Simple ML Algorithms and General Principles [1]

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[1] Partially based on Hastie, et al. (2009) ESL, and James, et al. (2013) ISLR

Clustering – an unsupervised learning method

- Goal: find subgroups of a sample observations
  - Not based on any single variable (e.g. gender, race)
  - Based on all given variables

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- Goal: find subgroups of a sample observations
  - Not based on any single variable (e.g. gender, race)
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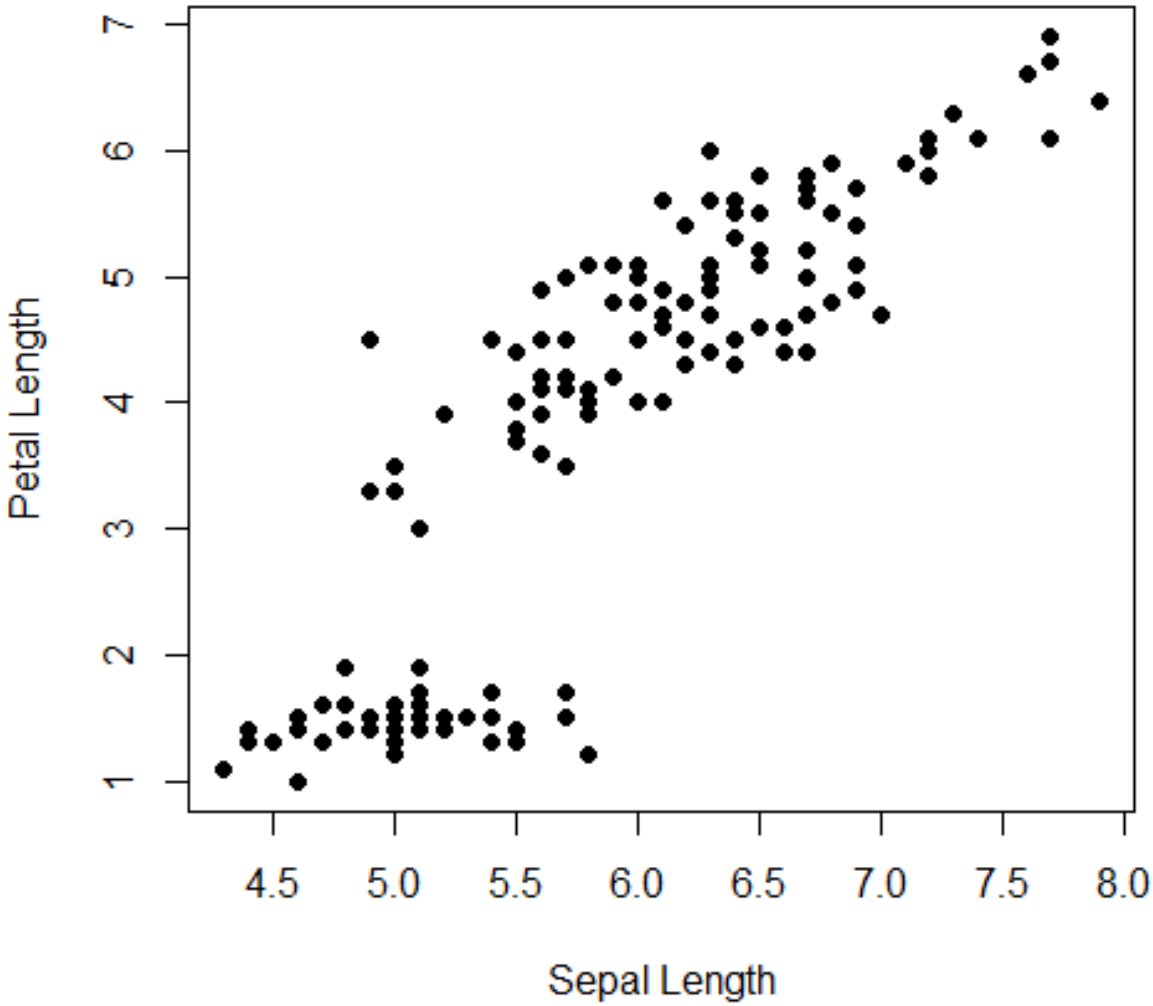
- The number of subgroup is subjective
- Approaches:
  - K-means clustering
  - Hierarchical clustering
  - Model-based clustering

