Lecture 2: Basics

Shuai Li

John Hopcroft Center, Shanghai Jiao Tong University

https://shuaili8.github.io

https://shuaili8.github.io/Teaching/VE445/index.html

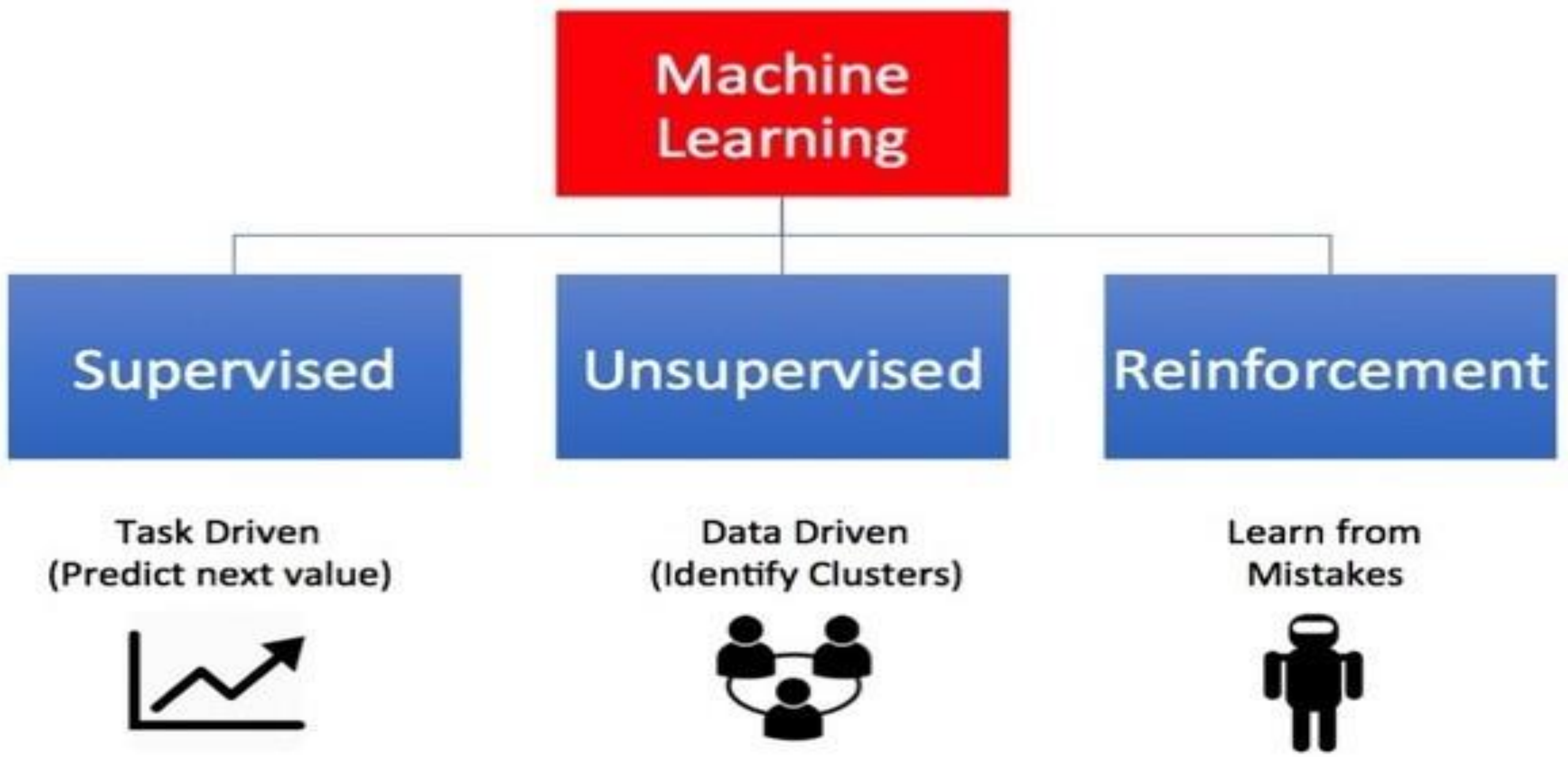
Last lecture

- What is Machine Learning and what is Artificial Intelligence
- An example of AI but not ML
  - A* algorithm
- History of ML
  - Deduction
  - Learning from samples (deep learning)
- Recent progress
  - Computer vision/speech recognition/natural language processing/game AI
- Many applications
  - Many industries/many aspects of life

Today’s lecture

- The classification of machine learning
  - Supervised/unsupervised/reinforcement
- Supervised learning
  - Evaluation metrics for classification
    - Accuracy/Precision/Recall/F1 score
  - Evaluation metrics for regression
    - Pearson coefficient/coefficient of determination
  - Model selection: bias/variance/generalization
  - Machine learning process
  - Generalization error bound (next time)

Types of Machine Learning



Machine Learning

Supervised

Unsupervised

Reinforcement

Task Driven
(Predict next value)

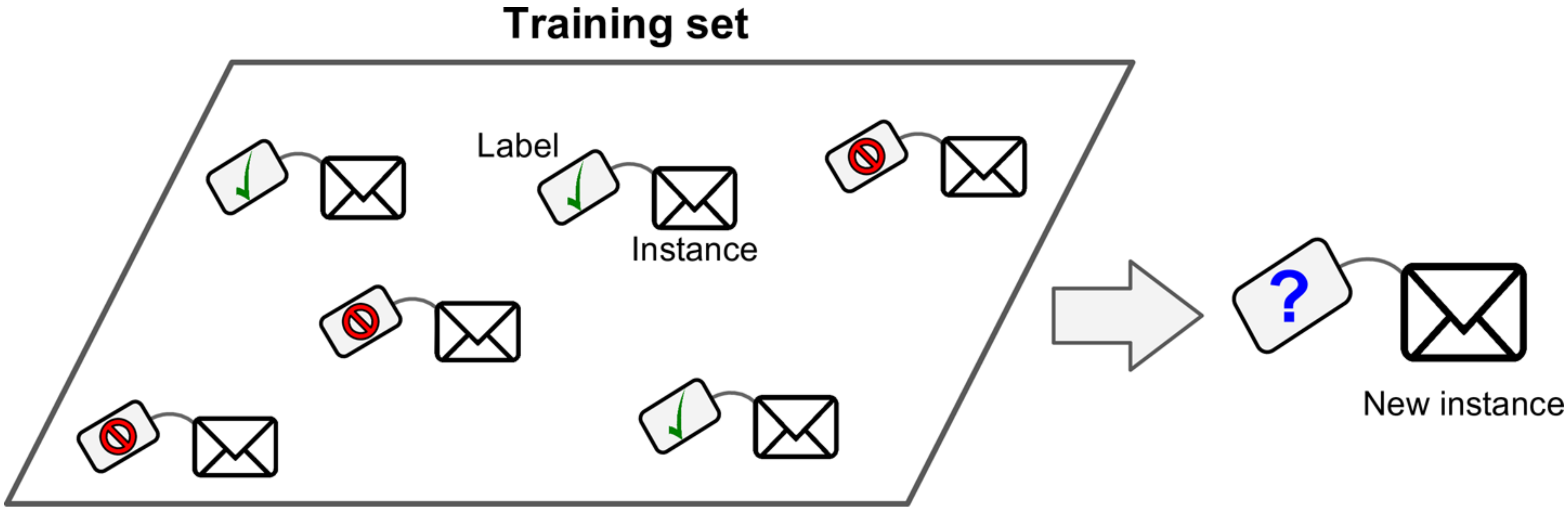
Data Driven
(Identify Clusters)

Learn from
Mistakes

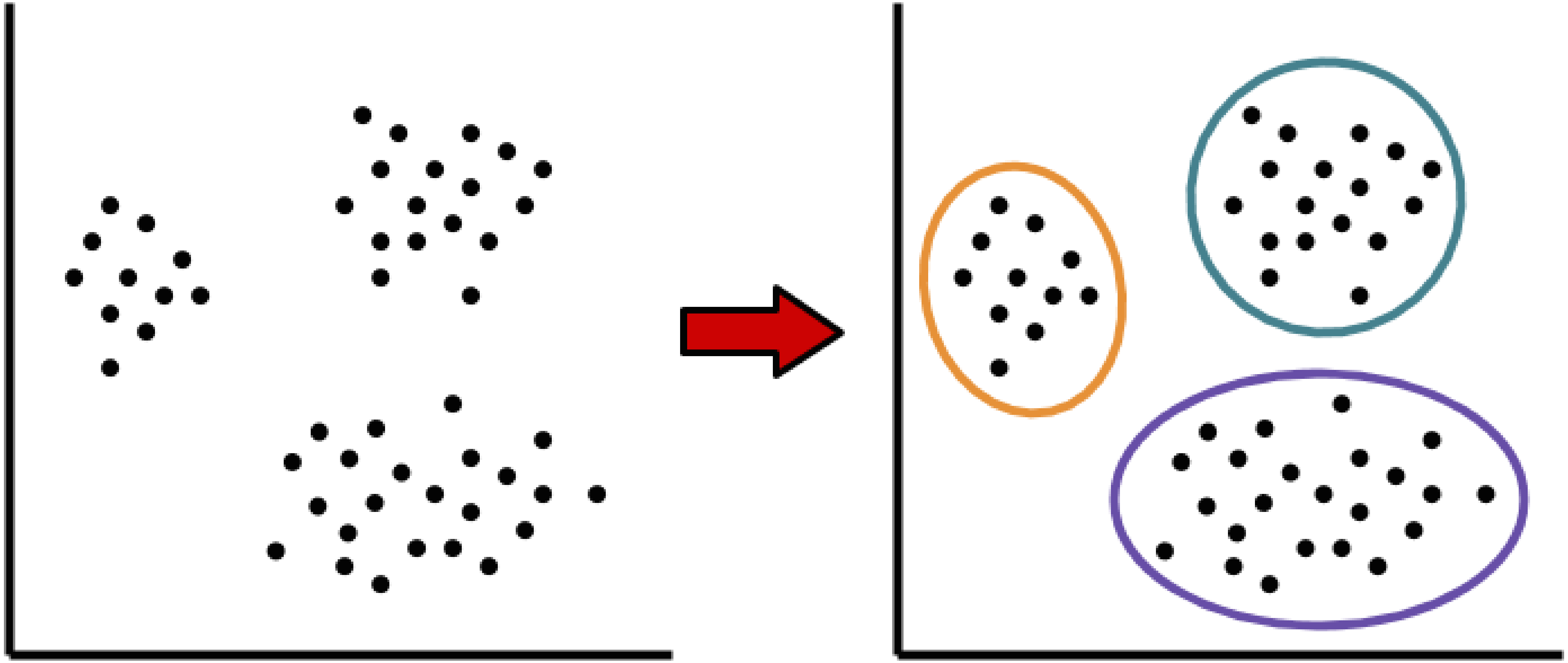
Machine Learning Categories

- Unsupervised learning
  - No labeled data
- Supervised learning
  - Use labeled data to predict on unseen points
- Semi-supervised learning
  - Use labeled data and unlabeled data to predict on unlabeled/unseen points
- Reinforcement learning
  - Sequential prediction and receiving feedbacks

