### Machine Learning Techniques (機器學習技法)



#### Lecture 16: Finale Hsuan-Tien Lin (林軒田) htlin@csie.ntu.edu.tw

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### Roadmap

- Embedding Numerous Features: Kernel Models
- 2 Combining Predictive Features: Aggregation Models
- Oistilling Implicit Features: Extraction Models

#### Lecture 15: Matrix Factorization

linear models of movies on extracted user features (or vice versa) jointly optimized with stochastic gradient descent

#### Lecture 16: Finale

- Feature Exploitation Techniques
- Error Optimization Techniques
- Overfitting Elimination Techniques
- Machine Learning in Practice

#### numerous features within some $\Phi$ :

### Exploiting Numerous Features via Kernel

#### numerous features within some $\Phi$ :

embedded in kernel  $K_{\Phi}$  with inner product operation

#### Polynomial Kernel

'scaled' polynomial transforms

#### numerous features within some $\Phi$ :

Polynomial Kernel	Gaussian Kernel
	infinite-dimensional
transforms	transforms

inale	le Feature Exploitation Techniques					
	Exploiting Numerous Features via Kernel					
numero	numerous features within some $\Phi$ : embedded in kernel $K_{\Phi}$ with inner product operation					
Polync	Polynomial Kernel Gaussian Kernel Stump Kernel					
Polynomial KernelGaussian KernelStump Kernel'scaled' polynomial transformsinfinite-dimensional transformsdecision-stumps as transforms						

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Polynomial Kernel	Gaussian Kernel	Stump Kernel
'scaled' polynomial	infinite-dimensional	decision-stumps as
transforms	transforms	transforms

#### Sum of Kernels

transform union

#### numerous features within some $\Phi$ :

Polynomial Kernel	Gaussian Kernel	Stump Kernel
'scaled' polynomial transforms	infinite-dimensional transforms	decision-stumps as transforms
Sum of Kernels	Product of Kernels	1
transform union	transform combination	

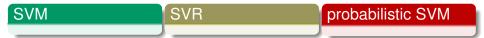
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SVM	<u> </u>	Ŭ T
	regression	regression probabilistic SVM

Feature Exploitation Techniques

### Exploiting Predictive Features via Aggregation predictive features within some $\Phi$ : $\phi_t(\mathbf{x}) = g_t(\mathbf{x})$

Feature Exploitation Techniques

# Exploiting Predictive Features via Aggregation predictive features within some $\Phi$ :

 $\phi_t(\mathbf{x}) = g_t(\mathbf{x})$ 

**Decision Stump** 

simplest perceptron; simplest DecTree

Feature Exploitation Techniques

### Exploiting Predictive Features via Aggregation

#### predictive features within some $\Phi$ :

 $\phi_t(\mathbf{x}) = g_t(\mathbf{x})$ 

#### Decision Stump

simplest perceptron; simplest DecTree Decision Tree branching (divide) + leaves (conquer)

Feature Exploitation Techniques

## Exploiting Predictive Features via Aggregation

#### predictive features within some **Φ**:

 $\phi_t(\mathbf{x}) = \mathbf{g}_t(\mathbf{x})$ 

Decision Stump	Decision Tree	(Gaussian) RBF
simplest perceptron;	branching (divide) +	prototype (center) +
simplest DecTree	leaves (conquer)	influence

Feature Exploitation Techniques

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#### predictive features within some $\Phi$ :

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Uniform	Non-Uniform	Conditional

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Bagging; Random Forest	AdaBoost; GradientBoost	Decision Tree;

Feature Exploitation Techniques

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Uniform	Non-Uniform	Conditional
Bagging;	AdaBoost;	Decision Tree;
Random Forest	GradientBoost	Nearest Neighbor

Feature Exploitation Techniques

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Bagging; Random Forest	AdaBoost; GradientBoost	Decision Tree; Nearest Neighbor
	probabilistic SVM	