An example – Iris data



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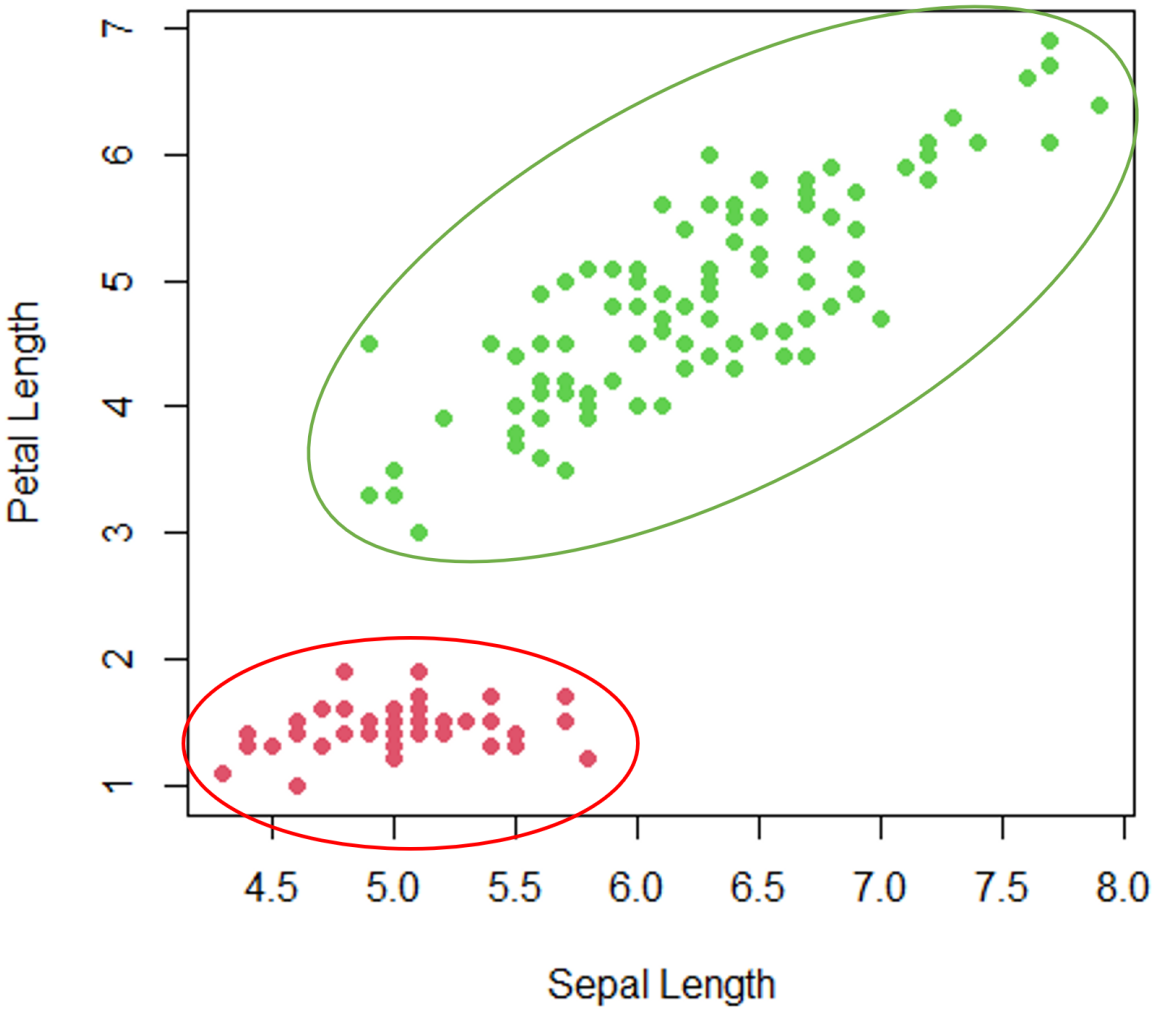

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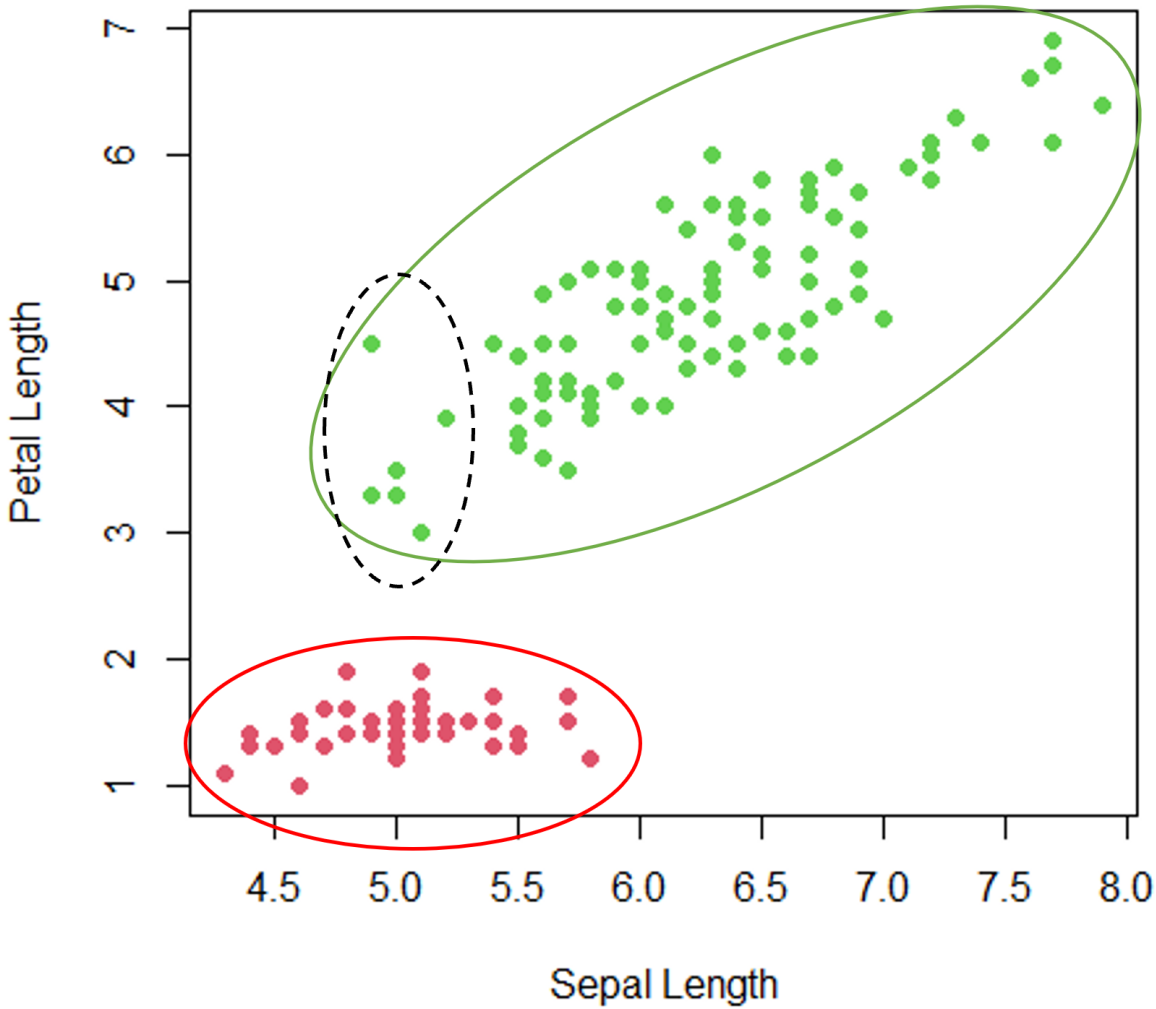


