Evaluating Machine-Learning Methods

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Computer Sciences 760
Spring 2018

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Some of the slides in these lectures have been adapted/borrowed from materials developed by Tom Dietterich, Pedro Domingos, Tom Mitchell, David Page, and Jude Shavlik

Goals for the lecture

you should understand the following concepts

- bias of an estimator
- test sets
- learning curves
- stratified sampling
- cross validation
- confusion matrices
- TP, FP, TN, FN
- ROC curves
- precision-recall curves
- recall/sensitivity/true positive rate (TPR)
- precision/positive predictive value (PPV)
- specificity and false positive rate (FPR or 1-specificity)

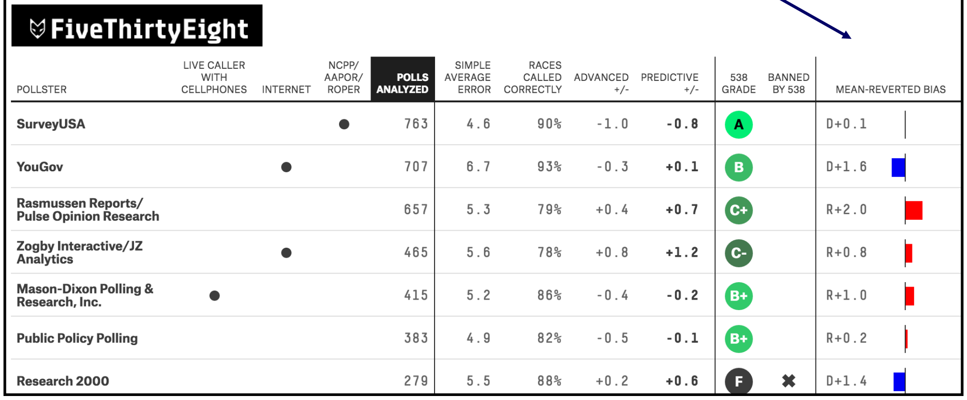
Bias of an estimator

θ true value of parameter of interest (e.g. model accuracy)

$\hat{\theta}$ estimator of parameter of interest (e.g. test set accuracy)

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

e.g. polling methodologies often have an inherent bias

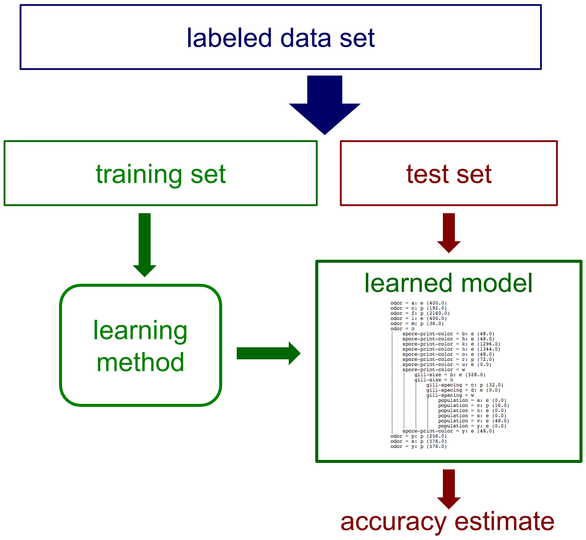


FiveThirtyEight

POLLSTER	LIVE CALLER WITH CELLPHONES	INTERNET	NCPP/ AAPOR/ ROPER	POLLS ANALYZED	SIMPLE AVERAGE ERROR	RACES CALLED CORRECTLY	ADVANCED +/-	PREDICTIVE +/-	538 GRADE	BANNED BY 538	MEAN-REVERTED BIAS
SurveyUSA			●	763	4.6	90%	-1.0	**-0.8**	A		D+0.1
YouGov		●		707	6.7	93%	-0.3	**+0.1**	B		D+1.6
Rasmussen Reports/ Pulse Opinion Research				657	5.3	79%	+0.4	**+0.7**	C+		R+2.0
Zogby Interactive/JZ Analytics		●		465	5.6	78%	+0.8	**+1.2**	C-		R+0.8
Mason-Dixon Polling & Research, Inc.	●			415	5.2	86%	-0.4	**-0.2**	B+		R+1.0
Public Policy Polling				383	4.9	82%	-0.5	**-0.1**	B+		R+0.2
Research 2000				279	5.5	88%	+0.2	**+0.6**	F	✖	D+1.4

