MACHINE LEARNING OVERVIEW



MACHINE LEARNING PROBLEMS



CLASSIFIER OVERVIEW

Representation	Evaluation	Optimization
Instances	Accuracy/Error rate	Combinatorial optimization
K-nearest neighbor	Precision and recall	Greedy search
Support vector machines	Squared error	Beam search
Hyperplanes	Likelihood	Branch-and-bound
Naive Bayes	Posterior probability	Continuous optimization
Logistic regression	Information gain	Unconstrained
Decision trees	K-L divergence	Gradient descent
Sets of rules	Cost/Utility	Conjugate gradient
Propositional rules	Margin	Quasi-Newton methods
Logic programs		Constrained
Neural networks		Linear programming
Graphical models		Quadratic programming
Bayesian networks		
Conditional random fields		

MANY CLASSIFIERS TO CHOOSE FROM

- **K-nearest neighbor**
- **Support Vector Machines**
- **Decision Trees**
- **Random Forrest**
- (Gradient) Boosted Decision Trees
- Logistic Regression
- Naïve Bayes
- **Bayesian network**
- RBMs
- • •

Which is the best one?

3-NEAREST NEIGHBOR



DECISION BOUNDARIES KNN

Assign label of nearest training data point to each test data point



from Duda et al.

Voronoi partitioning of feature space for two-category 2D and 3D data

MANY CLASSIFIERS TO CHOOSE FROM

K-nearest neighbor

- **Support Vector Machines**
- **Decision Trees**

Which is the best one?

Random Forrest

(Gradient) Boosted Decision Trees

- Logistic Regression
- Naïve Bayes
- **Bayesian network**

RBMs

• • • •

MAXIMUM MARGIN



The maximum margin linear classifier is the linear classifier with the, um, maximum margin. This is the simplest kind of SVM (Called an LSVM)

SUPPOSE WE'RE IN 1-DIMENSION





SUPPOSE WE'RE IN 1-DIMENSION

Not a big surprise



HARDER 1-DIMENSIONAL DATASET





THE KERNEL TRICK



V

THE KERNEL TRICK



[http://www.cs.berkeley.edu/~jordan/courses/281B-spring04/lectures/lec3.pdf]

SOFT MARGIN CLASSIFICATION



If the training data is not linearly separable, *slack variables* ξ_i (a regularization parameter) can be added to allow misclassification of difficult or noisy examples.

Still, try to minimize training set errors, and to place hyperplane "far" from each class (large margin)

Sec. 15.2.1

THE IMPACT OF REGULARIZATION





Right amount



Too much



SVM with a polynomial Kernel visualization

Created by: Udi Aharoni

https://www.youtube.com/watch?v=3liCbRZPrZA

MANY CLASSIFIERS TO CHOOSE FROM

- K-nearest neighbor
- **Support Vector Machines**
- **Decision Trees**

Which is the best one?

- **Random Forrest**
- (Gradient) Boosted Decision Trees
- **Logistic Regression**
- Naïve Bayes
- **Bayesian network**
- RBMs
- • •

TITANIC DATASET

survived	pclass	sex	age	sibsp	parch	fare	cabin	embarked
0	3	male	22	1	0	7.25		S
1	1	female	38	1	0	71.2833	C85	С
1	3	female	26	0	0	7.925		S
1	1	female	35	1	0	53.1	C123	S
0	3	male	35	0	0	8.05		S
0	3	male		0	0	8.4583		Q
0	1	male	54	0	0	51.8625	E46	S
0	3	male	2	3	1	21.075		S
1	3	female	27	0	2	11.1333		S
1	2	female	14	1	0	30.0708		С
1	3	female	4	1	1	16.7	G6	S
1	1	female	58	0	0	26.55	C103	S
0	3	male	20	0	0	8.05		S







```
IF sex='female' THEN survive=yes
ELSE IF sex='male' THEN survive = no
```

confusion matrix

no	yes	< classified a	as
468	109	no	
81	233	ves	

(468 + 233) / (468 + 109 + 81 + 233) = 79% correct (and 21% incorrect)

Not bad!

```
IF pclass='1' THEN survive=yes
ELSE IF pclass='2' THEN survive=yes
ELSE IF pclass='3' THEN survive=no
```

confusion matrix

no yes <-- classified as 372 119 | no 177 223 | yes

(372 + 223) / (372+119+223+177) = 67% correct (and 33% incorrect)

a little worse

ASIDE ON ENTROPY

Impurity/Entropy (informal)

Measures the level of impurity in a group of examples





Very impure group

Less impure





Minimum impurity



ENTROPY

• Entropy = $\prod_{i} \Box p_i \log_2 p_i$

p_i is the probability of class i Compute it as the proportion of class i in the set.

