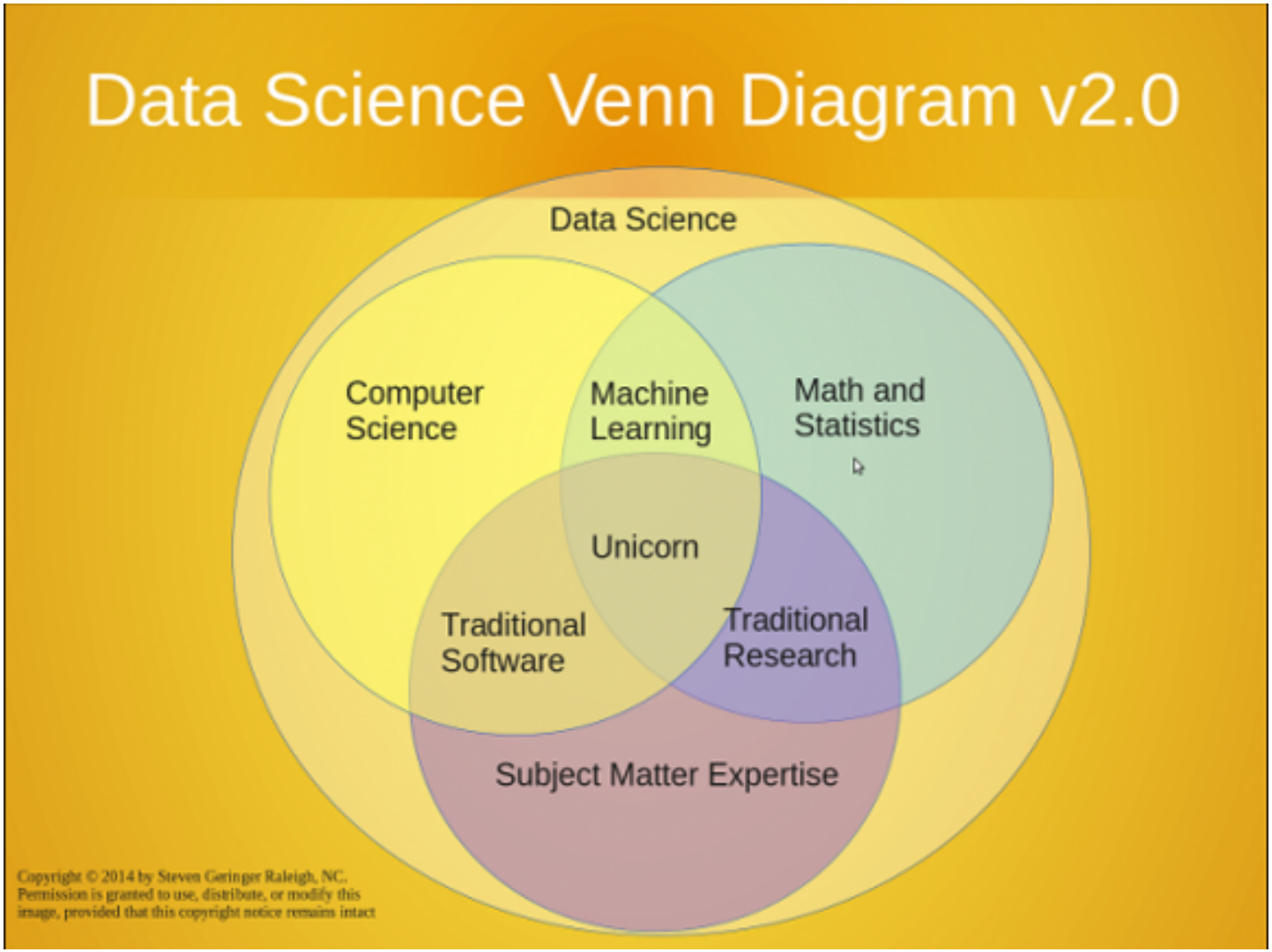
How much salary can a data scientist earn? (a report from indeed)

Machine Learning in Different Fields

Learning from data is essential in different scientific disciplines

- Predict stock returns in next six months based on historical data;
- Predict the probability of a loan default based on customer's information and historical records;
- Identify certain diseases based on medical image;
- Identify handwritten digits from image;
- Facial recognition;
- Natural language processing;
- Cluster customers based on their purchase behavior and other information
- .....

In practice, you need...