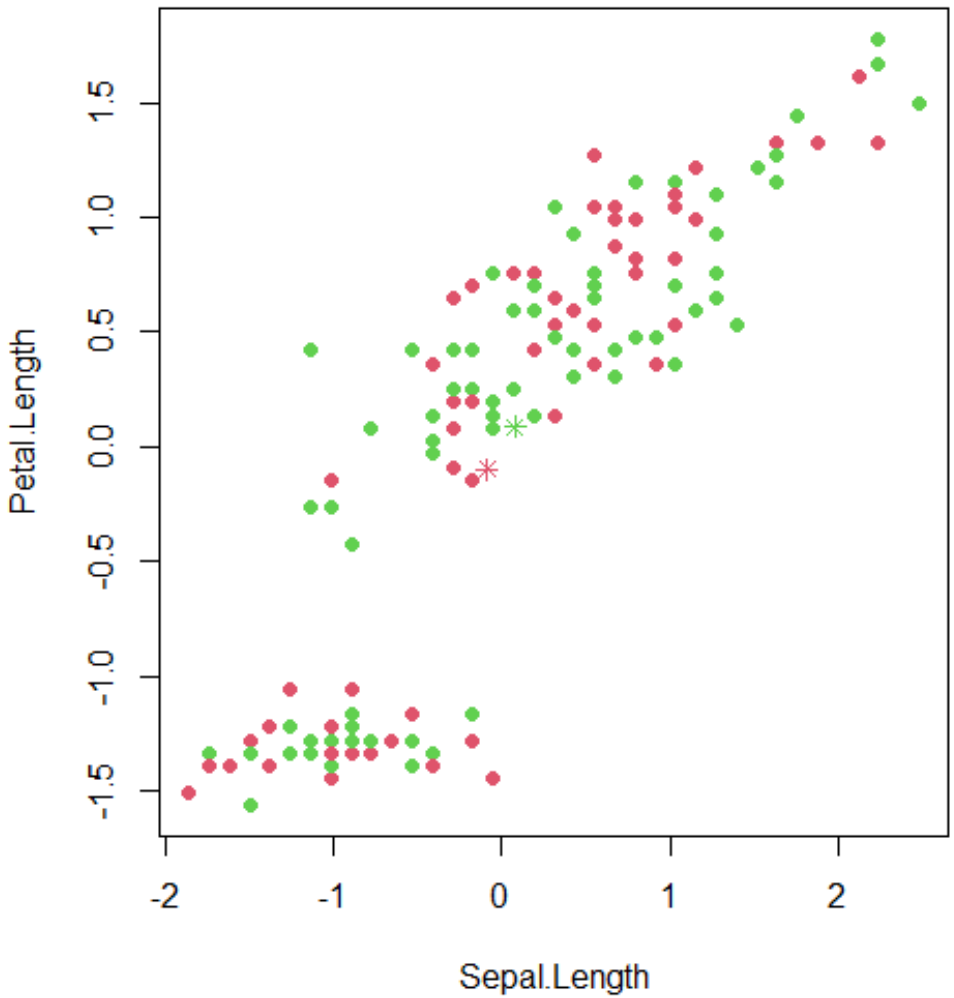
K-means clustering – step-by-step

Run the following R code, and see what it does.

```
iris1 <- scale(iris[,-c(2,4,5)])
n <- nrow(iris1)
index <- sample(2, n, replace = T)
iris.sub1 <- iris1[index==1,]
iris.sub2 <- iris1[index==2,]
mean.sub1 <- apply(iris.sub1, 2, mean)
mean.sub2 <- apply(iris.sub2, 2, mean)

plot(iris1, col=index+1, pch=16)
points(x=mean.sub1[1], y=mean.sub1[2], col=2, pch=8)
points(x=mean.sub2[1], y=mean.sub2[2], col=3, pch=8)
```

This is a random grouping (first step)