Feature Exploitation Techniques

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Uniform		Non-Uniform	Conditional	
Bagging; Random Fo	rest	AdaBoost; GradientBoost	Decision Tree; Nearest Neighbor	
		probabilistic SVM	J	
possibly Infinite Ensemble Learning, Decision Tree SVM,				
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as hidden variables to be 'jointly' optimized with usual weights

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-possibly with the help of unsupervised learning

Neural Network; Deep Learning

neuron weights

as hidden variables to be 'jointly' optimized with usual weights

Neural Network; Deep Learning	RBF Network
neuron weights	RBF centers

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Neural Network; Deep Learning	RBF Network	Matrix Factorization
neuron weights	RBF centers	user/movie factors

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Neural Network; Deep Learning	RBF Network	Matrix Factorization
neuron weights	RBF centers	user/movie factors
	k-Means	
	cluster centers	

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Neural Network; Deep Learning	RBF Network	Matrix Factorization
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	k-Means	Autoencoder; PCA

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Neural Network; Deep Learning	RBF Network	Matrix Factorization
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AdaBoost; GradientBoost	k-Means	Autoencoder; PCA
$g_t$ parameters	cluster centers	'basis' directions

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neuron weights	RBF centers	user/movie factors
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possibly GradientBoosted Neurons, NNet on Factorized Features,

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Machine Learning Techniques

Feature Exploitation Techniques

## Exploiting Low-Dim. Features via Compression low-dimensional features within some **Φ**:

compressed from original features

Feature Exploitation Techniques

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Decision Stump; DecTree Branching

'best' naïve projection to  $\mathbb R$ 

Feature Exploitation Techniques

## Exploiting Low-Dim. Features via Compression low-dimensional features within some **Φ**:

compressed from original features

Decision Stump;	Random Forest
DecTree Branching	Tree Branching
'best' naïve projection to ${\mathbb R}$	'random' low-dim. projection

Feature Exploitation Techniques

## Exploiting Low-Dim. Features via Compression low-dimensional features within some **Φ**:

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### Decision Stump; DecTree Branching

'best' naïve projection to  $\mathbb{R}$ 

Random Forest Tree Branching

'random' low-dim. projection

#### Autoencoder;PCA

info.-preserving compression

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'best' naïve projection to  $\mathbb{R}$ 

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'random' low-dim. projection

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info.-preserving compression

#### Matrix Factorization

projection from abstract to concrete

### Exploiting Low-Dim. Features via Compression low-dimensional features within some **Φ**:

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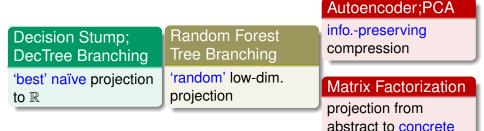


**Feature Selection** 

'most-helpful' low-dimensional projection

### Exploiting Low-Dim. Features via Compression low-dimensional features within some **Φ**:

compressed from original features



Feature Selection

'most-helpful' low-dimensional projection

#### possibly other 'dimension reduction' models

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Machine Learning Techniques

#### Fun Time

Consider running AdaBoost-Stump on a PCA-preprocessed data set. Then, in terms of the original features **x**, what does the final hypothesis  $G(\mathbf{x})$  look like?

- **1** a neural network with  $tanh(\cdot)$  in the hidden neurons
- 2 a neural network with sign( $\cdot$ ) in the hidden neurons
- 3 a decision tree
- 4 a random forest

#### Fun Time

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#### Reference Answer: (2)

PCA results in a linear transformation of  $\mathbf{x}$ . Then, when applying a decision stump on the transformed data, it is *as if* a perceptron is applied on the original data. So the resulting *G* is simply a linear aggregation of perceptrons.