Examples

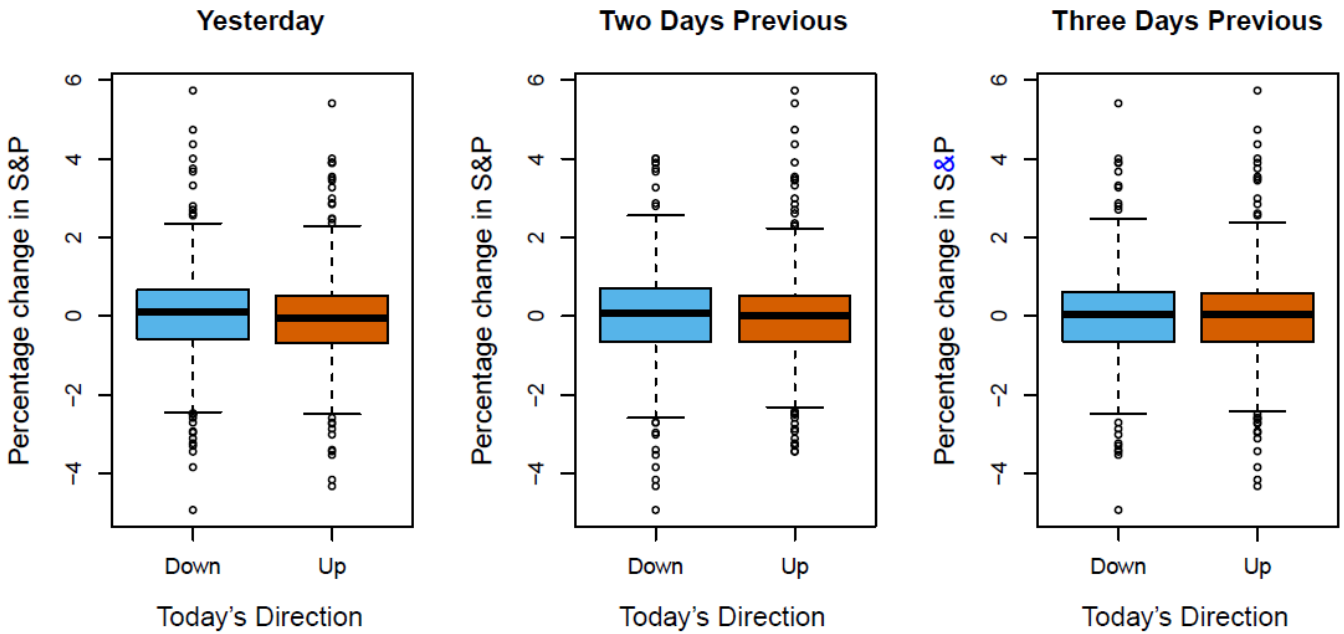
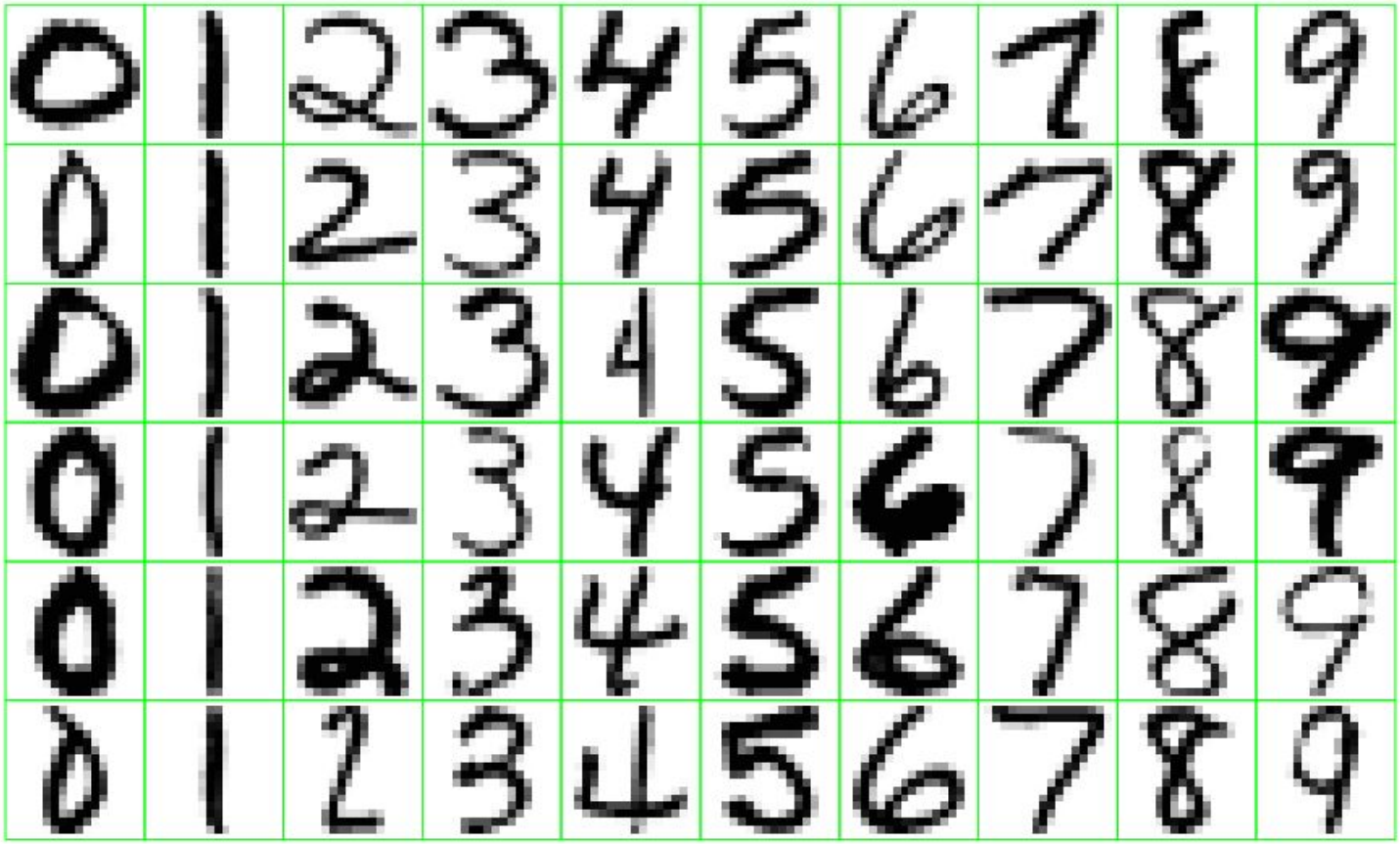


FIGURE 1.2. Left: *Boxplots of the previous day's percentage change in the S&P index for the days for which the market increased or decreased, obtained from the* `Smarket` *data.* Center and Right: *Same as left panel, but the percentage changes for 2 and 3 days previous are shown.*