Test sets revisited

How can we get an <u>unbiased</u> estimate of the accuracy of a learned model?



labeled data set

training set

test set

learning method

learned model

accuracy estimate

Test sets revisited

How can we get an unbiased estimate of the accuracy of a learned model?

- when learning a model, you should pretend that you don’t have the test data yet (it is “in the mail”)*
- if the test-set labels influence the learned model in any way, accuracy estimates will be biased

* In some applications it is reasonable to assume that you have access to the feature vector (i.e. x) but not the y part of each test instance.

Learning curves

How does the accuracy of a learning method change as a function of the training-set size?

this can be assessed by plotting *learning curves*

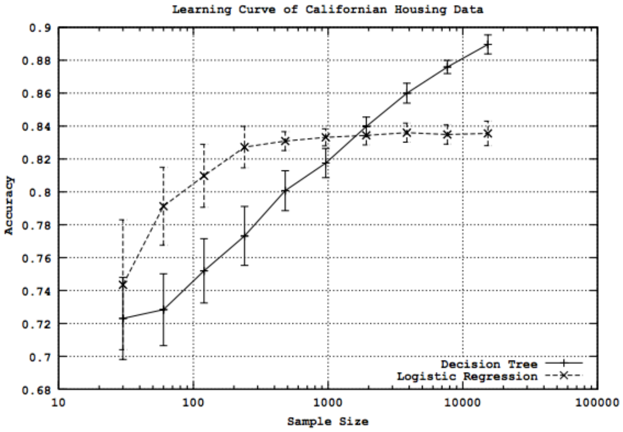
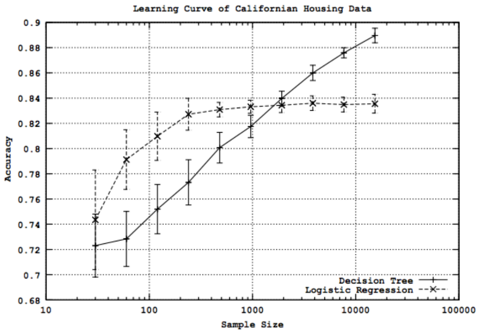


Figure from Perlich et al. *Journal of Machine Learning Research*, 2003

Learning curves

given training/test set partition

- for each sample size s on learning curve
  - (optionally) repeat n times
    - randomly select s instances from training set
    - learn model
    - evaluate model on test set to determine accuracy a
    - plot (s, a) or (s, avg. accuracy and error bars)



Limitations of using a single training/test partition

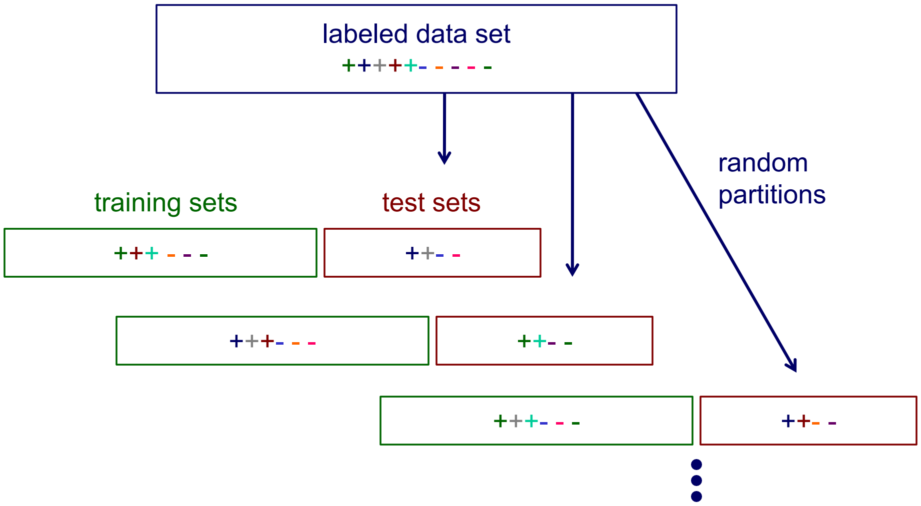
- we may not have enough data to make sufficiently large training and test sets
  - a <u>larger test set</u> gives us more reliable estimate of accuracy (i.e. a lower variance estimate)
  - but… a <u>larger training set</u> will be more representative of how much data we actually have for learning process
- a single training set doesn’t tell us how sensitive accuracy is to a particular training sample

