The Introduction To Artificial Intelligence

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The Introduction to Artificial Intelligence

- Part I Brief Introduction to AI & Different AI tribes
- Part II Knowledge Representation & Reasoning
- Part III AI GAMES and Searching
- Part IV Model Evaluation and Selection

Model Evaluation and Selection

- 1.1 Empirical Error and Overfitting
- 1.2 Evaluation Methods
- 1.3 Performance Measure
- 1.4 Summary

Model Evaluation and Selection

Solve two problems:
(1) How to make a model convincible?
(2) How to evaluate a model?

Model Evaluation and Selection

- 1.1 Empirical Error and Overfitting
- 1.2 Evaluation Methods
- 1.3 Performance Measure
- 1.4 Summary

1.1 Empirical Error and Overfitting

□ Definitions

Usually, if *m* samples totally, a model predict *a* samples incorrectly:

Error Rate: a/m, the proportion of wrong predictions;

Accuracy: 1- a/m, the proportion of right predictions.

Generally:

Error: the difference between the output of the model and the ground truth (real label).

Training Error/ Empirical Error: the error on training dataset.

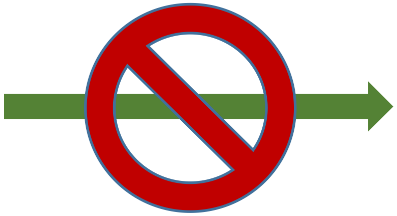
Generalization Error: the error on new data.

1.1 Empirical Error and Overfitting

Definitions

- Error Rate, Accuracy, Training error, Generalization error
- A best model:
  On training dataset: 0% Training error, 100% Accuracy,
  On new samples: 0% Generalization error, 100% Accuracy
- But:

0% Training error



0% Generalization error

1.1 Empirical Error and Overfitting

□ Overfitting and Underfitting

- Underfitting: A statistical model or a machine learning algorithm is said to have underfitting when it cannot capture the underlying trend of the data.

- In a nutshell, Underfitting refers to a model that can neither performs well on the training data nor generalize to new data.

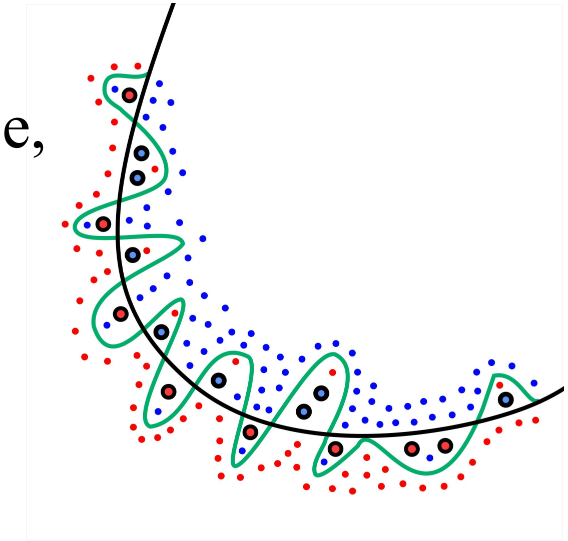
- Reasons for Underfitting:
  - High bias and low variance
  - The size of the training dataset used is not enough.
  - The model is too simple.
  - Training data is not cleaned and also contains noise in it.

1.1 Empirical Error and Overfitting

□ Overfitting and Underfitting

- Overfitting: In mathematical modeling, **overfitting** is “the production of an analysis that corresponds too closely or exactly to a particular set of data, and may therefore fail to fit to additional data or predict future observations reliably”.

- An overfitted model is a mathematical model that contains more parameters than can be justified by the data. In a mathematical sense, these parameters represent the degree of a polynomial. The essence of overfitting is to have unknowingly extracted some of the residual variation (i.e., the noise) as if that variation represented underlying model structure.



