Artificial Neural Network

# Part II: The Road Map of Machine Learning Algorithms

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## Introduction

- Kernel methods: Support vector machine
- Ensemble methods:
  - Random forest
  - Adaboost
  - Artificial Neural Network

Ensemble Methods

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## Kernel methods

• Feature mapping:  $\phi : \mathbb{R}^2 \to \mathbb{R}^3$ 

$$(x_1, x_2) \rightarrow (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$

• Inexplicit mapping:  $\phi$ 

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Kernel met	hods		
• Featu	ure mapping: $\phi:\mathbb{R}$ $(x_1,x_2)$	$\stackrel{2}{\longrightarrow} \mathbb{R}^{3}$ $\stackrel{1}{\longrightarrow} (x_{1}^{2}, \sqrt{2}x_{1}x_{2}, x_{2}^{2})$	ā., y.

- Inexplicit mapping:  $\phi$
- Kernel function:  $\kappa_{\phi}(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$
- Polynomial kenerl and Gaussian Kernel (RBF).

$$k_{q}(\underline{x}_{i},\underline{x}_{j}) = (C + \Im \underline{x}_{i},\underline{x}_{j}) \qquad k_{p}(\underline{x}_{i},\underline{x}_{j}) = e_{xp} \left\{ -\frac{\|\underline{x}_{i}-\underline{x}_{j}\|_{2}^{2}}{\sigma^{2}} \right\}$$

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- Polynomial kenerl and Gaussian Kernel (RBF).
- Kernel tricks: obtain a non-linear model by embedding kernel function into different linear algorithms.
- Kernel PCA, Kernel regression, Support vector machine.

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### Maximum Margin Classifier

• The margin of the decision boundary should be as large as possible.



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### Maximum Margin Classifier

• A statistical illustration of this idea:



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# Support Vectors



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## Support Vectors



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# Support Vectors



• Only the points on the boundary of margin have contributions to the final estimation results

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# Support Vectors



- Only the points on the boundary of margin have contributions to the final estimation results
- Kernelized MMC  $\rightarrow$  support vector machine



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# Over fitting in SVM



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# Soft Margin Classifier

- IDEA: We give up some high noise cases.
- For each observation, we introduce a fuzzy (Slackness) parameter, ξ<sub>i</sub> ≥ 0.
- Hyper-parameter: large *C*, less noise tolerance, high cost.



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## Summary of Kernel SVM

• SVM = MMC + Kernel trick.

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- RBF kernel SVM is the most popular one.
- The kernel parameter  $\sigma$  can be estimated from sample, see Caputo, Furesjo and Smola (2002).
- Tuning: exponential growing sequesces of C and  $\sigma$ , e.g.  $2^{-5}, 2^{-3}, ..., 2^{15}$ .

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#### Introduction to ensemble methods

• Whether Swedish national football team can qualify for the Euro Cup in 2020?



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- Uniform Aggregation. Bagging/Random forest.
- Give more weights to some experts.



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- Give more weights to some experts.
- Non-uniform Aggregation. Adaboost.



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BRB	BBB
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BRR	BBR
0	Δ
0	
	Δ
	BRB BRR O O

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	0		
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# Uniform Aggregation

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$$F(\mathbf{x}) = sign\left(\sum_{j=1}^{M} f_j(\mathbf{x})\right)$$
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$$V_{ar}(x) = E(x - E_{ar})^2$$

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## Bagging (Bootstrap Aggregation)

• Basic idea: Apply Bootstrap resampling technique to generate different bootstrap samples, such that the classifiers learned from each bootstrap sample have large diversity.



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#### Algorithm

- 1 Take a random sample with replacement from data set  $X^*$
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- S Repeat step 1 and 2(B) times, then perform uniform aggregation

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- **2** Train a classifier from this random sample
- S Repeat step 1 and 2 B times, then perform uniform aggregation
  - A strategy to enhance the existing algorithm. Any proper algorithm?