16/30 are green circles; 14/30 are pink crosses $log_2(16/30) = -.9;$ $log_2(14/30) = -1.1$ Entropy = -(16/30)(-.9) -(14/30)(-1.1) = .99

 Entropy comes from information theory. The higher the entropy the more the information content.

What does that mean for learning from examples?



What is the entropy if all examples belong to the same class?

- a) 0
- b) 1
- c) Infinite

2 CLASS EXAMPLE

 What is the entropy of a group in which all examples belong to the same class?

• What is the entropy of a group with 50% in either class?





EXAMPLE: ROLLING A DIE

$$p_1 = \frac{1}{6}, \ p_2 = \frac{1}{6}, \ p_3 = \frac{1}{6}, \ \dots$$

Entropy =
$$-\sum_{i} p_i \log_2 p_i$$

= $-6 \times \left(\frac{1}{6} \log_2 \frac{1}{6}\right)$

 ≈ 2.58



Has an unfair/weighted die a higher or lower entropy?

- A) Higher
- B) Lower

EXAMPLE: ROLLING A WEIGHTED DIE

$$p_1 = 0.1, p_2 = 0.1, p_3 = 0.1, \dots p_6 = 0.5$$

Entropy =
$$-\sum_{i} p_x \log_2 p_x$$

= $-5 \times (0.1 \log_2 0.1) - 0.5 \log_2 0.5$
= 2.16

The weighted die is has less uncertainty than a fair die

HOW UNCERTAIN IS YOUR DATA?

342/891 survivors in titanic training set

$$-\left(\frac{342}{891}\log_2\frac{342}{891} + \frac{549}{891}\log_2\frac{549}{891}\right) = 0.96$$

Say there were only 50 survivors

$$-\left(\frac{50}{891}\log_2\frac{50}{891} + \frac{841}{891}\log_2\frac{841}{891}\right) = 0.31$$

IN CLASS TASK

How can you use Entropy to build a decision tree.

Discuss with your neighbor(s)

Discuss the following ideas

Select the feature based on the highest entropy

Select the feature based on the lowest entropy

Stop splitting if the entropy is 0

Select the feature based on the entropy after the split

What if one group is under-/over represented

BACK TO DECISION TREES

Which attribute do we choose at each level?

The one with the highest information gain

• The one that reduces the uncertainty/impurity the most

We want to determine which attribute in a given set of training feature vectors is most useful for discriminating between the classes to be learned.

Information gain tells us how important a given attribute of the feature vectors is.

We will use it to decide the ordering of attributes in the nodes of a decision tree.

INFORMATION GAIN



Weighted Entropy: 466/1309 * 0.25 + 843 / 1309 * 0.21 = 0.22 Information Gain for split: 0.96 – 0.22 = 0.74
outlook	temperature	humidity	windy	play
overcast	cool	normal	TRUE	yes
overcast	hot	high	FALSE	yes
overcast	hot	normal	FALSE	yes
overcast	mild	high	TRUE	yes
rainy	cool	normal	TRUE	no
rainy	mild	high	TRUE	no
rainy	cool	normal	FALSE	yes
rainy	mild	high	FALSE	yes
rainy	mild	normal	FALSE	yes
sunny	hot	high	FALSE	no
sunny	hot	high	TRUE	no
sunny	mild	high	FALSE	no
sunny	cool	normal	FALSE	yes
sunny	mild	normal	TRUE	yes

$$-\left(\frac{9}{14}\log_2\frac{9}{14} + \frac{5}{14}\log_2\frac{5}{14}\right) = 0.94$$