1.1 Empirical Error and Overfitting

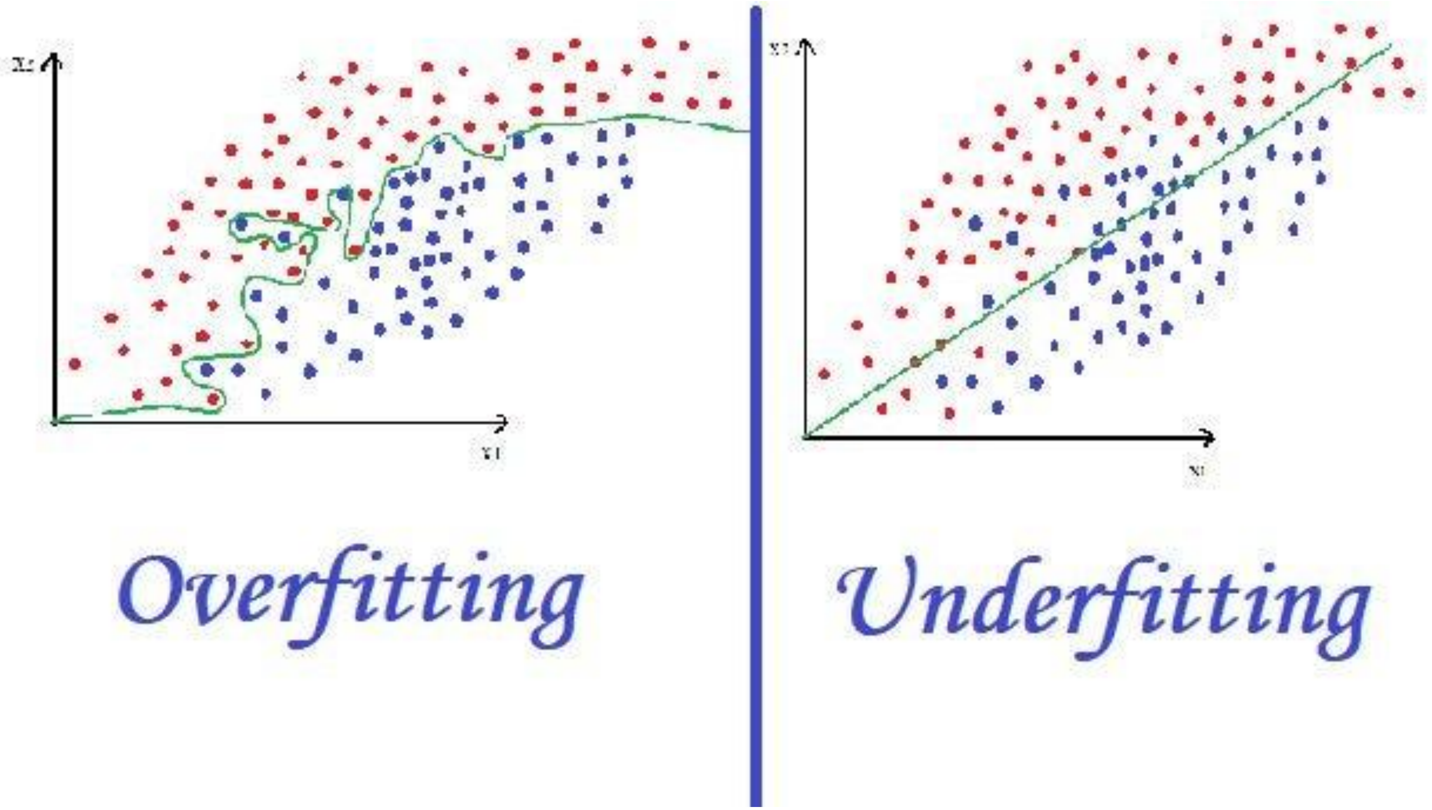
□ Overfitting and Underfitting

- In a nutshell, Overfitting is a problem where the evaluation of machine learning algorithms on training data is different from unseen data.

- Reasons for Overfitting are as follows:
  - High variance and low bias
  - The model is too complex
  - The size of the training data

1.1 Empirical Error and Overfitting

- Overfitting and Underfitting

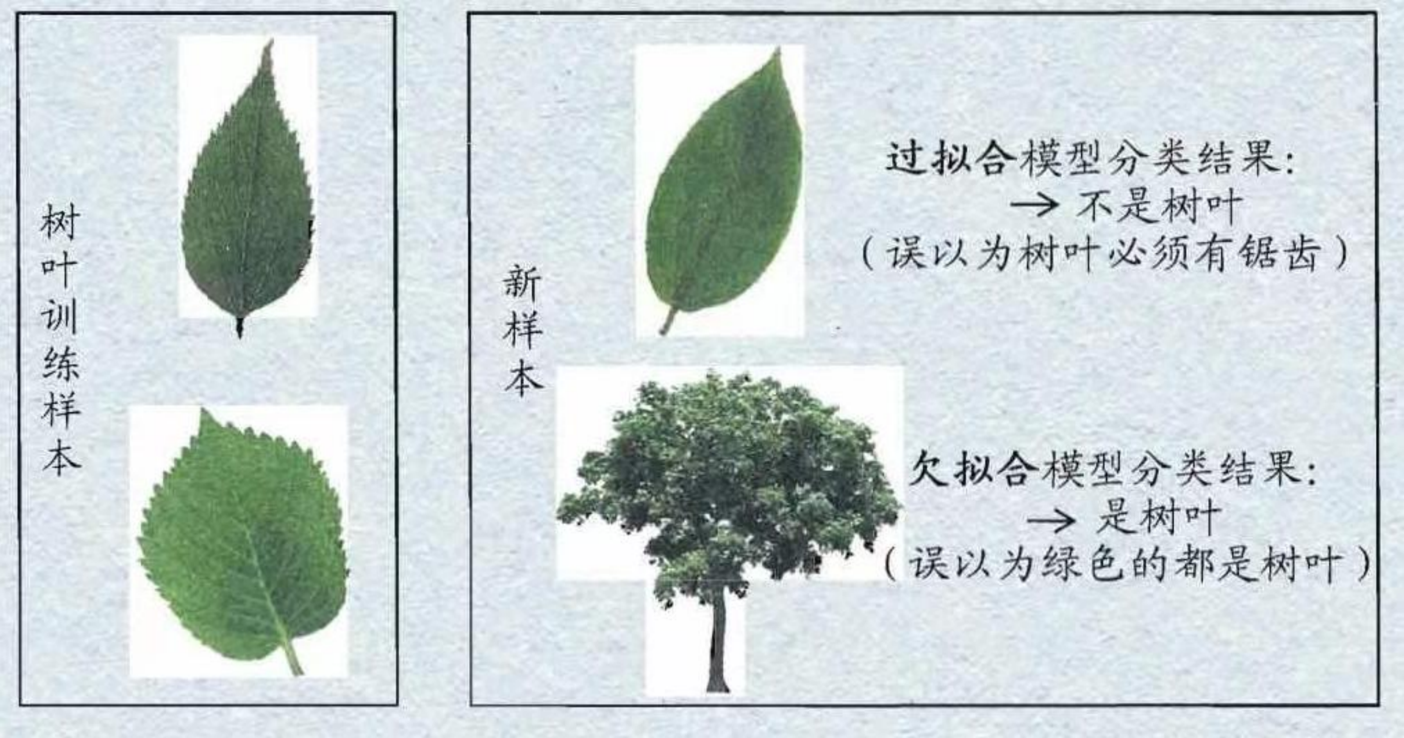


1.1 Empirical Error and Overfitting

Overfitting and Underfitting

Training samples

News samples



Overfitting

Underfitting

- Chapter 2 Model Evaluation and Selection, Machine Learning, Zhihua Zhou

1.1 Empirical Error and Overfitting

Overfitting and Underfitting

➢ Techniques to reduce underfitting:

- Increase model complexity
- Increase the number of features, performing feature engineering
- Remove noise from the data.
- Increase the number of epochs or increase the duration of training to get better results.

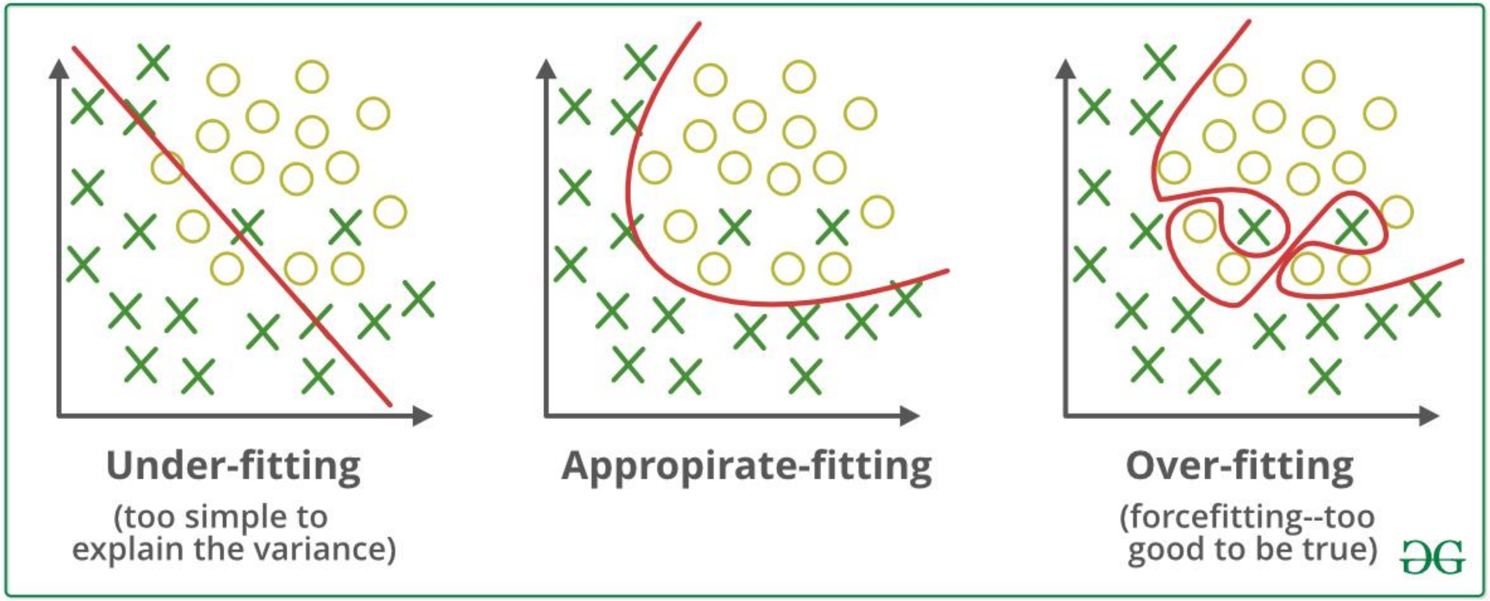
➢ Techniques to reduce overfitting:

- Increase training data.
- Reduce model complexity.
- Early stopping during the training phase (have an eye over the loss over the training period as soon as loss begins to increase stop training).
- Ridge Regularization and Lasso Regularization
- Use dropout for neural networks to tackle overfitting.

1.1 Empirical Error and Overfitting

□ Overfitting and Underfitting

- Overfitting: Good performance on the training data, poor generalization to other data.
- Underfitting: Poor performance on the training data and poor generalization to other data.


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

Model Evaluation and Selection

We already know:

What kind of model do we need?

→ Low training error, low generalization error, high Accuracy;

→ However, many methods could be utilized for one problem with different parameters.

→ how to select a model?