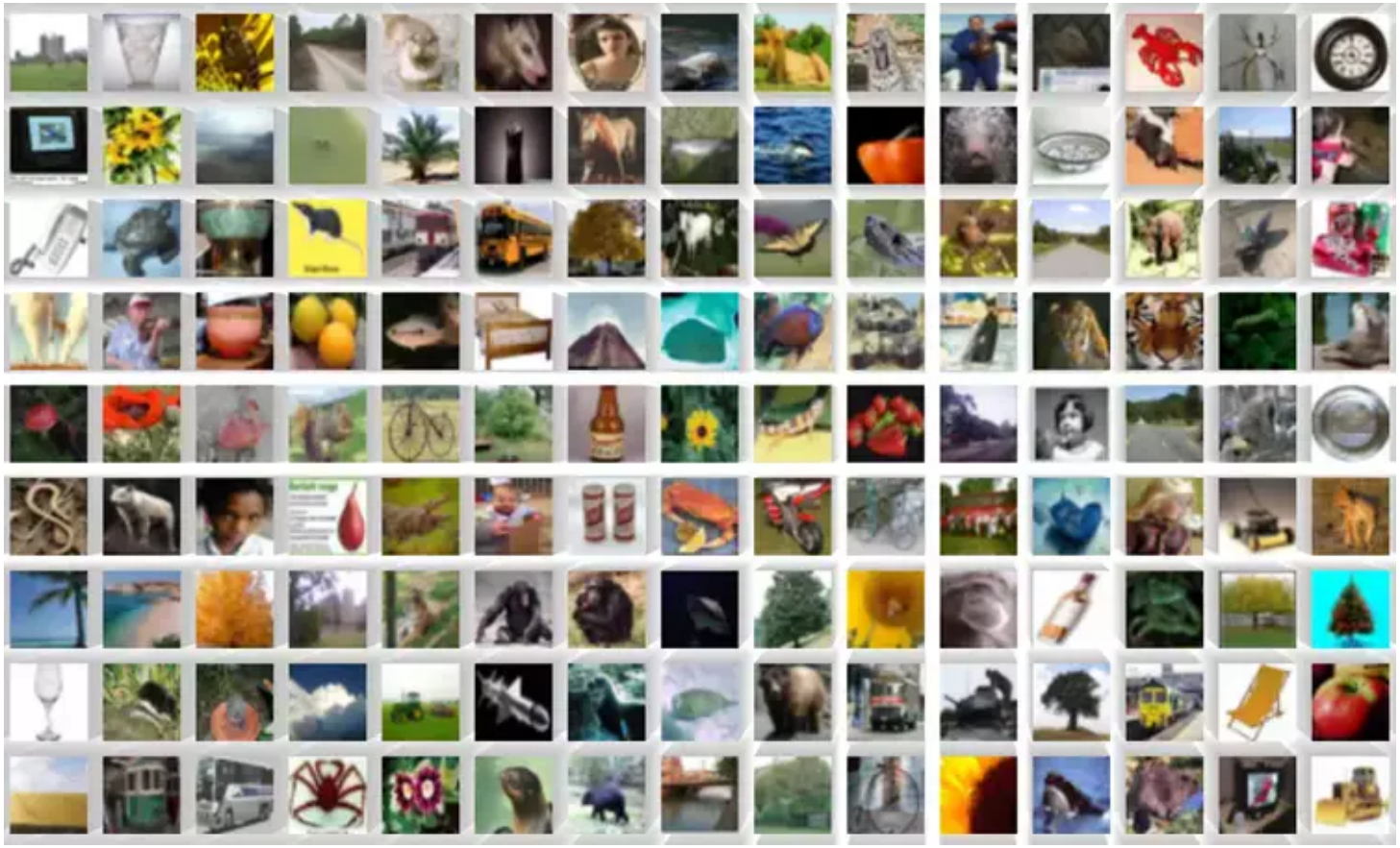
- This example is from ISLR page 3 (stock market data).
- Go to ChatGPT and ask it for a demonstrative example of analyzing the Smarket dataset from the textbook.

Examples



- This is part of the famous MNIST dataset for image recognition.
- Go to ChatGPT and ask it for a demonstrative example of analyzing the MNIST dataset.

Examples



- This is part of the famous CIFAR-100 dataset for image recognition.
- There are 100 classes labeled manually by researchers.
- Go to ChatGPT and ask it for a demonstrative example of analyzing the CIFAR-100 dataset.

Learning Types

- **Supervised learning**
  - There is specific response you need to predict
- **Unsupervised learning**
  - No response, instead, you need to create response based on some patterns
- **Semi-supervised learning**
  - Mixture of both

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- What type of learning is for large language model?

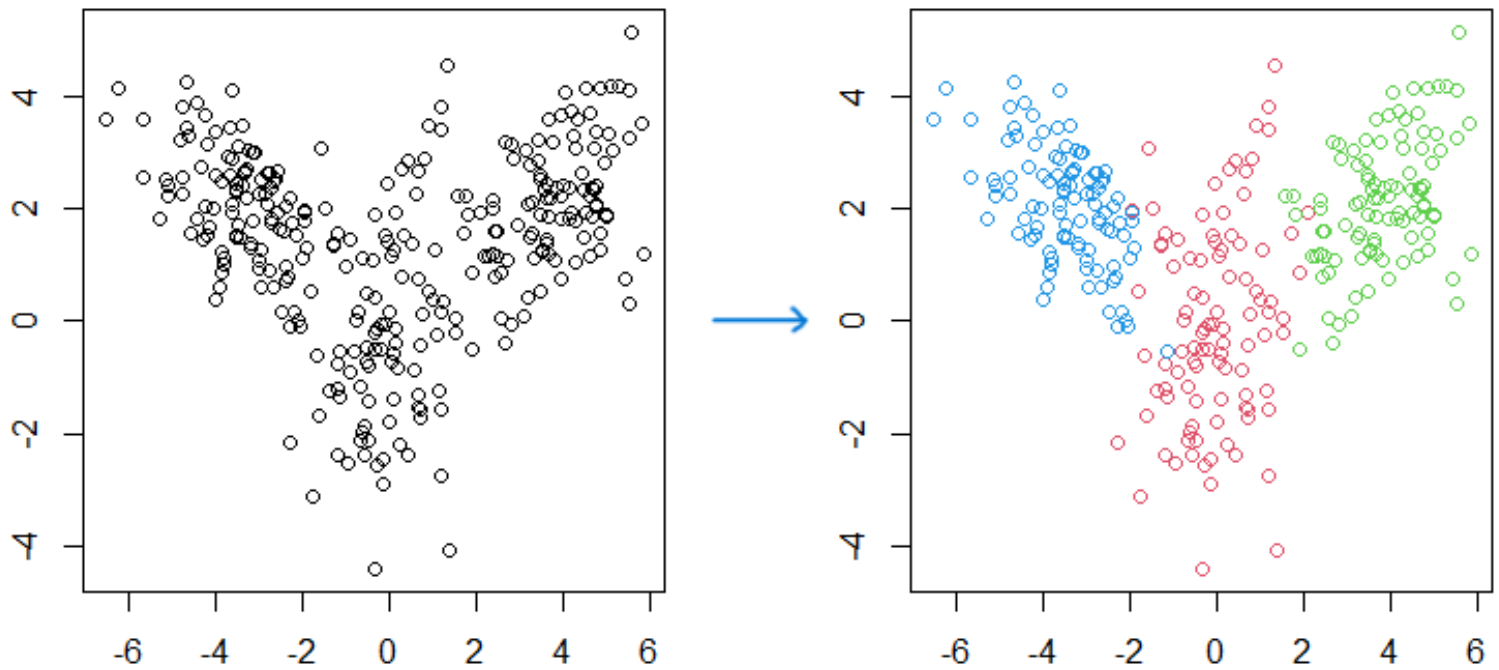
Unsupervised Learning

- Data is **unlabeled** (no Y's)
- Uncover patterns, groups among X's
- Subjective, no simple goal such as prediction
- Examples:
  - Marketing segmentation – clustering
  - Dimension reduction – principle component analysis (PCA)
  - Market basket analysis – association rules mining