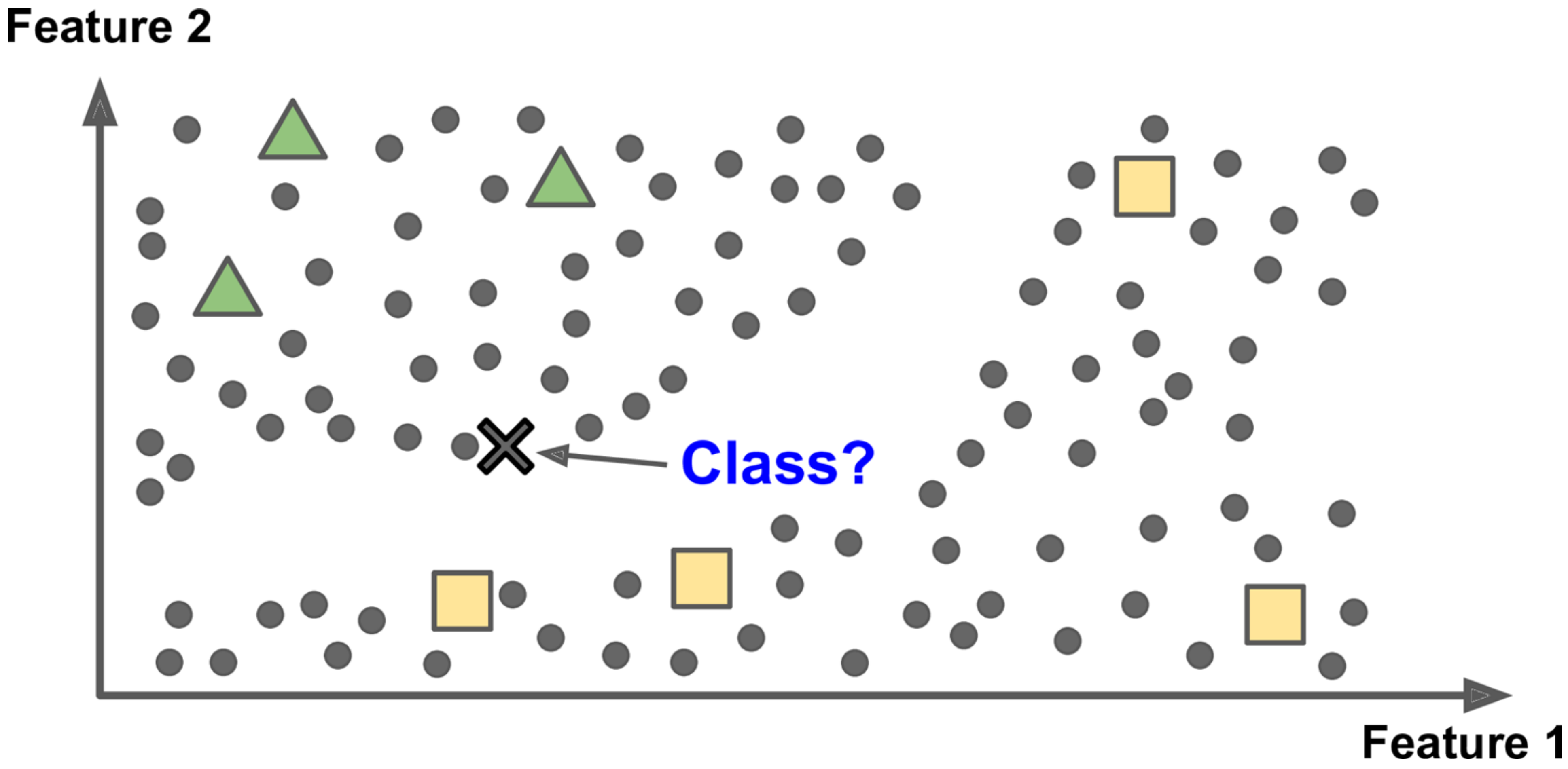
Supervised learning example



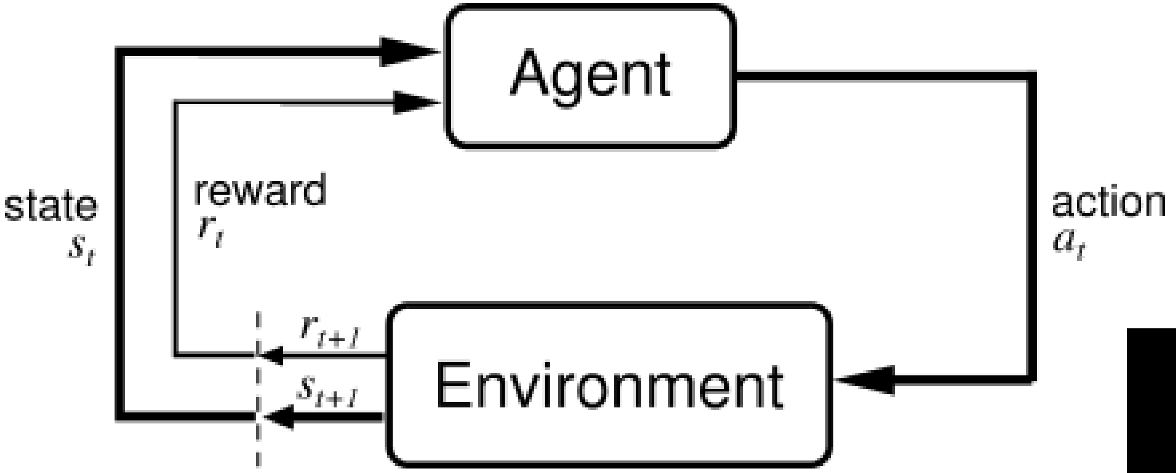
Unsupervised learning example

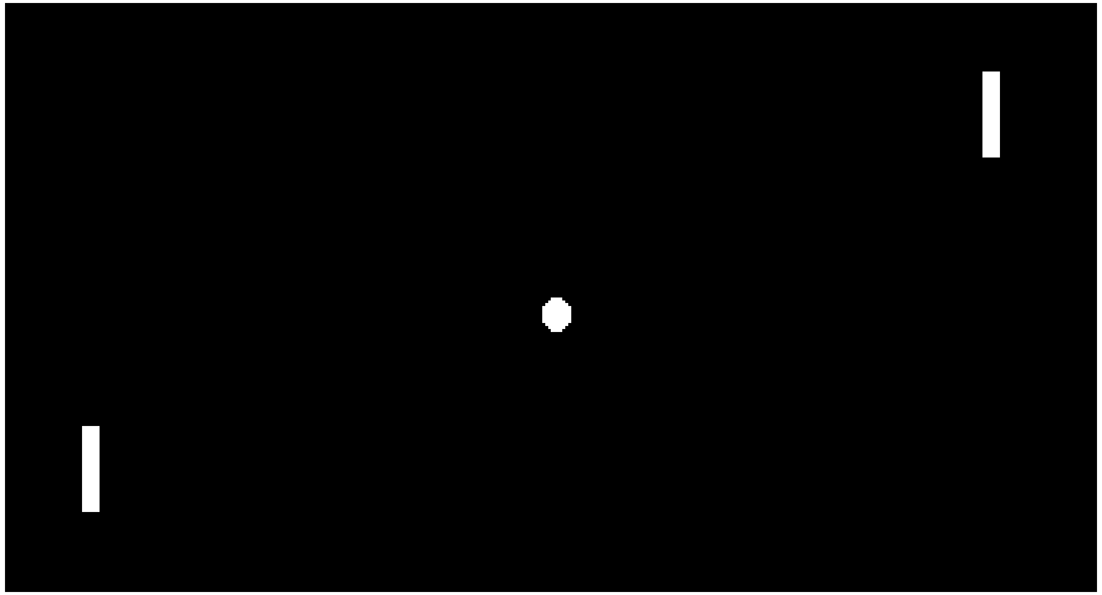


Semi-supervised learning example

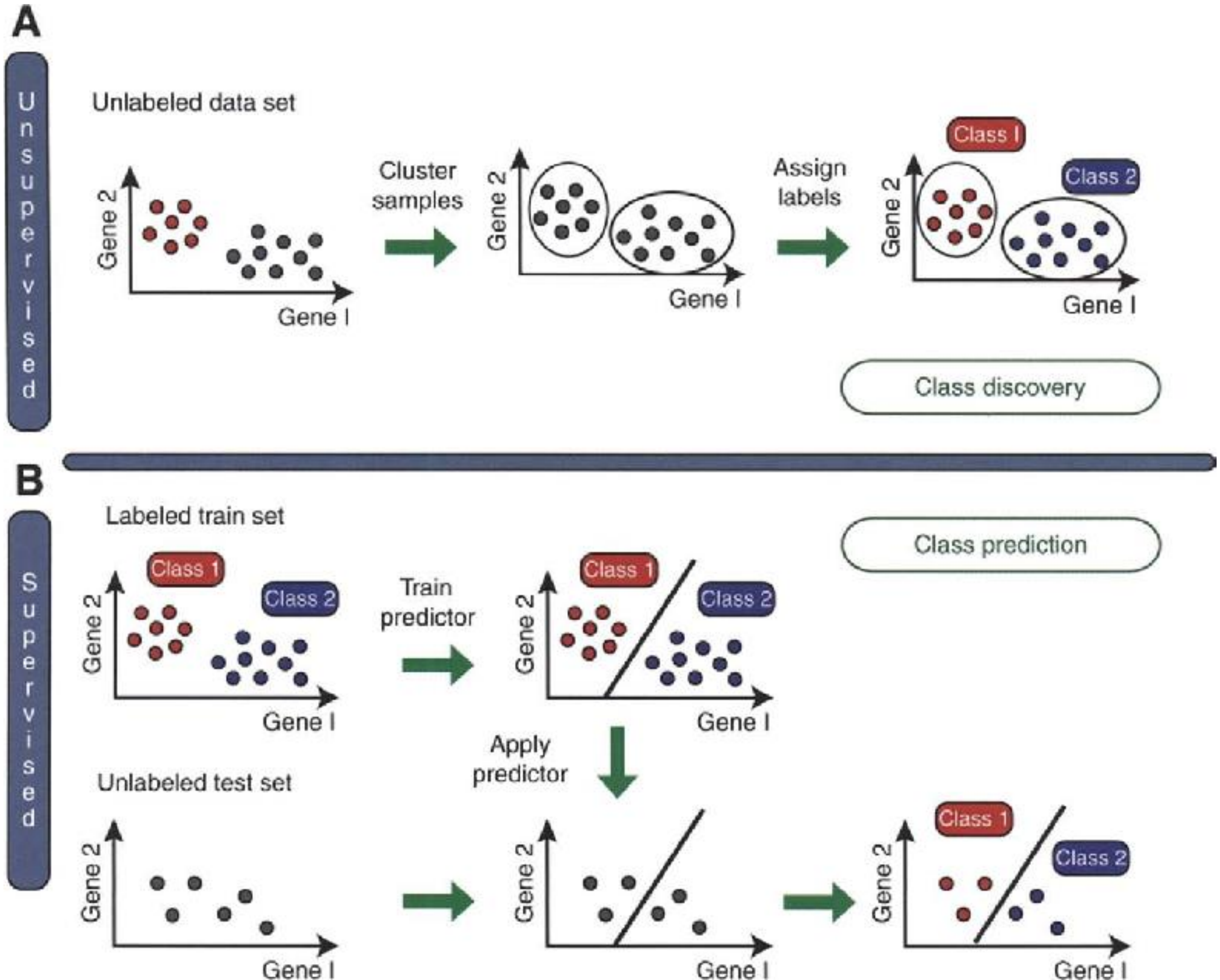


Reinforcement learning example





Supervised Learning	Unsupervised Learning
Input data is labelled	Input data is unlabeled
Uses training dataset	Uses just input dataset
Used for prediction	Used for analysis
Classification and regression	Clustering, density estimation and dimensionality reduction

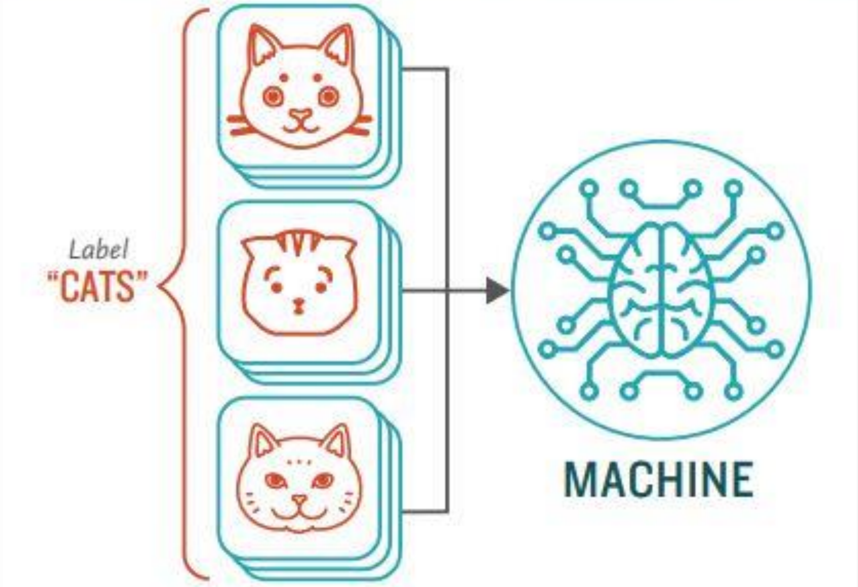

A
Unsupervised
Unlabeled data set
Gene 2
Gene I
Cluster samples
Gene 2
Gene I
Assign labels
Class I
Class 2
Gene 2
Gene I
Class discovery
B
Supervised
Labeled train set
Class 1
Class 2
Gene 2
Gene I
Train predictor
Class 1
Class 2
Gene 2
Gene I
Class prediction
Apply predictor
Unlabeled test set
Gene 2
Gene I
Gene 2
Gene I
Class 1
Class 2
Gene 2
Gene I

Supervised Learning

How Supervised Machine Learning Works

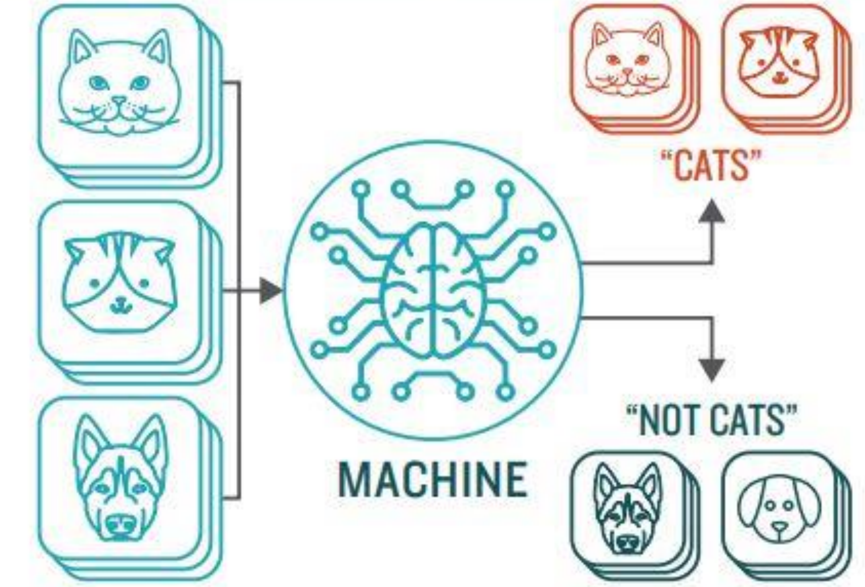
STEP I

Provide the machine learning algorithm categorized or "labeled" input and output data from to learn

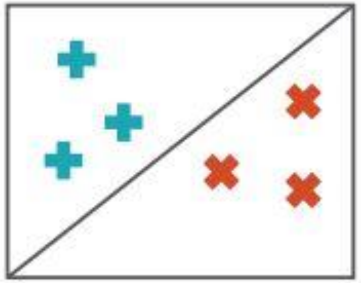


STEP 2

Feed the machine new, unlabeled information to see if it tags new data appropriately. If not, continue refining the algorithm