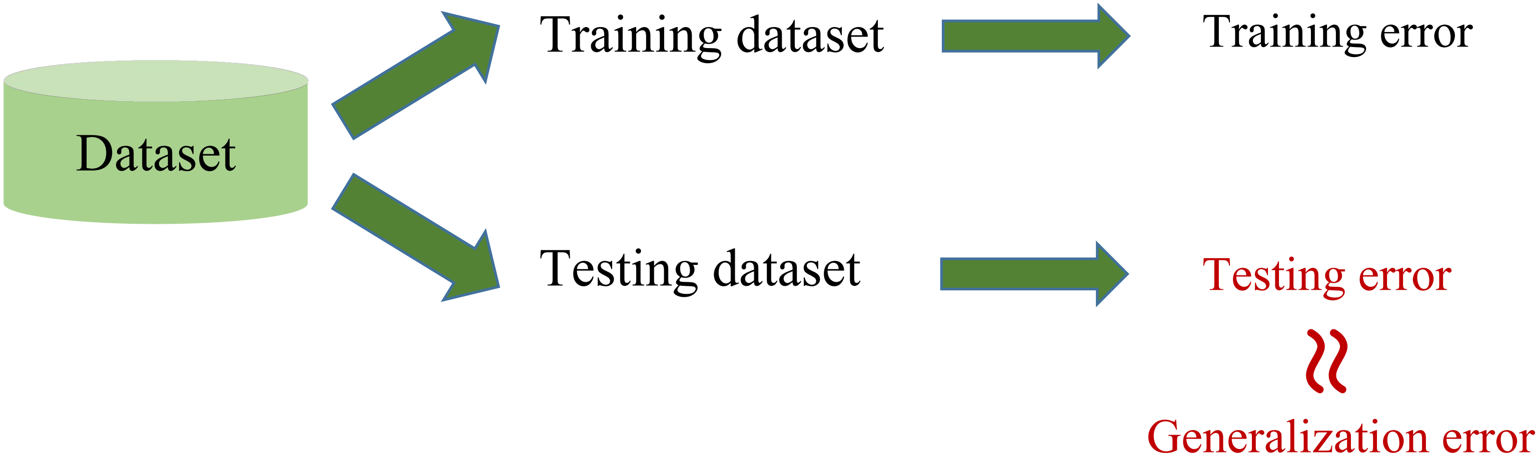
Model Evaluation and Selection

- 1.1 Empirical Error and Overfitting
- 1.2 Evaluation Methods
- 1.3 Performance Measure
- 1.4 Summary

1.2 Evaluation Methods

Evaluation Methods

- A model with low training error, low generalization error, high accuracy;
- How to compute generalization error?



Dataset

Training dataset

Training error

Testing dataset

Testing error

≈

Generalization error

How to divide training dataset and testing dataset?

1.2 Evaluation Methods

□ Evaluation Methods

- For example, m samples:

$$D = \{(x_1, y_1), (x_2, y_2), (x_3, y_3), \cdots, (x_m, y_m)\}$$

Training dataset: S Testing dataset: T

- $S \cap T = \emptyset$
- $S \cup T = D$

How to divide training dataset and testing dataset?

1.2 Evaluation Methods

Hold-out Method (留出法)

- Set a proportion r, like $r = 0.3$
- By sampling methods, make

$$T = r * D, S = (1 - r) * D$$

- Sampling methods:
  - Random sampling
  - Stratified sampling: keep the proportion rate of samples;

    For example, 500 positive samples, 500 negative samples in D and $r = 0.3$:

    S: 350 positive samples; 350 negative samples

    T: 150 positive samples; 150 negative samples

- Difficulty: r,

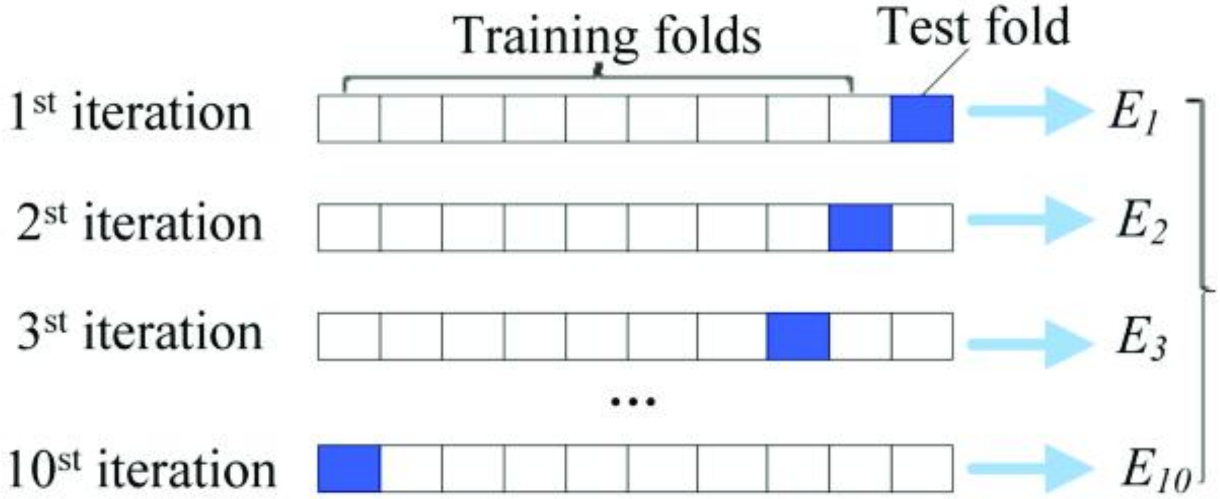
1.2 Evaluation Methods

Cross Validation (交叉验证法)

- Divided D dataset to k sub-dataset:

$$D = D_1 \cup D_2 \cup \cdots D_k, \quad D_i \cap D_j = \emptyset \ (i \neq j)$$

- Keep same distribution of each sub-dataset
- K-times test: (k-1) sub-dataset as S, 1 sub-dataset as T
- Average K-times test error as final results.