A simple ML algorithm – k-means clustering

- Clustering: group similar observations together
- k-means: one out of many algorithms for clustering
  - k: how many groups
  - means: the center of the group
- This is an iterative algorithm
  - making a little progress many times
- Similarity measures, or distances, are the key component behind the algorithm

An illustration



Supervised Learning

- Labeled data
- The goal is to predict or explain certain outcome
- Type of problem:
  - Regression: outcome is continuous
  - Classification: outcome is categorical
- Popular ML algorithms:
  - Least square, nearest neighbor, CART, gradient boosting, neural network, deep learning

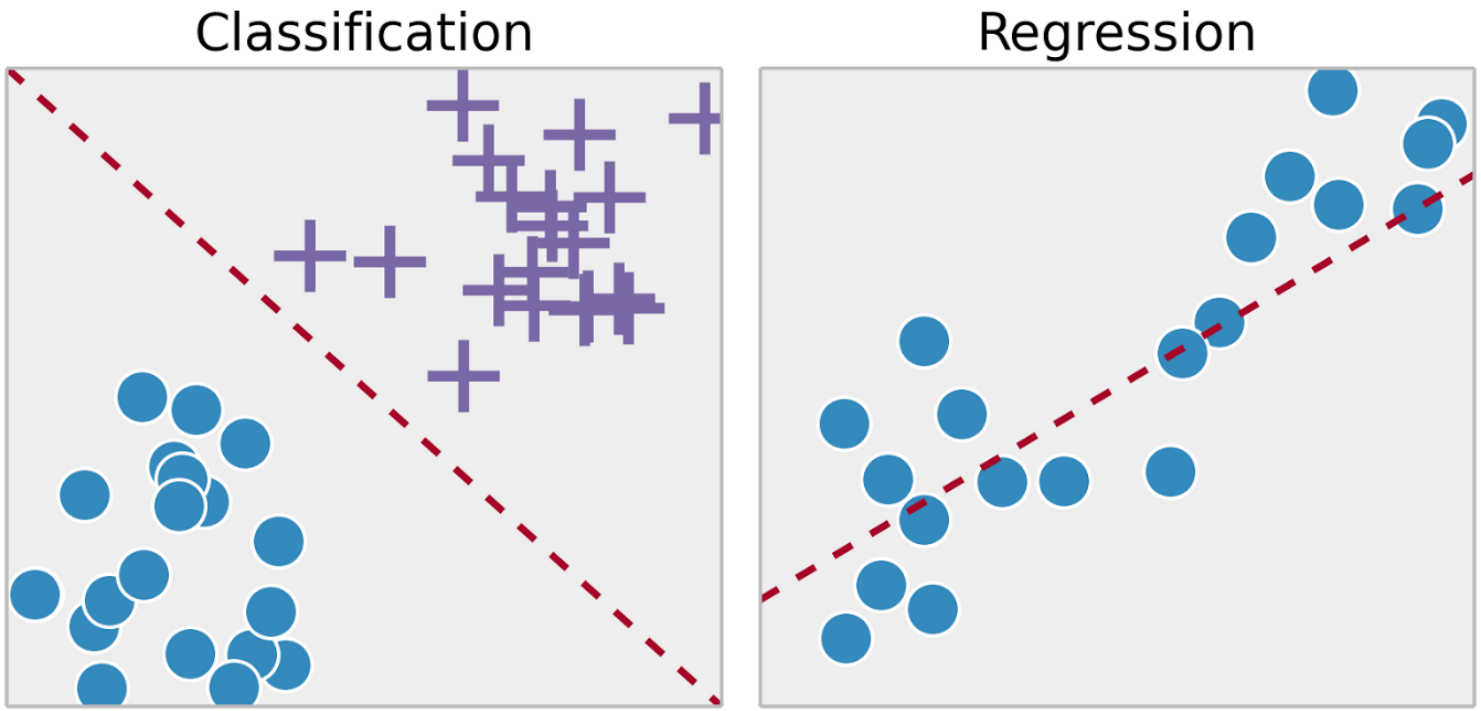
Supervised Learning

- Suppose we observe data Y_i and $\mathbf{x}_i = (X_{i1}, \ldots, X_{ip})$ for $i = 1, \ldots, n$.
- Y is the outcome (or response, dependent variable, target), and $\mathbf{x}$ is predictor (or independent variables, covariates, features, inputs)
- The learning problem can be modeled as

$$Y_i = f(\mathbf{x}_i) + \epsilon_i$$

  where $f(\cdot)$ is unknown function, and ϵ is random error.
- A general workflow: Learn from the **training data** and test the trained model on a holdout sample (**testing data**).

Regression and Classification



Regression

- Response variable is continuous
  - e.g., stock return, housing price, temperature
- Goal: prediction
- Learning methods:
  - Parametric methods, e.g., linear regression
  - Nonparametric methods, e.g., decision tree, neural network
- Commonly used evaluation metrics:
  - Mean squared error (MSE), mean absolute error (MAE), R-square

An example for regression

Can we predict Sales using ad media spending?

