Data Mining: Model Evaluation

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Model Evaluation

- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?
- Methods for Performance Evaluation
  - How to obtain reliable estimates?
- Methods for Model Comparison
  - How to compare the relative performance among competing models?

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Metrics for Performance Evaluation (1)

- Focus on the predictive capability of a model
  - Rather than how fast it takes to classify or build models, scalability, etc.
- Confusion Matrix:

	PREDICTED CLASS		
ACTUAL CLASS		Class=Yes	Class=No
	Class=Yes	TP	FN
	Class=No	FP	TN

TP: true positive

FN: false negative

FP: false positive

TN: true negative

- FP: falsely predicted to be positive (thus actual class is negative)
- FN: falsely predicted to be negative (thus actual class is positive)

Metrics for Performance Evaluation (2)

		PREDICTED CLASS	
ACTUAL CLASS		Class=Yes	Class=No
	Class=Yes	TP	FN
	Class=No	FP	TN

- Most widely-used metric:

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

Limitation of Accuracy

- Consider a 2-class problem
  - Number of Class 0 examples = 9990
  - Number of Class 1 examples = 10
- If model predicts everything to be class 0, the accuracy is 9990/10000 = 99.9 %
  - Accuracy is misleading because model does not detect any class 1 example
  - Should always at least compare with baseline accuracy!

Cost Matrix

	PREDICTED CLASS		
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	C(Yes|Yes)	C(No|Yes)
	Class=No	C(Yes|No)	C(No|No)

- $C(i|j)$: Cost of misclassifying class j example as class i
- Cost of misclassifying a healthy subject as a patient typically lower than vice versa

Computing Cost of Classification

Cost Matrix	PREDICTED CLASS		
ACTUAL CLASS	*C(i|j)*	**+**	**-**
	+	0	100
	-	2	1

Model M_1	PREDICTED CLASS		
ACTUAL CLASS		**+**	**-**
	+	90	10
	-	90	210

Accuracy = 75%

Cost = 1390

Model M_2	PREDICTED CLASS		
ACTUAL CLASS		**+**	**-**
	+	70	30
	-	50	250

Accuracy = 80%

Cost = 3350

Cost-Sensitive Measures

- Precision: of all samples predicted to be positive predictions, what fraction is actually positive? Biased towards *C*(Yes|Yes) & *C*(Yes|No)

$$\text{Precision (p)} = \frac{TP}{TP + FP}$$

- Recall: of all actually positive samples, what fraction is predicted to be positive? Biased towards *C*(Yes|Yes) & *C*(No|Yes)

$$\text{Recall (r)} = \frac{TP}{TP + FN}$$

- F-measure balances Precision and Recall

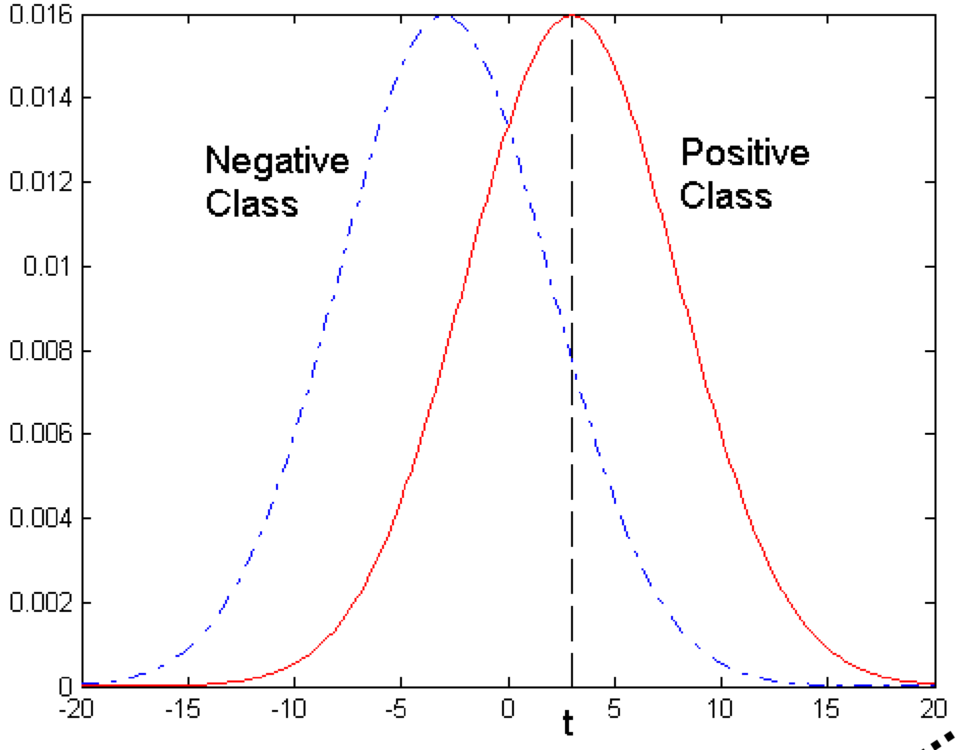
$$\text{F - measure (F)} = \frac{2rp}{r + p} = \frac{2TP}{2TP + FP + FN}$$