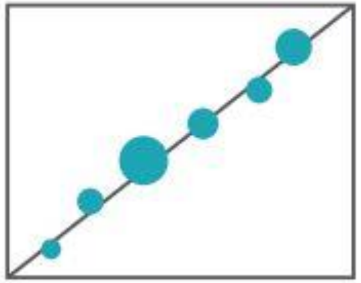


TYPES OF PROBLEMS TO WHICH IT'S SUITED



CLASSIFICATION

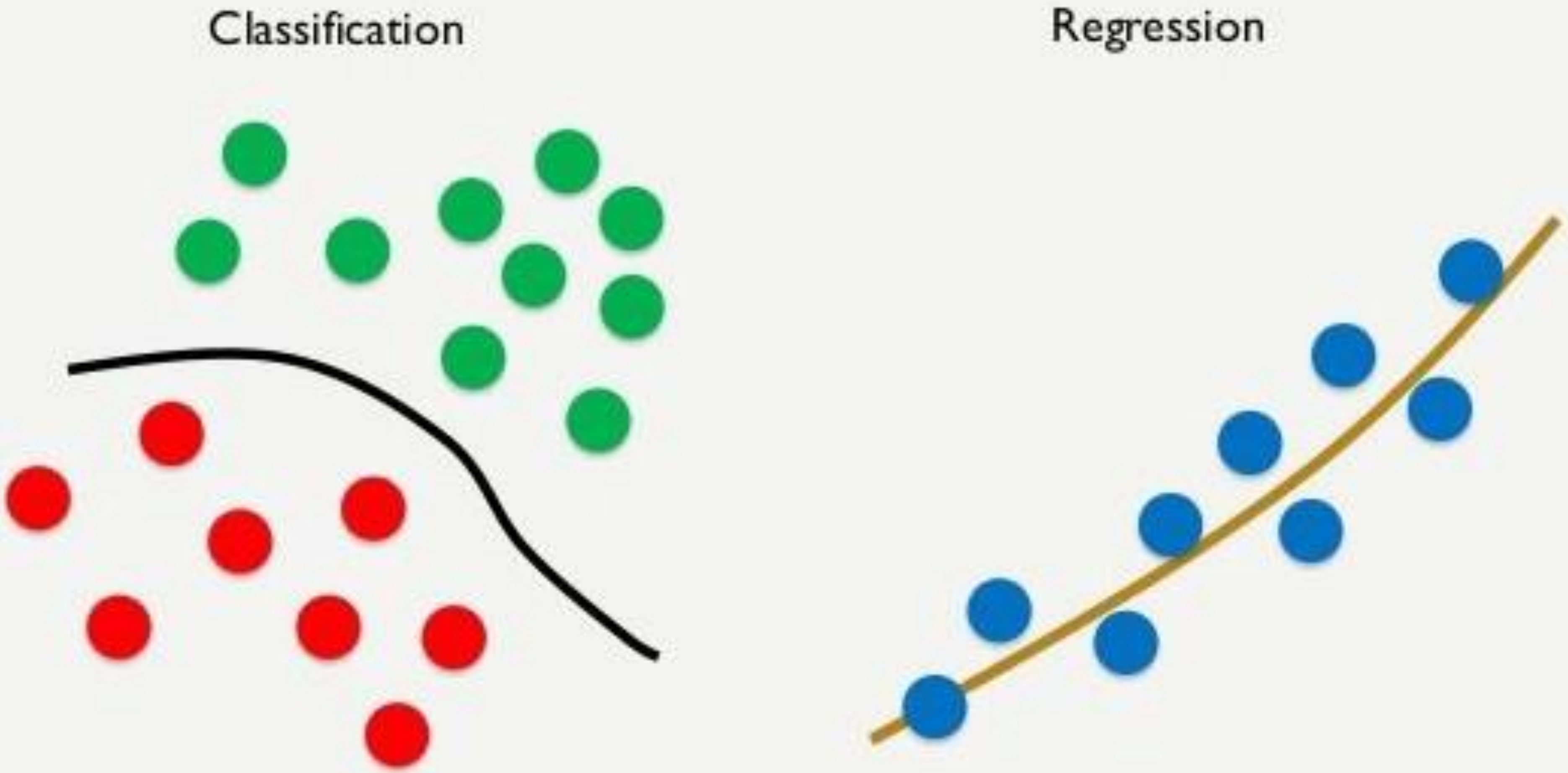
Sorting items into categories



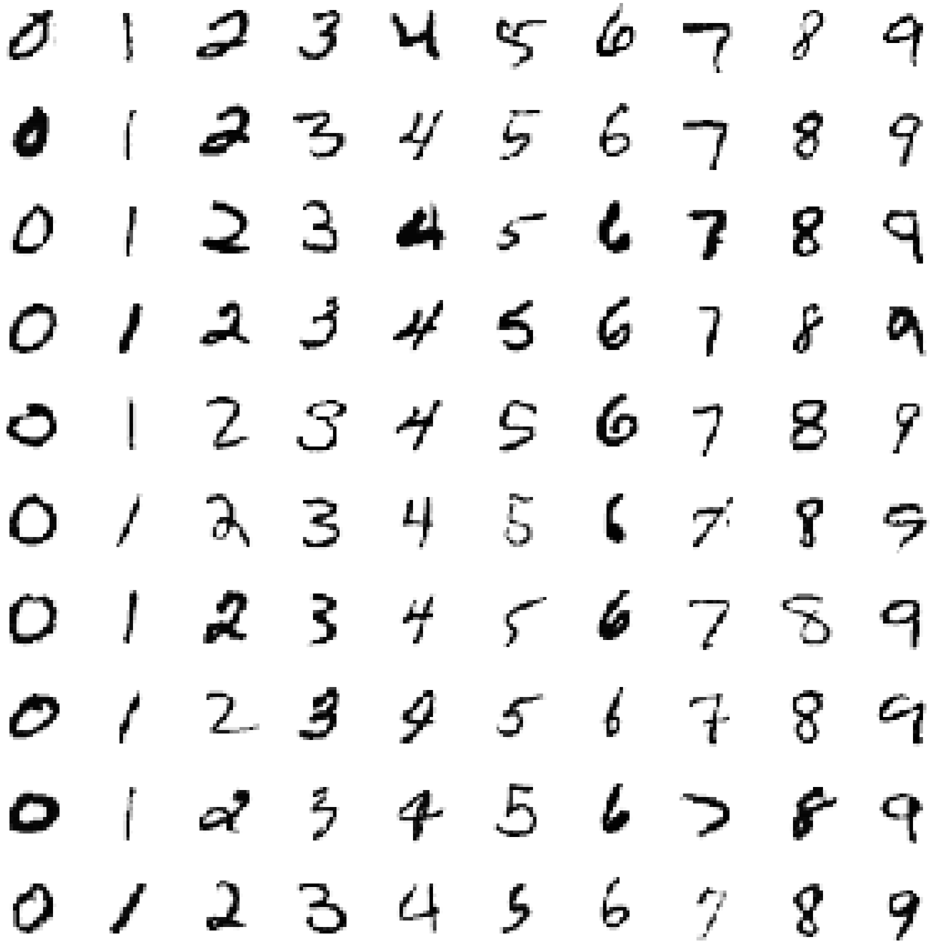
REGRESSION

Identifying real values (dollars, weight, etc.)

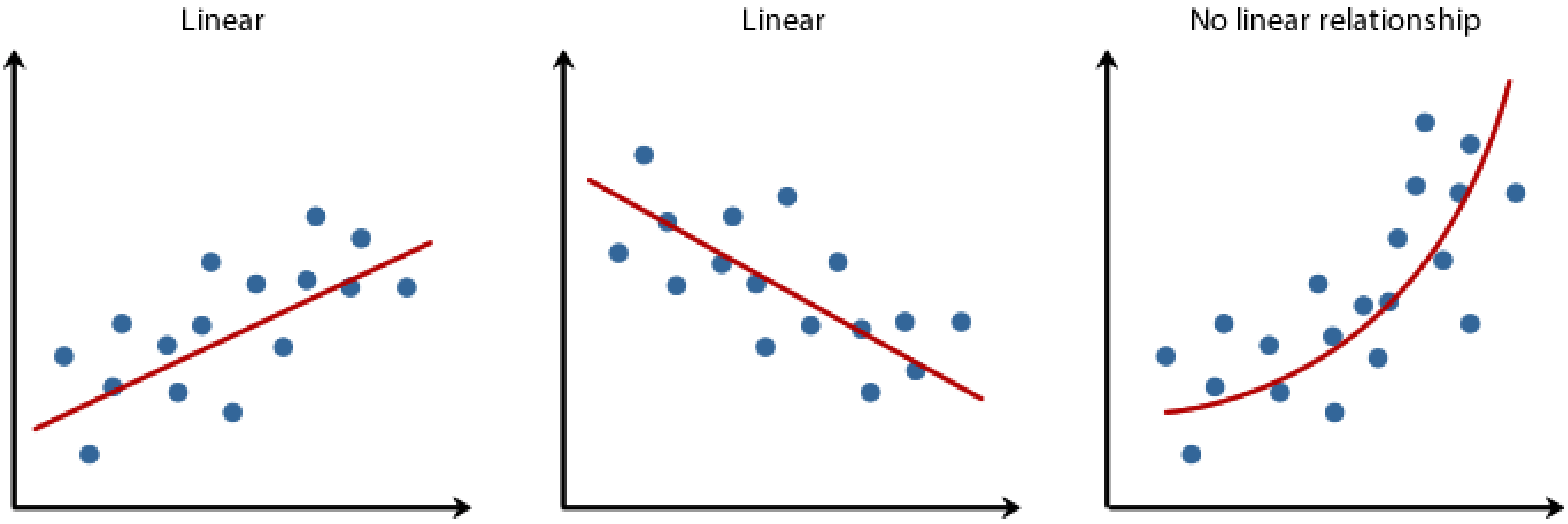
CLASSIFICATION VS REGRESSION



Classification -- Handwritten digits



Regression example



Linear

Linear

No linear relationship

Copyright 2014. Laerd Statistics.

Model Evaluations

Classification -- Model evaluations

- Confusion Matrix
  - TP – True Positive ; FP – False Positive
  - FN – False Negative; TN – True Negative

	Predicted Class		
Actual Class		Class = Yes	Class = No
	Class = Yes	a (TP)	b (FN)
	Class = No	c (FP)	d (TN)

$$\text{Accuracy} = \frac{a+d}{a+b+c+d} = \frac{TP+TN}{TP+TN+FP+FN}$$

Classification -- Model evaluations

- Given a set of records containing positive and negative results, the computer is going to classify the records to be positive or negative.

- Positive: The computer classifies the result to be positive
- Negative: The computer classifies the result to be negative
- True: What the computer classifies is true
- False: What the computer classifies is false

Classification -- Model evaluations

- Limitation of Accuracy
  - Consider a 2-class problem
    - Number of Class 0 examples = 9990
    - Number of Class 1 examples = 10
  - If a “stupid” model predicts everything to be class 0, accuracy is 9990/10000 = **99.9** %

- The accuracy is misleading because the model does not detect any example in class 1

Classification -- Model evaluations

- Cost-sensitive measures

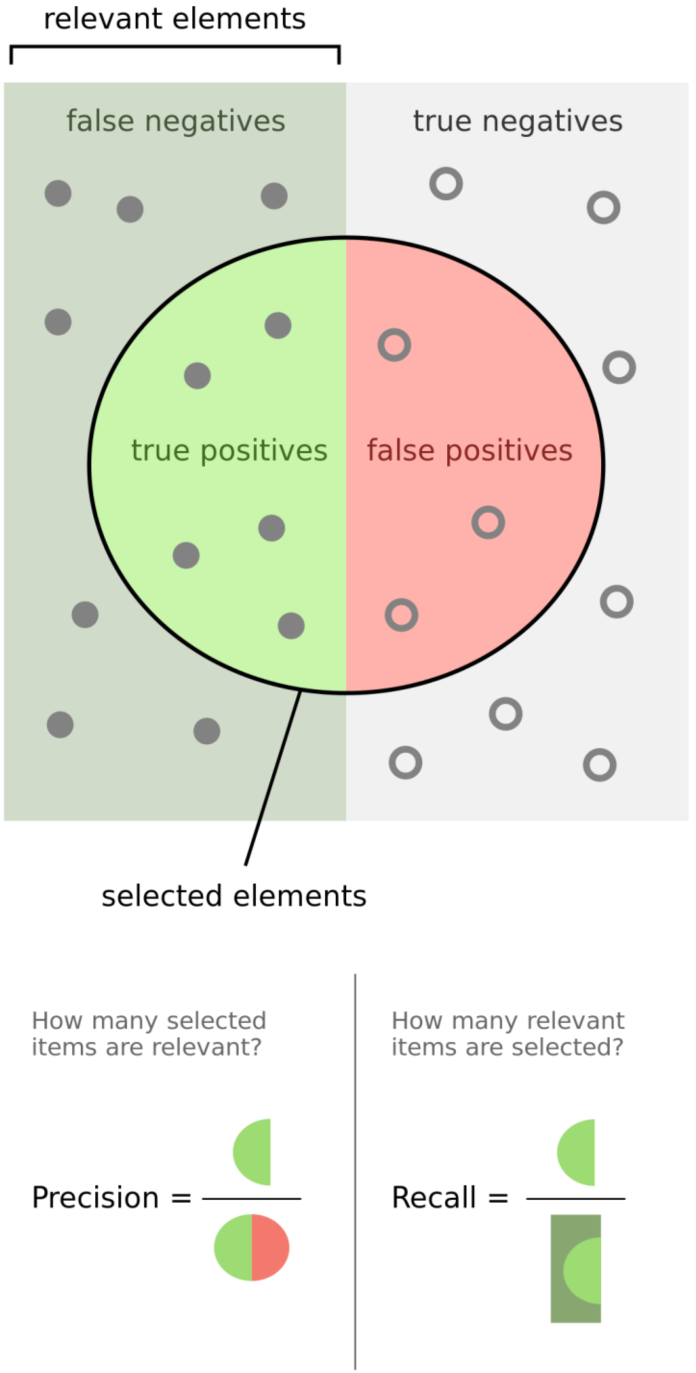
	Predicted Class		
Actual Class		Class = Yes	Class = No
	Class = Yes	a (TP)	b (FN)
	Class = No	c (FP)	d (TN)

$$\text{Precision (p)} = \frac{TP}{TP + FP} = \frac{a}{a + c}$$

$$\text{Recall (r)} = \frac{TP}{TP + FN} = \frac{a}{a + b}$$

$$\text{F - measure (F)} = \frac{2rp}{r + p} = \frac{2a}{2a + b + c}$$

Harmonic mean of Precision and Recall
(Why not just average?)



relevant elements

false negatives

true negatives

true positives

false positives

selected elements

How many selected items are relevant?

Precision =

How many relevant items are selected?

Recall =

How to understand

- A school is running a machine learning primary diabetes scan on all of its students
  - Diabetic (+) / Healthy (-)
  - False positive is just a false alarm
  - False negative
    - Prediction is healthy but is diabetic
    - Worst case among all 4 cases

- Accuracy
  - Accuracy = (TP+TN)/(TP+FP+FN+TN)
  - How many students did we correctly label out of all the students?

How to understand (cont.)

- A school is running a machine learning primary diabetes scan on all of its students
  - Diabetic (+) / Healthy (-)
  - False positive is just a false alarm
  - False negative
    - Prediction is healthy but is diabetic
    - Worst case among all 4 cases

- Precision
  - Precision = TP/(TP+FP)
  - How many of those who we labeled as diabetic are actually diabetic?

How to understand (cont.)

- A school is running a machine learning primary diabetes scan on all of its students
  - Diabetic (+) / Healthy (-)
  - False positive is just a false alarm
  - False negative
    - Prediction is healthy but is diabetic
    - Worst case among all 4 cases

- Recall (sensitivity)
  - Recall = TP/(TP+FN)
  - Of all the people who are diabetic, how many of those we correctly predict?

F1 score (F-Score / F-Measure)

- F1 Score = 2*(Recall * Precision) / (Recall + Precision)
- Harmonic mean (average) of the precision and recall
- F1 Score is best if there is some sort of balance between precision (p) & recall (r) in the system. Oppositely F1 Score isn’t so high if one measure is improved at the expense of the other.
- For example, if P is 1 & R is 0, F1 score is 0.

Which to choose

- Accuracy
  - A great measure
  - But only when you have symmetric datasets (FN & FP counts are close)
  - Also, FN & FP have similar costs
- F1 score
  - If the cost of FP and FN are different
  - F1 is best if you have an uneven class distribution
- Recall
  - If FP is far better than FN or if the occurrence of FN is unaccepted/intolerable
  - Would like more extra FP (false alarms) over saving some FN
  - E.g. diabetes. We'd rather get some healthy people labeled diabetic over leaving a diabetic person labeled healthy
- Precision
  - Want to be more confident of your TP
  - E.g. spam emails. We'd rather have some spam emails in inbox rather than some regular emails in your spam box.

Example

- Given 30 human photographs, a computer predicts 19 to be male, 11 to be female. Among the 19 male predictions, 3 predictions are not correct. Among the 11 female predictions, 1 prediction is not correct.

	Predicted Class		
Actual Class		Male	Female
	Male	a = TP = 16	b = FN = 1
	Female	c = FP = 3	d = TN = 10

Example

	Predicted Class		
Actual Class		Male	Female
	Male	a = TP = 16	b = FN = 1
	Female	c = FP = 3	d = TN = 10

- Accuracy = (16 + 10) / (16 + 3 + 1 + 10) = 0.867
- Precision = 16 / (16 + 3) = 0.842
- Recall = 16 / (16 + 1) = 0.941
- F-measure = 2 (0.842)(0.941) / (0.842 + 0.941)
  = 0.889

Discussion

- “In a specific case, precision cannot be computed.” Is the statement true? Why?
- If the statement is true, can F-measure be computed in that case?

	a	b	c
a	TP	FN	FN
b	FP	TN	TN
c	FP	TN	TN

←Classified as

a: positive
b: negative
c: negative

- How about if b is positive, a and c are negative, or if c is positive, a and b are negative ?