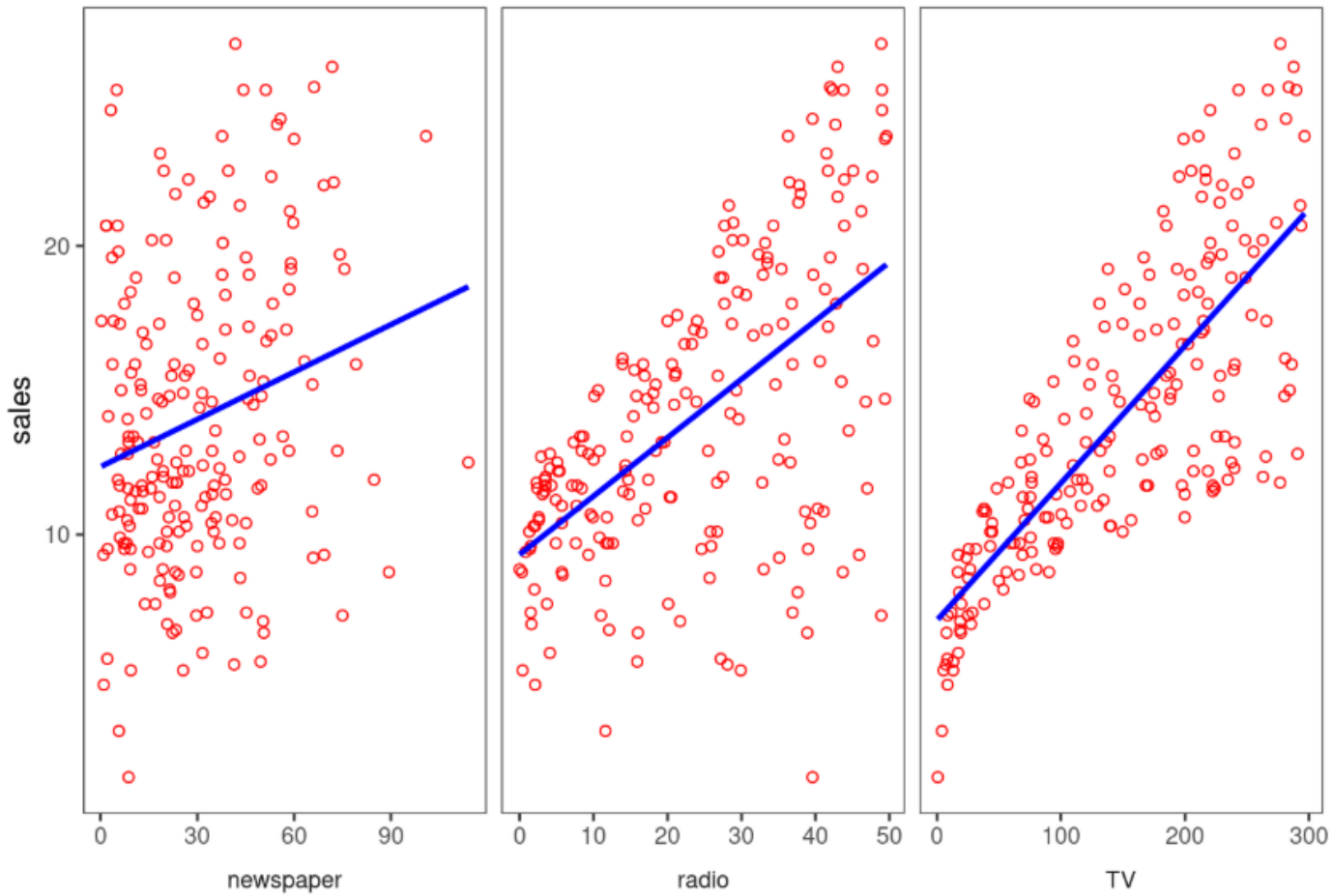
- Three channels of media: TV, radio, and newspaper
  - Spending on these channels are predictors, often denoted by X
- The outcome variable is sales, often denoted by Y
- Because our intuition is higher ads spending leads to higher sales. Thus, a linear regression can be developed to predict sales:

$$Y = \beta_0 + \beta_1 * X_1 + \beta_2 * X_2 + \beta_3 * X_3 + \epsilon$$

- Here the unknown function is a linear function, that is
  - $f(x) = \beta_0 + \beta_1 * X_1 + \beta_2 * X_2 + \beta_3 * X_3$
- The model needs to "learn" from the data to figure out the parameters: $\beta_0, \beta_1, \beta_2, \beta_3$. How?

Visualizing the data

Exploratory data analysis (EDA) is always important and a necessary step before building any models



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Now practice time. Let's play with this data!

Prediction accuracy for regression problem

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Prediction accuracy for regression problem

- How good is the model?
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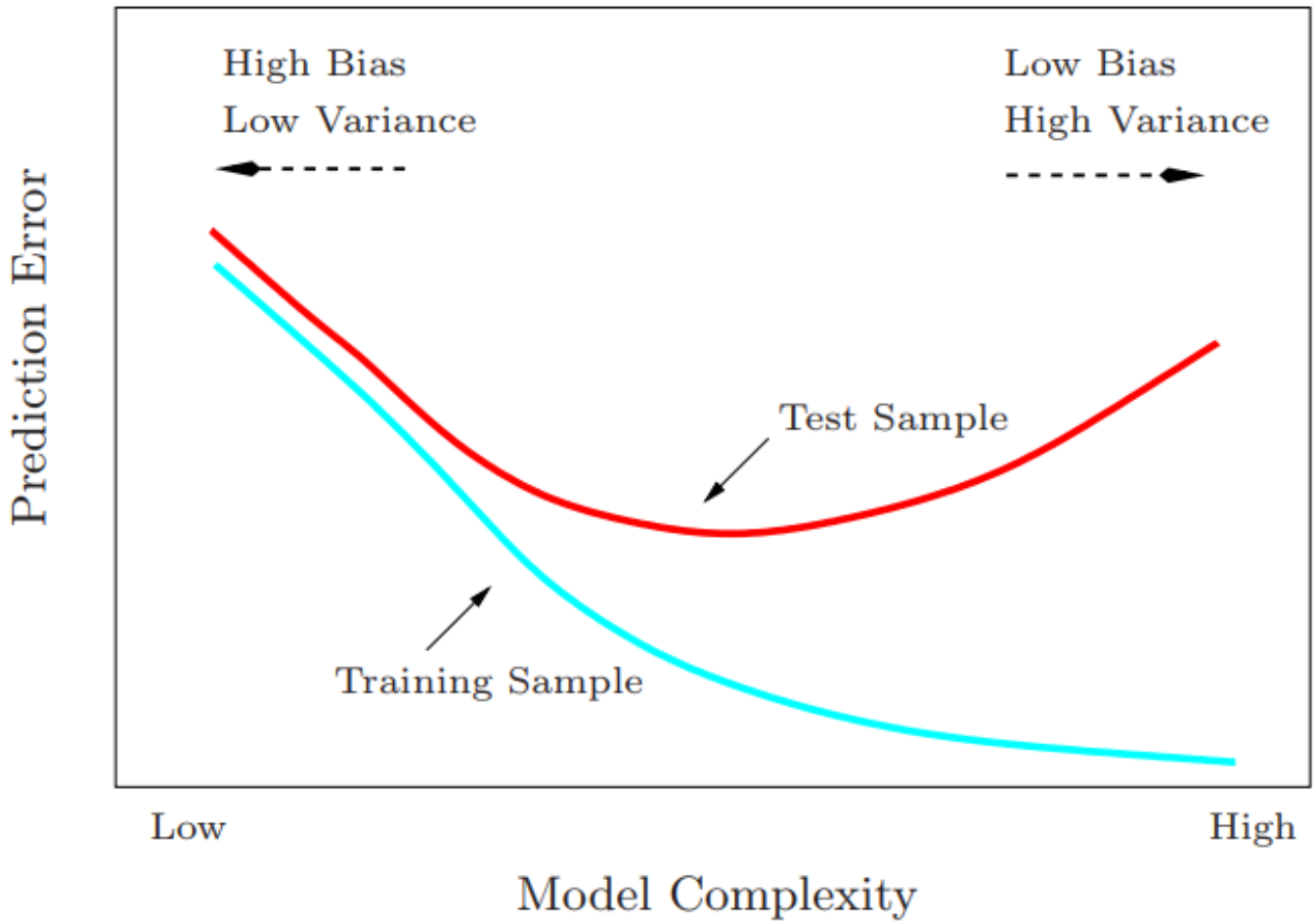
- One of the most common metrics is the *mean squared error*
- Denote training set $Tr = \{x_i, y_i\}_1^N$, and testing set $Te = \{x_i, y_i\}_1^M$