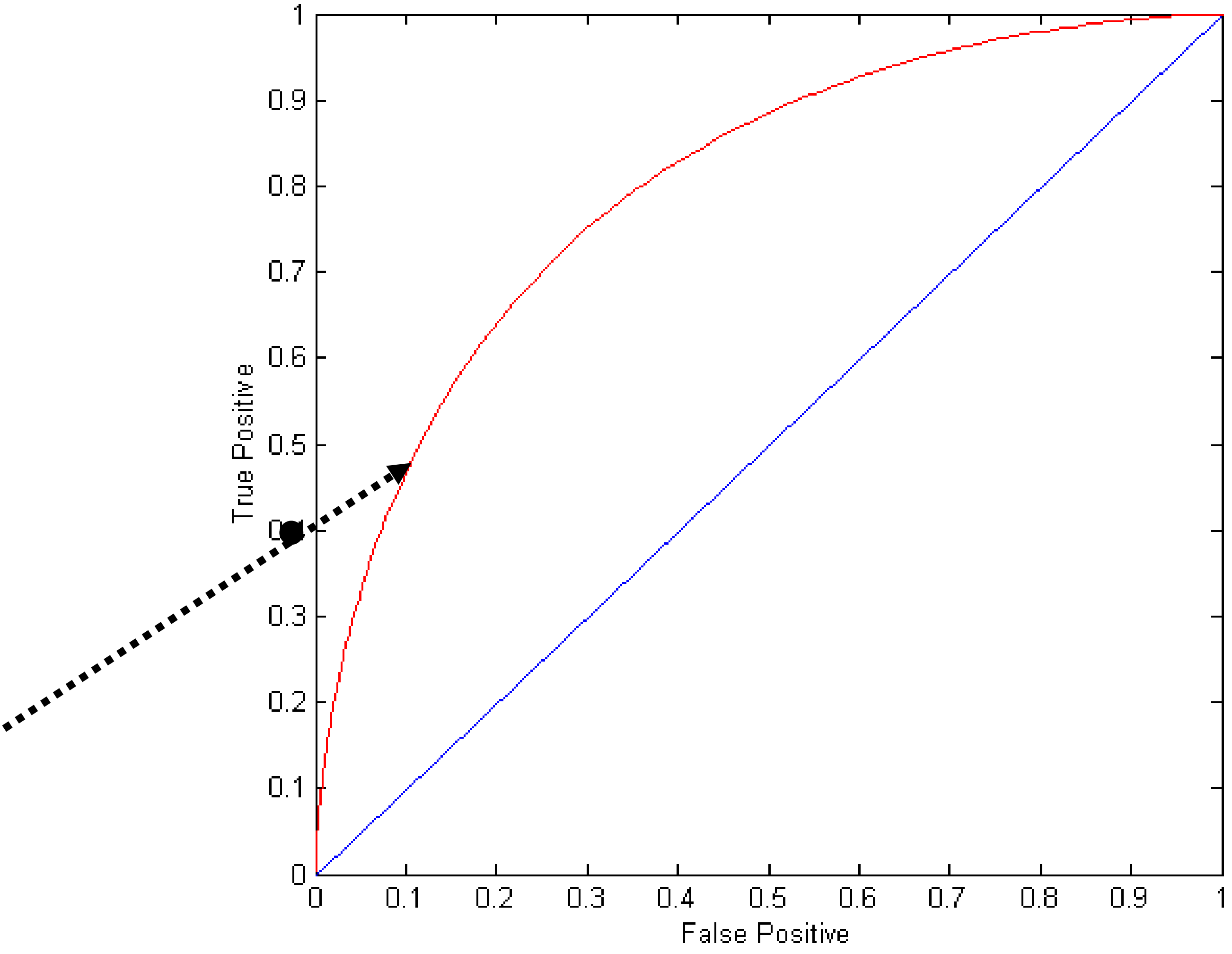
Receiver Operating Characteristics (ROC)

- Developed in 1950s for signal detection theory to analyze noisy signals
  - Characterizes the trade-off between positive hits and false alarms
- ROC curve plots TP rate (on the y-axis) against FP rate (on the x-axis)
- TP rate = TP/(TP + FN) = recall = sensitivity
  fraction of positive examples correctly classified as positive
- FP rate = FP/(FP + TN) = 1 – specificity
  fraction of negative examples incorrectly classified as positive
- Performance of each classifier represented as a point on the ROC curve
- Changing the threshold of the algorithm changes the location of the point

ROC Curve (1)

- One-dimensional data set containing 2 classes (positive and negative)
- Points located at *x* > *t* classified as positive

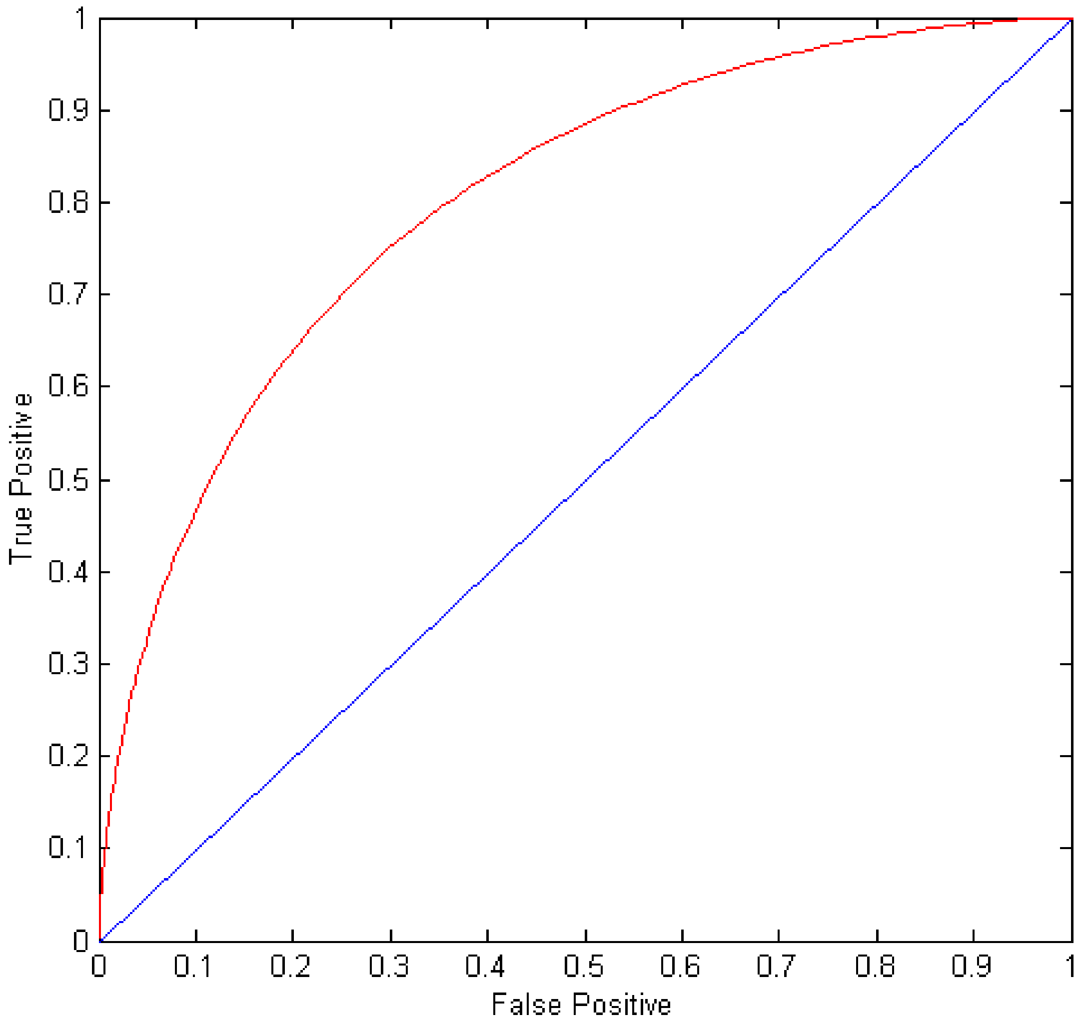




At threshold t:

TP rate=0.5, FN rate=0.5,
FP rate=0.12, TN rate=0.88

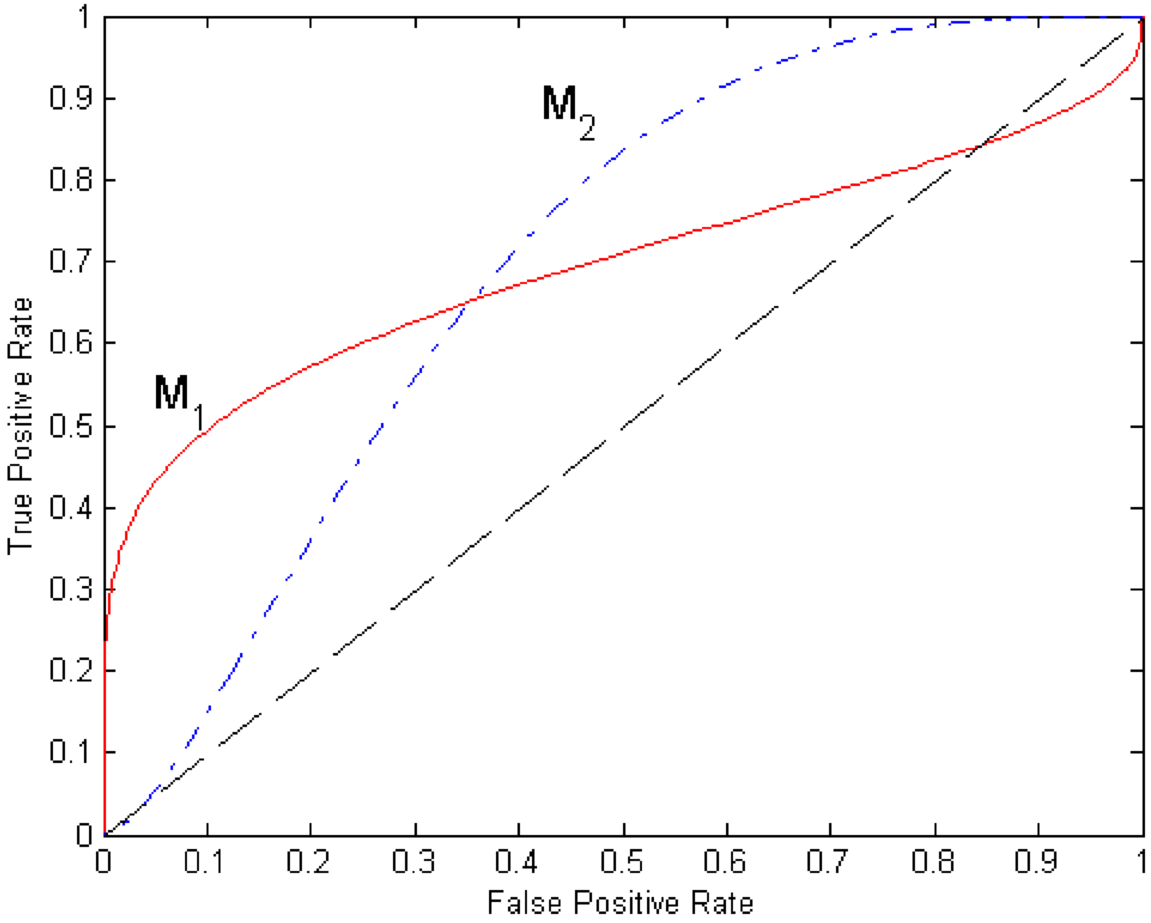
ROC Curve (2)



- (TP,FP):
  - (0,0): declare everything to be negative class
  - (1,1): declare everything to be positive class
  - (1,0): ideal
- Diagonal line:
  - Random guessing
- Below diagonal line:
  - Prediction is opposite of the true class

Using ROC for Model Comparison

- No model consistently outperforms the other
  - M_1 is better for small FPR
  - M_2 is better for large FPR



- Area Under the ROC Curve (AUC)
  - Ideal: area = 1
  - Random guess: area = 0.5

How to Construct an ROC curve (1)

Instance	*P*(+|*A*)	True Class
1	1	+
2	0.93	+
3	0.87	-
4	0.85	+
5	0.85	-
6	0.85	-
7	0.76	-
8	0.53	+
9	0.43	-
10	0.25	+

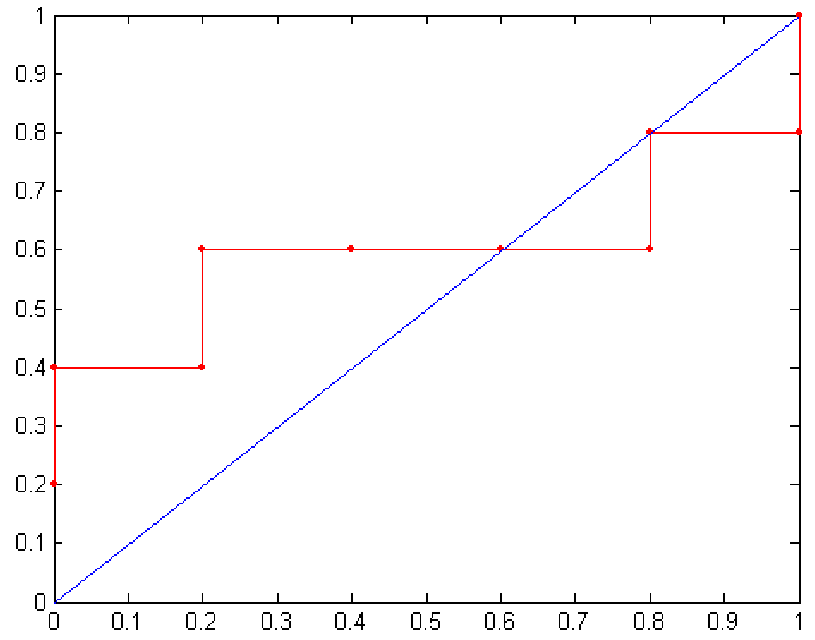
- Use classifier that produces posterior probability for each test instance *P*(+|*A*)
- Sort the instances according to *P*(+|*A*) in decreasing order
- Apply threshold at each unique value of *P*(+|*A*)
- Count the number of TP, FP, TN, FN at each threshold
- TP rate, TPR = TP/(TP + FN)
- FP rate, FPR = FP/(FP + TN)