The next step

Run the following R code, and see what it does.

```
Eudist <- function(x, y) sqrt(sum((x-y)^2))

d1<-sapply(1:n,function(i) Eudist(mean.sub1,iris1[i,]))
d2<-sapply(1:n,function(i) Eudist(mean.sub2,iris1[i,]))
index.new <- apply(cbind(d1, d2), 1, which.min)
iris.sub1 <- iris1[index.new==1,]
iris.sub2 <- iris1[index.new==2,]
mean.sub1 <- apply(iris.sub1, 2, mean)
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plot(iris1, col=index.new+1, pch=16)
points(x=mean.sub1[1], y=mean.sub1[2], col=2, pch=8)
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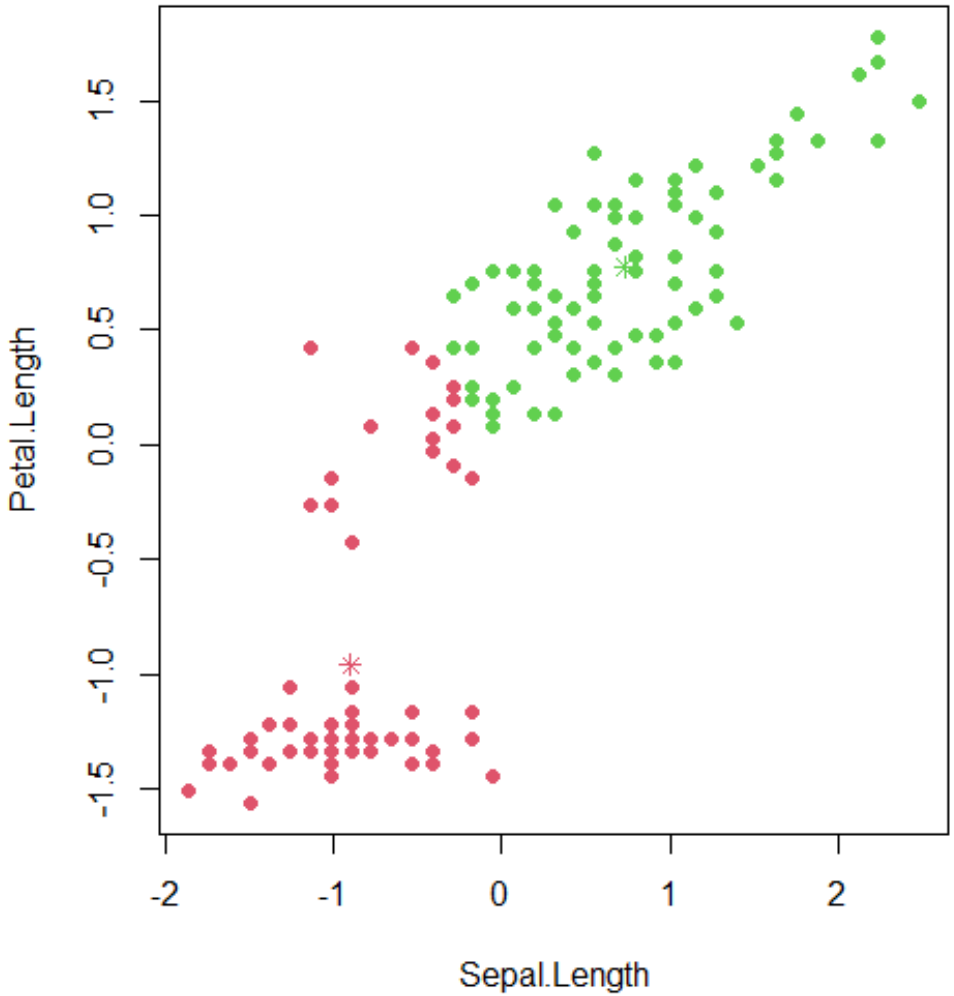
```

Data points are regrouped (second step)



How does this happen?