$$\text{MSE}_{Tr} = \frac{1}{N} \sum_{i \in Tr} (y_i - \hat{f}(x_i))^2$$

$$\text{MSE}_{Te} = \frac{1}{M} \sum_{i \in Te} (y_i - \hat{f}(x_i))^2$$

- Training error, MSE_{Tr}, may be biased due to overfitting
- In this course, we denote *MSE* as training error, and *MSPE* as testing error

Prediction error – a tradeoff

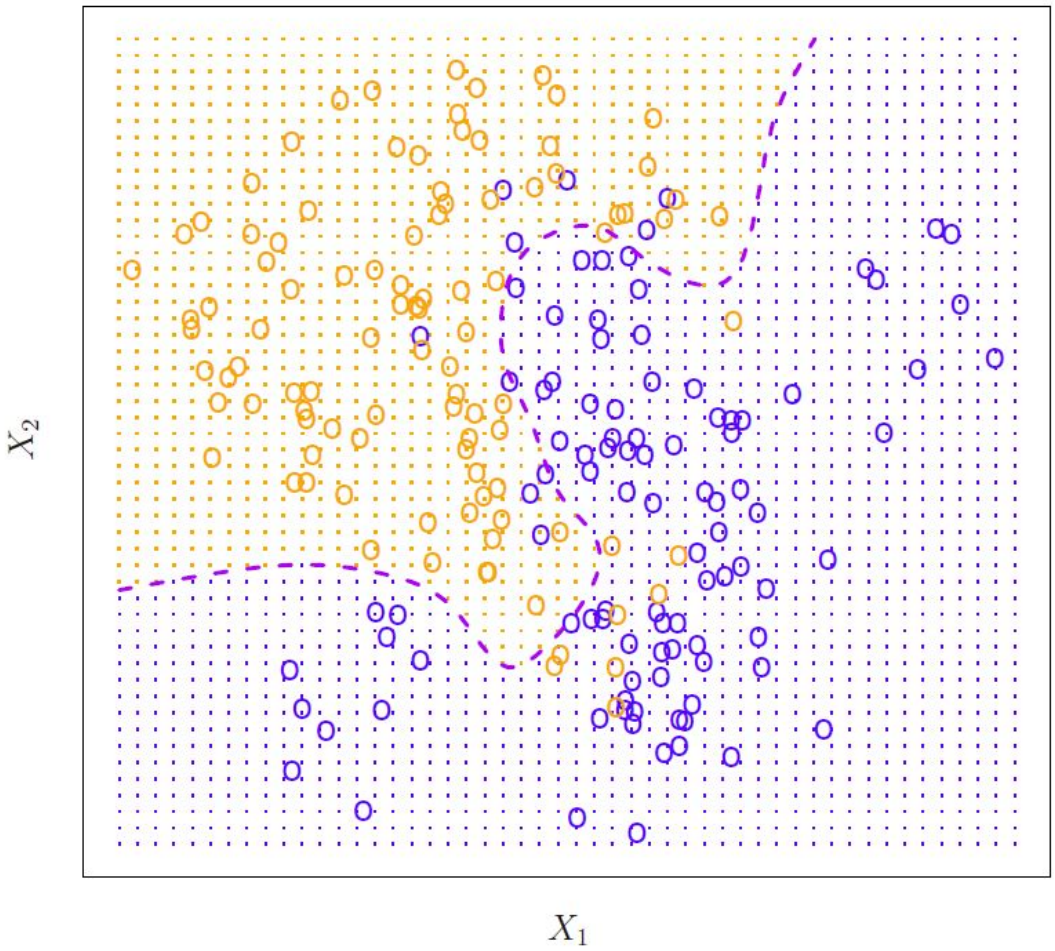



HOW MUCH ACCURACY DID YOU GET ?
I GOT 99%
AND WHAT WAS THE PROPORTION OF YOUR TEST SET ?
I TESTED WITH THE SAME TRAINING SET
imgflip.com

Classification

- Response variable is categorical
  - e.g., {A, B, C}, {dog, cat}, {0, 1}
- Goal: prediction (classification)
- Learning methods:
  - Parametric methods, e.g., logistic regression
  - Nonparametric methods, e.g., decision tree, neural network
- an example of neural networks: [link]
- Commonly used evaluation metrics:
  - misclassification error, false positive rate (FPR), false negative rate (FNR), AUC, F1 score, pseudo R-square, etc.