Using multiple training/test partitions

- two general approaches for doing this
  - random resampling
  - cross validation

Random resampling

We can address the second issue by repeatedly randomly partitioning the available data into training and set sets.



labeled data set

+++++- - - - -

random partitions

training sets

test sets

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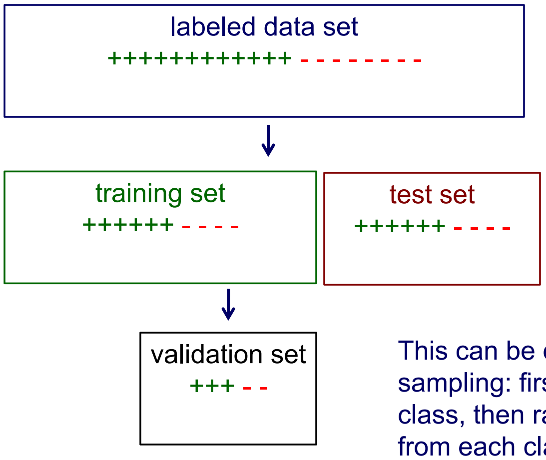
Stratified sampling

When randomly selecting training or validation sets, we may want to ensure that class proportions are maintained in each selected set



labeled data set
++++++++++++ - - - - - - - - -

training set
++++++ - - - -

test set
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validation set
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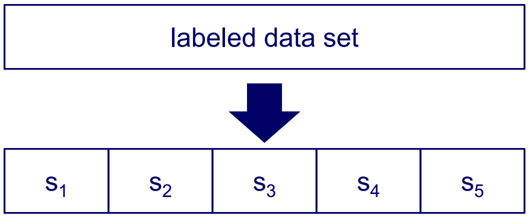
This can be done via stratified sampling: first stratify instances by class, then randomly select instances from each class proportionally.

Cross validation

partition data into *n* subsamples



labeled data set

s_1 s_2 s_3 s_4 s_5

iteratively leave one subsample out for the test set, train on the rest

iteration	train on	test on
1	s_2 s_3 s_4 s_5	s_1
2	s_1 s_3 s_4 s_5	s_2
3	s_1 s_2 s_4 s_5	s_3
4	s_1 s_2 s_3 s_5	s_4
5	s_1 s_2 s_3 s_4	s_5

Cross validation example

Suppose we have 100 instances, and we want to estimate accuracy with cross validation

iteration	**train on**	**test on**	**correct**
1	s_2 s_3 s_4 s_5	s_1	11 / 20
2	s_1 s_3 s_4 s_5	s_2	17 / 20
3	s_1 s_2 s_4 s_5	s_3	16 / 20
4	s_1 s_2 s_3 s_5	s_4	13 / 20
5	s_1 s_2 s_3 s_4	s_5	16 / 20