How to Construct an ROC curve (2)

Class	**+**	**-**	**+**	**-**	**-**	**-**	**+**	**-**	**+**	**+**	
Threshold ≥	**0.25**	**0.43**	**0.53**	**0.76**	**0.85**	**0.85**	**0.85**	**0.87**	**0.93**	**0.95**	**1.00**
TP	**5**	**4**	**4**	**3**	**3**	**3**	**3**	**2**	**2**	**1**	**0**
FP	**5**	**5**	**4**	**4**	**3**	**2**	**1**	**1**	**0**	**0**	**0**
TN	**0**	**0**	**1**	**1**	**2**	**3**	**4**	**4**	**5**	**5**	**5**
FN	**0**	**1**	**1**	**2**	**2**	**2**	**2**	**3**	**3**	**4**	**5**
TPR	**1**	**0.8**	**0.8**	**0.6**	**0.6**	**0.6**	**0.6**	**0.4**	**0.4**	**0.2**	**0**
FPR	**1**	**1**	**0.8**	**0.8**	**0.6**	**0.4**	**0.2**	**0.2**	**0**	**0**	**0**

Instance	***P*(+|*A*)**	**True Class**
1	1	+
2	0.93	+
3	0.87	-
4	0.85	+
5	0.85	-
6	0.85	-
7	0.76	-
8	0.53	+
9	0.43	-
10	0.25	+

ROC Curve:



ROC in MATLAB

```
% t: actual outputs (targets)
% y: continuous predictions


% compute true/false positive rates and thresholds

[tpr,fpr,th] = roc(t,y)

% directly plot ROC curve

plotroc(t,y)
```

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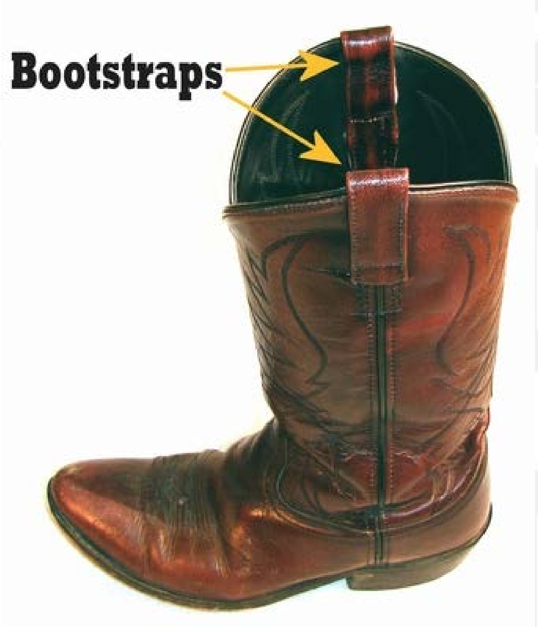
Methods of Estimation

- Holdout
  - Reserve, e.g., 2/3 for training and 1/3 for testing
  - Fine for huge data sets
- Random subsampling
  - Repeated holdout
- Cross-validation
  - Partition data into *k* disjoint subsets
  - k-fold: train on *k*-1 partitions, test on the remaining one
  - Leave-one-out: *k*=*n* with *n* the number of samples
  - Better than holdout for small data sets
- Bootstrap
  - Sampling with replacement



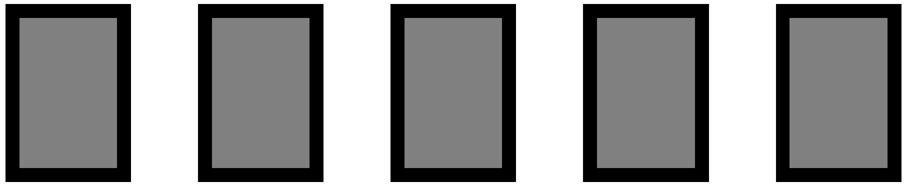
“pull oneself over a fence
by one's bootstraps”

Cross-Validation

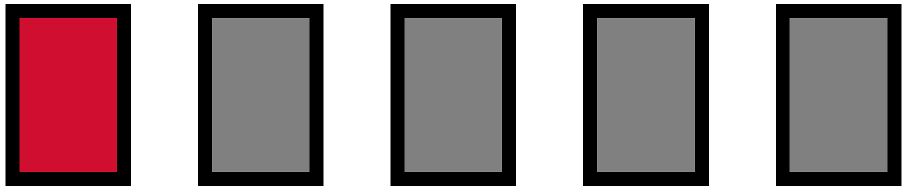
- Advantage over holdout: all data used for training and testing
- Predictions on test folds can be concatenated and can then be treated as if they are predictions on an independent test set, e.g., for making an ROC curve
- Ideal for comparing classifiers on relatively small data sets
- Make sure to use the same splits for all classifiers
- Can make use of sign test to check significance of difference in performance between classifiers (more later)

Cross-validation Example

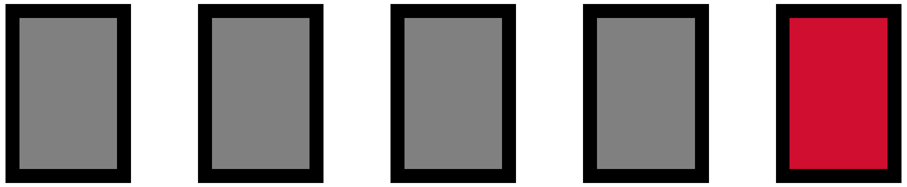
- Break up data into groups of the same size