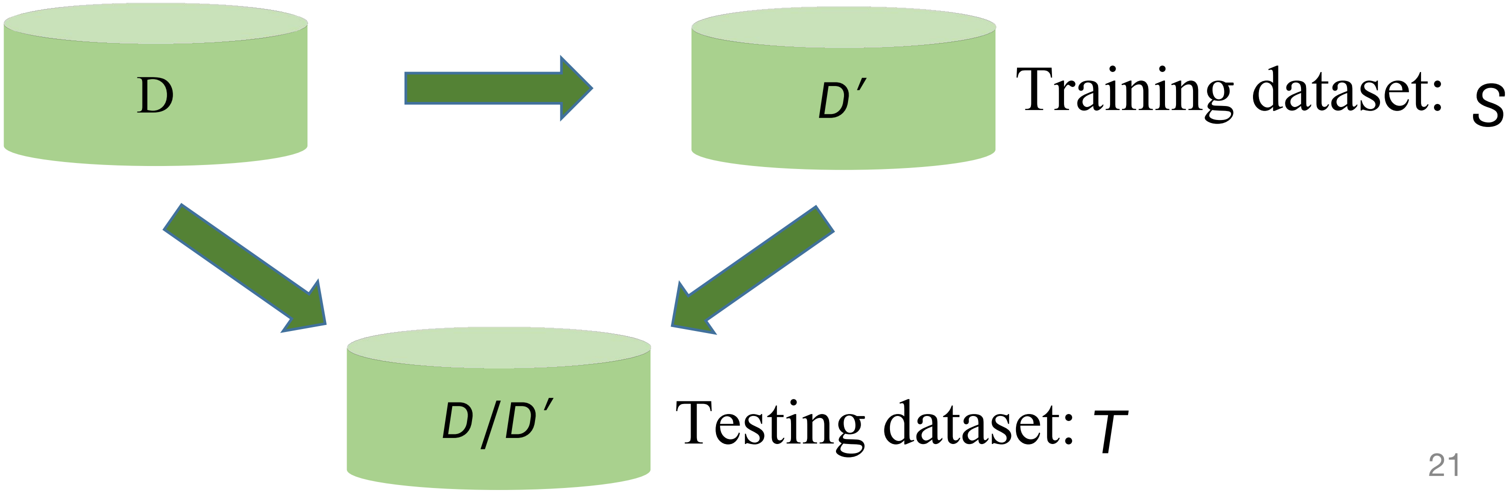


$$E = \frac{1}{k}\sum_{i=1}^{k} E_i$$

1.2 Evaluation Methods

Bootstrapping (自助法)

- Based on Bootstrapping Sampling
  - Randomly select 1 sample from D and copy it to D';
  - Repeat m times
  - Obviously, some of the samples in D will be repeated in D', and some will not.
  - Suitable for small datasets！



Model Evaluation and Selection

- 1.1 Empirical Error and Overfitting
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1.3 Performance Measure

Performance Measure

- For dataset D, with x_i as input, y_i as true label,

$$D = \{(x_1, y_1), (x_2, y_2), (x_3, y_3), \cdots, (x_m, y_m)\}$$

- The predicted output of a model (f),

$$outputs = \{y_1^*, y_2^*, y_3^*, \cdots, y_m^*\}$$

How to measure the predictions of different models?

1.3 Performance Measure

- Two different tasks
  - For regression tasks: Mean Squared Error

$$E(f,D) = \frac{1}{m}\sum_{i=1}^{m}(y_i^* - y_i)^2$$

  - The classification task: Error Rate, Accuracy

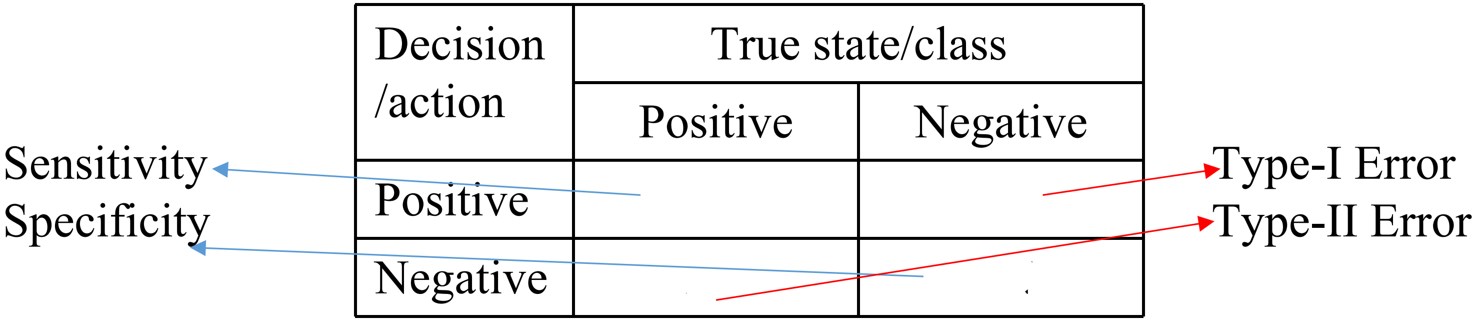
$$E(f,D) = \frac{1}{m}\sum_{i=1}^{m}\prod(y_i^* \neq y_i)$$

$$Acc(f,D) = \frac{1}{m}\sum_{i=1}^{m}\prod(y_i^* = y_i) = 1 - E(f,D)$$

1.3 Performance Measure

Confusion matrix

- For binary classification tasks



Decision /action	True state/class	
	Positive	Negative
Positive		
Negative		

Sensitivity
Specificity

Type-I Error
Type-II Error

Correct classification
TP: the number of samples belonging to positive decided positive
TN: the number of samples belonging to negative decided negative

