For written notes on this lecture, please read chapter 3 of *The Practical Bioinformatician,*

CS2220: Introduction to Computational Biology

Unit 1a: Essence of Knowledge Discovery

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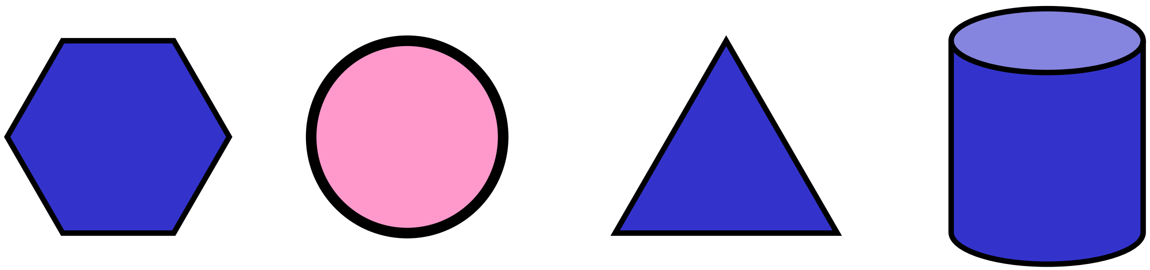
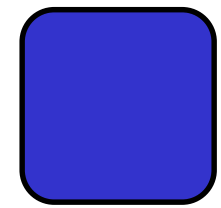
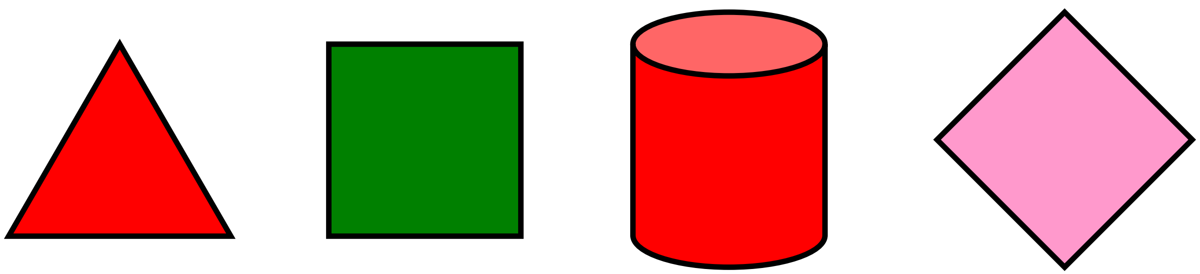
What is knowledge discovery?

Jonathan’s blocks





Jessica’s blocks



Whose block is this?

Jonathan’s rules : Blue or Circle
Jessica’s rules : All the rest

What is knowledge discovery?




Question: Can you explain how?

Key steps

- **Training data gathering**
- **Feature generation**
  - k-grams, colour, texture, domain know-how, ...
- **Feature selection**
  - Entropy, $\chi 2$, CFS, t-test, domain know-how...
- **Feature integration**
  - SVM, ANN, PCL, CART, C4.5, kNN, ...

Some classifiers / machine learning methods

What is accuracy?

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What is accuracy?

	predicted as positive	predicted as negative
positive	TP	FN
negative	FP	TN

$$\text{Accuracy} = \frac{\text{No. of correct predictions}}{\text{No. of predictions}}$$

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

Examples (Balanced population)

classifier	TP	TN	FP	FN	Accuracy
A	25	25	25	25	50%
B	50	25	25	0	75%
C	25	50	0	25	75%
D	37	37	13	13	74%

- **Clearly, B, C, D are all better than A**
- **Is B better than C, D?**
- **Is C better than B, D?**
- **Is D better than B, C?**

Accuracy may not tell the whole story

Examples (Unbalanced population)

classifier	TP	TN	FP	FN	Accuracy
A	25	75	75	25	50%
B	0	150	0	50	75%
C	50	0	150	0	25%
D	30	100	50	20	65%

- **Clearly, D is better than A**
- **Is B better than A, C, D?**

Exercise: What is B's Prediction strategy?

High accuracy is meaningless if population is unbalanced

What is sensitivity (aka recall)?

	predicted as positive	predicted as negative
positive	TP	FN
negative	FP	TN

$$\underset{\text{wrt positives}}{\text{Sensitivity}} = \frac{\text{No. of correct positive predictions}}{\text{No. of positives}}$$

$$= \frac{TP}{TP + FN}$$

Sometimes sensitivity wrt negatives is termed **specificity**

Exercise: Write down the formula for specificity

What is precision?

	predicted as positive	predicted as negative
positive	TP	FN
negative	FP	TN

$$\underset{\text{wrt positives}}{\text{Precision}} = \frac{\text{No. of correct positive predictions}}{\text{No. of positives predictions}}$$

$$= \frac{\text{TP}}{\text{TP} + \text{FP}}$$

Unbalanced population revisited

classifier	TP	TN	FP	FN	Accuracy	Sensitivity	Precision
A	25	75	75	25	50%	50%	25%
B	0	150	0	50	75%		
C	50	0	150	0	25%		
D	30	100	50	20	65%	60%	38%

- **What are the sensitivity and precision of B and C?**
- **Is B better than A, C, D?**

Exercise #1

Abstract model of a classifier

- **Given a test sample *S***
- **Compute scores *p(S)*, *n(S)***
- **Predict *S* as negative if $p(S) / n(S) < t$**
- **Predict *S* as positive if $p(S) / n(S) \geq t$**

t is the decision threshold of the classifier

changing *t* affects the recall and precision, and hence accuracy, of the classifier