- Hold aside one group for testing and use the rest to build model



- Repeat



Stratified Ten-fold Cross-validation

- Standard method for evaluation: stratified ten-fold cross-validation
- Why ten? Works fine in practice and not too computationally intensive
- Stratification, i.e., keeping the same class distribution across folds, reduces the estimate's variance
- Even better: repeated stratified cross-validation
  - E.g. ten-fold cross-validation is repeated ten times and results are averaged (reduces the variance)

The Bootstrap

- CV uses sampling without replacement
  - The same instance, once selected, cannot be selected again for a particular training/test set

- The bootstrap uses sampling with replacement to form the training set
  - Sample a dataset of *n* instances *n* times with replacement to form a new dataset of *n* instances
  - Use this data as the training set
  - Use the instances from the original dataset that don’t occur in the new training set for testing

- A particular instance has a probability of 1–1/*n* of not being picked
  - Thus its probability of ending up in the test data is: $\left(1-\frac{1}{n}\right)^n \approx e^{-1} = 0.368$
  - This means the training data will contain approximately 63.2% of the instances

Estimating Error with the Bootstrap

- The error estimate on the test data will be very pessimistic
  - Trained on just ~63% of the instances
- Therefore, combine it with the training error:

$$err = 0.632 \cdot e_{\text{test}} + 0.368 \cdot e_{\text{training}}$$

- The training error gets less weight than the error on the test data
- Repeat process several times with different replacement samples; average the results
- Referred to as the 0.632 bootstrap estimator

General Issues

- Unbalanced data
- Tuning “hyperparameters”
- Learning curves

Unbalanced Data

- Sometimes, classes have very unequal frequency
  - medical diagnosis: 90% healthy, 10% disease
  - eCommerce: 99% don't buy, 1% buy
  - Security: >99.99% of Americans are not terrorists
- Majority class classifier can be very close to 100% correct, but is still completely useless…
- Measuring performance by ROC at least helps a bit
- Alternative is to construct balanced train and test sets, and train model on a balanced set
  - consider all minority class instances
  - add equal number of randomly selected samples from the majority class

Tuning Hyperparameters

- Many classification methods contain "hyperparameters", e.g., the maximum depth of the tree, the number of hidden units in a neural network, the regularization parameter in support vector machines, the number of nearest neighbors in *k* nearest neighbors

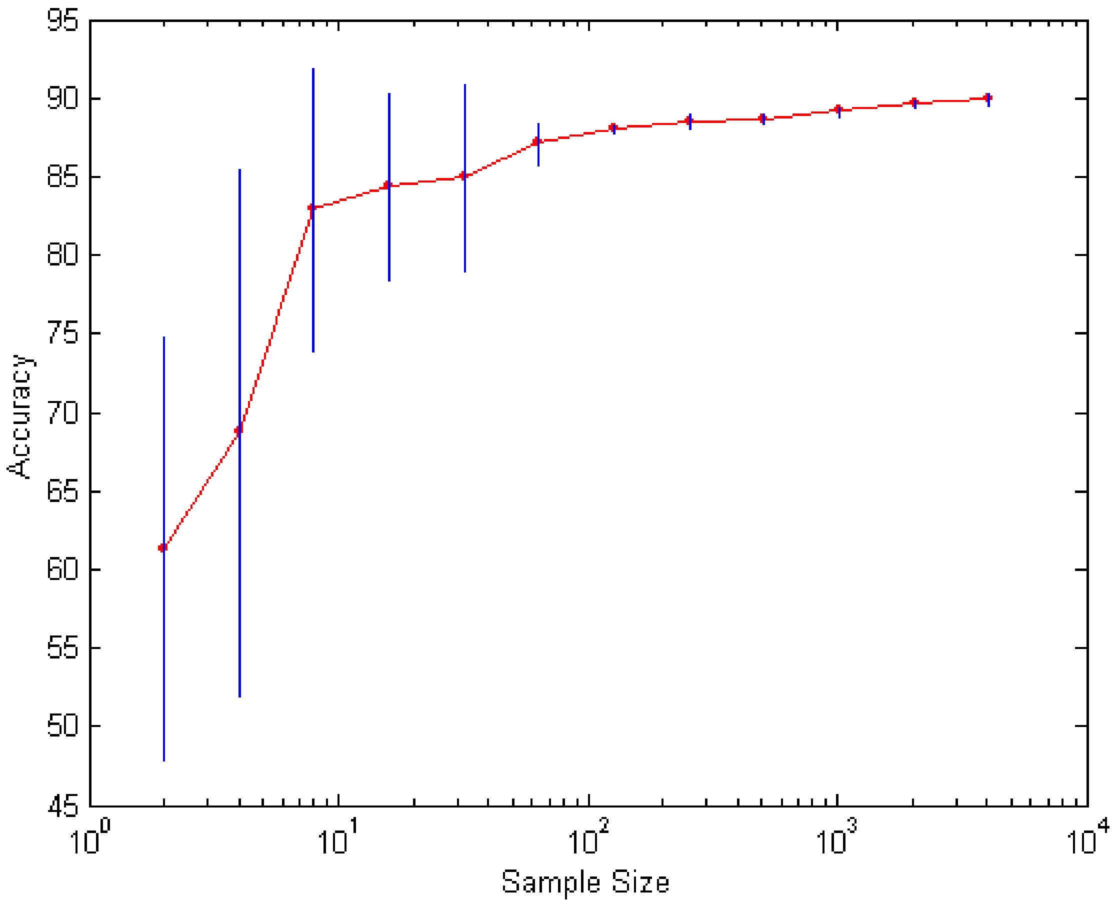
- Test data should not be used in any way to tune the hyperparameters!

- Proper procedure uses three sets: training data, validation data, and test data, e.g., ten-fold cross-validation with
  - 9 folds for combined training and validation and 1 fold for testing
  - within the data available for training and validation another ten-fold cross-validation to tune the hyperparameters

- Conceptually, you use "inner" cross-validation to optimize the hyperparameters and "outer" cross-validation to estimate the generalization of the whole procedure (including the optimization of the hyperparameters)

Learning Curves

- Learning curve shows how accuracy changes with varying sample size
- Can be constructed by subsampling smaller data sets from the full data set
- Useful to check whether collecting more data may still further improve performance



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Two Classifiers, Single Test Set

- Given a test set with the true class and the predictions of the two models:

Instance	M_1	M_2	True Class
1	+	+	+
2	+	+	+
3	+	-	-
4	-	-	-
5	-	-	-
6	+	-	+
7	-	+	-
8	-	-	+
9	+	+	-
…	…	….	…

- Translate to table with correct/wrong:

$\mathbf{M_2}$

$\mathbf{M_1}$

	correct	wrong	
correct	50	6	56
wrong	14	30	44
	64	36	

NB: this part deviates from the book, which considers two classifiers on different test sets, which is silly and hardly ever occurs in practice

Example 1

M_2

		correct	wrong	
M_1	correct	50	9	59
	wrong	11	30	41
		61	39	

- Is M_2 significantly better than M_1 at significance level 0.05?