accuracy = 73/100 = 73%

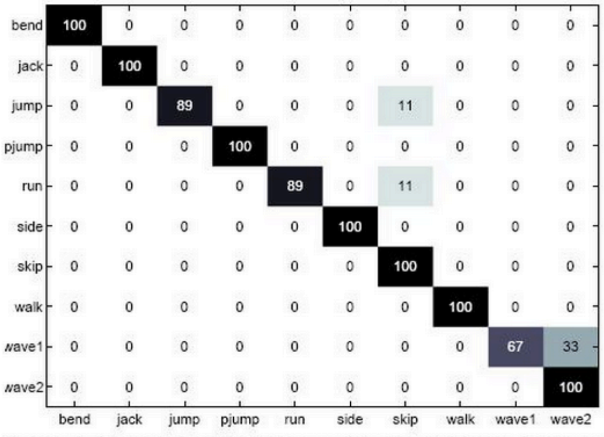
Cross validation

- 10-fold cross validation is common, but smaller values of *n* are often used when learning takes a lot of time
- in *leave-one-out* cross validation, *n* = # instances
- in *stratified* cross validation, stratified sampling is used when partitioning the data
- CV makes efficient use of the available data for testing
- note that whenever we use multiple training sets, as in CV and random resampling, we are evaluating a learning method as opposed to an individual learned model

Confusion matrices

How can we understand what types of mistakes a learned model makes?

task: activity recognition from video



actual class

	bend	jack	jump	pjump	run	side	skip	walk	wave1	wave2
bend	100	0	0	0	0	0	0	0	0	0
jack	0	100	0	0	0	0	0	0	0	0
jump	0	0	89	0	0	0	11	0	0	0
pjump	0	0	0	100	0	0	0	0	0	0
run	0	0	0	0	89	0	11	0	0	0
side	0	0	0	0	0	100	0	0	0	0
skip	0	0	0	0	0	0	100	0	0	0
walk	0	0	0	0	0	0	0	100	0	0
wave1	0	0	0	0	0	0	0	0	67	33
wave2	0	0	0	0	0	0	0	0	0	100

predicted class

figure from vision.jhu.edu

Confusion matrix for 2-class problems

actual class

predicted class		positive	negative
	positive	true positives (TP)	false positives (FP)
	negative	false negatives (FN)	true negatives (TN)

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

$$\text{error} = 1 - \text{accuracy} = \frac{\text{FP} + \text{FN}}{\text{TP} + \text{FP} + \text{FN} + \text{TN}}$$

Is accuracy an adequate measure of predictive performance?

accuracy may not be useful measure in cases where

- there is a large class skew
  - Is 98% accuracy good when 97% of the instances are negative?
- there are differential misclassification costs – say, getting a positive wrong costs more than getting a negative wrong
  - Consider a medical domain in which a false positive results in an extraneous test but a false negative results in a failure to treat a disease
- we are most interested in a subset of high-confidence predictions

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Other accuracy metrics

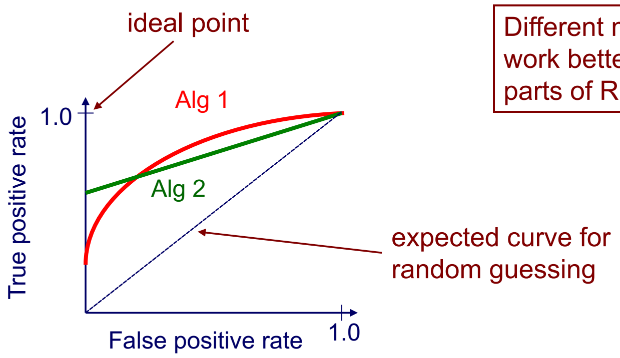
		actual class	
		positive	negative
predicted class	positive	true positives (TP)	false positives (FP)
	negative	false negatives (FN)	true negatives (TN)

$$\text{true positive rate (recall)} = \frac{\text{TP}}{\text{actual pos}} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$\text{false positive rate} = \frac{\text{FP}}{\text{actual neg}} = \frac{\text{FP}}{\text{TN} + \text{FP}}$$

ROC curves

A *Receiver Operating Characteristic* (*ROC*) curve plots the TP-rate vs. the FP-rate as a threshold on the confidence of an instance being positive is varied



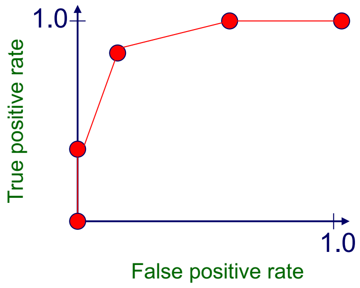
Different methods can work better in different parts of ROC space.