Example

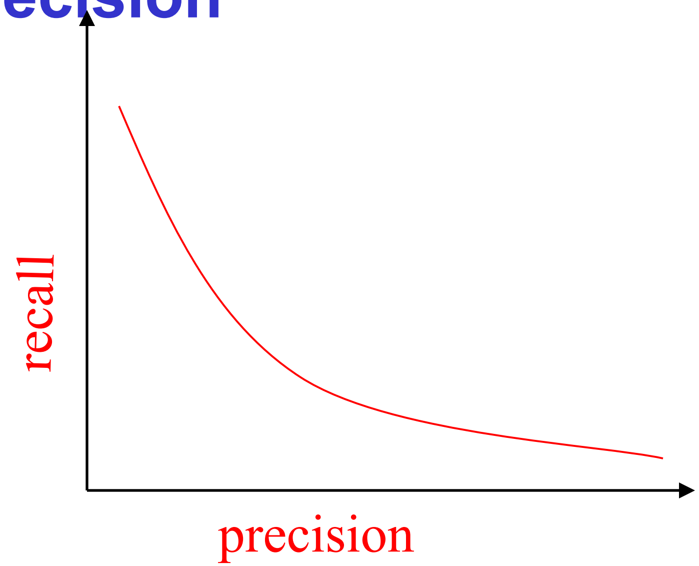
S	P(S)	N(S)	Actual Class	Predicted Class @ t = 3	Predicted Class @ t = 2
2	0.961252	0.038748	P	P	P
3	0.435302	0.564698	N	N	N
6	0.691596	0.308404	P	N	P
7	0.180885	0.819115	N	N	N
8	0.814909	0.185091	P	P	P
10	0.887220	0.112780	P	P	P
			accuracy	5 / 6	6/6
			recall	3 / 4	4/4
			precision	3 / 3	4/4

Recall that …

- **Predict *S* as negative if $p(S) / n(S) < t$**
- **Predict *S* as positive if $p(S) / n(S) \geq t$**

Precision-recall trade-off

- A predicts better than B if A has better recall and precision than B
- There is a trade-off between recall and precision



- In some apps, once you reach satisfactory precision, you optimize for recall
- In some apps, once you reach satisfactory recall, you optimize for precision

Comparing prediction performance

- **Accuracy is the obvious measure**
  – But it conveys the right intuition only when the positive and negative populations are roughly equal in size

- **Recall and precision together form a better measure**
  – But what do you do when A has better recall than B and B has better precision than A?

F-measure (Used in info extraction)

- **Take the harmonic mean of recall and precision**

$$F = \frac{2 * \text{recall} * \text{precision}}{\text{recall} + \text{precision}} \quad \text{(wrt positives)}$$

classifier	TP	TN	FP	FN	Accuracy	F-measure
A	25	75	75	25	50%	33%
B	0	150	0	50	75%	undefined
C	50	0	150	0	25%	40%
D	30	100	50	20	65%	46%

Does not accord with intuition:
C predicts everything as +ve, but still rated better than A

Adjusted accuracy

- **Weigh by the importance of the classes**

$$\text{Adjusted accuracy} = \alpha * \text{Sensitivity} + \beta * \text{Specificity}$$

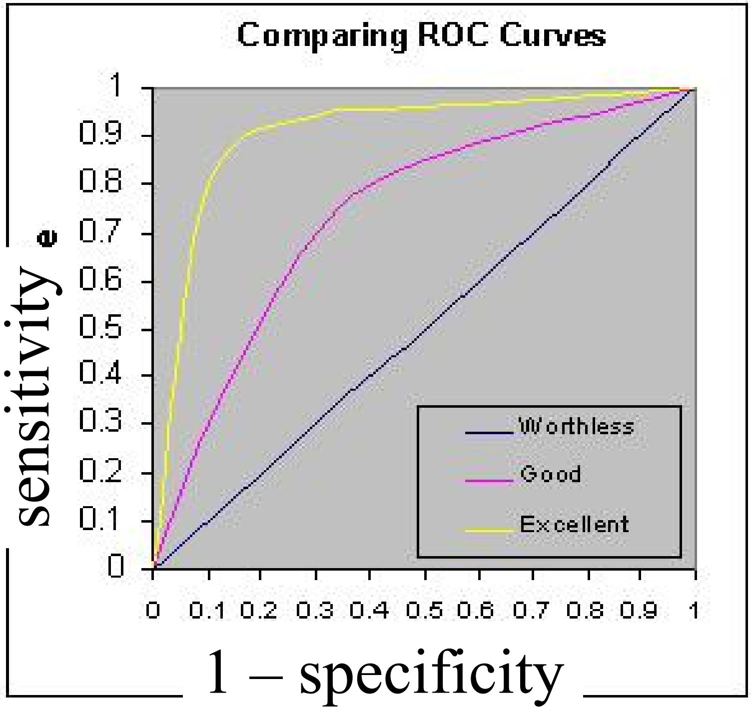
where $\alpha + \beta = 1$

typically, $\alpha = \beta = 0.5$

classifier	TP	TN	FP	FN	Accuracy	Adj Accuracy
A	25	75	75	25	50%	50%
B	0	150	0	50	75%	50%
C	50	0	150	0	25%	50%
D	30	100	50	20	65%	63%

ROC curves

- By changing t, we get a range of sensitivities and specificities of a classifier
- A predicts better than B if A has better sensitivities than B at most specificities
- Leads to ROC curve that plots sensitivity vs. (1 – specificity)
- Then the larger the area under the ROC curve, the better



Food for thought

- **You have a classifier. On a test set having 20% +ve and 80% -ve cases, the classifier’s recall and precision are both 80%**
- **Suppose you test it on a new test set having 80% +ve and 20% -ve cases. What do you expect its accuracy to be?**

- You may assume that the +ve (resp. –ve) cases in both test sets are equally sufficiently representative of the +ve (resp. –ve) real-world population

- **What lesson have you learned?**

Exercise #2

What is cross validation?