Example 2

$\mathbf{M_2}$

		correct	wrong	
$\mathbf{M_1}$	correct	5000	900	5900
	wrong	1100	3000	4100
		6100	3900	

- Is M_2 significantly better than M_1 at significance level 0.05?

Example 3

$\mathbf{M_2}$

		correct	wrong	
$\mathbf{M_1}$	correct	50	0	50
	wrong	10	40	50
		60	40	

- Is M_2 significantly better than M_1 at significance level 0.05?

Example 4

$\mathbf{M_2}$

		correct	wrong	
$\mathbf{M_1}$	correct	80	0	80
	wrong	10	10	20
		90	10	

- Is M_2 significantly better than M_1 at significance level 0.05?

Example 5

		$\mathbf{M_2}$		
		correct	wrong	
$\mathbf{M_1}$	correct	5	0	5
	wrong	2	3	5
		7	3	

- Is M_2 significantly better than M_1 at significance level 0.05?

Example 6

$\mathbf{M_2}$

$\mathbf{M_1}$

	correct	wrong	
correct	50	6	56
wrong	14	30	44
	64	36	

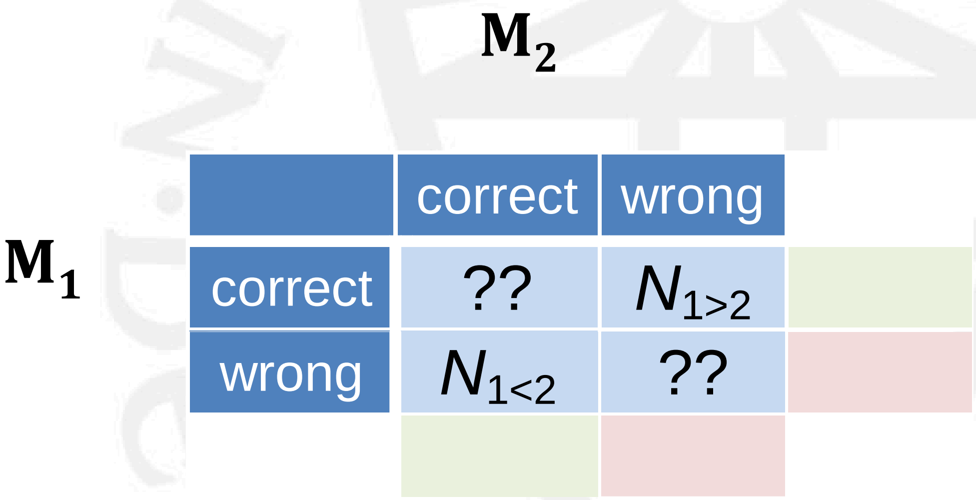
- Is M_2 significantly better than M_1 at significance level 0.05?

Sign Test (1)

- General test for difference in the median between paired samples
- Non-parametric: makes no assumptions about distribution
- x_1 = 1 if M_1 is correct, x_1 = 0 if M_1 is wrong; similar for x_2
- Is the median of x_2 larger than the median of x_1?
- Null hypothesis: for a random pair of samples, x_1 and x_2 are equally likely to be larger than the other

Sign Test (2)

- Call $N_{1<2}$ the number of samples for which M_2 is correct and M_1 is incorrect
- Samples for which $x_1 = x_2$ can be omitted: only $N_{1<2}$ and $N_{1>2}$ matter!
- Boils down to a binomial test:
  - Null hypothesis: fair "coin", $p = 0.5$
  - Test statistic: $W = N_{1<2}$
  - Under the null hypothesis, the test statistic follows a binomial distribution with number of draws $N = N_{1<2} + N_{1>2}$
- One-sided alternative: $M_2 > M_1$, i.e., $p > 0.5$
- Two-sided alternative: $M_2 \neq M_1$, i.e., $p \neq 0.5$



$\mathbf{M_2}$

		correct	wrong	
$\mathbf{M_1}$	correct	??	$N_{1>2}$	🟩
	wrong	$N_{1<2}$	??	🟥
		🟩	🟥	

Example 1

$\mathbf{M}_2$

$\mathbf{M}_1$

	correct	wrong	
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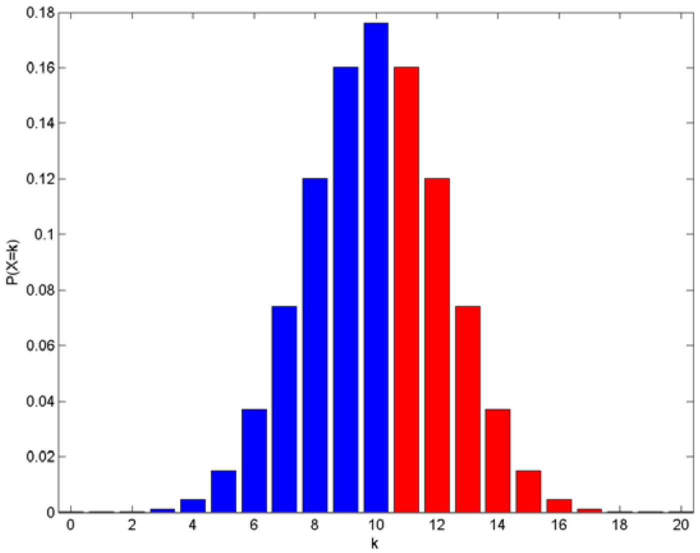
	61	39	



`Binocdf(10,20,0.5)`

$P(W \geq 11)$

- $N = 20$ draws
- P-value = $P(W \geq 11)$ = `1-Binocdf(10,20,0.5)`= 0.4199 > 0.05
- Clearly not significant