If we choose **outlook**: overcast : 4 records, 4 are "yes" $-\left(\frac{4}{4}\log_2\frac{4}{4}\right) = 0$

rainy : 5 records, 3 are "yes" $-\left(\frac{3}{5}\log_2\frac{3}{5} + \frac{2}{5}\log_2\frac{2}{5}\right) = 0.97$

sunny : 5 records, 2 are "yes"

 $-\left(\frac{2}{5}\log_2\frac{2}{5} + \frac{3}{5}\log_2\frac{3}{5}\right) = 0.97$

Expected new entropy:

$$\frac{4}{14} \times 0.0 + \frac{5}{14} \times 0.97 + \frac{5}{14} \times 0.97$$

= 0.69

37

outlook	temperature	humidity	windy	play
overcast	cool	normal	TRUE	yes
overcast	hot	high	FALSE	yes
overcast	hot	normal	FALSE	yes
overcast	mild	high	TRUE	yes
rainy	cool	normal	TRUE	no
rainy	mild	high	TRUE	no
rainy	cool	normal	FALSE	yes
rainy	mild	high	FALSE	yes
rainy	mild	normal	FALSE	yes
sunny	hot	high	FALSE	no
sunny	hot	high	TRUE	no
sunny	mild	high	FALSE	no
sunny	cool	normal	FALSE	yes
sunny	mild	normal	TRUE	yes

$$-\left(\frac{9}{14}\log_2\frac{9}{14} + \frac{5}{14}\log_2\frac{5}{14}\right) = 0.94$$

Clicker:

If we choose windy, what is the expected entropy?

a) 0.81

```
= - (6/8 \log(6/8) + 2/8 \log(2/8))
```

```
b) 0.89
= 6/14 * 1 +
    (-8/14* (6/8 log(6/8) + 2/8 log(2/8)))
```

c) 1
= - (0.5 * log(0.5)+0.5 * log(0.5))

outlook	temperature	humidity	windy	play
overcast	cool	normal	TRUE	yes
overcast	hot	high	FALSE	yes
overcast	hot	normal	FALSE	yes
overcast	mild	high	TRUE	yes
rainy	cool	normal	TRUE	no
rainy	mild	high	TRUE	no
rainy	cool	normal	FALSE	yes
rainy	mild	high	FALSE	yes
rainy	mild	normal	FALSE	yes
sunny	hot	high	FALSE	no
sunny	hot	high	TRUE	no
sunny	mild	high	FALSE	no
sunny	cool	normal	FALSE	yes
sunny	mild	normal	TRUE	yes

$$-\left(\frac{9}{14}\log_2\frac{9}{14} + \frac{5}{14}\log_2\frac{5}{14}\right) = 0.94$$

If we choose windy: FALSE: 8 records, 6 are "yes" 0.81 = -(6/8*log(6/8)+2/8*log(2/8))

TRUE: 6 records, 3 are "yes"

1

Expected new entropy:

0.81(8/14) + 1 (6/14)

temperature	humidity	windy	play	
cool	normal	TRUE	yes	
hot	high	FALSE	yes	
hot	normal	FALSE	yes	
mild	high	TRUE	yes	
cool	normal	TRUE	no	
mild	high	TRUE	no	
cool	normal	FALSE	yes	
mild	high	FALSE	yes	
mild	normal	FALSE	yes	
hot	high	FALSE	no	
hot	high	TRUE	no	
mild	high	FALSE	no	
cool	normal	FALSE	yes	
mild	normal	TRUE	yes	
	temperature cool hot hot cool mild cool mild cool mild hot hot hot mild cool mild	temperaturehumiditycoolnormalhothighhotnormalhotnormalmildhighcoolnormalmildhighcoolnormalmildhighcoolnormalmildhighhothighhothighhothighmildhighnormalhighmildnormalmildhighmildnormalmildnormalmildnormalmildnormal	temperaturehumiditywindycoolnormalTRUEhothighFALSEhotnormalFALSEmildhighTRUEcoolnormalTRUEcoolnormalTRUEmildhighTRUEcoolnormalFALSEmildhighFALSEmildhighFALSEmildhighFALSEhothighFALSEhothighTRUEmildhighTRUEmildhighFALSEhothighFALSEmildhighFALSEmildnormalFALSEmildnormalFALSEmildnormalFALSEmildnormalTRUEmildnormalFALSEmildnormalTRUE	temperaturehumiditywindyplaycoolnormalTRUEyeshothighFALSEyeshotnormalFALSEyesmildhighTRUEyescoolnormalTRUEnomildhighTRUEnomildhighTRUEnocoolnormalFALSEyesmildhighFALSEyesmildhighFALSEyesmildnormalFALSEyeshothighTRUEnohothighTRUEnomildhighFALSEyesmildhighFALSEnomildhighFALSEyesmildhighFALSEyesmildhighFALSEyesmildhighFALSEyesmildnormalFALSEyesmildnormalFALSEyesmildnormalFALSEyesmildnormalFALSEyesmildnormalFALSEyesmildnormalFALSEyesmildnormalFALSEyesmildnormalFALSEyesmildnormalFALSEyesmildnormalFALSEyesmildnormalFALSEyesmildnormalFALSEyesmildnormalFALSEyes