Regression-Model Evaluation

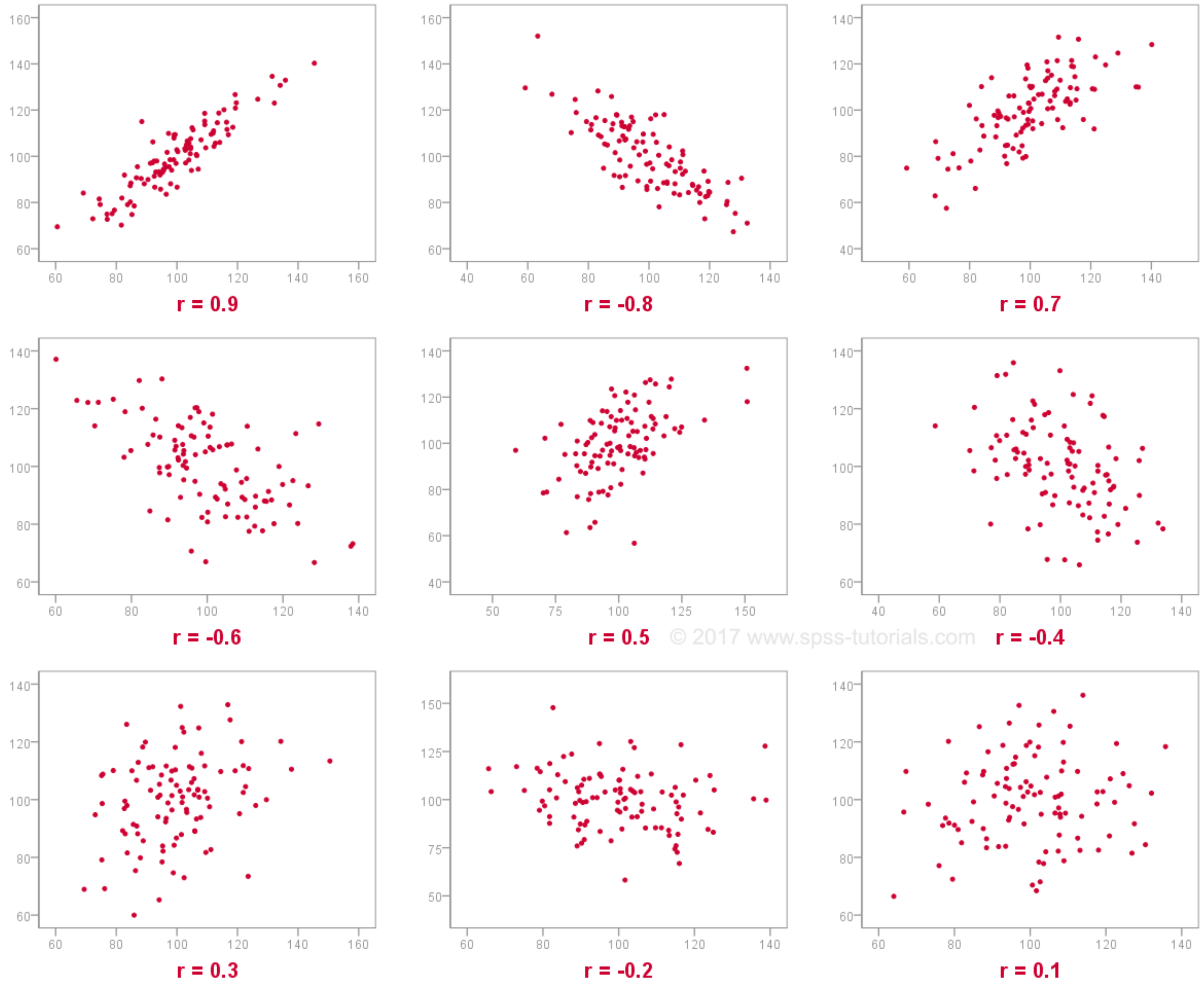
- Pearson correlation measures the linear association between continuous variables
  - Quantifies the degree to which a relationship between two variables can be described by a line.

$$r_{XY} = \frac{\sum_{i=1}^{n}(X_i - \overline{X})(Y_i - \overline{Y})}{\sqrt{\sum_{i=1}^{n}(X_i - \overline{X})^2}\sqrt{\sum_{i=1}^{n}(Y_i - \overline{Y})^2}}$$

- Remember the definition of cosine between vectors:

$$\cos(\theta) = \frac{\mathbf{A} \cdot \mathbf{B}}{\|\mathbf{A}\|\|\mathbf{B}\|} = \frac{\sum\limits_{i=1}^{n} A_i B_i}{\sqrt{\sum\limits_{i=1}^{n} A_i^2}\sqrt{\sum\limits_{i=1}^{n} B_i^2}},$$

Examples of Pearson correlation



r = 0.9 r = -0.8 r = 0.7

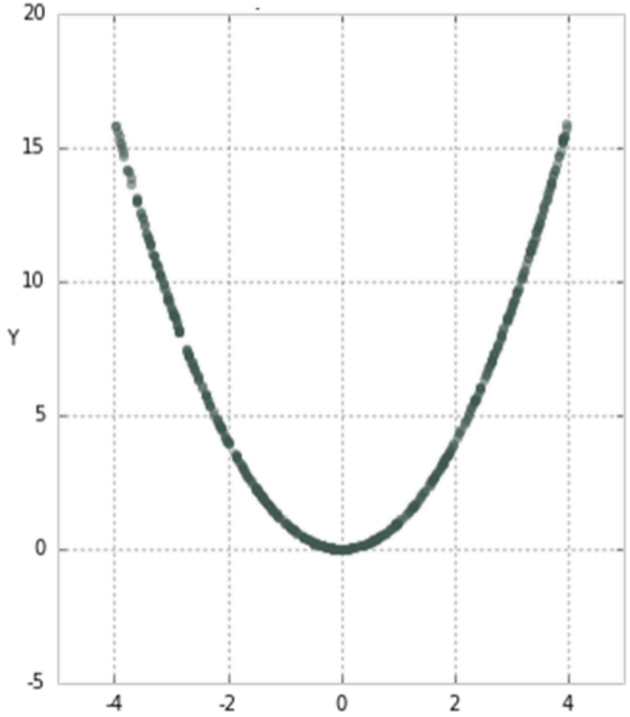
r = -0.6 r = 0.5 r = -0.4

© 2017 www.spss-tutorials.com

r = 0.3 r = -0.2 r = 0.1

Limitation

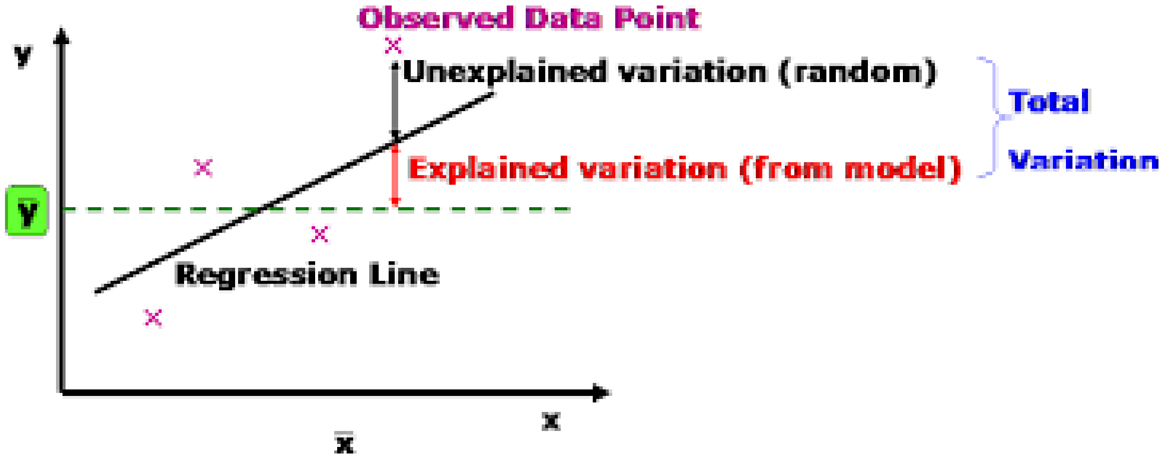
- Only linear correlation can be detected.
- Clearly, there are some relationship between X and Y, but the correlation is only 0.02.



Coefficient of determination

- Coefficient of determination (R^2) is the proportion of the variance in the dependent variable that is predictable from the independent variable.

- It measures how much of the residue can be explained by the regression line



Regression -- Model evaluation

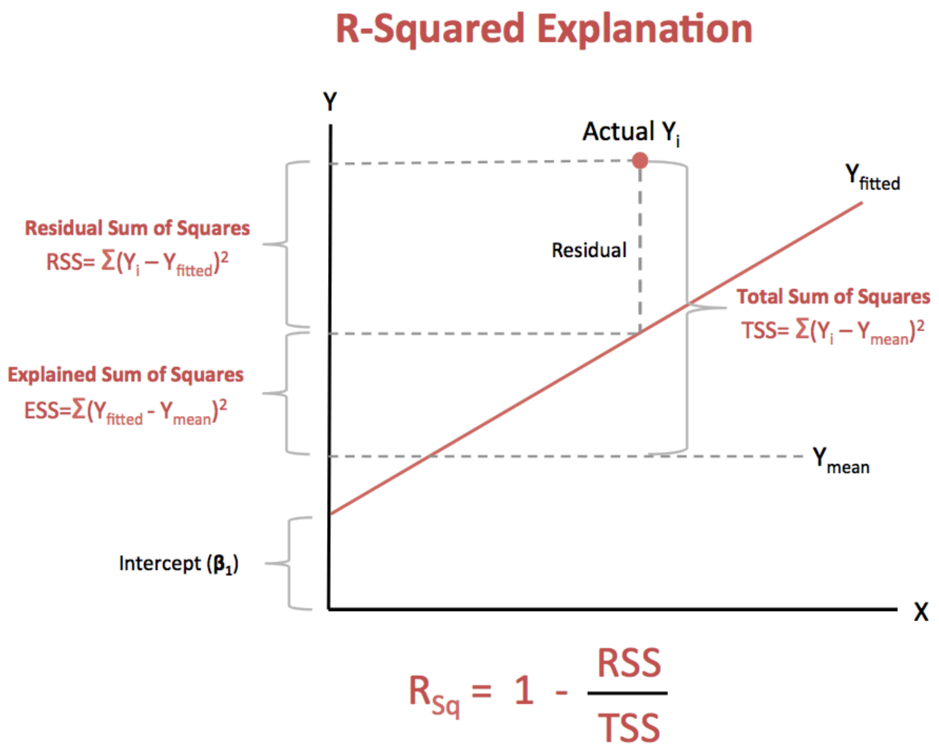
- $R^2 = \dfrac{explained\ variance}{total\ variance}$

- Total variance: $SS_{\text{tot}} = \sum_i (y_i - \bar{y})^2$

- Explained variance: $SS_{\text{reg}} = \sum_i (f_i - \bar{y})^2$

- Or, it can be computed as:

$$R^2 \equiv 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}} \quad \text{where} \quad SS_{\text{res}} = \sum_i (y_i - f_i)^2 = \sum_i e_i^2$$

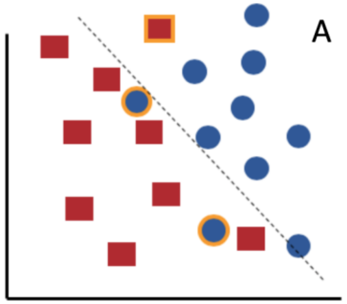


Model Selections

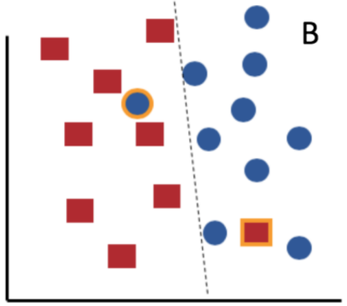
Minimize the error rate?

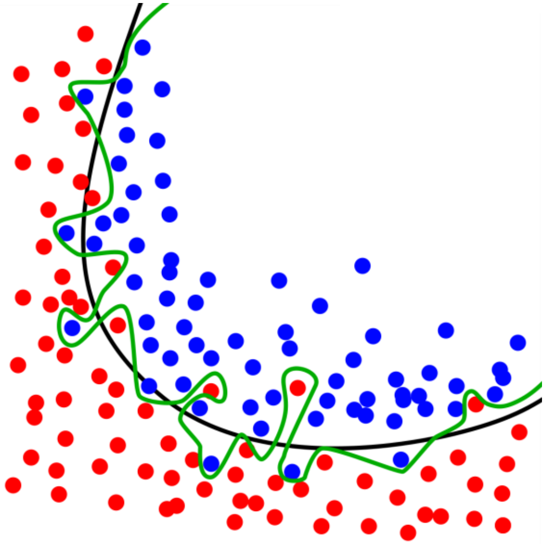
- Given a data set S
- Error rate = $\frac{\#\text{ of Errors}}{\#\text{ of Total Samples}}$
- Accuracy = 1 - Error rate

Error rate = $\frac{3}{19}$



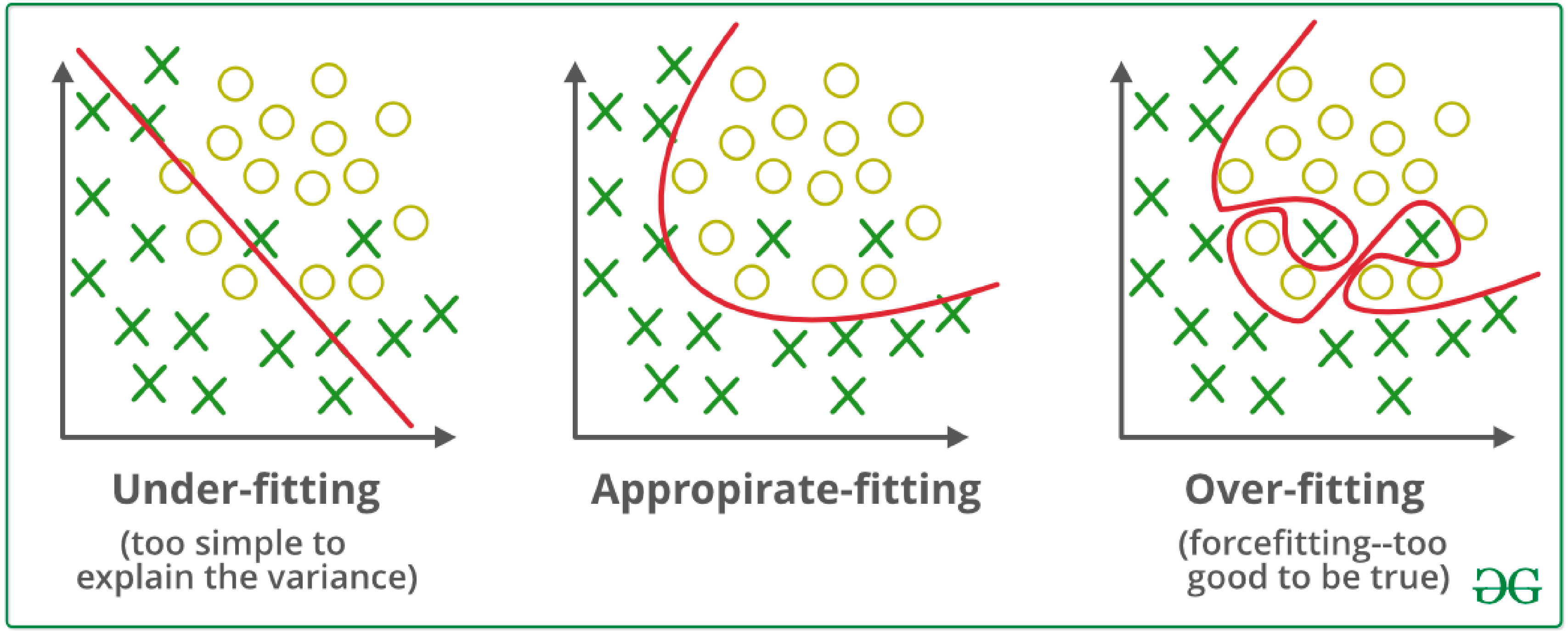
Error rate = $\frac{2}{19}$





https://malware.news/uploads/default/original/3X/6/d/6df12e50b7f97cdba92697ce164cbe4a5502a349.png
https://upload.wikimedia.org/wikipedia/commons/thumb/1/19/Overfitting.svg/1200px-Overfitting.svg.png