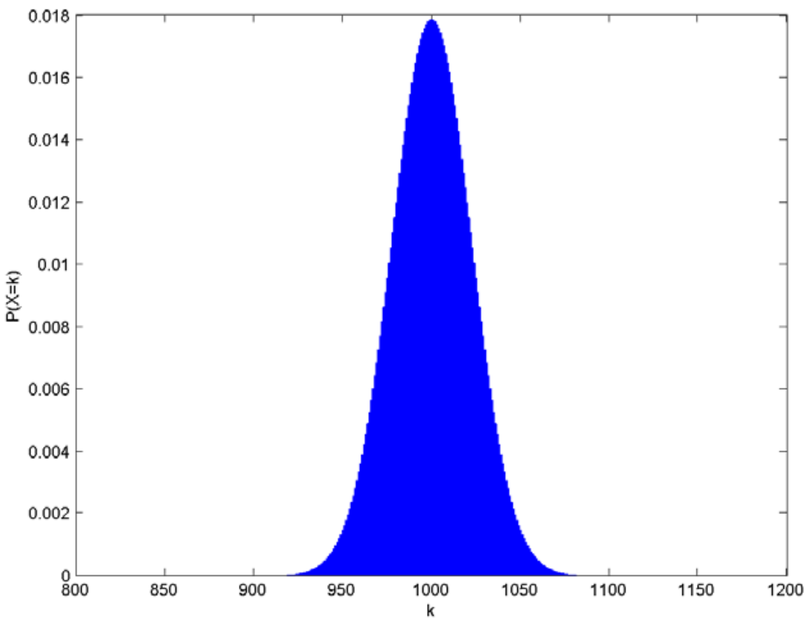
null hypothesis: $p = 0.5$

Example 2

$\mathbf{M}_2$

$\mathbf{M}_1$

	correct	wrong	
correct	5000	900	5900
wrong	1100	3000	4100
	6100	3900	



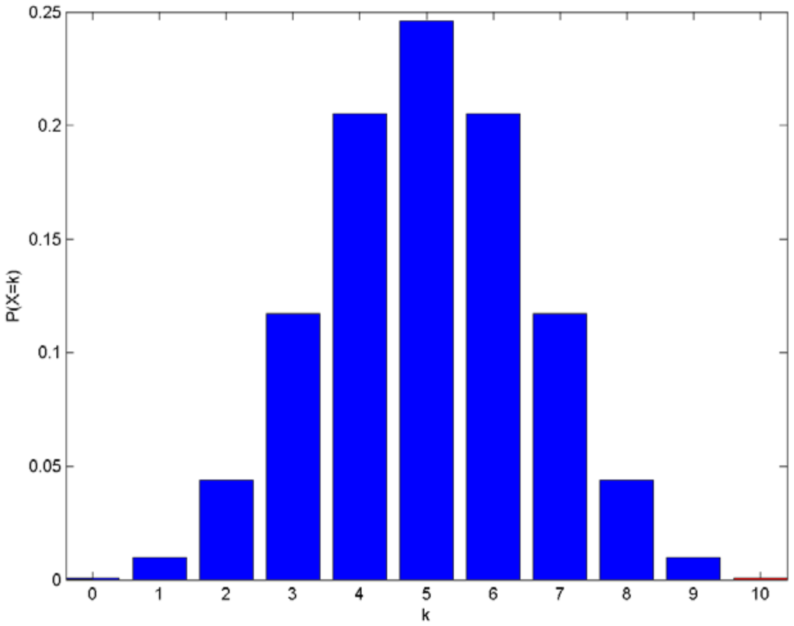
- N = 2000 draws
- P-value = $P(W \geq 1100)$ = `1-Binocdf(1099,2000,0.5)`= $4.23 \times 10^{-6} < 0.05$
- Clearly significant

Example 3

$\mathbf{M_2}$

$\mathbf{M_1}$

	correct	wrong	
correct	50	0	50
wrong	10	40	50
	60	40	

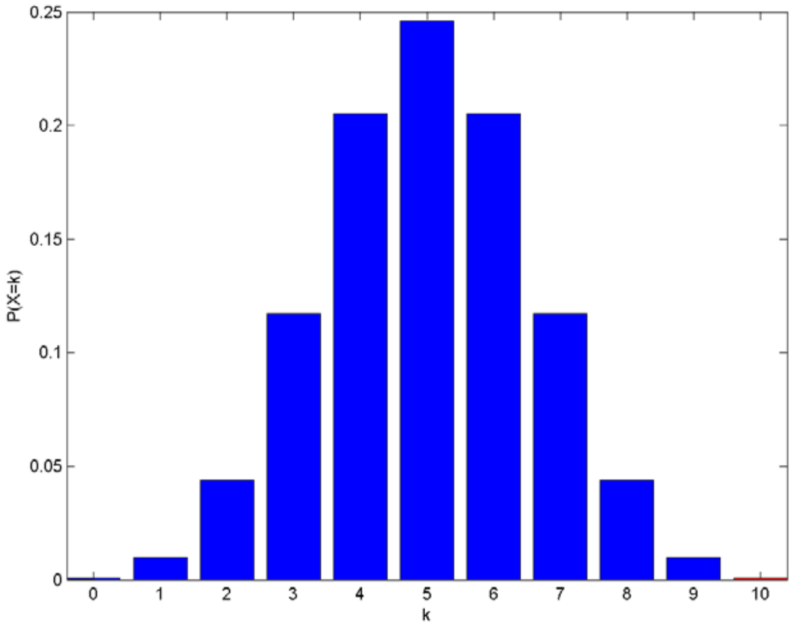


- $N = 10$ draws
- P-value = $P(W \geq 10)$ = `1-Binocdf(9,10,0.5)`= 9.77×10^{-4} (= 2^{-10}) < 0.05
- Clearly significant