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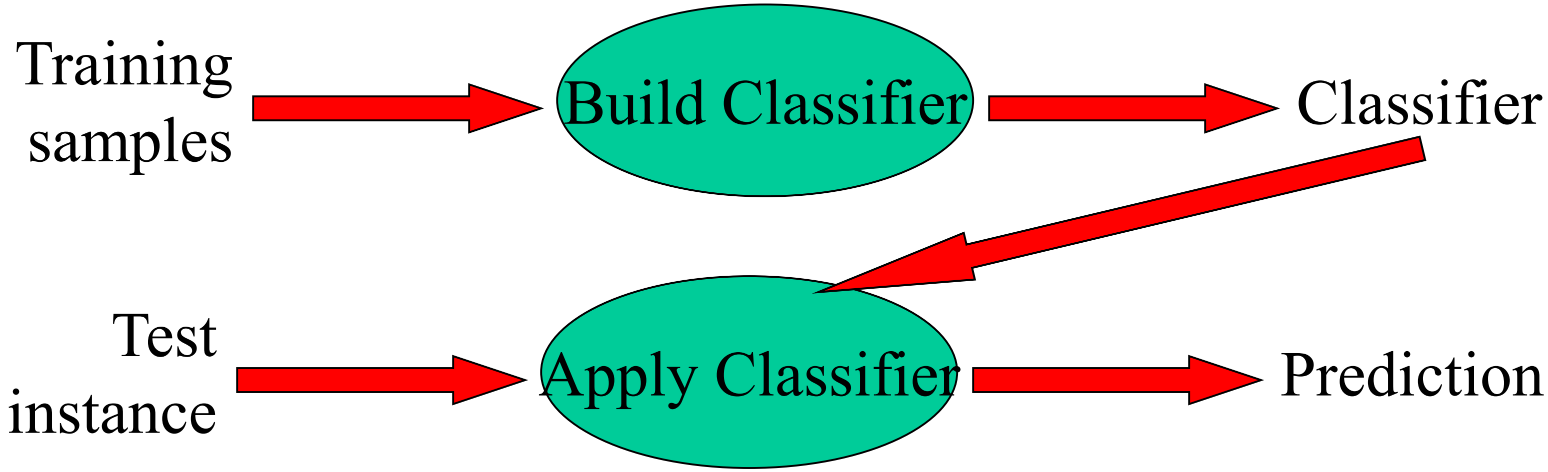
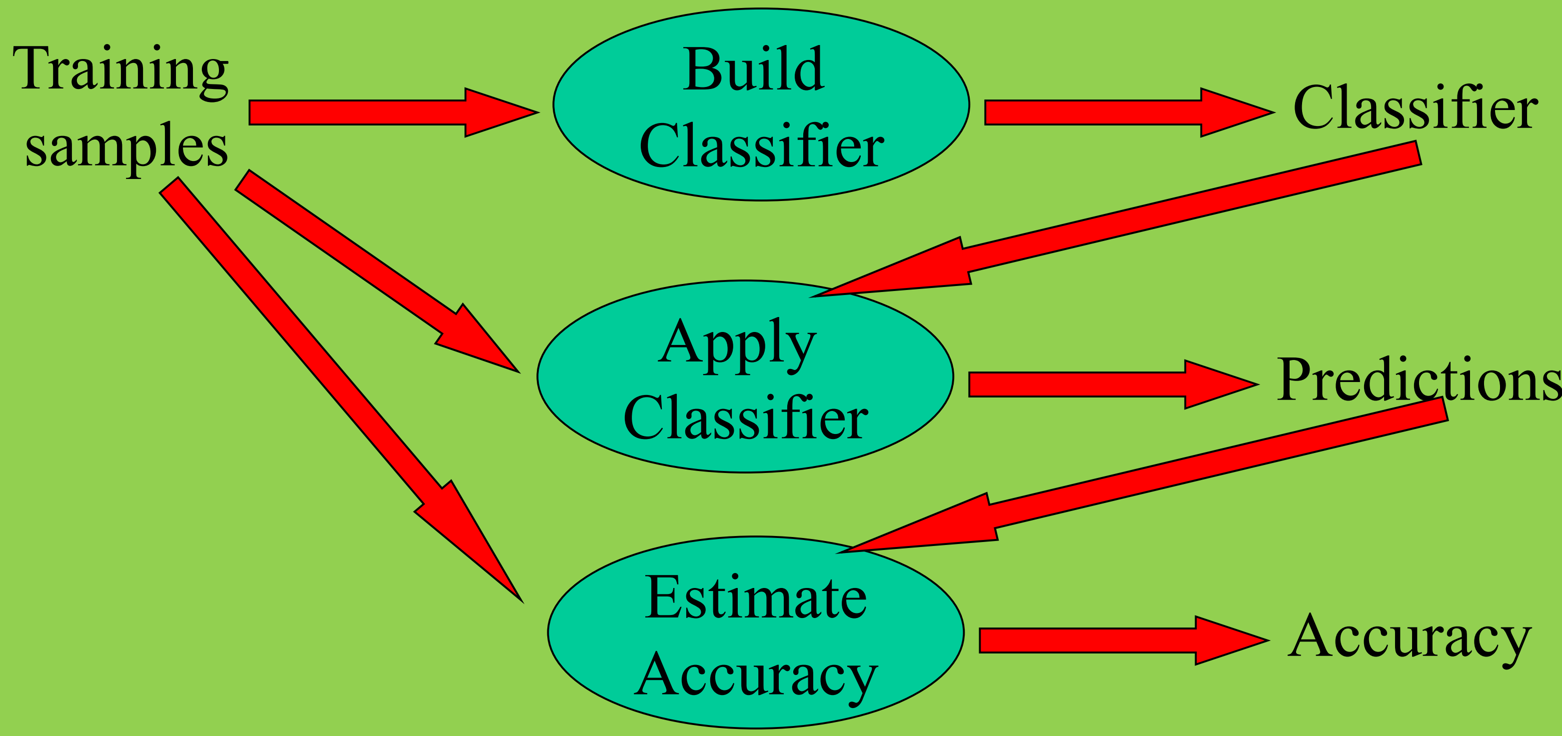
Construction of a classifier



Estimate accuracy: Wrong way



- **Why is this way of estimating accuracy wrong?**

Exercise #3

Recall ...