Classification – an illustration[1]

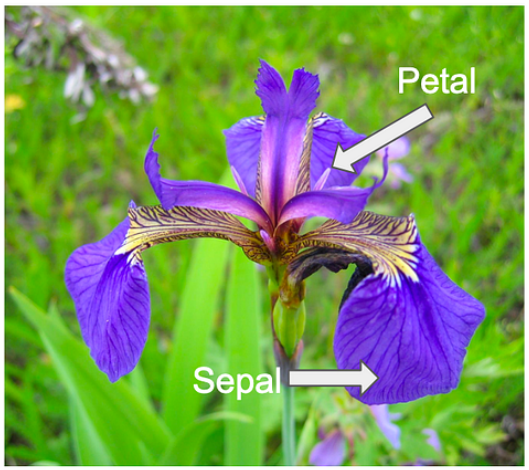


[1]Source: ISLR pp.38, Figure 2.13

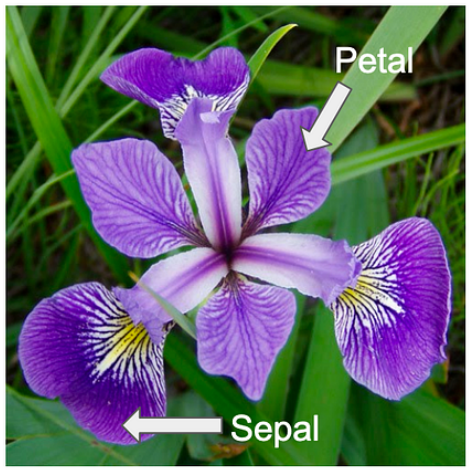
An example for classification

Suppose we want to classify types of flowers by measuring their sizes.

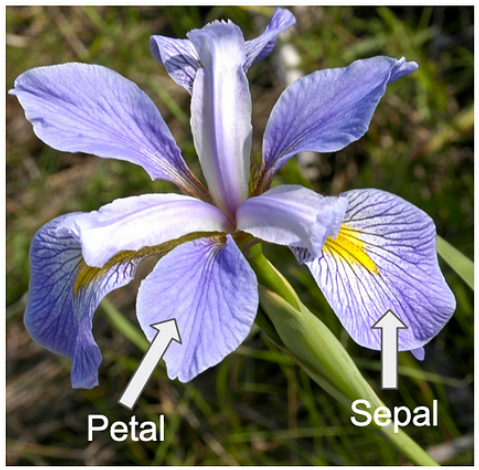
Iris setosa



Iris versicolor



Iris virginica



- Predictors (X): sepal width and length, petal width and length
- Label (Y): {setosa, versicolor, virginica}
- Learning goal: what kind of X more likely belongs to what class

A simple classifier: K-nearest neighbor

- Model:

$$\hat{Y} = \hat{f}(\mathbf{x}) = \frac{1}{k} \sum_{\mathbf{x}_i \in N_k(\mathbf{x})} y_i$$

  where $N_k(\mathbf{x})$ is the neighborhood of $\mathbf{x}$ defined by the k closest points $\mathbf{x}_i$.

- k: size of the neighbor
  - smaller or bigger neighbor is better?
- How to find the neighbor of any point $\mathbf{x}$?

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- Response variable is **qualitative**, which has no numeric meaning
- A classifier $\hat{C}(x)$ either correctly predict x or not
- A commonly used prediction error: Misclassification rate (MR)

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- Most classifier $\hat{C}(x)$ involves certain decision rule
  - As a learning outcome, the machine may say "a flower with characteristics x is more likely to be setosa than other types."

K-fold cross-validation

- Instead of doing train and test once, we can do it K times

Folder 1	Folder 2	Folder 3	Folder 4	Folder 5
Test	Train	Train	Train	Train
Train	Test	Train	Train	Train
Train	Train	Test	Train	Train
Train	Train	Train	Test	Train
Train	Train	Train	Train	Test

- Use 2,3,4,5 as training and 1 as testing
- Use 1,3,4,5 as training and 2 as testing
- Keep doing this loop...
- Average 5 testing errors, that is CV score
- In practice, $K = 5$ or 10 is recommended

Bias-Variance Tradeoff

- This is a very important tradeoff that governs the choice of statistical learning methods.
- **Bias**: how far the estimated model $\hat{f}(x)$ is to the true model $f(x)$.
  - Unbiased estimate is defined as: $\mathbb{E}\hat{f}(x) = f(x)$
  - Usually, we calculate the squared bias: $(\mathbb{E}\hat{f}(x) - f(x))^2$
- **Variance**: the variation of estimated model $\hat{f}(x)$ based on different training set.

Bias-Variance Tradeoff

Source: link

Bias-Variance Tradeoff

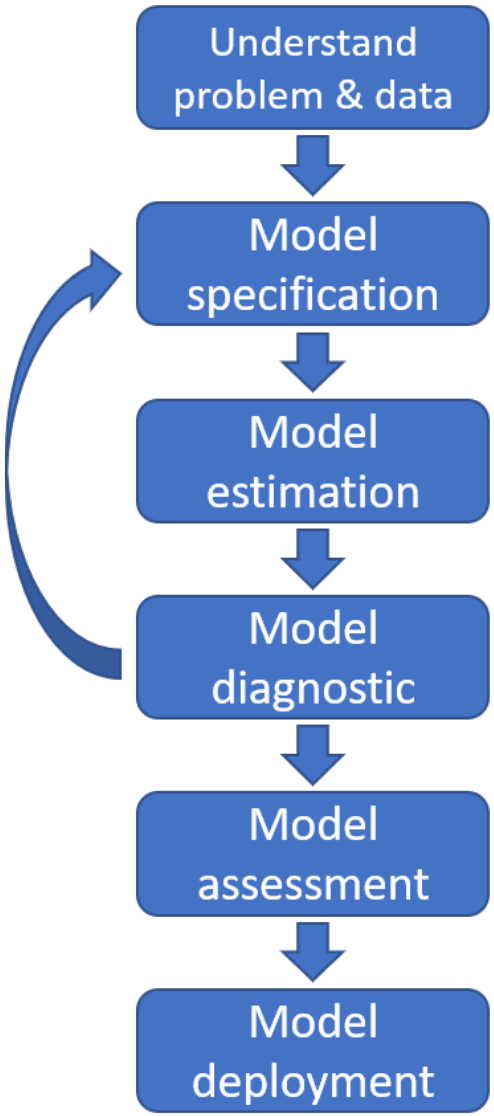
- Suppose the data arise from a model $Y = f(x) + \epsilon$, with $\mathbb{E}(\epsilon) = 0$ and $Var(\epsilon) = \sigma^2$.
- Suppose $\hat{f}(x)$ is trained based on some training data, and let (x_0, y_0) be a test observation from the same population.
- The *expected prediction error* can be decomposed to:

$$\mathbb{E}[y_0 - \hat{f}(x_0)]^2 = \sigma^2 + Bias^2(\hat{f}(x_0)) + Var(\hat{f}(x_0))$$

(Challenge yourself: Show it.)