Let's repeat the second step

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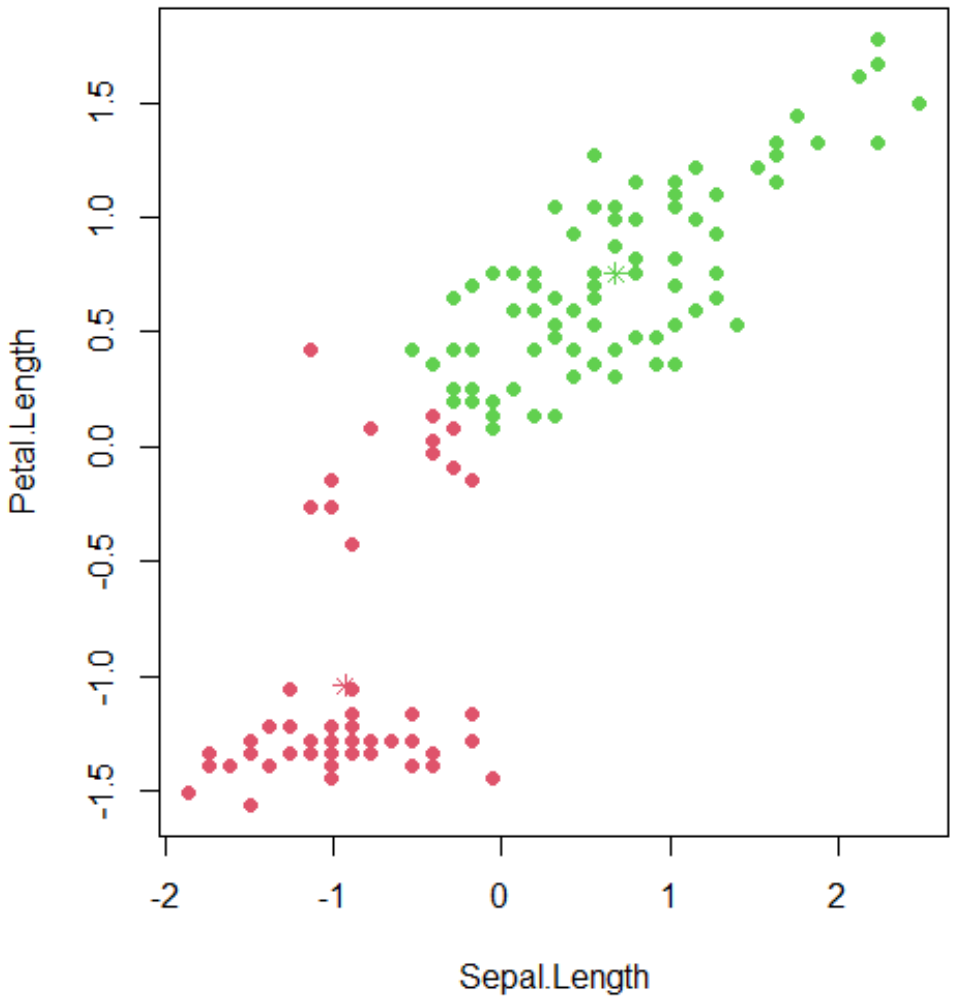
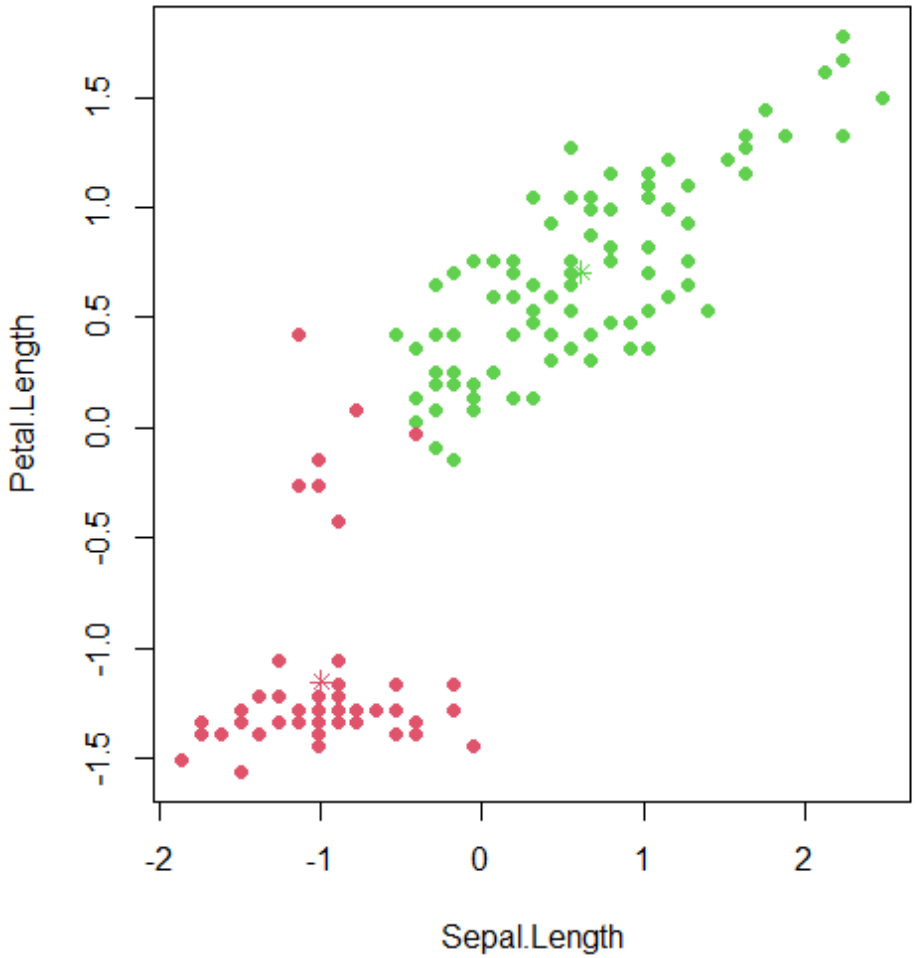
points(x=mean.sub2[1], y=mean.sub2[2], col=3, pch=8)
```

Note that the code does not change at all. Why?

Data points are regrouped again



We can keep repeating this step, until...



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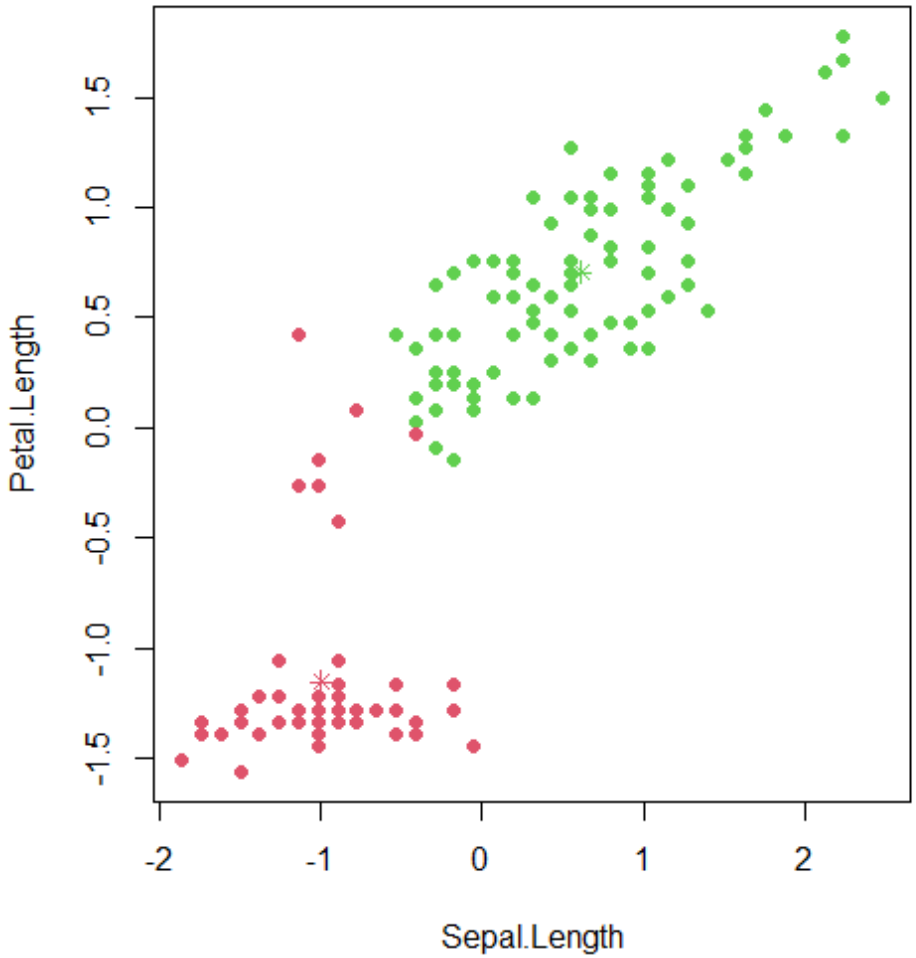

Members in each cluster do not change, which means the algorithm converges. How can we translate it into some numeric scores?

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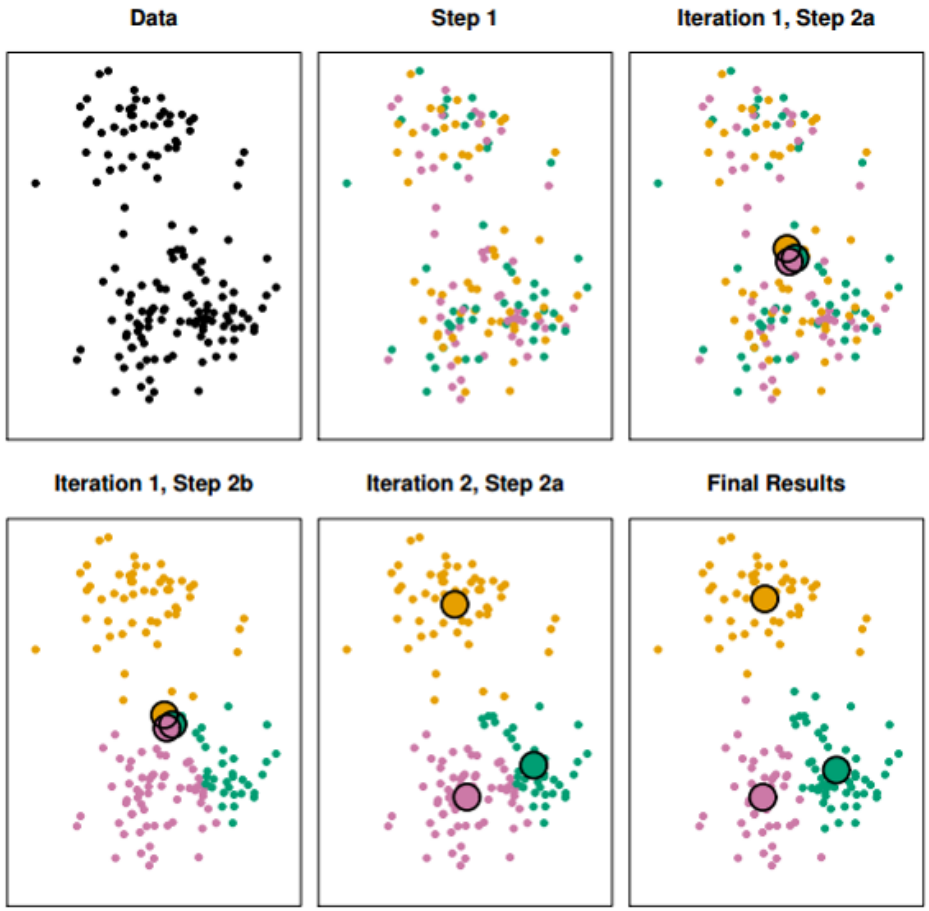
- Between-group sum square:
  the difference between total SS and sum of within SS.

- Exercise:
  Revisit the algorithm we just performed. Compute the above three measures at the end of each step. How are they changing over iterations?

Recap



- Here is a very good animation to illustrate k-means clustering algorithm. [link]

K-means algorithm

1. Randomly find k data points (observations) as the initial centers