$$-\left(\frac{9}{14}\log_2\frac{9}{14} + \frac{5}{14}\log_2\frac{5}{14}\right) = 0.94$$



40

outlook	temperature	humidity	windy	play	
overcast	cool	normal	TRUE	yes	
overcast	hot	high	FALSE	yes	
overcast	hot	normal	FALSE	yes	
overcast	mild	high	TRUE	yes	
rainy	cool	normal	TRUE	no	
rainy	mild	high	TRUE	no	
rainy	cool	normal	FALSE	yes	
rainy	mild	high	FALSE	yes	
rainy	mild	normal	FALSE	yes	
sunny	hot	high	FALSE	no	
sunny	hot	high	TRUE	no	
sunny	mild	high	FALSE	no	
sunny	cool	normal	FALSE	yes	
sunny	mild	normal	TRUE	yes	

$$-\left(\frac{9}{14}\log_2\frac{9}{14} + \frac{5}{14}\log_2\frac{5}{14}\right) = 0.94$$

If we choose **humidity**: normal : 7 records, 6 are "yes"

0.59

high : 7 records, 2 are "yes"

0.86

Expected new entropy:

0.59(7/14) + 0.86(7/14)

= <u>0.725</u>

outlook	temperature	humidity	windy	play
overcast	cool	normal	TRUE	yes
overcast	hot	high	FALSE	yes
overcast	hot	normal	FALSE	yes
overcast	mild	high	TRUE	yes
rainy	cool	normal	TRUE	no
rainy	mild	high	TRUE	no
rainy	cool	normal	FALSE	yes
rainy	mild	high	FALSE	yes
rainy	mild	normal	FALSE	yes
sunny	hot	high	FALSE	no
sunny	hot	high	TRUE	no
sunny	mild	high	FALSE	no
sunny	cool	normal	FALSE	yes
sunny	mild	normal	TRUE	yes

$$-\left(\frac{9}{14}\log_2\frac{9}{14} + \frac{5}{14}\log_2\frac{5}{14}\right) = 0.94$$

outlook

0.94 - 0.69 = 0.25	highest gain
--------------------	--------------

temperature

0.94 - 0.91 = 0.03

humidity

0.94 - 0.725 = 0.215

windy

0.94 - 0.87 = 0.07

DOCUMENT CLASSIFICATION



Clicker Question (assuming equal size):a) Falcon's Information Gain is higherb) Mars' Information Gain is higher

BUILDING A DECISION TREE (ID3 ALGORITHM)

Assume attributes are discrete

• Discretize continuous attributes

Choose the attribute with the highest Information Gain

Create branches for each value of attribute

Examples partitioned based on selected attributes

Repeat with remaining attributes

Stopping conditions

- All examples assigned the same label
- No examples left



Expensive to train

Prone to overfitting

- Drive to perfection on training data, bad on test data
- Pruning can help: remove or aggregate subtrees that provide little discriminatory power (C45)