…the abstract model of a classifier

- **Given a test sample S**
- **Compute scores p(S), n(S)**
- **Predict S as negative if p(S) / n(S) < t**
- **Predict S as positive if p(S) / n(S) ≥ t**

t is the decision threshold of the classifier

K-nearest neighbour classifier (k-NN)

- **Given a sample S, find the k observations S_i in the known data that are "closest" to it, and take majority vote of their responses**
- **Assume S is well approximated by its neighbours**

$$p(S) = \sum_{S_i \in N_k(S) \cap D^P} 1 \qquad n(S) = \sum_{S_i \in N_k(S) \cap D^N} 1$$

where $N_k(S)$ is the neighbourhood of S defined by the k nearest samples to it.

Assume distance between samples is Euclidean distance for now

Illustration of kNN (k=8)

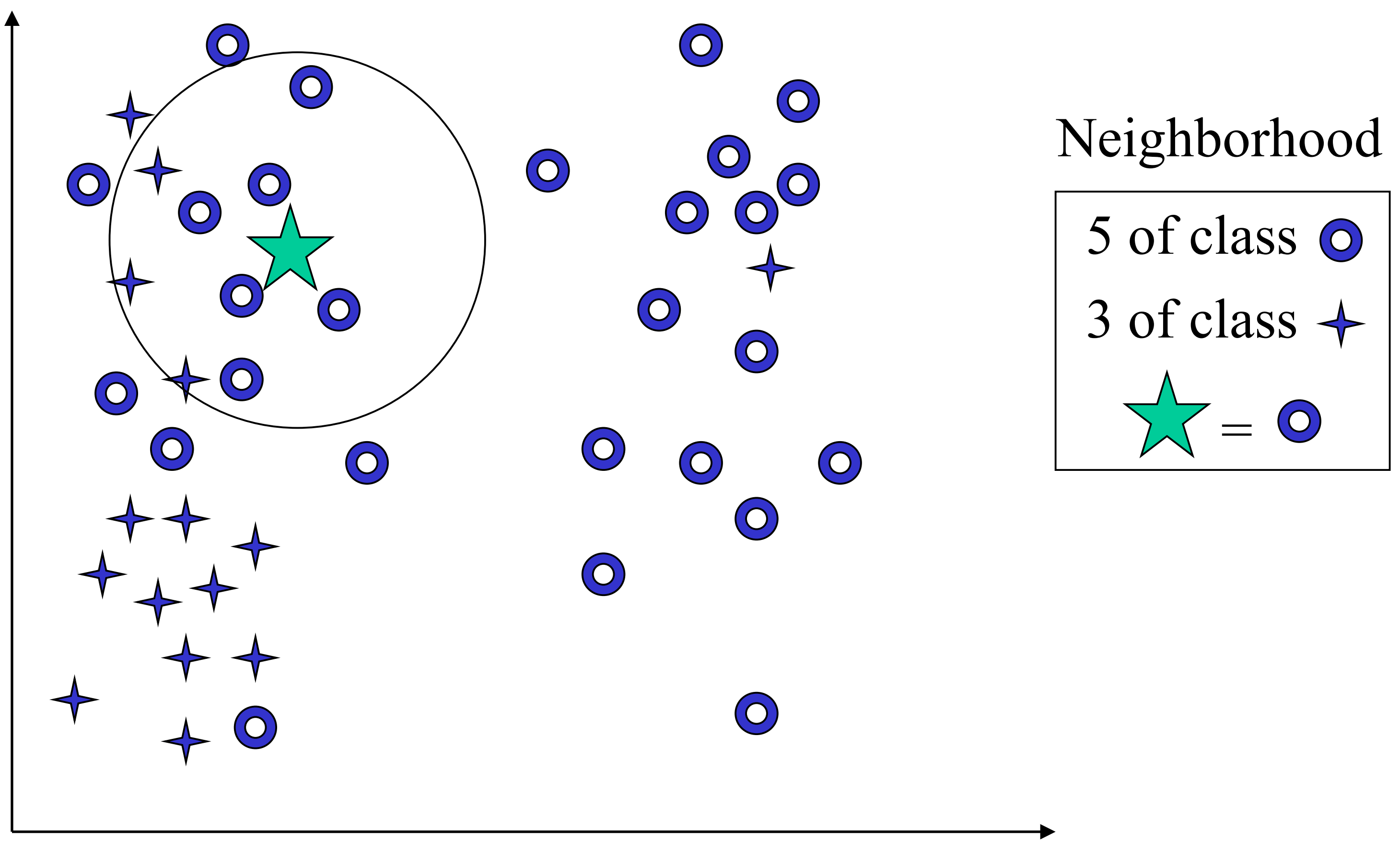
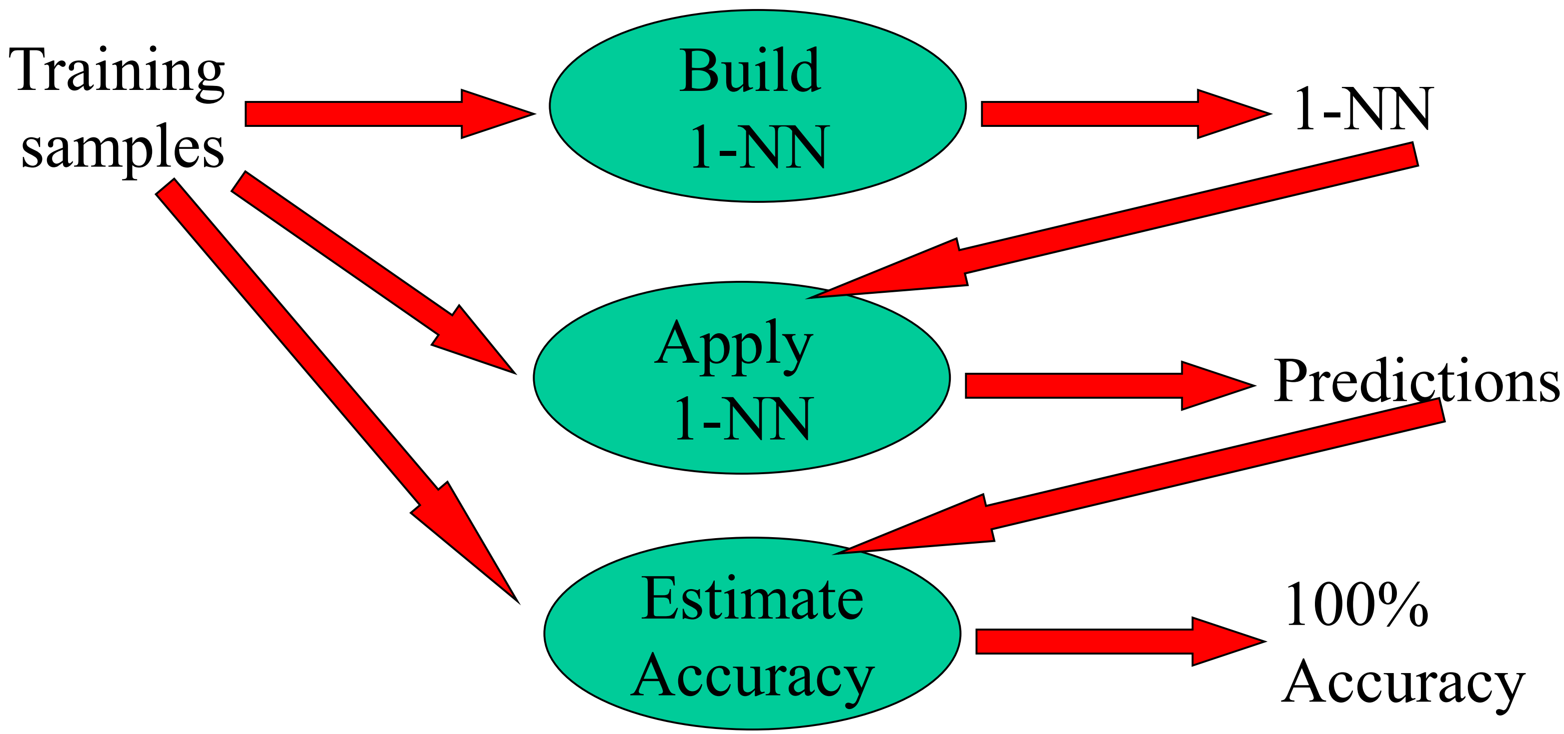