2. For each data point, find the closest center and label it (e.g., using different colors). Now you have k clusters
3. Re-calculate the centers of current clusters
4. Repeat step 2 and 3 until the centers do not change

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 – Least Squares

- Linear regression model

$$Y = \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p + \epsilon$$

- The estimated model is

$$\hat{Y} = \hat{f}(\mathbf{x}) = \hat{\beta}^T \mathbf{x}$$

- Solve $\hat{\beta}$ using least square

$$\hat{\beta} = \arg\min_{\beta} \sum_{i=1}^{n} (y_i - \beta^T \mathbf{x}_i)^2$$

Supervised Learning – Nearest Neighbor

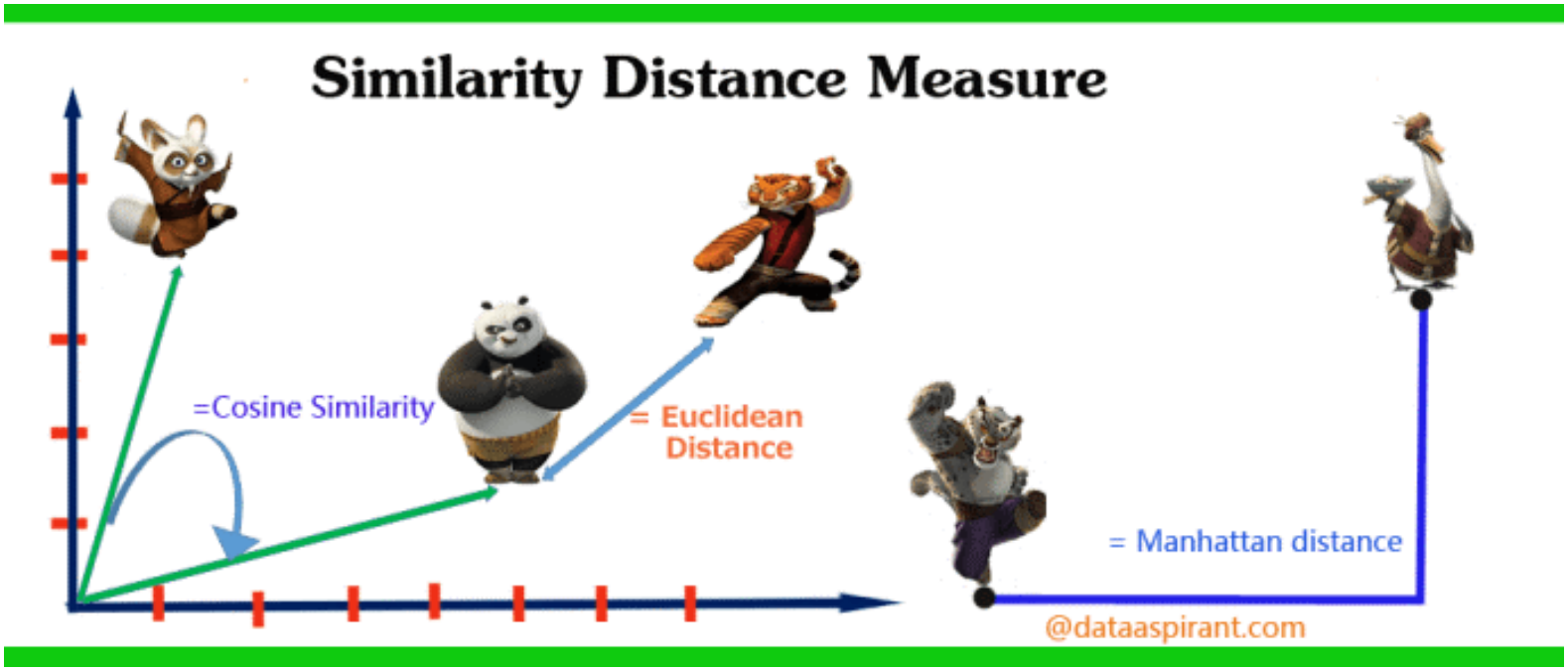
- Model:

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

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

- k determines the flexibility of the model (should larger k or smaller k results in more flexible model?)
- How to define the neighbor? (How to find closest points to $\mathbf{x}_i$?) - Similarity measures

Distance-based Similarity Measures



An example[2]

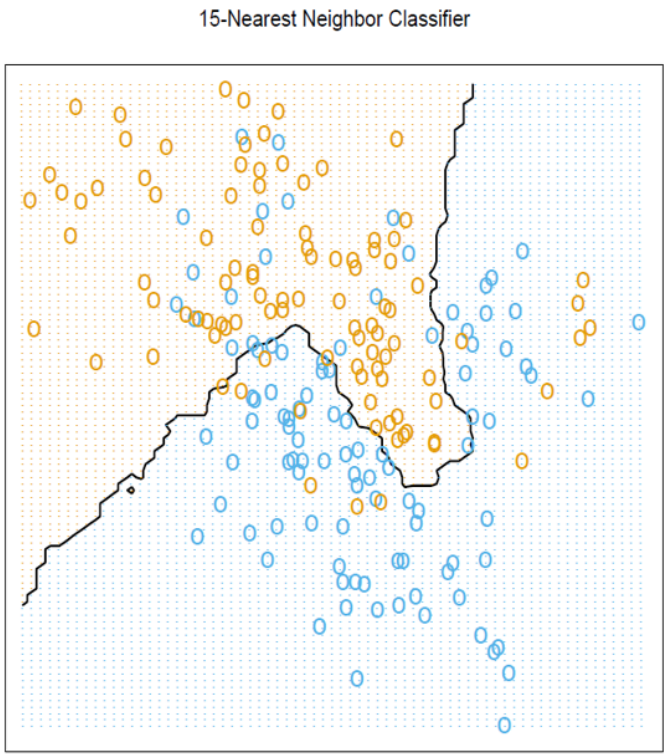