#### Numerical Optimization via Gradient Descent when $\nabla E$ 'approximately' defined, use it for 1st order approximation:

new variables = old variables –  $\eta \nabla E$ 

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#### SGD/Minibatch/GD

(Kernel) LogReg;

- Neural Network [backprop];
- Matrix Factorization;

Linear SVM (maybe)

# Numerical Optimization via Gradient Descent when $\nabla E$ 'approximately' defined, use it for 1st order approximation:

new variables = old variables –  $\eta \nabla E$ 

#### SGD/Minibatch/GD (Kernel) LogReg; Neural Network [backprop]; Matrix Factorization; Linear SVM (maybe)

### Functional GD AdaBoost; GradientBoost

# Numerical Optimization via Gradient Descent when $\nabla E$ 'approximately' defined, use it for 1st order approximation:

new variables = old variables –  $\eta \nabla E$ 

SGD/Minibatch/GD	Steepest Descent	Functional GD
(Kernel) LogReg;	AdaBoost;	AdaBoost;
Neural Network [backprop];	GradientBoost	GradientBoost
Matrix Factorization;		
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# Numerical Optimization via Gradient Descent when $\nabla E$ 'approximately' defined, use it for 1st order approximation:

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SGD/Minibatch/GD	Steepest Descent	Functional GD
(Kernel) LogReg;	AdaBoost;	AdaBoost;
Neural Network [backprop];	GradientBoost	GradientBoost
Matrix Factorization;		
Linear SVM (maybe)		

possibly 2nd order techniques, GD under constraints, ....

### when difficult to solve original problem, seek for equivalent solution

#### Indirect Optimization via Equivalent Solution

### when difficult to solve original problem, seek for equivalent solution

#### Dual SVM

equivalence via convex QP

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### when difficult to solve original problem, seek for equivalent solution

Dual SVM	Kernel LogReg Kernel RidgeReg
equivalence via	equivalence via
convex QP	representer

when difficult to solve original problem, seek for equivalent solution

Dual SVM	Kernel LogReg Kernel RidgeReg	PCA
equivalence via convex QP	equivalence via representer	equivalence to eigenproblem

when difficult to solve original problem, seek for equivalent solution

Dual SVM	Kernel LogReg Kernel RidgeReg	PCA
equivalence via convex QP	equivalence via representer	equivalence to eigenproblem

some other boosting models and modern solvers of kernel models rely on such a technique heavily

#### when difficult to solve original problem, seek for 'easier' sub-problems

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#### Multi-Stage

probabilistic SVM;

linear blending;

stacking;

RBF Network;

DeepNet pre-training

### when difficult to solve original problem, seek for 'easier' sub-problems

Multi-Stage	Alternating Optim.
probabilistic SVM;	<i>k</i> -Means;
linear blending;	alternating LeastSqr;
stacking;	
RBF Network;	
DeepNet pre-training	

### when difficult to solve original problem, seek for 'easier' sub-problems

Multi-Stage	Alternating Optim.
probabilistic SVM;	<i>k</i> -Means;
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RBF Network;	
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### Complicated Optimization via Multiple Steps when difficult to solve original problem,

#### seek for 'easier' sub-problems

Multi-Stage	Alternating Optim.	Divide & Conquer
probabilistic SVM;	<i>k</i> -Means;	decision tree;
linear blending;	alternating LeastSqr;	
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#### Complicated Optimization via Multiple Steps when difficult to solve original problem,

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probabilistic SVM;	<i>k</i> -Means;	decision tree;
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RBF Network;		
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#### useful for complicated models

#### Fun Time

When running the DeepNet algorithm introduced in Lecture 213 on a PCA-preprocessed data set, which optimization technique is used?

- 1 variants of gradient-descent
- 2 locating equivalent solutions
- 3 multi-stage optimization
- 4 all of the above

#### Fun Time

When running the DeepNet algorithm introduced in Lecture 213 on a PCA-preprocessed data set, which optimization technique is used?