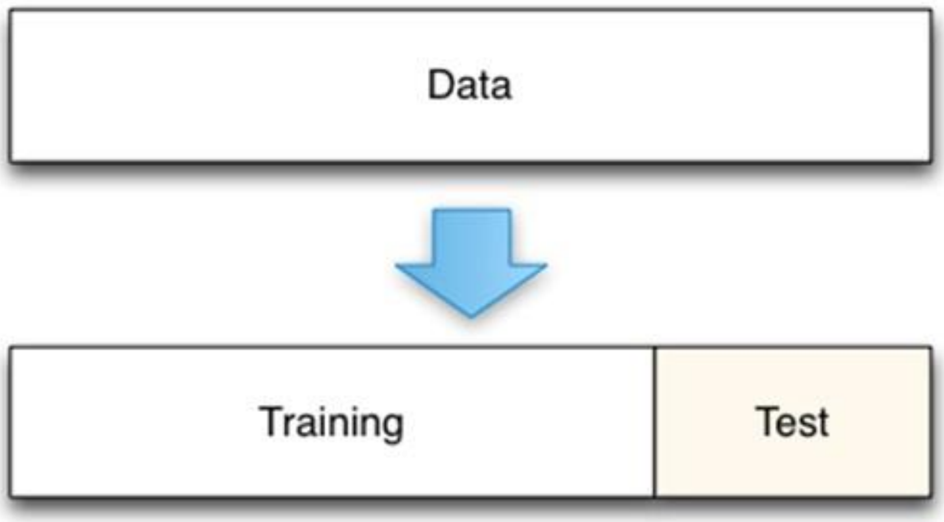
Fitting


Under-fitting
(too simple to explain the variance)
Appropirate-fitting
Over-fitting
(forcefitting--too good to be true)

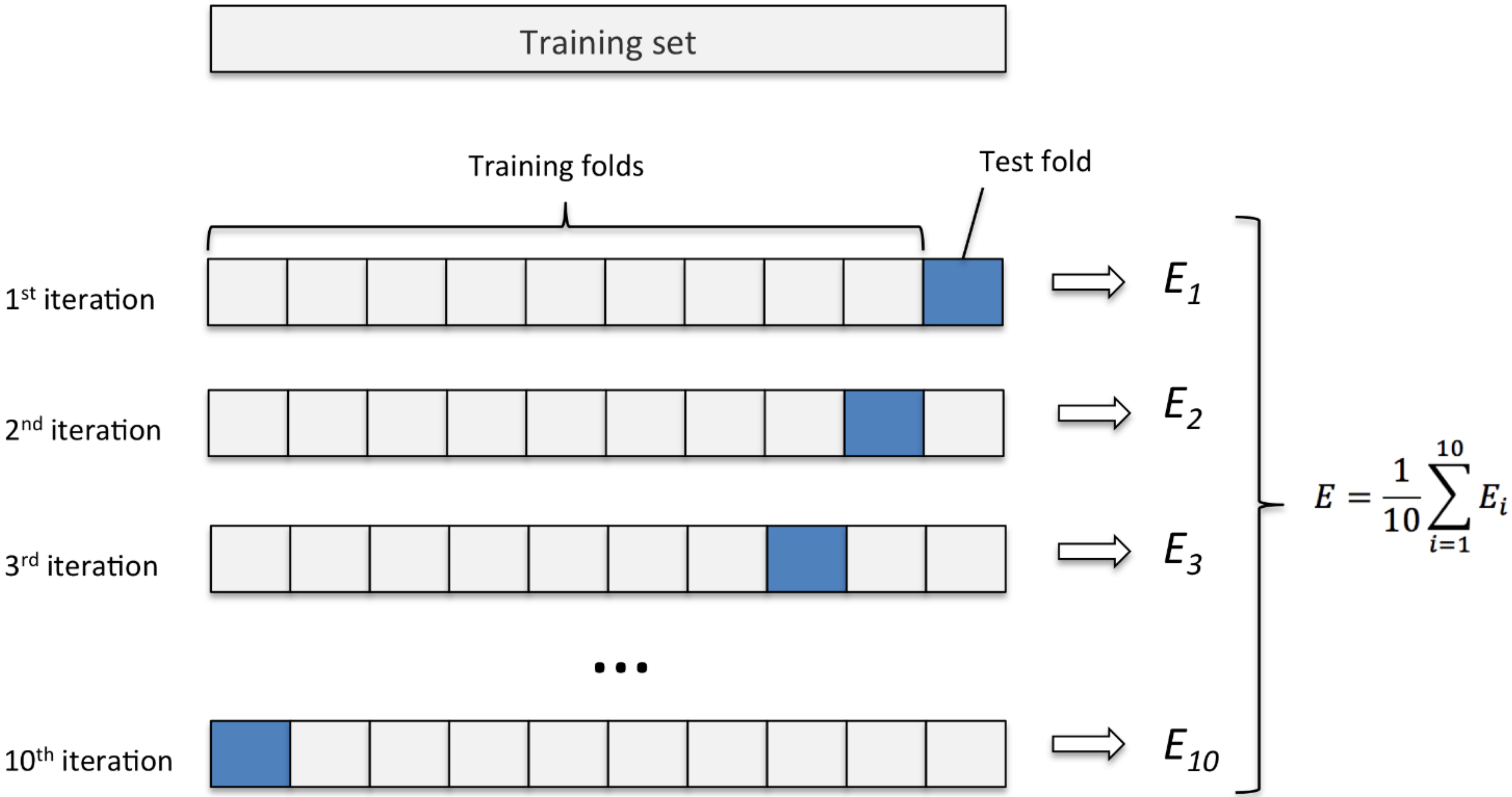
https://media.geeksforgeeks.org/wp-content/cdn-uploads/20190523171258/overfitting_2.png

Split training and test

- Split dataset to training and test
- Train models on training dataset
- The evaluation of the model is the error on test dataset
- Might overfit the training dataset

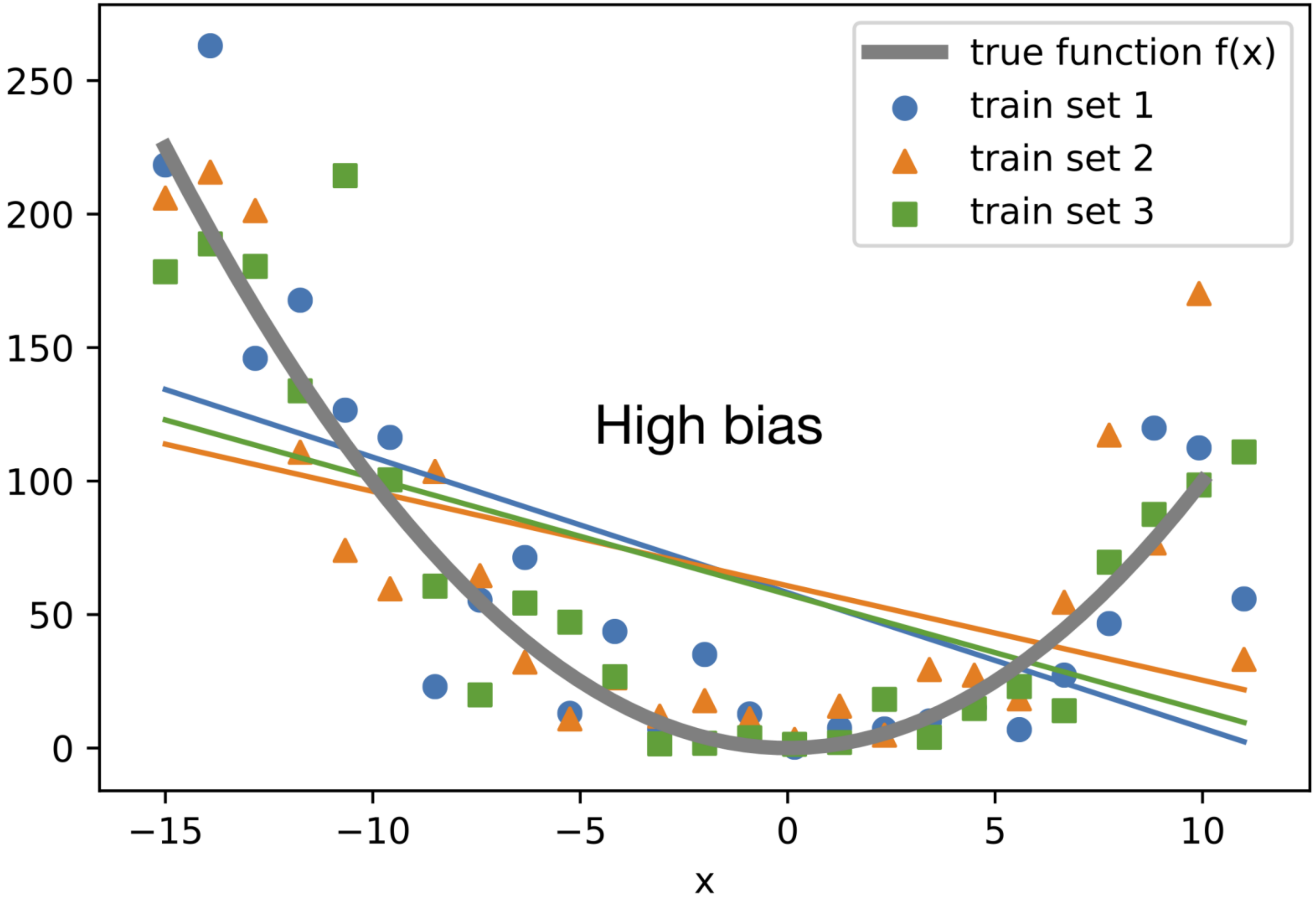


Cross validation

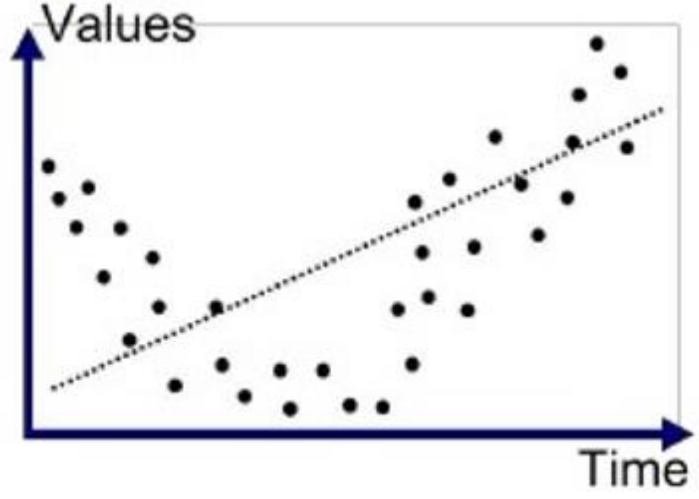


Bias

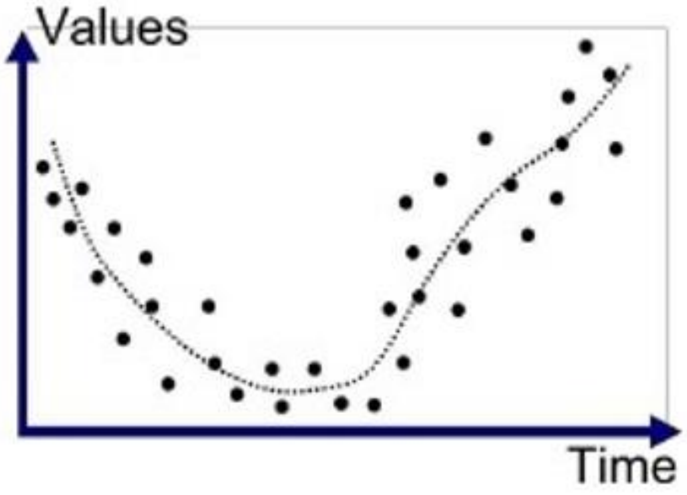
$$\text{Bias} = E[\hat{\theta}] - \theta.$$