Algorithm for creating an ROC curve

```
let $\left(\left(y^{(1)}, c^{(1)}\right) \ldots \left(y^{(m)}, c^{(m)}\right)\right)$ be the test-set instances sorted according to predicted confidence $c^{(i)}$ that each instance is positive
let $num\_neg$, $num\_pos$ be the number of negative/positive instances in the test set
$TP = 0$, $FP = 0$
$last\_TP = 0$
for $i = 1$ to $m$
    // find thresholds where there is a pos instance on high side, neg instance on low side
    if ($i > 1$) and ( $c^{(i)} \neq c^{(i-1)}$ ) and ( $y^{(i)}$ == neg ) and ( $TP > last\_TP$ )
            $FPR = FP \,/\, num\_neg$,   $TPR = TP \,/\, num\_pos$
        output ($FPR$, $TPR$) coordinate
        $last\_TP = TP$
    if $y^{(i)}$ == pos
        $++TP$
    else
        $++FP$
$FPR = FP \,/\, num\_neg$,  $TPR = TP \,/\, num\_pos$
output ($FPR$, $TPR$) coordinate
```

Plotting an ROC curve

instance	confidence positive		correct class
Ex 9	.99		+
Ex 7	.98	TPR= 2/5, FPR= 0/5	+
Ex 1	.72		-
Ex 2	.70		+
Ex 6	.65	TPR= 4/5, FPR= 1/5	+
Ex 10	.51		-
Ex 3	.39		-
Ex 5	.24	TPR= 5/5, FPR= 3/5	+
Ex 4	.11		-
Ex 8	.01	TPR= 5/5, FPR= 5/5	-



ROC curve example

task: recognizing genomic units called operons

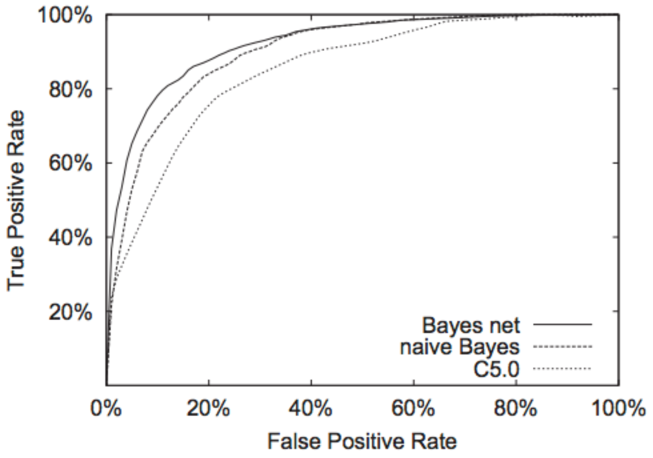
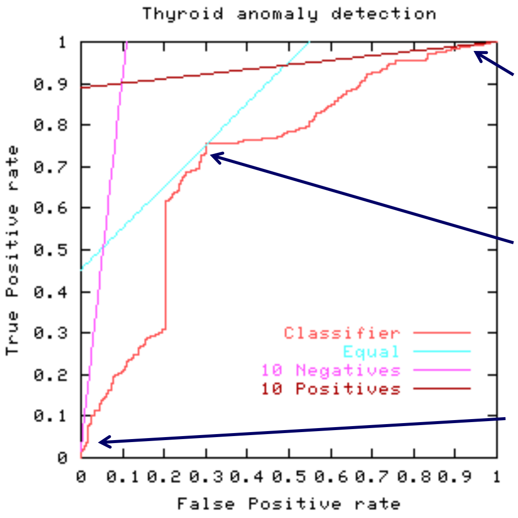