Example 4

$\mathbf{M_2}$

		correct	wrong	
$\mathbf{M_1}$	correct	80	0	80
	wrong	10	10	20
		90	10	

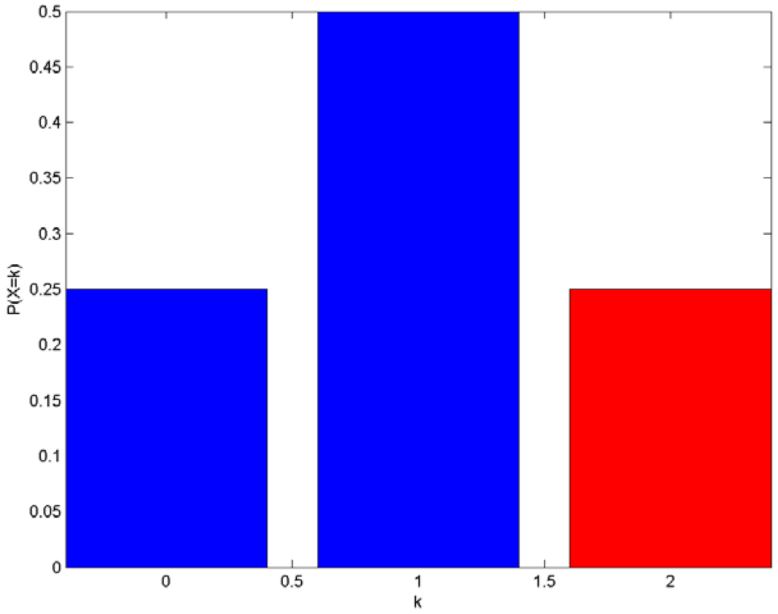


- N = 10 draws: same as before
- P-value = $P(W \geq 10)$ = `1-Binocdf(9,10,0.5)`= 9.77×10^{-4} (= 2^{-10}) < 0.05
- Clearly significant

Example 5

$\mathbf{M}_2$

		correct	wrong	
$\mathbf{M}_1$	correct	5	0	5
	wrong	2	3	5
		7	3	



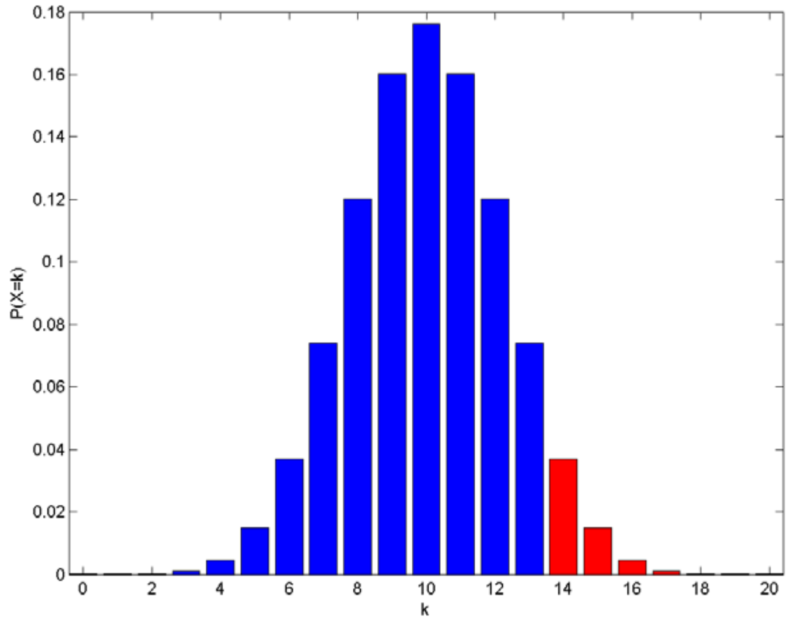
- $N = 2$ draws
- P-value = $P(W \geq 2)$ = `1-Binocdf(1,2,0.5)`= 0.25 (= 2^{-2}) > 0.05
- Clearly not significant

Example 6

$\mathbf{M}_2$

$\mathbf{M}_1$

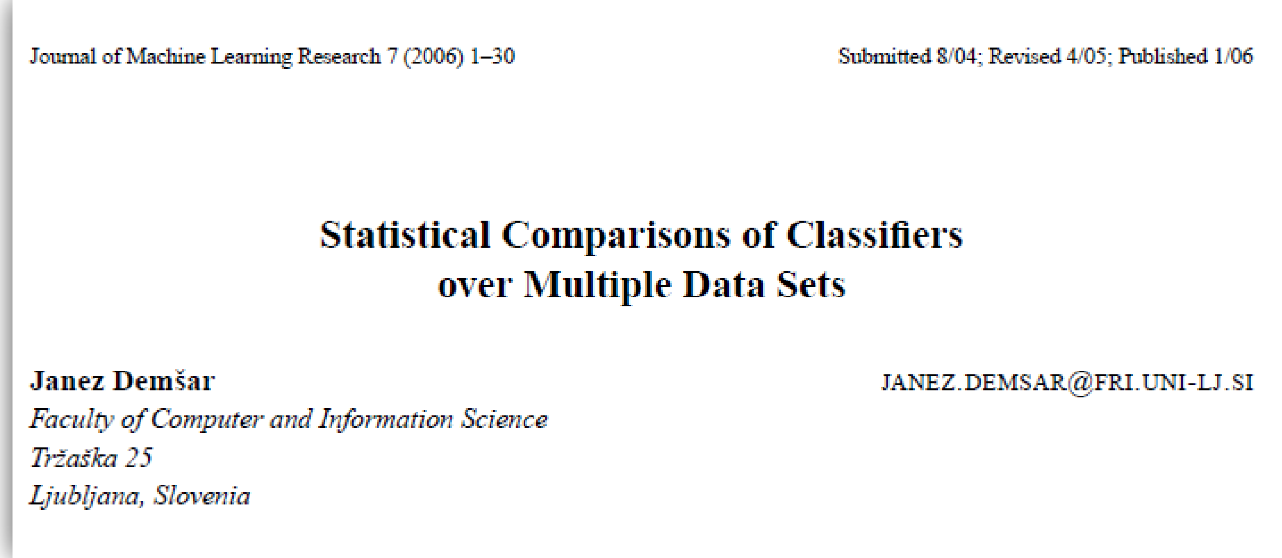
	correct	wrong	
correct	50	6	56
wrong	14	30	44
	64	36	



- $N = 20$ draws
- P-value = $P(W \geq 14)$ = `1-Binocdf(13,20,0.5)`= 0.0577 > 0.05
- Just not significant

Two Classifiers, Multiple Test Sets

- Standard practice: compare different classifiers on a whole range of problems, e.g., from the UCI repository
- Simplest idea: use the sign test, but now on complete test sets instead of test samples
- Now $N_{1<2}$ is the number of test sets on which M_2 does better than M_1
- The Wilcoxon signed-rank test also takes into account how much better a classifier does
- Demšar, JMLR 2006, is the key reference, also for comparing multiple classifiers on multiple test sets



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Statistical Comparisons of Classifiers over Multiple Data Sets

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