- variants of gradient-descent
- 2 locating equivalent solutions
- 3 multi-stage optimization
- 4 all of the above

#### Reference Answer: (4)

minibatch GD for training; equivalent eigenproblem solution for PCA; multi-stage for pre-training

Overfitting Elimination Techniques

## Overfitting Elimination via Regularization when model too 'powerful':

add brakes somewhere

Overfitting Elimination Techniques

### Overfitting Elimination via Regularization when model too 'powerful':

#### add brakes somewhere



SVM;

AdaBoost (indirectly)

Overfitting Elimination Techniques

## Overfitting Elimination via Regularization when model too 'powerful':

#### add brakes somewhere

large-margin	L2
SVM;	SVR;
AdaBoost (indirectly)	kernel models;
	NNet [weight-decay]

Overfitting Elimination Techniques

## Overfitting Elimination via Regularization when model too 'powerful':

#### add brakes somewhere

large-margin	L2	voting/averaging
SVM;	SVR;	uniform blending;
AdaBoost (indirectly)	kernel models;	Bagging;
	NNet [weight-decay]	Random Forest

Overfitting Elimination Techniques

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#### denoising

autoencoder

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autoencoder

#### pruning

#### decision tree

Overfitting Elimination Techniques

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SVM;	SVR;	uniform blending;
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denoising	weight-elimination
autoencoder	NNet

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decision tree

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denoising	weight-elimination
autoencoder	NNet

pruning	early stopping
decision tree	NNet (any GD-like)

Overfitting Elimination Techniques

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SVM;	SVR;	uniform blending;
AdaBoost (indirectly)	kernel models;	Bagging;
	NNet [weight-decay]	Random Forest
denoising	weight-elimination	constraining

autoencoder	NNet	autoenc. [weights];
		RBF [# centers];
pruning	early stopping	
decision tree	NNet (any GD-like)	

**Overfitting Elimination Techniques** 

#### Overfitting Elimination via Regularization when model too 'powerful':

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arguably most important techniques

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Machine Learning Techniques

### Overfitting Elimination via Validation

#### when model too 'powerful':

check performance carefully and honestly

## Overfitting Elimination via Validation when model too 'powerful':

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# SV	OOB
SVM/SVR	Random Forest

# Overfitting Elimination via Validation when model too 'powerful':

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# SV	OOB	Internal Validation
SVM/SVR	Random Forest	blending;
		DecTree pruning

## Overfitting Elimination via Validation when model too 'powerful':

#### check performance carefully and honestly

# SV	OOB	Internal Validation
SVM/SVR	Random Forest	blending;
		DecTree pruning

simple but necessary

#### Fun Time

What is the major technique for eliminating overfitting in Random Forest?

- voting/averaging
- 2 pruning
- early stopping
- weight-elimination

#### Fun Time

What is the major technique for eliminating overfitting in Random Forest?

- voting/averaging
- 2 pruning
- early stopping
- weight-elimination

#### Reference Answer: (1)

Random Forest, based on uniform blending, relies on voting/averaging for regularization.

Feature engineering and classifier ensemble for KDD Cup 2010, Yu et al., KDDCup 2010

linear blending of

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linear blending of

Logistic Regression + many rawly encoded features

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Logistic Regression + many rawly encoded features Random Forest + human-designed features

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linear blending of

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yes, you've learned everything! :-)

#### NTU KDDCup 2011 Track 1 World Champion Model

A linear ensemble of individual and blended models for music rating prediction, Chen et al., KDDCup 2011

NNet, DecTree-like, and then linear blending of

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Matrix Factorization variants, including probabilistic PCA

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#### NNet, DecTree-like, and then linear blending of

- Matrix Factorization variants, including probabilistic PCA
- Restricted Boltzmann Machines: an 'extended' autoencoder

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#### NNet, DecTree-like, and then linear blending of

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- Probabilistic Latent Semantic Analysis:

an extraction model that has 'soft clusters' as hidden variables

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- Probabilistic Latent Semantic Analysis: an extraction model that has 'soft clusters' as hidden variables
- linear regression, NNet, & GBDT

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#### yes, you can 'easily' understand everything! :-)

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Machine Learning Techniques

A two-stage ensemble of diverse models for advertisement ranking in KDD Cup 2012, Wu et al., KDDCup 2012

NNet, GBDT-like, and then linear blending of

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- Linear Regression variants, including linear SVR
- Logistic Regression variants

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- Linear Regression variants, including linear SVR
- Logistic Regression variants
- Matrix Factorization variants

• . . .