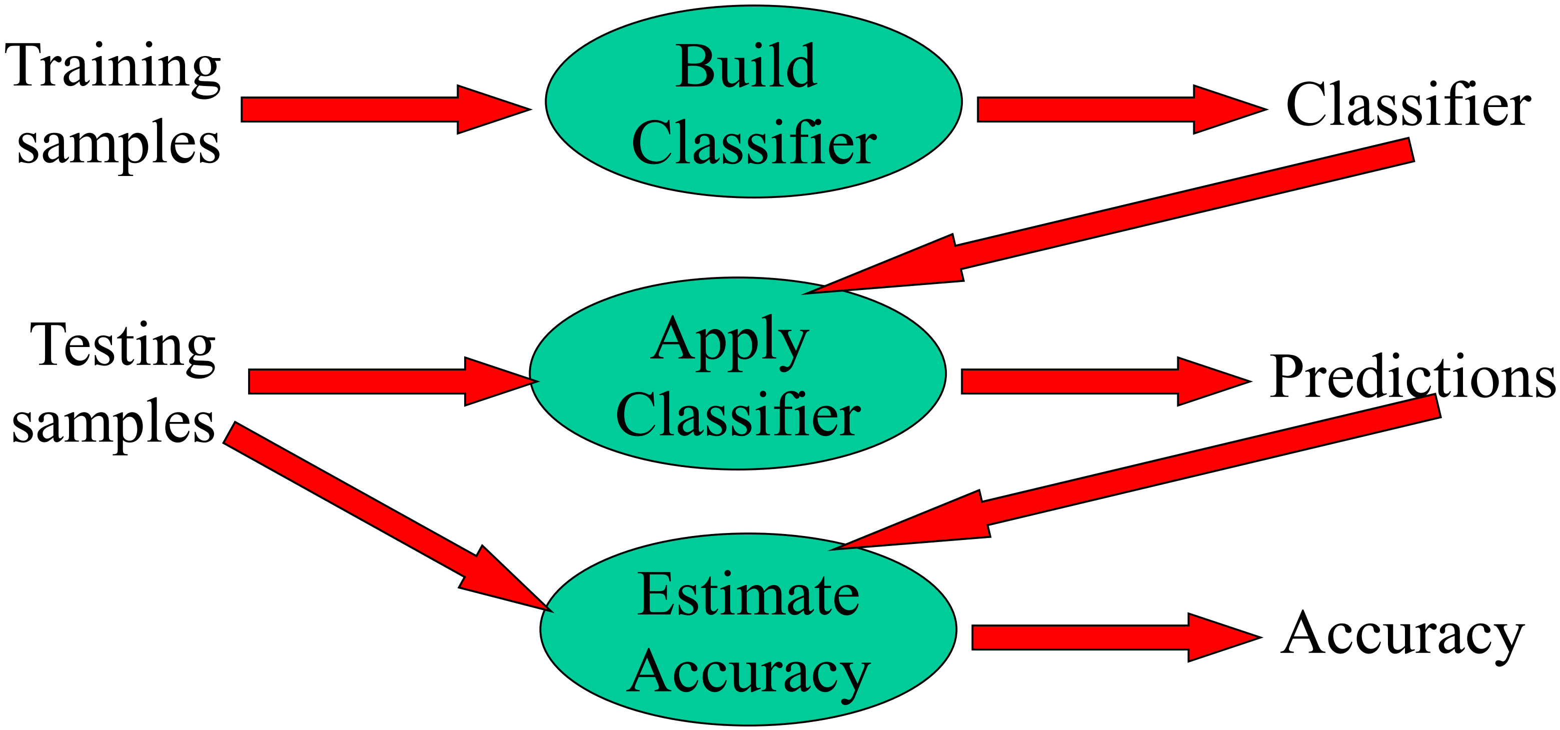
Image credit: Zaki

Estimate accuracy: Wrong way



For sure k-NN (k = 1) has 100% accuracy (Why?) in the "accuracy estimation" procedure above. Does this accuracy generalize to new test instances?