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#### Decision Tree

ID	Unable	Estate	Marital	Income
1	0	1	S	125
2	0	0	М	100
3	0	0	S	70
4	0	1	М	120
5	1	0	D	95
6	0	0	М	60
7	0	1	D	220
8	1	0	S	85
9	0	0	М	75
10	1	0	S	90



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#### Decision Tree

Key: Sequentially split the feature space into small pieces.

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3	0	0	S	70	
4	0	1	М	120	able Marital
5	1	0	D	95	No Yes
6	0	0	М	60	Income (able)
7	0	1	D	220	>80 <80
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### Motivations

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- Large variation! Bagging!

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- The main weaknesses of decision tree is unstable and very sensitive to the data.
- Large variation! Bagging!
- Random forest = Decision tree + bagging

**1** Draw a bootstrap sample from original data.

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- In literature, it is called random subspace, also a kind of feature mapping.
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- **3** Repeat these procedure B times.
- Apply uniform aggregation method on those trees, then we have our random forest model.

Kernel Methods 20000000 Ensemble Methods

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## Out of Bagging Errors

• Out of bagging samples: a set of samples which is not included in the bootstrap sample.

# Out of Bagging Errors

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- The probability of an example is not included in a Bootstrap sample:

$$\left(1-\frac{1}{N}\right)^{N} \rightarrow \frac{1}{e} \approx 0.37$$

$$60^{0}/6 40^{0}/6$$

$$1 = 10^{10}$$

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- Self-validation.

Kernel Methods 00000000 Ensemble Methods

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#### Feature Importance

• Measure the importance for each features,  $\mathcal{I}(x_i)$ 

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- Replace the feature  $x_i$  by permuted  $x_i^P$
- Then we can measure the importance of x<sub>i</sub> by the difference of performance

 $\mathcal{I}(x_j) = Err_{OOB}(x_j) - Err_{OOB}(x_i^p)$ 

### Turning Random Forest

• Two hyper-parameters: the number of trees,  $N_t$  and the number of features randomly selected on each spliting,  $N_f$ .

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  - Fix N<sub>t</sub> and choose different numbers around the squar root of the total number of feature variables.
  - Build up the classifier, then select the best given OOB errors.

Ensemble Methods

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### Boosting and Adaboosting

• Uniform aggregation: Bagging, Random Forest.

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## Boosting and Adaboosting

- Uniform aggregation: Bagging, Random Forest.
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- Adaboost, Freund Y. and Schapire R.E. (1997): Learn from failures and mistakes.

Ensemble Methods

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### Adaboost

• Teach kids to distinguish apple from other fruits.



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### Adaboost

• Teach kids to distinguish apple from other fruits.

Circle



Ensemble Methods

Artificial Neural Network

### Adaboost

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Circle



Ensemble Methods

Artificial Neural Network

### Adaboost

• Teach kids to distinguish apple from other fruits.

Circle + Red



Ensemble Methods

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### Adaboost

• Teach kids to distinguish apple from other fruits.

Circle + Red



Introd	

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### Adaboost

- Teach kids to distinguish apple from other fruits.
- Circle + Red + Green



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Adaboost			

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	Kernel Methods 0000000	Ensemble Methods 000000000000000000000000000000000000	Artificial Neural Network
Adaboost			

- Teach kids to distinguish apple from other fruits.
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# Weighted Classifer

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#### Example

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- Adaboost: a reweight scheme, such that the mis-classified examples get more weights in the next round.

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Ensemble Methods

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### ANN in Ensemble methods

• Uniform aggregation:  $F(\mathbf{x}) = Sign\left(\sum_{j=1}^{J} f_j(\mathbf{x})\right)$ 

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### ANN in Ensemble methods

- Uniform aggregation:  $F(\mathbf{x}) = Sign\left(\sum_{j=1}^{J} f_j(\mathbf{x})\right)$
- Random forest = Bagging + Decision tree

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## ANN in Ensemble methods

- Uniform aggregation:  $F(\mathbf{x}) = Sign\left(\sum_{j=1}^{J} f_j(\mathbf{x})\right)$
- Random forest = Bagging + Decision tree
- Question: Can we learn  $f_j$  as a perceptron,  $f_j = Sign(\mathbf{w}^T \mathbf{x} + w_0)$ ?
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# ANN in Ensemble methods