C4.5 EXTENSIONS

Continuous Attributes

outlook	temperature	humidity	windy	play
overcast	cool	60	TRUE	yes
overcast	hot	80	FALSE	yes
overcast	hot	63	FALSE	yes
overcast	mild	81	TRUE	yes
rainy	cool	58	TRUE	no
rainy	mild	90	TRUE	no
rainy	cool	54	FALSE	yes
rainy	mild	92	FALSE	yes
rainy	mild	59	FALSE	yes
sunny	hot	90	FALSE	no
sunny	hot	89	TRUE	no
sunny	mild	90	FALSE	no
sunny	cool	60	FALSE	yes
sunny	mild	62	TRUE	yes

Consider every possible binary partition; choose the partition with the highest gain



Expect = $10/14*0.47 + 4/14*0^{\bigcirc}$ = 0.33

PERFORMANCE OF DIFFERENT ML MODEL FAMILIES



IN-CLASS TASK



How would you draw the expected decision boundary for

- Random Forrest
- SVM w/ kernel and regularization
- 1-KNN





The decision boundary looks like the one of:

- a) Random Forrest
- b) SVM w/ kernel and regularization
- c) 1-KNN





The decision boundary looks like the one of:

- a) Random Forrest
- b) SVM w/ kernel and regularization
- c) 1-KNN

RANDOM FORREST



The decision boundary looks like the one of:

- a) Random Forrest
- b) SVM w/ kernel and regularization
- c) 1-KNN

MACHINE LEARNING PROBLEMS



LINEAR REGRESSION



POLYNOMIAL REGRESSION



С С

DECISION TREE - REGRESSION





PERFORMANCE



Machine Learnin



What if you model has an high error?

- Try getting more training examples
- Try smaller sets of features
- Try getting additional features
- Try creating features from existing features (kernels)
- Try decrease regularization
- Try increase regularization

What Error/Quality Metric to use?

Classification:

- Accuracy
- F-score
- F1-micro
- F1-macro
- ROC AUC (micro, macro)
- ...

Regression

- Mean-Squared Error
- Root-Mean Squared Error
- Mean absolute Error
- R²
- Cohen Kappa
- •

••

Precision, Recall, Accuracy

	True	False
True	tp	fp
False	fn	tn

- Precision: correctly identified positive cases
 Precision P = tp/(tp + fp)
- **Recall**: correctly identified positive cases from all the actual positive cases.

Recall R = tp/(tp + fn)

• Accuracy: measure of all the correctly identified cases Accuracy R = (tp+tn)/(tp + fp + fn + tn)

Evaluation: Accuracy isn't always enough

• How do you interpret 90% accuracy?

Evaluation: Accuracy isn't always enough

- How do you interpret 90% accuracy?
 - You can't; it depends on the problem
- Need a baseline:
 - Base Rate
 - Accuracy of trivially predicting the most-frequent class
 - Random Rate
 - Accuracy of making a random class assignment
 - Might apply prior knowledge to assign random distribution
 - Naïve Rate
 - Accuracy of some simple default or pre-existing model
 - Ex: "All females survived"

Why Optimize? Pitfalls



What Error/Quality Metric to use?

Classification:

- Accuracy
- F-score
- F1-micro
- F1-macro
- ROC AUC (micro, macro)
- ...

Regression

- Mean-Squared Error
- Root-Mean Squared Error
- Mean absolute Error
- R²
- Cohen Kappa

•

. .

Precision, Recall, Accuracy

		True Label		
		True	False	
Predicted	True	tp	fp	
Label	False	fn	tn	

- Precision: correctly identified positive cases
 Precision P = tp/(tp + fp)
- **Recall**: correctly identified positive cases from all the actual positive cases.