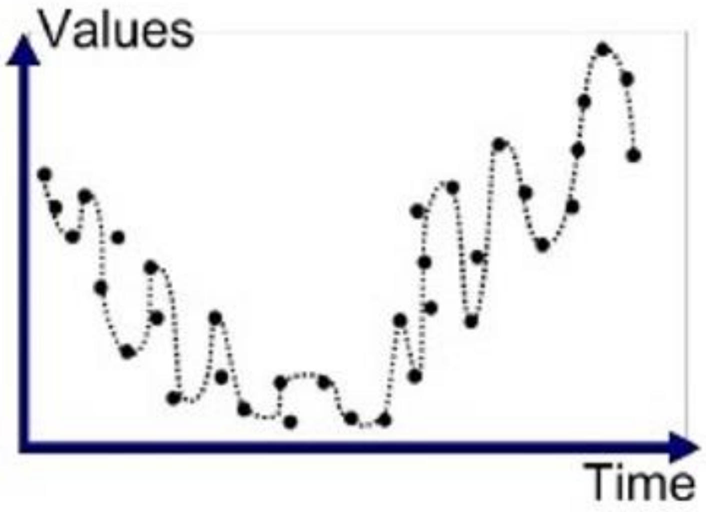
Underfitting



Underfitted



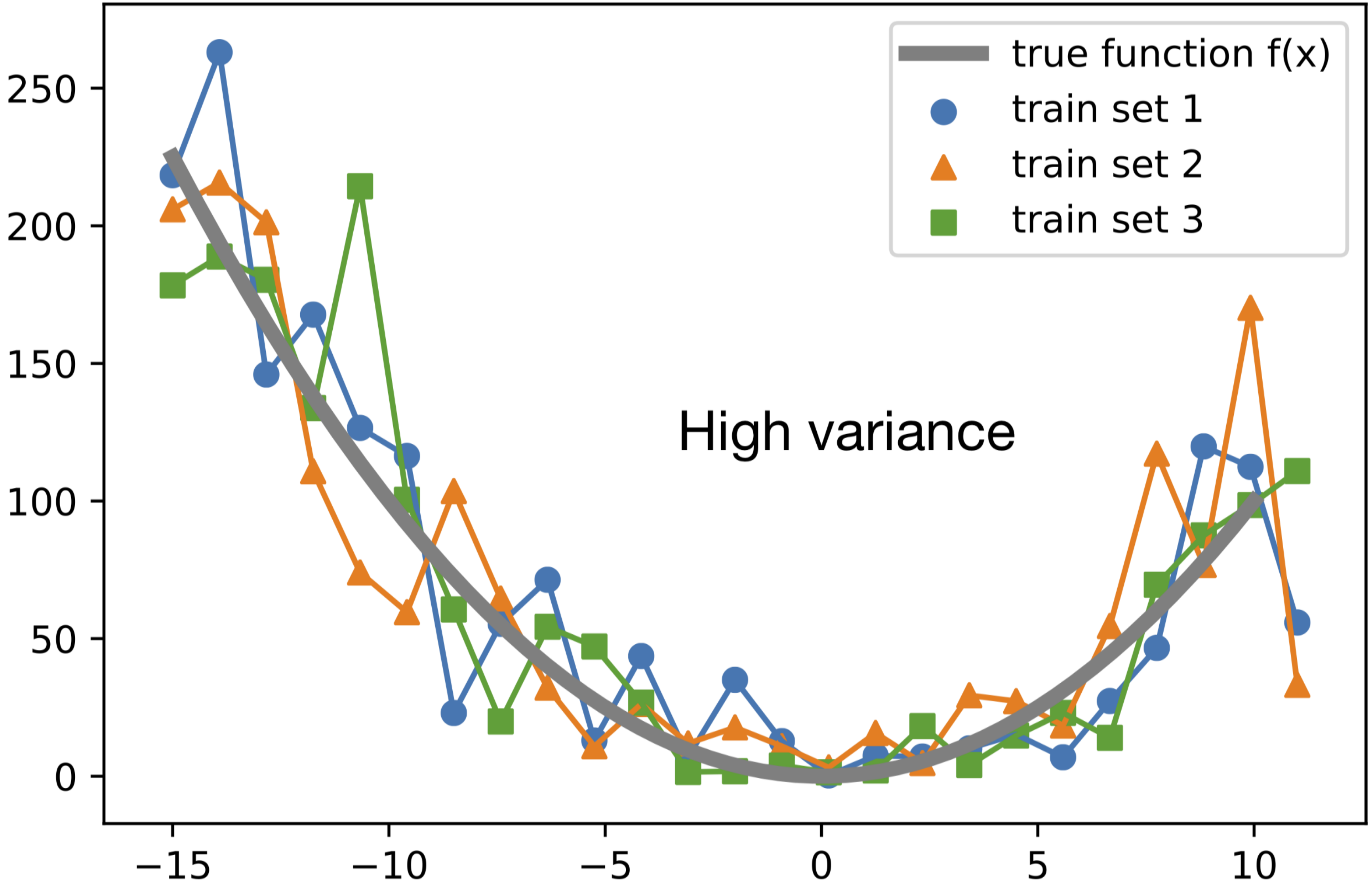
Good Fit/Robust



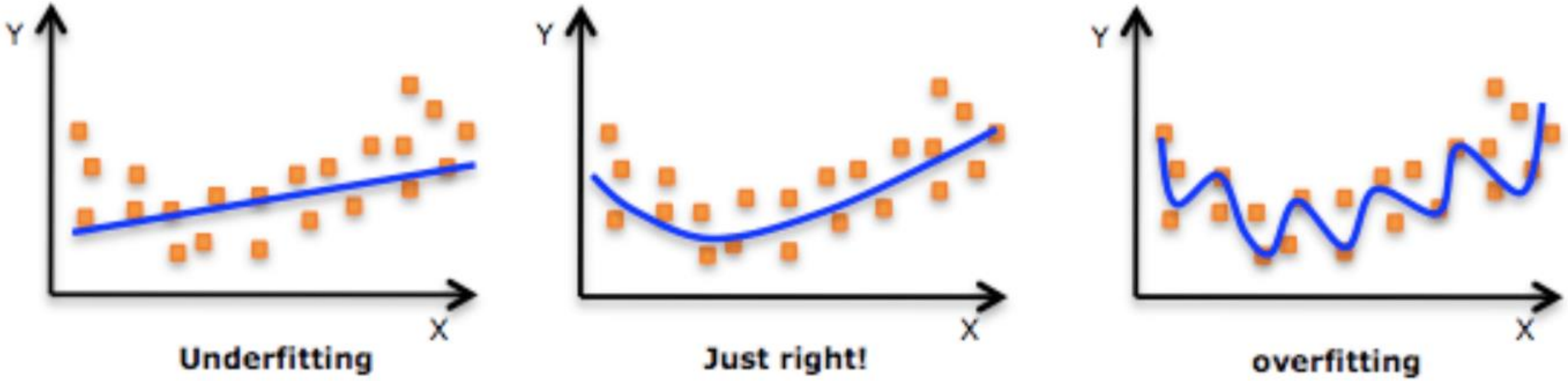
Overfitted

Variance

$$\mathrm{Var}(\hat{\theta}) = E[(E[\hat{\theta}] - \hat{\theta})^2].$$



Overfitting



Bias-variance decomposition

$$S = (\overset{\text{True value}}{y} - \overset{\text{Estimated value}}{\hat{y}})^2$$

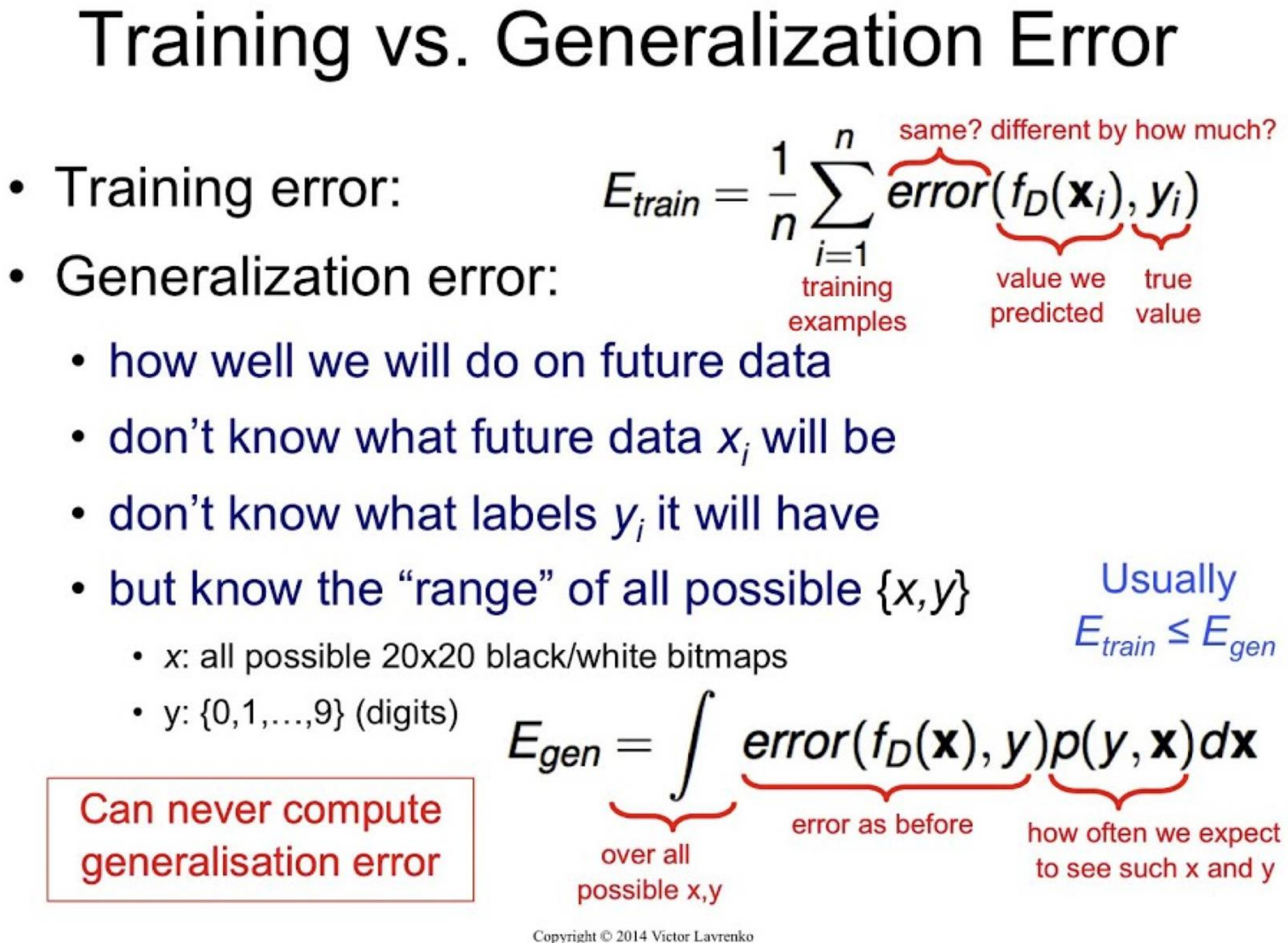
$$\begin{aligned}(y - \hat{y})^2 &= (y - E[\hat{y}] + E[\hat{y}] - \hat{y})^2 \\ &= (y - E[\hat{y}])^2 + (E[\hat{y}] - y)^2 + 2(y - E[\hat{y}])(E[\hat{y}] - \hat{y}).\end{aligned}$$

$$\begin{aligned}E[2(y - E[\hat{y}])(E[\hat{y}] - \hat{y})] &= 2E[(y - E[\hat{y}])(E[\hat{y}] - \hat{y})] \\ &= 2(y - E[\hat{y}])E[(E[\hat{y}] - \hat{y})] \\ &= 2(y - E[\hat{y}])(E[E[\hat{y}]] - E[\hat{y}]) \\ &= 2(y - E[\hat{y}])(E[\hat{y}] - E[\hat{y}]) \\ &= 0.\end{aligned}$$

$$E[S] = E[(y - \hat{y})^2]$$

$$\begin{aligned}E[(y - \hat{y})^2] &= (y - E[\hat{y}])^2 + E[(E[\hat{y}] - \hat{y})^2] \\ &= [\text{Bias}]^2 + \text{Variance}.\end{aligned}$$

Can be understood by replacing y and $\hat{y}$ with model parameters θ and $\hat{\theta}$



Training vs. Generalization Error

- Training error:

$$E_{train} = \frac{1}{n}\underset{\text{training examples}}{\sum_{i=1}^{n}} \overbrace{error}^{\text{same? different by how much?}}(\underbrace{f_D(\mathbf{x}_i)}_{\text{value we predicted}}, \underbrace{y_i}_{\text{true value}})$$

- Generalization error:
  - how well we will do on future data
  - don't know what future data x_i will be
  - don't know what labels y_i it will have
  - but know the "range" of all possible $\{x,y\}$
    - x: all possible 20x20 black/white bitmaps
    - y: {0,1,…,9} (digits)

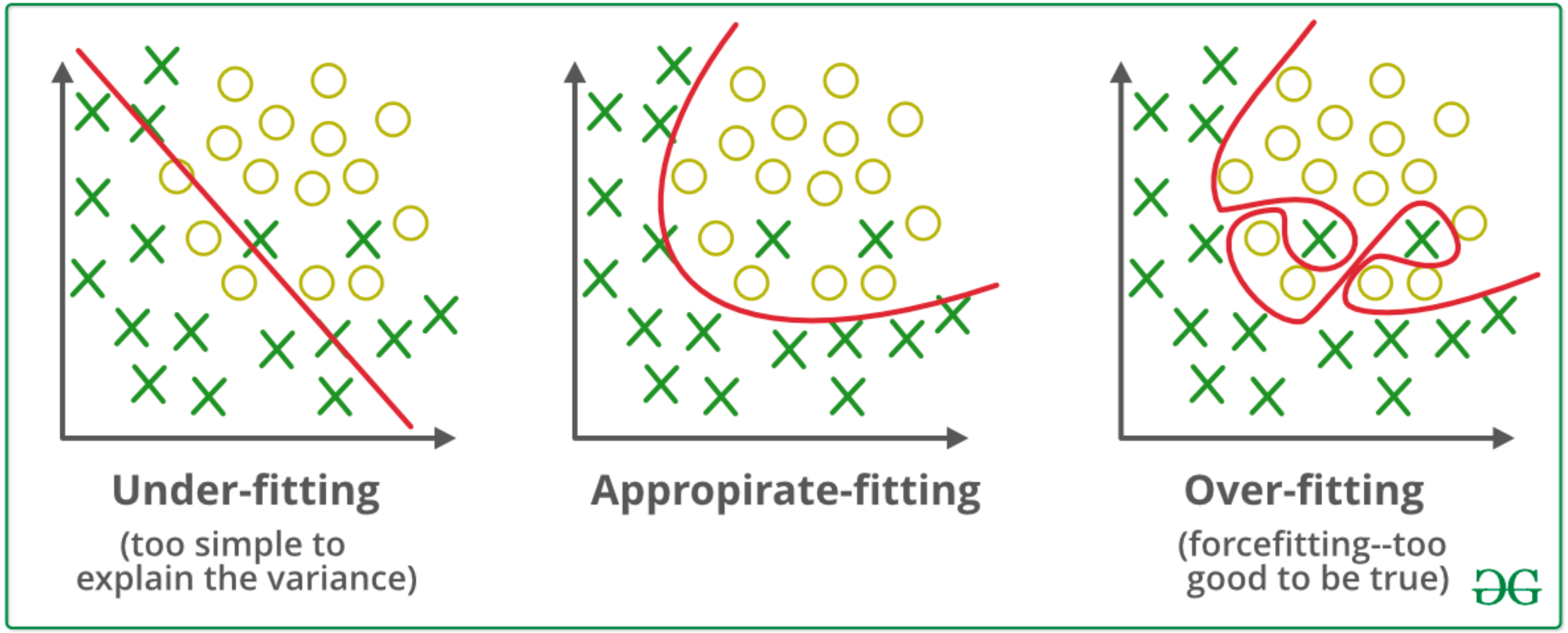
Usually $E_{train} \leq E_{gen}$

$$E_{gen} = \underbrace{\int}_{\text{over all possible x,y}} \underbrace{error(f_D(\mathbf{x}), y)}_{\text{error as before}}\underbrace{p(y,\mathbf{x})}_{\text{how often we expect to see such x and y}}d\mathbf{x}$$