FIGURE 2.2. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable* (BLUE $= 0$, ORANGE $= 1$) *and then fit by 15-nearest-neighbor averaging as in (2.8). The predicted class is hence chosen by majority vote amongst the 15-nearest neighbors.*

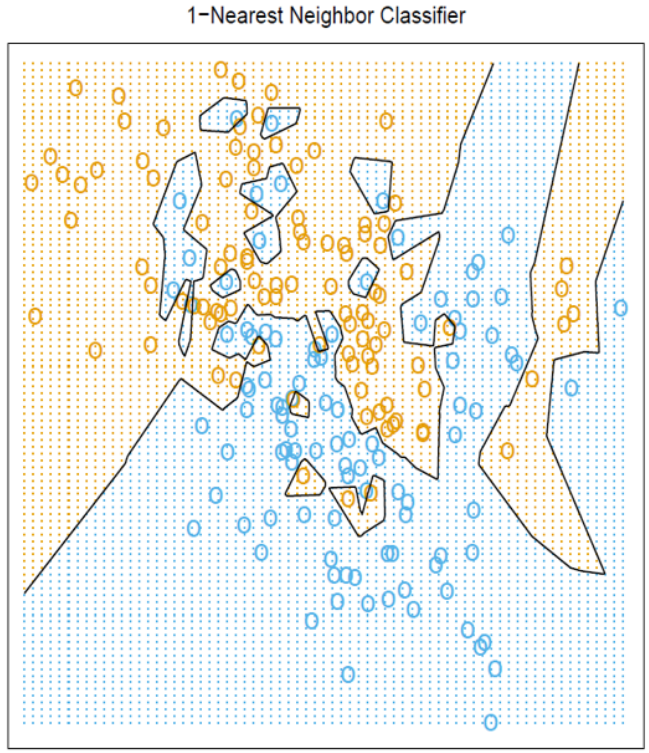


FIGURE 2.3. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable* (BLUE $= 0$, ORANGE $= 1$), *and then predicted by 1-nearest-neighbor classification.*

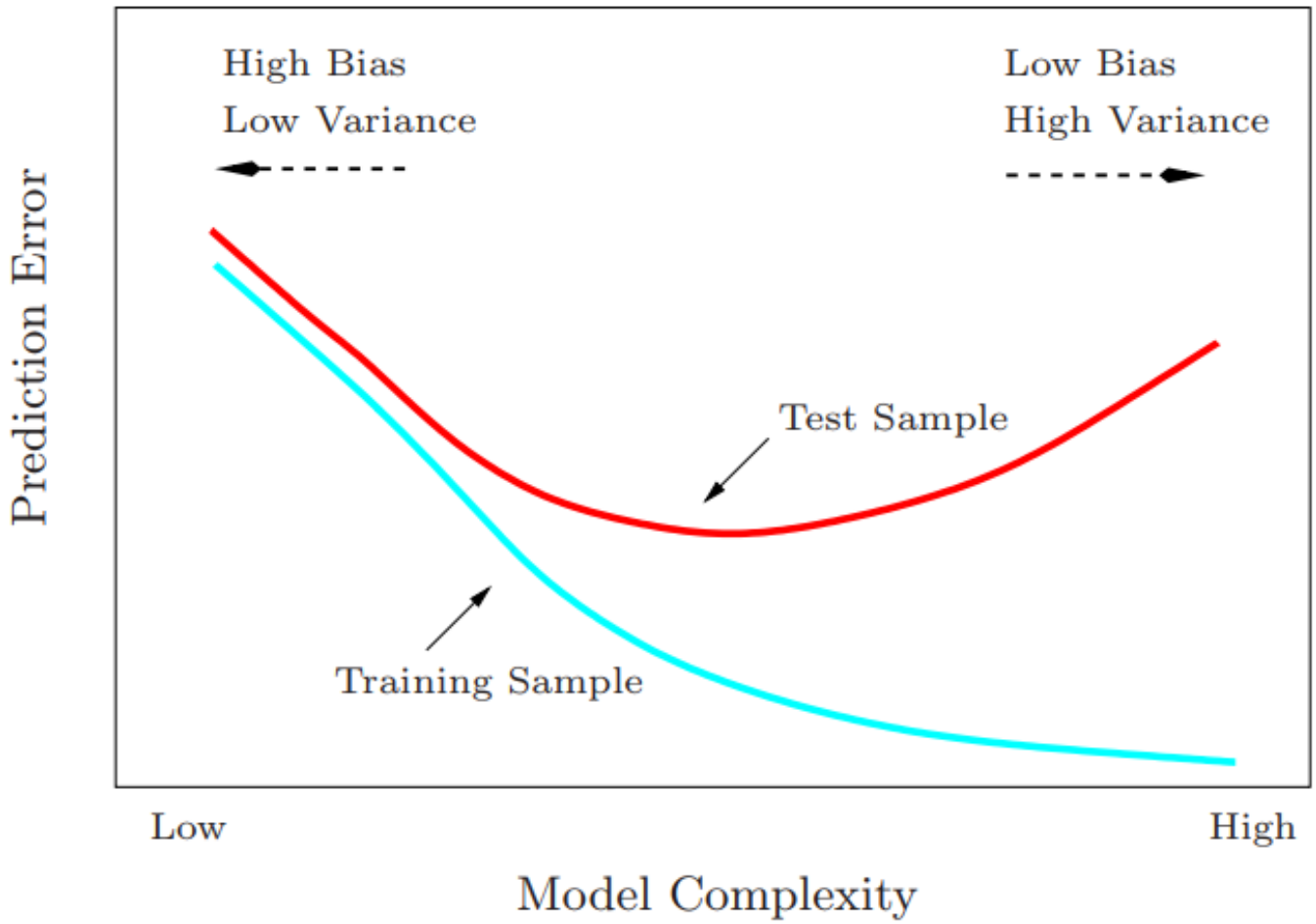
[2] ESL pg.15-16

Model Assessment (for supervised learning)

How do we know if the estimated model $\hat{f}(x)$ is **useful**?

- We never know the true $f(x)$
- Split sample to training and testing sets
- Train the model (learning algorithm) based on training sample by minimizing *training error*
- Apply the estimated model on the testing sample to calculate the *prediction (testing) error*
- We care more about testing error rather than training error

Prediction Error



Prediction Error

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


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 Problems

- Response variable is **qualitative**
- Train a classifier $\hat{C}(x)$ that can label any new input data x
- It usually involves certain decision rule
- Prediction (testing) error: Misclassification rate (MR)

$$MR_{Te} = \frac{1}{M} \sum_{i \in Te} \mathbb{I}[y_i \neq \hat{C}(x_i)]$$

K-Fold Cross-validation

- Instead of doing training vs. testing once, we 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

Leave-one-out Cross-validation

- By the name, it requires to repeat training-testing procedure n times
- However, for least square linear model, there is a short cut that makes LOOCV the same that of a single model fit

$$CV_n = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - \hat{y}_i}{1 - h_i}\right)^2$$

  where h_i is the diagonal element of "hat" matrix.
- In general, the estimates from LOOCV are highly correlated hence their average can have high variance
- In practice, $K = 5$ or 10 is recommended
- Exercise: write your own code to perform 10-fold CV for knn (try different k) model on the "iris" dataset.

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.