Misclassification
FP: the number of samples belonging to negative decided positive incorrectly. (False Alarm)
FN: the number of samples belonging to positive decided negative incorrectly.(Missed Detection)

1.3 Performance Measure

- Sensitivity (TP rate)
  - $S_n = \frac{TP}{TP+FN}$
- Specificity (TN rate)
  - $S_p = \frac{TN}{TN+FP}$
- FP rate (Type-I Error)
  - FP rate = $\frac{FP}{FP+TN}$
- FN rate (Type-II Error)
  - FN rate = $\frac{FN}{FN+TP}$
- Accuracy

$$accuracy = \frac{TP + TN}{TP + FP + TN + FN}$$

- Precision

$$precision = \frac{TP}{TP + FP}$$

Decision/ action	True state/class	
	Positive	Negative
Positive	TP	FP
Negative	FN	TN

$TP + FP + TN + FN =$
$Total\ number\ of\ samples\ in\ dataset$

1.3 Performance Measure

- Sensitivity (TP rate)
  - $S_n = \frac{TP}{TP+FN}$
- Specificity (TN rate)
  - $S_p = \frac{TN}{TN+FP}$
- FP rate (Type-I Error)
  - $\text{FP rate} = \frac{FP}{FP+TN}$
- FN rate (Type-II Error)
  - $\text{FN rate} = \frac{FN}{FN+TP}$

Decision/ action	True state/class	
	Positive	Negative
Positive	TP	FP
Negative	FN	TN

$TP + FP + TN + FN =$
$Total\ number\ of\ samples\ in\ dataset$

- Accuracy

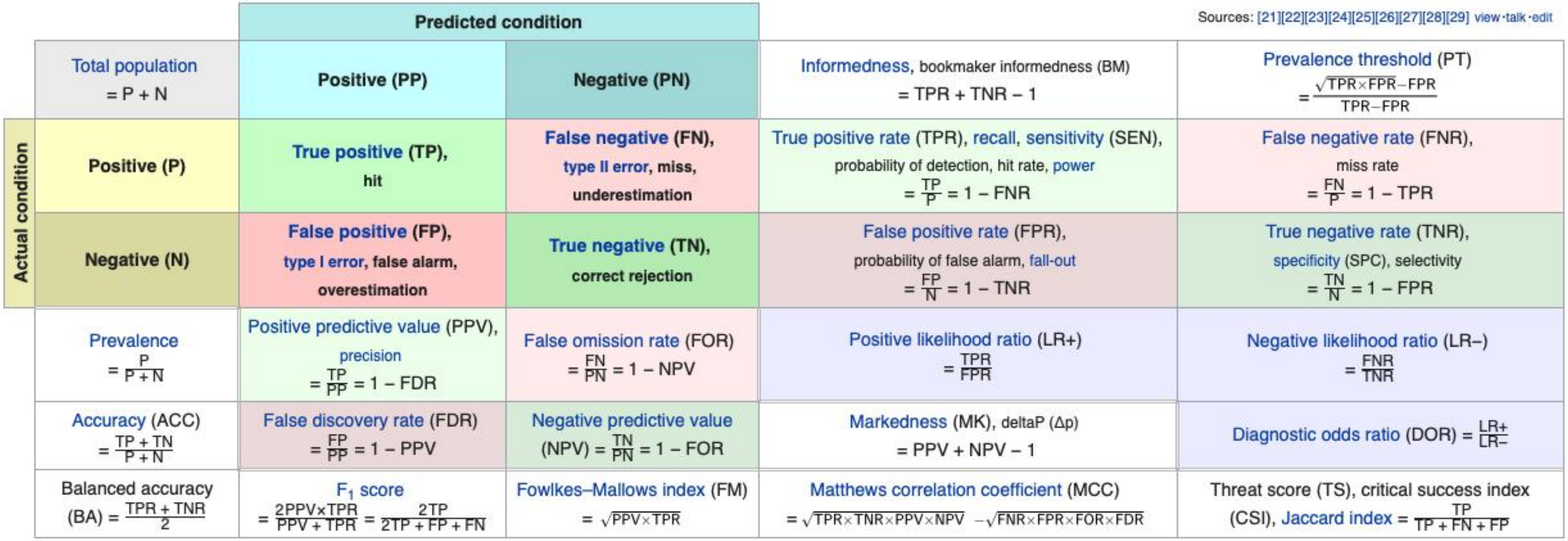
$$accuracy = \frac{TP + TN}{TP + FP + TN + FN}$$