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NNet, GBDT-like, and then linear blending of

- Linear Regression variants, including linear SVR
- Logistic Regression variants
- Matrix Factorization variants

#### 'key' is to blend properly without overfitting

. . .

Machine Learning in Practice

#### NTU KDDCup 2013 Track 1 World Champion Model

Combination of feature engineering and ranking models for paperauthor identification in KDD Cup 2013, Li et al., KDDCup 2013

linear blending of

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- Random Forest with many many many trees
- GBDT variants

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Combination of feature engineering and ranking models for paperauthor identification in KDD Cup 2013, Li et al., KDDCup 2013

- linear blending of
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  - GBDT variants

with tons of efforts in designing features

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Combination of feature engineering and ranking models for paperauthor identification in KDD Cup 2013, Li et al., KDDCup 2013

- linear blending of
  - Random Forest with many many many trees
  - GBDT variants

with tons of efforts in designing features

'another key' is to construct features with domain knowledge

## 1 C4.5: another decision tree

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C4.5: another decision tree
2 k-Means

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- SVM

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- Apriori: for frequent itemset mining

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- 6 EM: 'alternating optimization' algorithm for some models

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- 2 k-Means
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- EM: 'alternating optimization' algorithm for some models

PageRank: for link-analysis, similar to matrix factorization

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- AdaBoost
- 8 k Nearest Neighbor

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- Apriori: for frequent itemset mining
- EM: 'alternating optimization' algorithm for some models

- PageRank: for link-analysis, similar to matrix factorization
- AdaBoost
- 8 k Nearest Neighbor
- Naive Bayes: a simple linear model with 'weights' decided by data statistics

- C4.5: another decision tree
- 2 k-Means
- 3 SVM
- Apriori: for frequent itemset mining
- EM: 'alternating optimization' algorithm for some models

- PageRank: for link-analysis, similar to matrix factorization
- AdaBoost
- 8 k Nearest Neighbor
- Naive Bayes: a simple linear model with 'weights' decided by data statistics

🕕 C&RT

- 1 C4.5: another decision tree
- 2 k-Means
- 3 SVM
- Apriori: for frequent itemset mining
- 5 EM: 'alternating optimization' algorithm for some models

- PageRank: for link-analysis, similar to matrix factorization
- AdaBoost
- 8 k Nearest Neighbor
- Naive Bayes: a simple linear model with 'weights' decided by data statistics

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personal view of five missing ML competitors: LinReg, LogReg, Random Forest, GBDT, NNet

#### Machine Learning Jungle

bagging support vector machine decision tree neural network kernel sparsity autoencoder aggregation functional gradient AdaBoost deep learning nearest neighbor uniform blending decision stump dual SVR quadratic programming prototype kernel LogReg large-margin GBDT matrix factorization Gaussian kernel PCA random forest **RBF network** probabilistic SVM k-means OOB error soft-margin

welcome to the jungle!

#### Fun Time

#### Which of the following is the official lucky number of this class?

- 9876
- 2 1234
- 3 1126
- 4 6211

#### Fun Time

#### Which of the following is the official lucky number of this class?



- 2 1234
- 3 1126
- 4 6211

#### Reference Answer: (3)

May the luckiness always be with you!

#### Summary

- Embedding Numerous Features: Kernel Models
- 2 Combining Predictive Features: Aggregation Models
- 8 Distilling Implicit Features: Extraction Models

#### Lecture 16: Finale

- Feature Exploitation Techniques
  kernel, aggregation, extraction, low-dimensional
- Error Optimization Techniques

gradient, equivalence, stages

Overfitting Elimination Techniques

(lots of) regularization, validation

• Machine Learning in Practice

welcome to the jungle

next: happy learning!