- Uniform aggregation:  $F(\mathbf{x}) = Sign\left(\sum_{j=1}^{J} f_j(\mathbf{x})\right)$
- Random forest = Bagging + Decision tree
- Question: Can we learn  $f_j$  as a perceptron,  $f_j = Sign(\mathbf{w}^T \mathbf{x} + w_0)$ ?
- Question: Can we learn different weights for different perceptrons from the target variable y, such that the final model F(x), is a non-uniform aggregation of those perceptrons?

$$F(\mathbf{x}) = Sign\left(\alpha_0 + \sum_{j=1}^J \alpha_j Sign(\mathbf{w}_j^T \mathbf{x} + w_0)\right)$$

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## Motivations

• 'AND' operator:  $AND(f_1, f_2)$ 



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- 'AND' operator: AND(f<sub>1</sub>, f<sub>2</sub>)
- Find a line split the space.

 $\alpha_0 + \alpha_1 f_1 + \alpha_2 f_2 = \mathbf{0}$ 



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• The final classifier is

 $Sign(-1 + f_1(x) + f_2(x))$ 



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$$Sign\left(\alpha_{0} + \sum_{j=1}^{2} \alpha_{j} Sign\left(\mathbf{w}_{j}^{T} \mathbf{x} + w_{j0}\right)\right)$$



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• 'OR' and 'NOT'



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- 'OR' and 'NOT'
- Any convex set can be approximated by this model if *J* is large enough.



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#### Non-uniform Aggregation of Perceptrons

• Non-uniform Aggregation of Perceptrons can be presented as

$$F(\mathbf{x}) = Sign\left(w_0^{(2)} + \sum_{j=1}^{J} w_j^{(2)} Sign\left(\sum_{i=1}^{d} w_{j,i}^{(1)} x_i + w_{j,0}^{(1)}\right)\right)$$

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Input Layer

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Input Layer Hidden Layers

Artificial Neural Network

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Input Layer Hidden Layers Output Layer

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## Motivations

A non-convex set.



 $x_1$ 

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## Motivations

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- A non-convex set.
- 'XOR' operator.



# Motivations



• 'XOR' operator.



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- Not linear separable... Any idear?



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There is nothing difficulty cann't be solved by eating a hamburg at MÄX, if so, just eat one more.

# Motivations

- A non-convex set.
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There is nothing difficulty cann't be solved by Multi-layers perceptron, if so, just add one more layer

Kernel Methods 20000000 Ensemble Methods

Artificial Neural Network

#### Multi-Layers Perceptron



## From MLP to Artificial Neural Network

• The general MLP can be represented as

$$\begin{aligned} z_{j}^{(1)} &= Sign\left(\mathbf{w}_{j}^{(1)T}\mathbf{x}\right) \\ &\vdots \\ z_{j}^{(L)} &= Sign\left(\mathbf{w}_{j}^{(L)T}\mathbf{z}^{(L-1)}\right) \\ y &= Sign\left(\mathbf{w}_{j}^{(L+1)T}\mathbf{z}^{(L)}\right) \end{aligned}$$



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- Neurons:  $z_j^{(L)}$ , latent variable.



# From MLP to Artificial Neural Network

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$$\vdots$$
  

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$$y = Sign \left( \mathbf{w}_{j}^{(L+1)T} \mathbf{z}^{(L)} \right)$$

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- Activation function, σ(·), Sign(·), Identity function, logit function and so on.



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Artificial Neural Network

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- Output layer: *y*, objective function → regression or classification.



Artificial Neural Network

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Feed-foward Neural Network

Kernel Methods 00000000 Ensemble Methods

Artificial Neural Network

### ANN, an integrated learning process





Kernel Methods 20000000 Ensemble Methods

Artificial Neural Network

### ANN, an integrated learning process



Kernel Methods 20000000 Ensemble Methods

Artificial Neural Network

### ANN, an integrated learning process



- The last layer of neurons can be viewed as a set of extracted features from the raw data.
- ANN can be viewed as an integrated learning process.