- Precision

$$precision = \frac{TP}{TP + FP}$$

1.3 Performance Measure

- Confusion matrix from Wiki

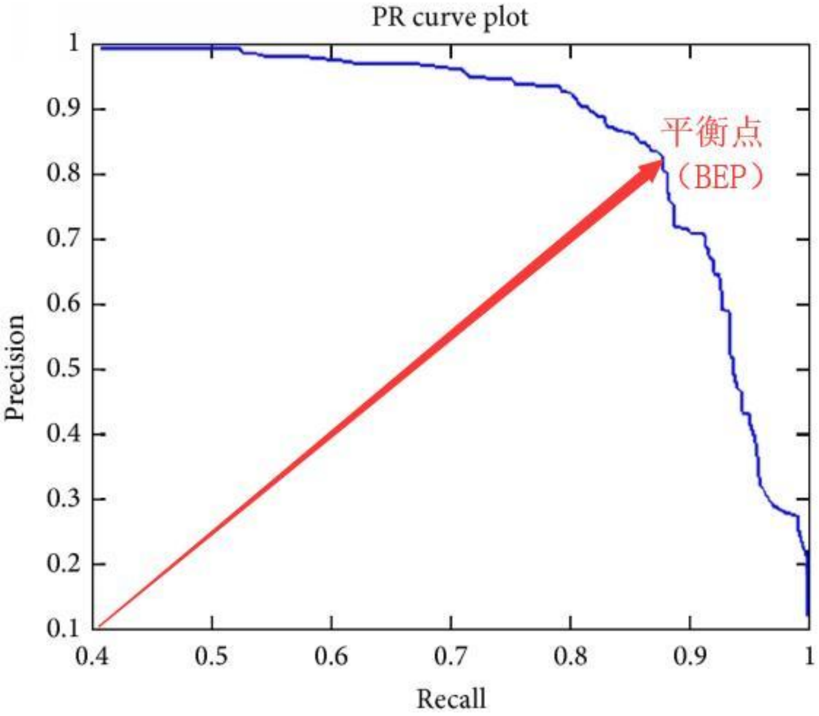


Sources: [21][22][23][24][25][26][27][28][29] view · talk · edit

		Predicted condition			
	Total population $= P + N$	Positive (PP)	Negative (PN)	Informedness, bookmaker informedness (BM) $= TPR + TNR - 1$	Prevalence threshold (PT) $= \frac{\sqrt{TPR \times FPR} - FPR}{TPR - FPR}$
Actual condition	Positive (P)	**True positive (TP),** **hit**	**False negative (FN),** **type II error, miss,** **underestimation**	True positive rate (TPR), recall, sensitivity (SEN), probability of detection, hit rate, power $= \frac{TP}{P} = 1 - FNR$	False negative rate (FNR), miss rate $= \frac{FN}{P} = 1 - TPR$
	Negative (N)	**False positive (FP),** **type I error, false alarm,** **overestimation**	**True negative (TN),** **correct rejection**	False positive rate (FPR), probability of false alarm, fall-out $= \frac{FP}{N} = 1 - TNR$	True negative rate (TNR), specificity (SPC), selectivity $= \frac{TN}{N} = 1 - FPR$
	Prevalence $= \frac{P}{P + N}$	Positive predictive value (PPV), precision $= \frac{TP}{PP} = 1 - FDR$	False omission rate (FOR) $= \frac{FN}{PN} = 1 - NPV$	Positive likelihood ratio (LR+) $= \frac{TPR}{FPR}$	Negative likelihood ratio (LR−) $= \frac{FNR}{TNR}$
	Accuracy (ACC) $= \frac{TP + TN}{P + N}$	False discovery rate (FDR) $= \frac{FP}{PP} = 1 - PPV$	Negative predictive value (NPV) $= \frac{TN}{PN} = 1 - FOR$	Markedness (MK), deltaP (Δp) $= PPV + NPV - 1$	Diagnostic odds ratio (DOR) $= \frac{LR+}{LR-}$
	Balanced accuracy (BA) $= \frac{TPR + TNR}{2}$	F_1 score $= \frac{2 PPV \times TPR}{PPV + TPR} = \frac{2TP}{2TP + FP + FN}$	Fowlkes–Mallows index (FM) $= \sqrt{PPV \times TPR}$	Matthews correlation coefficient (MCC) $= \sqrt{TPR \times TNR \times PPV \times NPV} - \sqrt{FNR \times FPR \times FOR \times FDR}$	Threat score (TS), critical success index (CSI), Jaccard index $= \frac{TP}{TP + FN + FP}$

1.3 Performance Measure

- P-R Curve: Precision- Recall
  - A PR curve is simply a graph with Precision values on the y-axis and Recall （ Sensitivity ） values on the x-axis.



- The point is called “Break-Even Point, BEP”, when precision= recall.
- If the BEP value of model A is bigger than it of model B, we can say model A is better than model B based on BEP.

1.3 Performance Measure

- Sensitivity (Recall, R)
  - $S_n = \frac{TP}{TP+FN}$

- Precision (P)
  - $precision = \frac{TP}{TP+FP}$

Decision/ action	True state/class	
	Positive	Negative
Positive	TP	FP
Negative	FN	TN

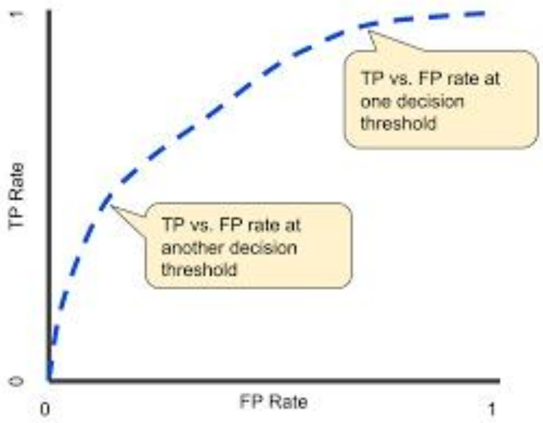
$TP + FP + TN + FN =$
$Total\ number\ of\ samples\ in\ dataset$