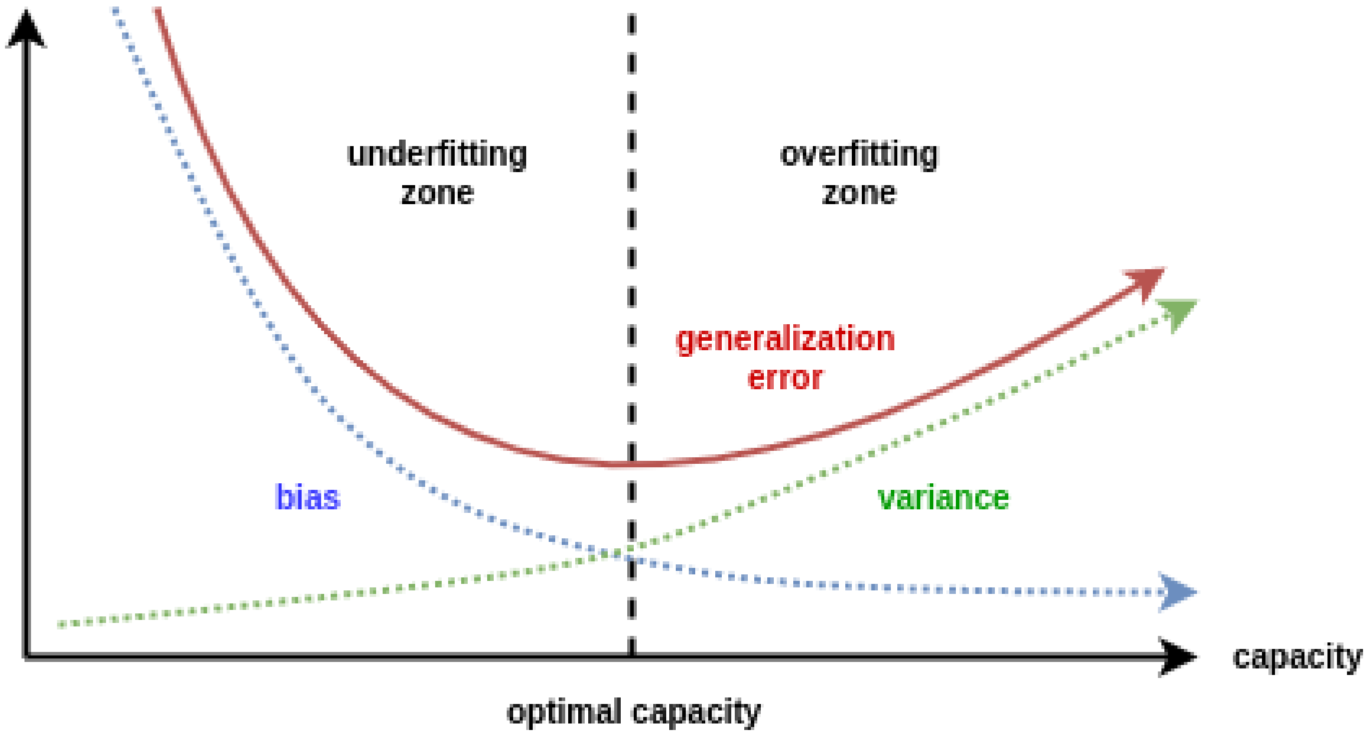
Can never compute generalisation error

Generalization

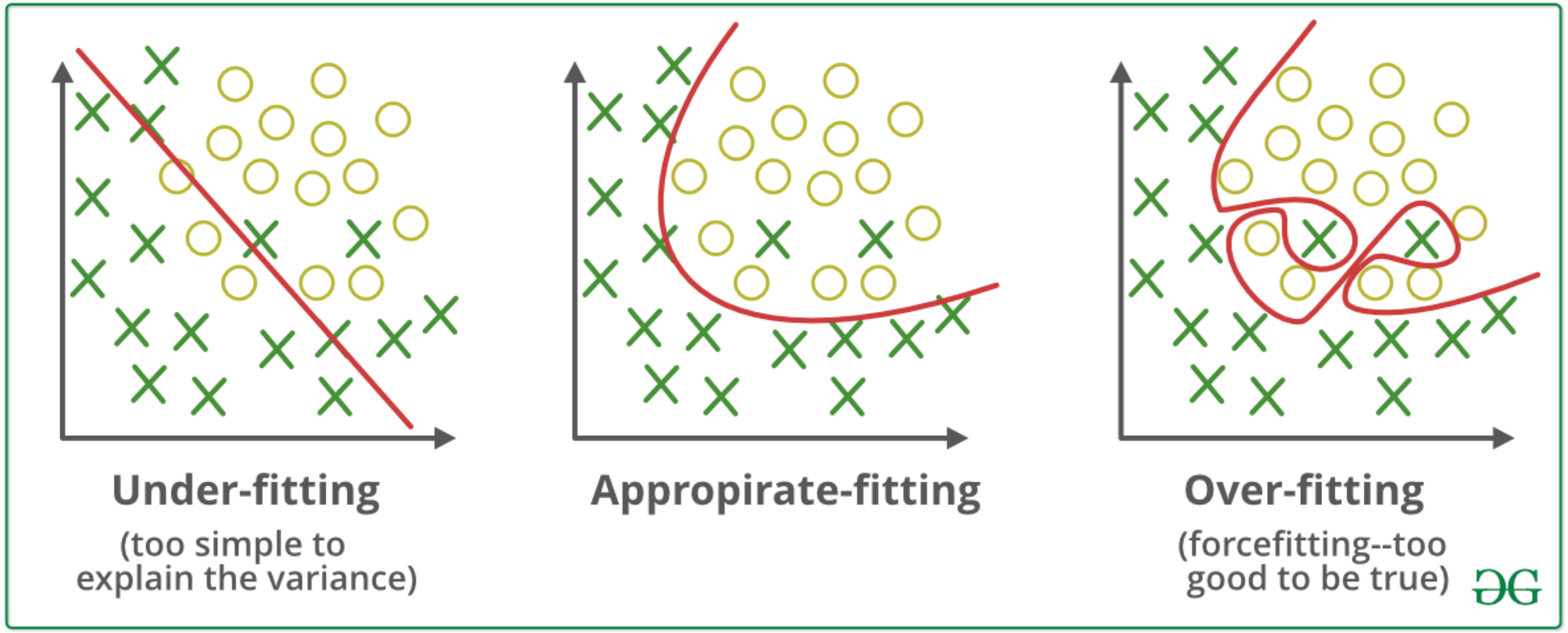
- Observations:
  - The best hypothesis on the sample may not be the best overall
  - Complex rules (very complex separation surfaces) can be poor predictors
  - trade-off: complexity of hypothesis set vs sample size (underfitting/overfitting)


Under-fitting
(too simple to explain the variance)
Appropirate-fitting
Over-fitting
(forcefitting--too good to be true)

Balance bias-variance trade-off

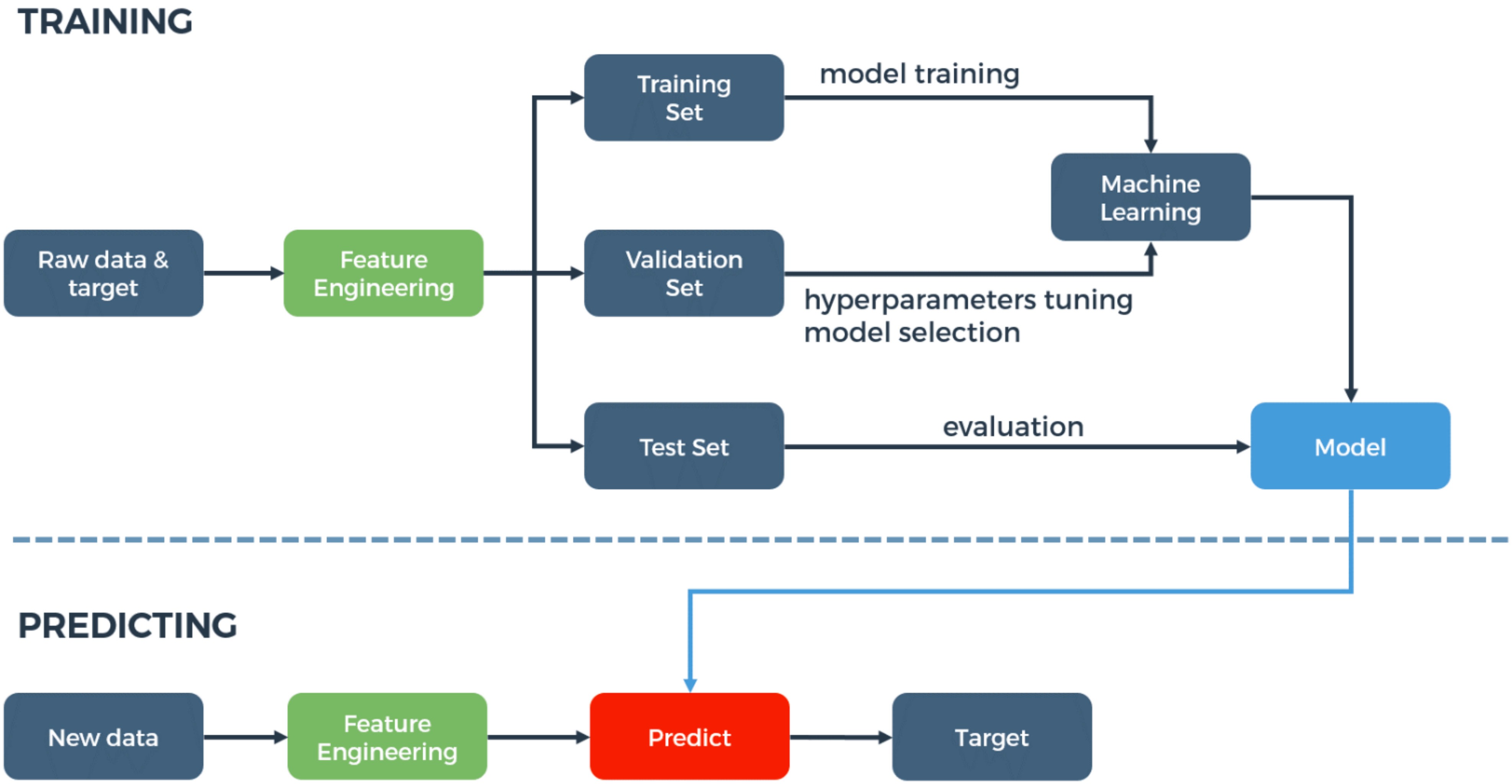


Learning ≠ Fitting


Under-fitting
(too simple to explain the variance)
Appropirate-fitting
Over-fitting
(forcefitting--too good to be true)

- Notion of simplicity/complexity
- How to define complexity
- Model selection

Machine Learning Process

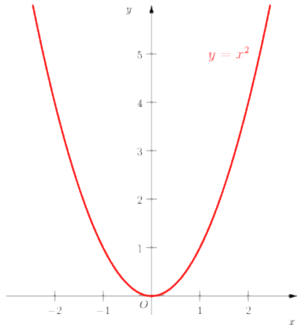


https://techblog.cdiscount.com/assets/images/DataScience/automl/ML_process.png

Problem Formulation

Problem Definition

- Spaces:
  - Input space (feature space) X, output space (labeled space) Y
- Loss function: $L: Y \times Y \to \mathbb{R}$
  - $L(\hat{y}, y)$: loss of predicting $\hat{y}$ when the true output is y
  - Binary classification: $L(\hat{y}, y) = 1_{\hat{y} \neq y}$
  - Regression: $L(\hat{y}, y) = \frac{1}{2}(\hat{y} - y)^2$



- Hypothesis set: $H \subseteq Y^X$(mappings from X to Y)
  - Space of possible models, e.g. all linear functions
  - Depends on feature structure and prior knowledge about the problem

Set-up

- Training data:
  - Sample S of size N drawn i.i.d. from $\mathrm{X} \times Y$ according to distribution D:
$$S = \{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$$
- Objective:
  - Find hypothesis $h \in H$ with small generalization error

- Generalization error
$$R(h) = \mathbb{E}_{(x,y)\sim D}[L(h(x), y)]$$
- Empirical error
$$\hat{R}(h) = \frac{1}{N}\sum_{i=1}^{N} L(h(x_i), y_i)$$

Model Selection

- For any $h \in H$

$$R(h) - \min_{h'} R(h') = \overbrace{\left(R(h) - \min_{h' \in H} R(h')\right)}^{\text{estimation}} + \overbrace{\left(\min_{h' \in H} R(h') - \min_{h'} R(h')\right)}^{\text{approximation}}$$

  - Approximation: only depends on H
  - Estimation
    - Recall $R(h) = \mathbb{E}_{(x,y)\sim D}[L(h(x), y)]$
    - Empirical error: $\hat{R}(h) = \frac{1}{N}\sum_{i=1}^{N} L(h(x_i), y_i)$
- Empirical risk minimization:

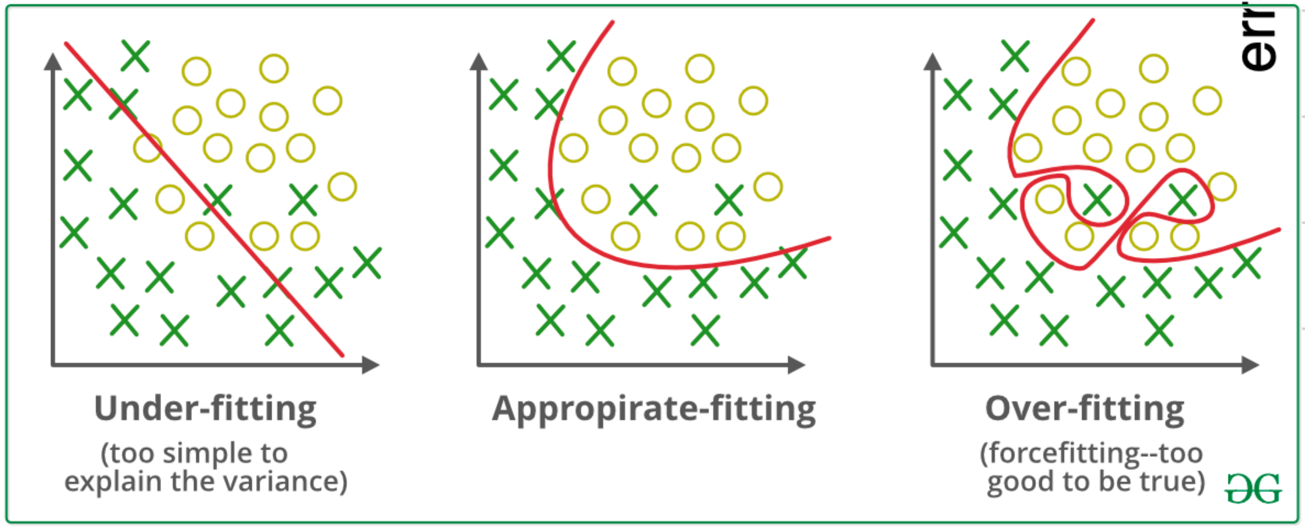
$$h = \text{argmin}_{h \in H} \hat{R}(h)$$

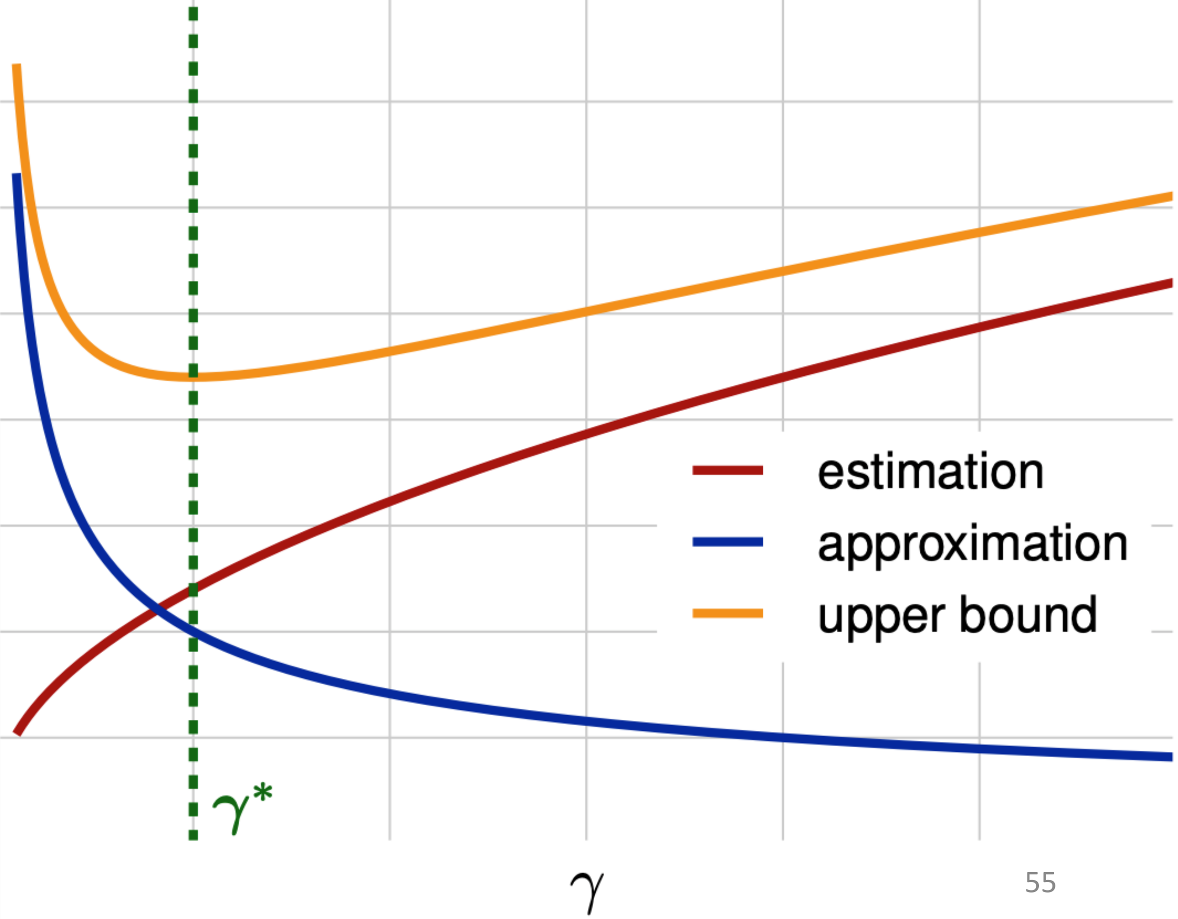
Model Selection

estimation

approximation

- $R(h) - \min_{h'} R(h') = \left(R(h) - \min_{h' \in H} R(h')\right) + \left(\min_{h' \in H} R(h') - \min_{h'} R(h')\right)$
- ERM $h = \text{argmin}_{h \in H} \hat{R}(h)$