Estimate accuracy: Right way



Testing samples are NOT to be used during "Build Classifier"

How many training and testing samples?

- **No fixed ratio between training and testing samples; but typically 2:1 ratio**
- **Proportion of instances of different classes in testing samples should be similar to proportion in the real world, and preferably also to proportion in the training samples**
- **What if there are insufficient samples to reserve 1/3 for testing?**

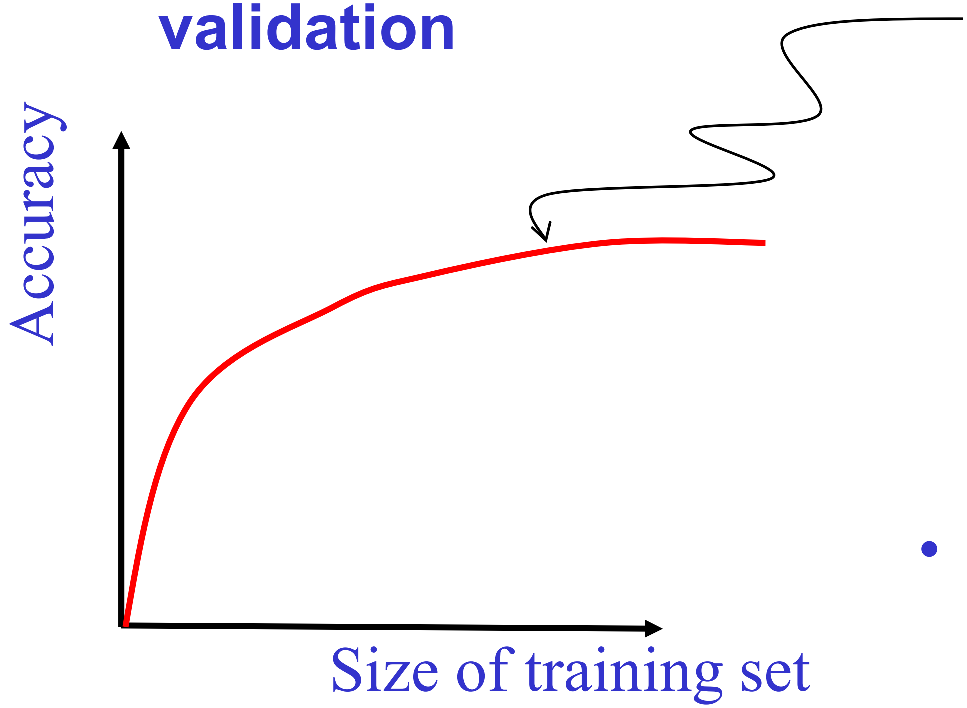
Cross validation

1.Test	2.Train	3.Train	4.Train	5.Train
1.Train	2.Test	3.Train	4.Train	5.Train
1.Train	2.Train	3.Test	4.Train	5.Train
1.Train	2.Train	3.Train	4.Test	5.Train
1.Train	2.Train	3.Train	4.Train	5.Test

- Divide samples into k roughly equal parts
- Each part has similar proportion of samples from different classes
- Use each part to test other parts
- Total up accuracy

How many fold?

- **If samples are divided into k parts, we call this k-fold cross validation**



- **Choose k so that**
  - the k-fold cross validation accuracy does not change much from k-1 fold
  - each part within the k-fold cross validation has similar accuracy

- **k = 5 or 10 are popular choices for k**

Food for thought

- **What is the logical basis of cross validation?**
- Hint: Central limit theorem