- Typically as the **flexibility** of $\hat{f}$ increases, its variance increases, and its bias decreases.

Model building process



- Describe the problem by stating the goal and purpose of statistical analysis.
- Given the dataset, conduct exploratory data analysis to maximize the knowledge of information carried by the data.

- Identify relevant variables and do necessary data cleaning and transformation. These include missing data imputation, variable recoding and transformation, etc.
- Identify appropriate statistical models to achieve the purpose of analysis.

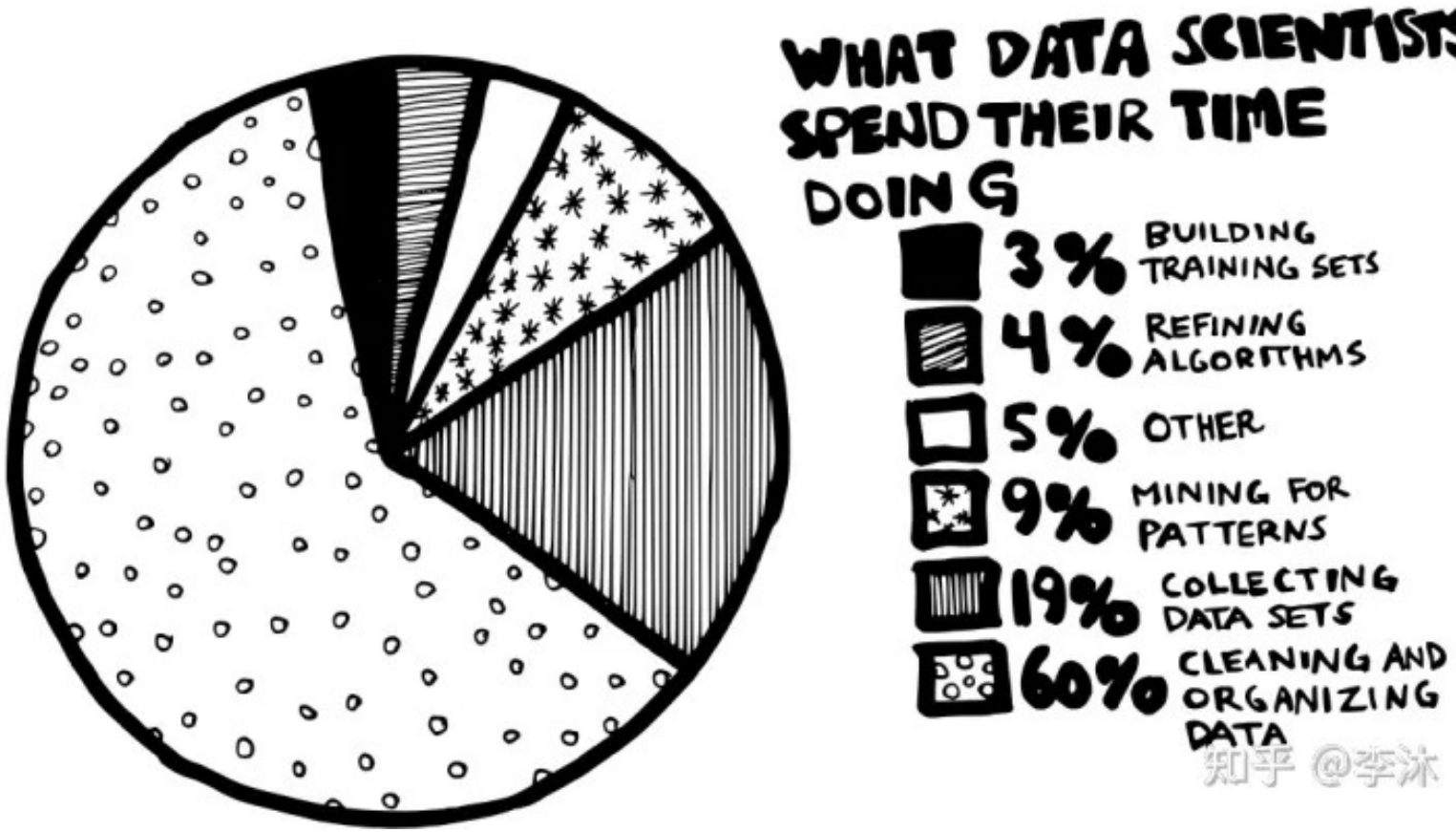
- Use software to estimate the model. This process may involve debugging.
- Understand the main components of the output.
- Statistical inference needs to be conducted.

- Check if there is any model assumption violation. (For more ML oriented methods such as neural networks, this step is often skipped due to less assumptions.)
- If violation is identified, go back and re-specify the model. For example, if residual plots show quadratic pattern, then the quadratic term of one or more predictors needs to be included. Graphical inspections are needed in this procedure.

- Typically, various models are estimated, including a certain type of model with different sets of variables (determined by variable selection), and different types of model such as linear regression, regression tree, and neural networks.
- Compare all estimated models in terms of certain criteria, such as cross-validation error, AIC and BIC, etc.

- At the end of analysis, a final model needs to be determined for deployment.
- Depending on different scenarios, the final model may be a set of models that include several different models.
- Inference and model interpretation should be part of the deployment.

The reality


WHAT DATA SCIENTISTS SPEND THEIR TIME DOING
3% BUILDING TRAINING SETS
4% REFINING ALGORITHMS
5% OTHER
9% MINING FOR PATTERNS
19% COLLECTING DATA SETS
60% CLEANING AND ORGANIZING DATA
知乎 @李沐