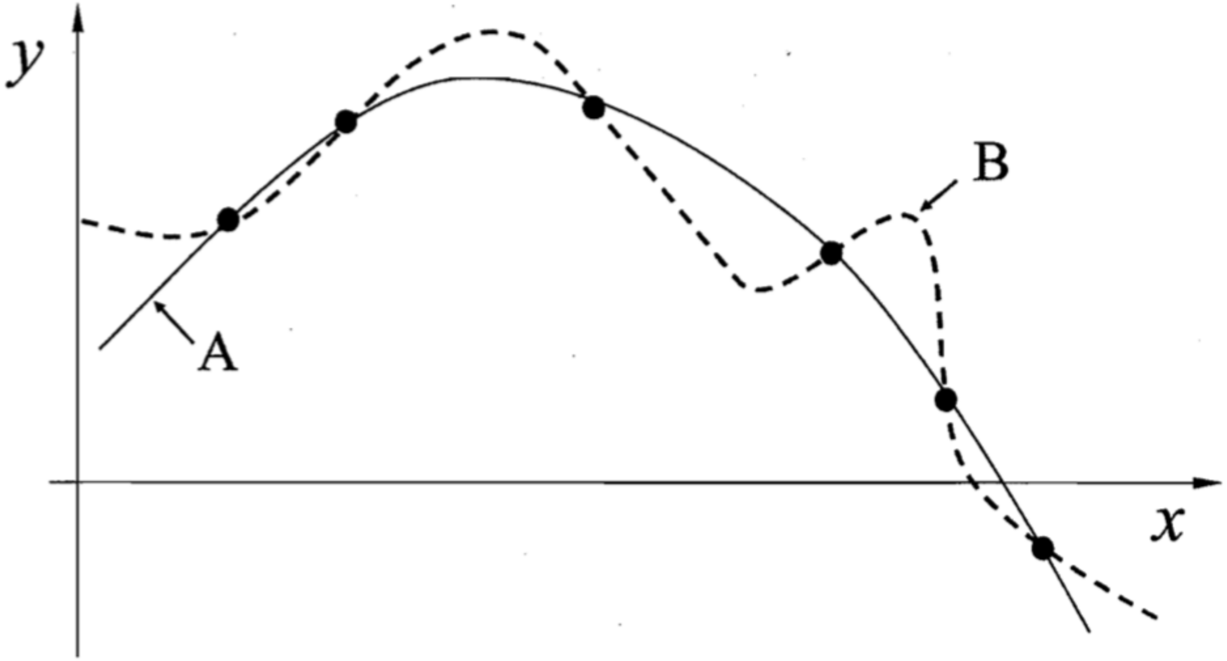

Under-fitting
(too simple to explain the variance)
Appropirate-fitting
Over-fitting
(forcefitting--too good to be true)
∂G



Principle of Occam’s Razor

Suppose there exist two explanations for an occurrence.

The one that requires the least assumptions is usually correct.



存在多条曲线与有限样本训练集一致

Figure credit: Zhihua Zhou

Regularization

- Recall empirical risk minimization(ERM):

$$h = \text{argmin}_{h \in H} \hat{R}(h)$$

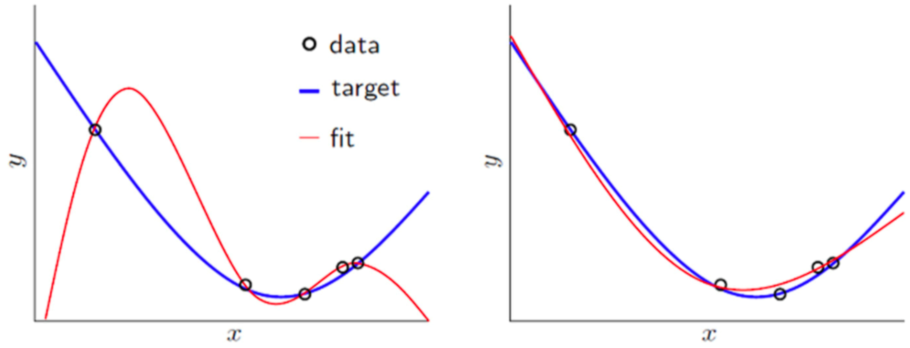
The above equation can be over-optimized.

- Regularization-based algorithms

$$h = \text{argmin}_{h \in H} \hat{R}(h) + \lambda \Omega(h)$$

regularization parameter

Complexity of h



(a) without regularization

(b) with regularization

Figure credit: Weinan Zhang

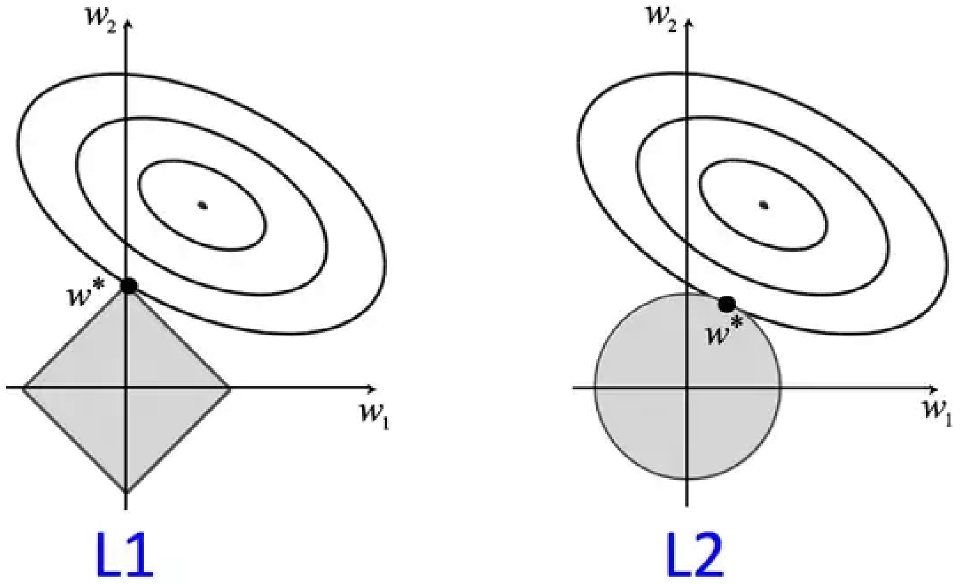
Regularization (cont.)

- E.g. L^2-norm (Ridge):

$$\Omega(h = ax + b) = a^2 + b^2$$

- E.g. L^1-norm (Lasso):

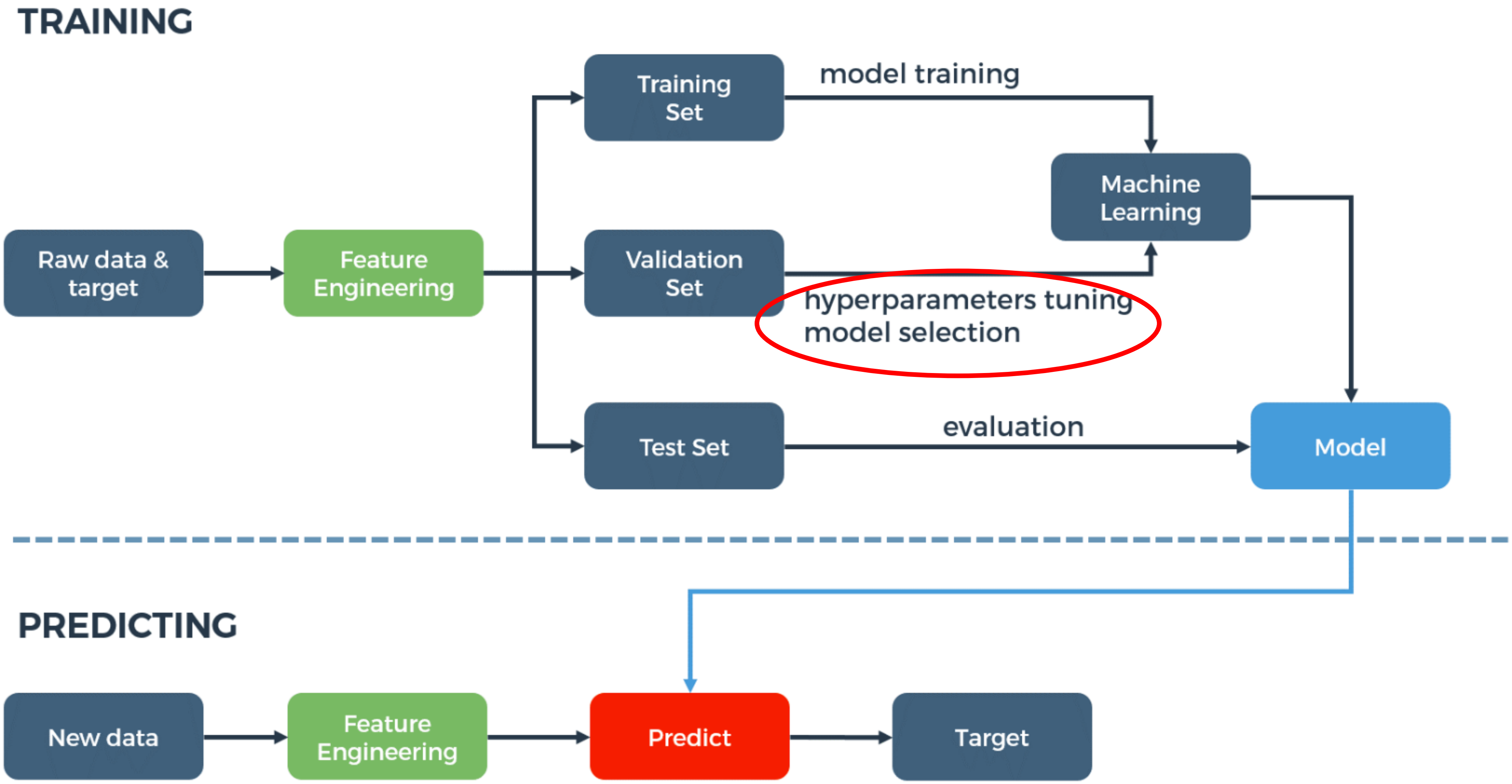
$$\Omega(h = ax + b) = |a| + |b|$$



L1 L2

https://miro.medium.com/max/1200/1*o6H_R3Do1zpch-3MZk_fjQ.png

Machine Learning Process



https://techblog.cdiscount.com/assets/images/DataScience/automl/ML_process.png

Generalization Error Bound

A Simple Case Study on Generalization Error

- Finite hypothesis set $\mathcal{F} = \{f_1, f_2, \dots, f_d\}$
- Theorem of generalization error bound:

  For any function $f \in \mathcal{F}$, with probability no less than $1 - \delta$, it satisfies

$$R(f) \leq \hat{R}(f) + \epsilon(d, N, \delta)$$

  where

$$\epsilon(d, N, \delta) = \sqrt{\frac{1}{2N}\left(\log d + \log \frac{1}{\delta}\right)}$$

  - *N*: number of training instances
  - *d:* number of functions in the hypothesis set

Section 1.7 in Dr. Hang Li's text book.

Lemma: Hoeffding Inequality

Let $X_1, X_2, \ldots, X_n$ be bounded independent random variables $X_i \in [a, b]$, the average variable *Z* is

$$Z = \frac{1}{n} \sum_{i=1}^{n} X_i$$

Then the following inequalities satisfy:

$$P(Z - \mathbb{E}[Z] \geq t) \leq \exp\left(\frac{-2nt^2}{(b-a)^2}\right)$$

$$P(\mathbb{E}[Z] - Z \geq t) \leq \exp\left(\frac{-2nt^2}{(b-a)^2}\right)$$

http://cs229.stanford.edu/extra-notes/hoeffding.pdf

Proof of Generalized Error Bound

- Assume the bounded loss function $L(y, f(x)) \in [0,1]$
- Based on Hoeffding Inequality, for $\epsilon > 0$, we have

$$P(R(f) - \hat{R}(f) \geq \epsilon) \leq \exp(-2N\epsilon^2)$$

- As $\mathcal{F} = \{f_1, f_2, \ldots, f_d\}$ is a finite set, it satisfies

$$\begin{aligned} P(\exists f \in \mathcal{F} : R(f) - \hat{R}(f) \geq \epsilon) &= P\Big(\bigcup_{f \in \mathcal{F}} \{R(f) - \hat{R}(f) \geq \epsilon\}\Big) \\ &\leq \sum_{f \in \mathcal{F}} P(R(f) - \hat{R}(f) \geq \epsilon) \\ &\leq d \exp(-2N\epsilon^2) \end{aligned}$$

Proof of Generalized Error Bound

- Equivalence statements

$$P(\exists f \in \mathcal{F} : R(f) - \hat{R}(f) \geq \epsilon) \leq d \exp(-2N\epsilon^2)$$

$$\Updownarrow$$

$$P(\forall f \in \mathcal{F} : R(f) - \hat{R}(f) < \epsilon) \geq 1 - d \exp(-2N\epsilon^2)$$

- Then setting

$$\delta = d \exp(-2N\epsilon^2) \quad \Leftrightarrow \quad \epsilon = \sqrt{\frac{1}{2N} \log \frac{d}{\delta}}$$

The generalized error is bounded with the probability

$$P(R(f) < \hat{R}(f) + \epsilon) \geq 1 - \delta$$

□

Generalization error bound revisit

- Finite hypothesis set $\mathcal{F} = \{f_1, f_2, \ldots, f_d\}$
- Theorem of generalization error bound:

  For any function $f \in \mathcal{F}$, with probability no less than $1 - \delta$, it satisfies

  $$R(f) \leq \hat{R}(f) + \epsilon(d, N, \delta)$$

  where

  $$\epsilon(d, N, \delta) = \sqrt{\frac{1}{2N}\Big(\log d + \log \frac{1}{\delta}\Big)}$$

  - *N*: number of training instances
  - *d:* number of functions in the hypothesis set

Summary

- The classification of machine learning
  - Supervised/unsupervised/reinforcement
- Supervised learning
  - Evaluation metrics for classification
    - Accuracy/Precision/Recall/F1 score
  - Evaluation metrics for regression
    - Pearson coefficient/coefficient of determination
  - Model selection: bias/variance/generalization
  - Machine learning process
  - Generalization error bound

Next Lecture

Linear Regression

Shuai Li

https://shuaili8.github.io

Questions?

https://shuaili8.github.io/Teaching/VE445/index.html