- **What / whose accuracy does it really estimate?**

Exercise #4

Curse of dimensionality

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Recall kNN …

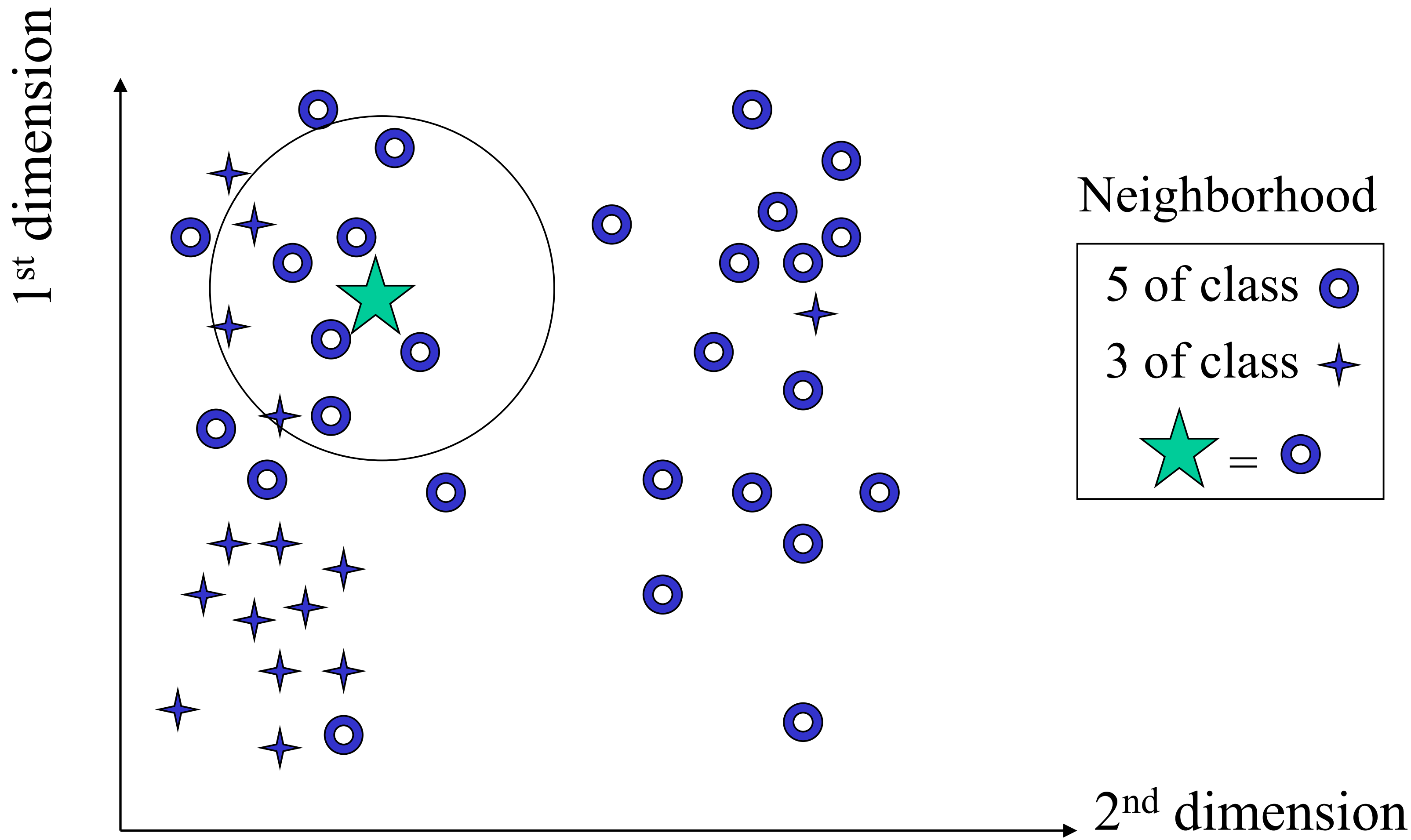
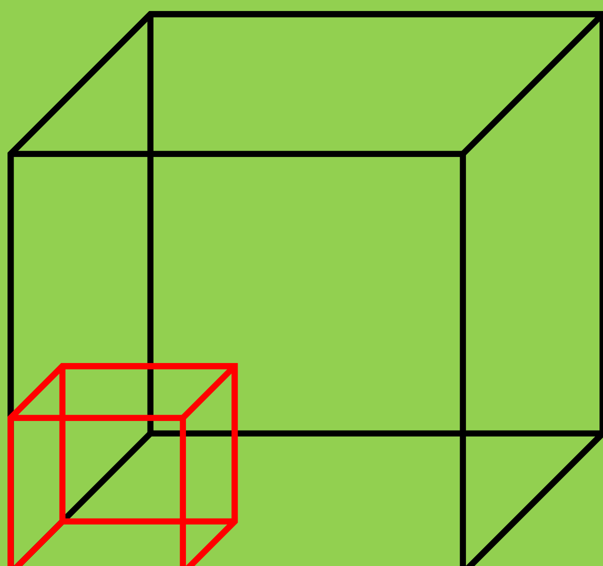


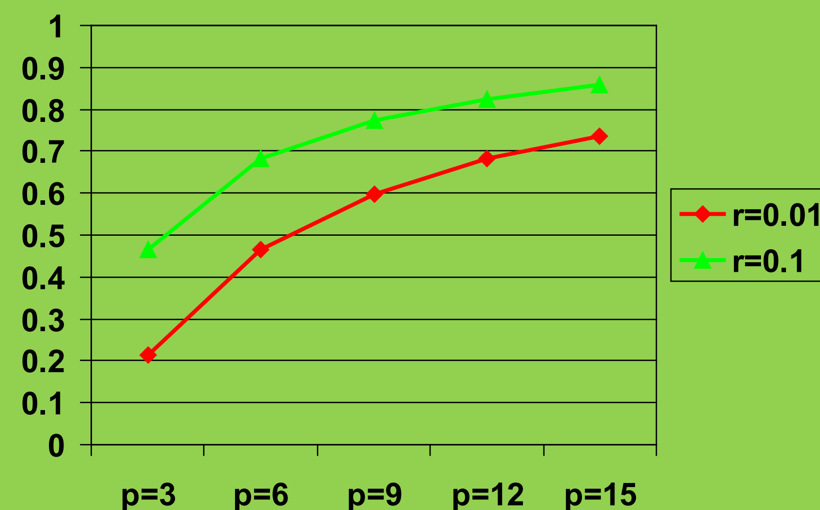
Image credit: Zaki

Curse of dimensionality

- **How much of each dimension is needed to cover a proportion r of a p-dimensional sample space?**



- **Calculate by $e_p(r) = r^{1/p}$. Why?**
- **So, to cover 10% of a 15-D space, need 85% of each dimension!**



Exercise #5

Consequence of the curse

- Suppose the number of samples given to us in the total sample space is fixed
- Let the dimension increase
- Then the distance of the k nearest neighbours of any point increases
- Then the k nearest neighbours are less and less useful for prediction, and can confuse the k-NN classifier

What is feature selection?