Recall R = tp/(tp + fn)

• **F-Score:** is the harmonic mean of precision and recall

$$F = \frac{2}{\frac{1}{R} + \frac{1}{P}} = \frac{tp}{tp + \frac{1}{2}(fp + fn)}$$

F1 Micro

		True Label		
		L1	L2	L3
Predicted	L1	7	1	4
Label	L2	0	1	12
	L3	1	6	6

Precision micro: true positives for all the classes divided by the all positive predictions Precision Score Micro = TP / (TP + FP) TP = (7 + 1 + 6)FP = 1 + 4 + 0 + 12 + 1 + 6

Recall micro: Sum of **true positives for all the classes** divided by the actual positives. Recall Score Micro: TP / (TP + FN)

F1 Score:
$$\frac{tp}{tp+\frac{1}{2}(fp+fn)}$$

Macro

F1 Macro

		True Label		
		L1	L2	L3
Predicted	L1	7	1	4
Label	L2	0	1	12
	L3	1	6	6

Precision micro: arithmetic mean of all the precision scores of different classes Precision Score Macro = ((7/8) + (1/8) + (6/22))/3

Recall micro: arithmetic mean of all the recall scores .

When to use F1 Micro and when to use F1 Macro?

F1 Macro

		True Label		
		L1	L2	L3
Predicted Label	L1	7	1	4
	L2	0	1	12
	L3	1	6	6

Precision micro: **arithmetic mean of all the precision scores** of different classes Precision Score Macro = ((7/8) + (1/8) + (6/22))/3

Recall micro: arithmetic mean of all the recall scores .

When to use F1 Micro and when to use F1 Macro?

- Micro weights each instance or prediction equally.
- Macro weights each class equally (better for imbalance of labels)
- Use weighted macro-averaging score in case of class imbalances (different number of instances related to different class labels).

ROC AUC

(usually used for models with a threshold)



False Positive Rate (FP / FP + TN)

What would be the ideal ROC curve? How would a random guess look like

ROC AUC

(usually used for models with a threshold)



What if your model has a high error?

- Try getting more training examples
- Try smaller sets of features
- Try getting additional features
- Try creating features from existing features (kernels)
- Try decrease regularization
- Try increase regularization


Training set M















Training set M





Training set M





Training set M





Training set M

Training Set (m)



Clicker:

Test error

- a) decreases with M
- b) increases with M
- c) stays constant





Training set M



Training Set (m)



High Bias



Training set M

High Bias



Training set M

Clicker: If you have high-bias, does more data help?

- a) No
- b) Yes

High Variance



Clicker: If you have high-variance, does more data help?

- a) No
- b) Yes

1. Get more training examples

- 2. Try smaller sets of features
- 3. Try getting additional features
- 4. Try adding polynomial features (kernels)
- 5. Try increase regularization
- 6. Try decrease regularization

- A. High Variance
- B. High Bias
- C. Both
- D. None

- 1. Get more training examples
- 2. Try smaller sets of features
- 3. Try getting additional features
- 4. Try adding polynomial features (kernels)
- 5. Try increase regularization
- 6. Try decrease regularization

- A. High Variance
- B. High Bias
- C. Both
- D. None

- 1. Get more training examples
- 2. Try smaller sets of features
- 3. Try getting additional features
- 4. Try adding polynomial features (kernels)
- 5. Try increase regularization
- 6. Try decrease regularization

- A. High Variance
- B. High Bias
- C. Both
- D. None

- 1. Get more training examples
- 2. Try smaller sets of features
- 3. Try getting additional features
- 4. Try adding polynomial features (kernels)
- 5. Try increase regularization
- 6. Try decrease regularization

- A. High Variance
- B. High Bias
- C. Both
- D. None

- 1. Get more training examples
- 2. Try smaller sets of features
- 3. Try getting additional features
- 4. Try adding polynomial features (kernels)
- 5. Try increase regularization
- 6. Try decrease regularization

- A. High Variance
- B. High Bias
- C. Both
- D. None

- 1. Get more training examples
- 2. Try smaller sets of features
- 3. Try getting additional features
- 4. Try adding polynomial features (kernels)
- 5. Try increase regularization
- 6. Try decrease regularization

- A. High Variance
- B. High Bias
- C. Both
- D. None

Cross-validation

k-fold: split the data into k groups, train on every group except for one, which you test on.

Repeat for all groups



Parameter Tuning

Grid Search







Training set size



Training set size





Training set size





Can we prune now?



Algorithm 1 training error > Algorithm 2 validation error

Northstar's (now Einblick) AutoML

Built for *interactive results*, unlike all other Auto-ML tools, which can take hours to produce results



https://staging.einblick.ai/?w=6228f27140d515321ee4d967