figure from Bockhorst et al., *Bioinformatics* 2003

ROC curves and misclassification costs

The best operating point depends on the relative costs of FN and FP misclassifications



best operating point when FN costs 10× FP

best operating point when cost of misclassifying positives and negatives is equal

best operating point when FP costs 10× FN

ROC curves

Does a low false-positive rate indicate that most positive predictions (i.e. predictions with confidence > some threshold) are correct?

suppose our TPR is 0.9, and FPR is 0.01

fraction of instances that are positive	fraction of positive predictions that are correct
0.5	0.989
0.1	0.909
0.01	0.476
0.001	0.083

Other accuracy metrics

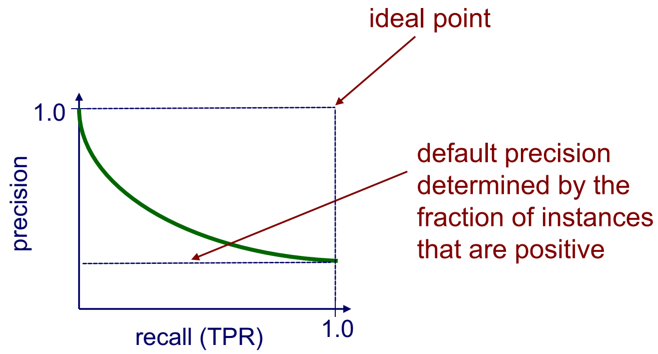
		actual class	
		positive	negative
predicted class	positive	true positives (TP)	false positives (FP)
	negative	false negatives (FN)	true negatives (TN)

$$\text{recall (TP rate)} = \frac{\text{TP}}{\text{actual pos}} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$\text{precision (positive predictive value)} = \frac{\text{TP}}{\text{predicted pos}} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$

Precision/recall curves

A *precision/recall curve* plots the precision vs. recall (TP-rate) as a threshold on the confidence of an instance being positive is varied



ideal point

default precision determined by the fraction of instances that are positive

Precision/recall curve example

predicting patient risk for VTE

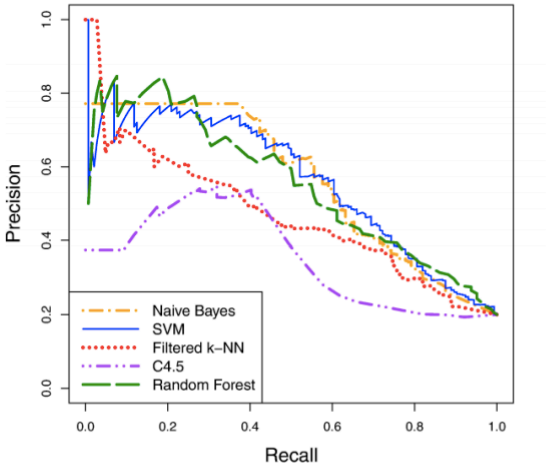


figure from Kawaler et al., *Proc. of AMIA Annual Symosium,* 2012

How do we get one ROC/PR curve when we do cross validation?

Approach 1

- make assumption that confidence values are comparable across folds
- pool predictions from all test sets
- plot the curve from the pooled predictions

Approach 2 (for ROC curves)

- plot individual curves for all test sets
- view each curve as a function
- plot the average curve for this set of functions

Comments on ROC and PR curves

both

- allow predictive performance to be assessed at various levels of confidence
- assume binary classification tasks
- sometimes summarized by calculating *area under the curve*

ROC curves

- insensitive to changes in class distribution (ROC curve does not change if the proportion of positive and negative instances in the test set are varied)
- can identify optimal classification thresholds for tasks with differential misclassification costs

precision/recall curves

- show the fraction of predictions that are false positives
- well suited for tasks with lots of negative instances