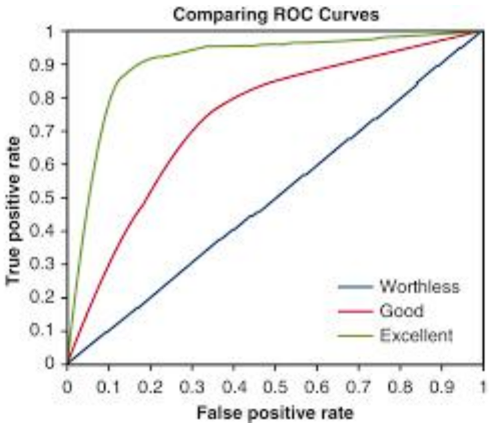
- F1

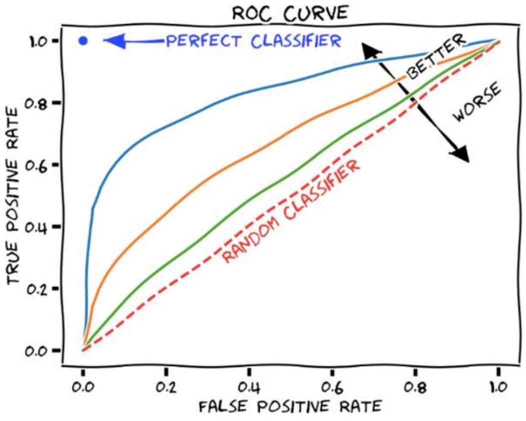
$$F1 = \frac{2 \times P \times R}{P + R}$$

1.3 Performance Measure

ROC Curve (Receiver Operating Characteristic)







- ➢ An ROC curve (receiver operating characteristic curve) is a graph showing the performance of a classification model at all classification thresholds.

2.3 Type-I Error Probability & Type-II Error Probability

□ ROC Curve (Receiver Operating Characteristic)

➢ For a binary classification,

- 5 positive samples, and prediction probability: (0.9,0.8,0.5,0.4,0.3)
- 5 negative samples: (0.7,0.6,0.2,0.1,0.01)
- Ranking:(0.9,0.8,0.7,0.6,0.5,0.4,0.3,0.2,0.1,0.01)

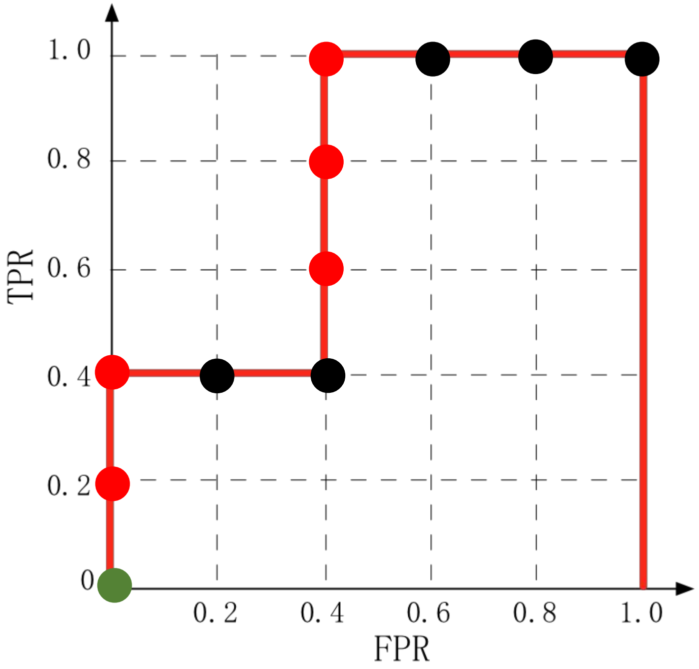
Thresholds	0.9	0.8	0.7	0.6	0.5	0.4	0.3	0.2	0.1	0.01
TPR = TP/(TP+FN)	0.2	0.4	0.4	0.4	0.6	0.8	1.0	1.0	1.0	1.0
FPR = FP/(FP+TN)	0	0	0.2	0.4	0.4	0.4	0.4	0.6	0.8	1.0

- TP: number of true positive samples; FP: number of false positive samples
- TN: number of true negative samples; FN: number of false negative samples

2.3 Type-I Error Probability & Type-II Error Probability

ROC Curve (Receiver Operating Characteristic)

Thresholds	0.9	0.8	0.7	0.6	0.5	0.4	0.3	0.2	0.1	0.01
TPR	0.2	0.4	0.4	0.4	0.6	0.8	1.0	1.0	1.0	1.0
FPR	0	0	0.2	0.4	0.4	0.4	0.4	0.6	0.8	1.0



- Area Under Curve: AUC
- AUC:

$$AUC = \frac{1}{2}\sum_{i=1}^{m-1}(x_{i+1} - x_i) \cdot (y_i + y_{i+1})$$

- AUC =1; perfect!
- 0.5<AUC<1, better than randomly classification;
- AUC = 0.5, same as randomly classification;

Test

ROC Curve (Receiver Operating Characteristic)

样本编号	真实标签	模型输出概率	样本编号	真实标签	模型输出概率
1	p	0.9	11	p	0.4
2	p	0.8	12	n	0.39
3	n	0.7	13	p	0.38
4	p	0.6	14	n	0.37
5	p	0.55	15	n	0.36
6	p	0.54	16	n	0.35
7	n	0.53	17	p	0.34
8	n	0.52	18	n	0.33
9	p	0.51	19	p	0.30
10	n	0.505	20	n	0.10

- p : positive sample, n: negative sample

Summary

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Model Evaluation and Selection

Solve two problems:
(1) How to make a model convincible?
(2) How to evaluate a model?

Summary

- How to make a model convincible?
  - Error, Training error, Generalization error
  - Overfitting and Underfitting
  - Evaluation Methods: Hold-out method, Cross Validation, Bootstrapping
- How to evaluate a model?
  - Measure metrics: ACC, Recall, F1,AUC…