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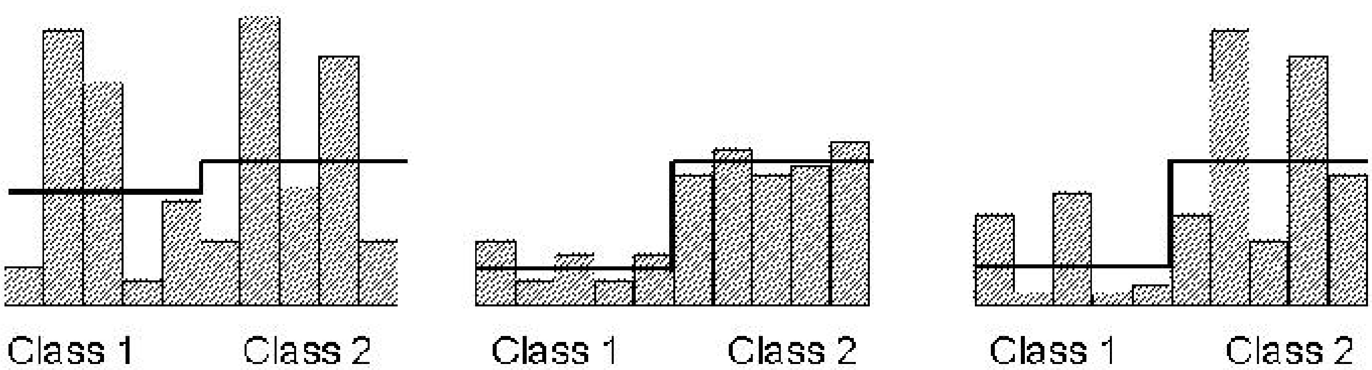
Tackling the curse

- **Given a sample space of p dimensions**
- **It is possible that some dimensions are irrelevant**
- **Need to find ways to separate those dimensions (aka features) that are relevant (aka signals) from those that are irrelevant (aka noise)**

Signal selection (Basic idea)

- **Choose a feature w/ low intra-class distance**
- **Choose a feature w/ high inter-class distance**



Signal selection (e.g., t-statistics)

The t-stats of a signal is defined as

$$t = \frac{|\mu_1 - \mu_2|}{\sqrt{(\sigma_1^2/n_1) + (\sigma_2^2/n_2)}}$$

where σ_i^2 is the variance of that signal in class i, μ_i is the mean of that signal in class i, and n_i is the size of class i.

Food for thought

- **How is the t-statistic typically used?**
- **What are the assumptions required for this way of using the t-statistic?**

Exercise #6

Self-fulfilling oracle

- Construct artificial dataset with 100 samples, each with 100,000 randomly generated features and randomly assigned class labels

- Select 20 features with the best t-statistics (or other methods)

- Evaluate accuracy by cross validation using the 20 selected features

- The resulting accuracy can be ~90%

- But the true accuracy should be 50%, as the data were derived randomly

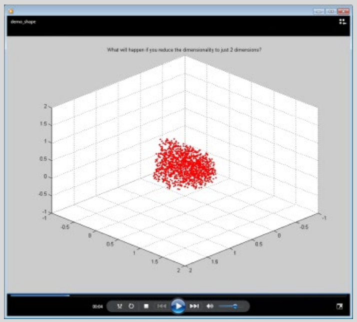
What went wrong?

- **The 20 features were selected from whole dataset**
- **Information in the held-out testing samples has thus been "leaked" to the training process**
- **The correct way is to re-select the 20 features at each fold; better still, use a totally new set of samples for testing**

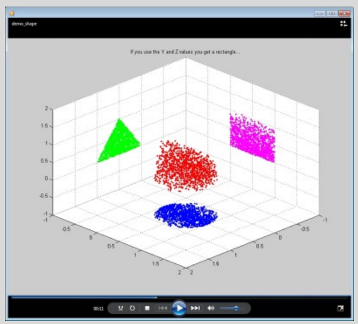
While **dimensionality reduction** is an important tool in machine learning/data mining, we must always be aware that it can distort the data in misleading ways.

Above is a two dimensional projection of an intrinsically three dimensional world….

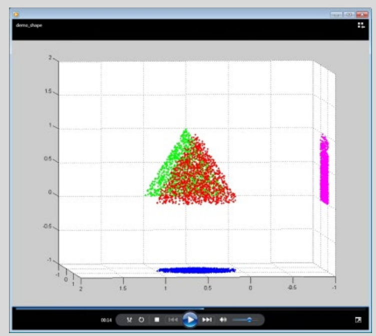
A cloud of points in 3D



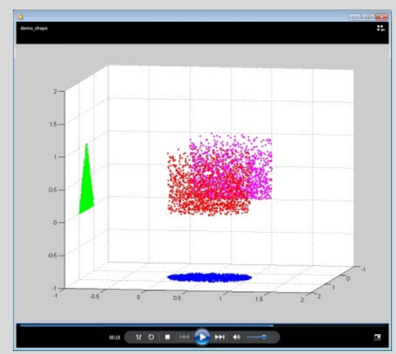
Can be projected into 2D
XY or XZ or YZ



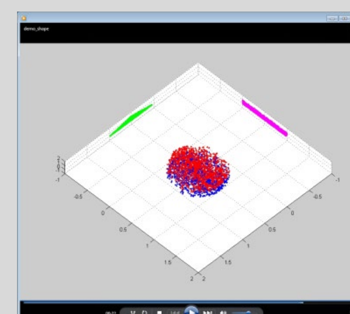
In 2D XZ we see
a triangle



In 2D YZ we see
a square



In 2D XY we see
a circle



Screen dumps of a short video from
www.cs.gmu.edu/~jessica/DimReducDanger.htm

Concluding remarks

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What have we learned?

- **Methodology of data mining**
  - Feature generation, feature selection, feature integration
- **Evaluation of classifiers**
  - Accuracy, sensitivity, precision
  - Cross validation
- **Curse of dimensionality**
  - Feature selection concept
  - Self-fulfilling oracle

Any questions?

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Acknowledgements

- **The first two slides were shown to WLS 20+ years ago by Tan Ah Hwee**
- **The three slides on the dangers of dimensionality reduction were created by Eamonn Keogh**

References

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