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**

Wong Limsoon
What is knowledge discovery?

Jonathan’s blocks
- Hexagon
- Circle
- Triangle
- Cylinder

Jessica’s blocks
- Triangle
- Square
- Cylinder
- Diamond

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

Whose block is this?
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?
What is accuracy?

<table>
<thead>
<tr>
<th></th>
<th>predicted as positive</th>
<th>predicted as negative</th>
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</thead>
<tbody>
<tr>
<td>positive</td>
<td>TP</td>
<td>FN</td>
</tr>
<tr>
<td>negative</td>
<td>FP</td>
<td>TN</td>
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</tbody>
</table>

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

= \( \frac{TP + TN}{TP + TN + FP + FN} \)
Examples (Balanced population)

<table>
<thead>
<tr>
<th>classifier</th>
<th>TP</th>
<th>TN</th>
<th>FP</th>
<th>FN</th>
<th>Accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>25</td>
<td>25</td>
<td>25</td>
<td>25</td>
<td>50%</td>
</tr>
<tr>
<td>B</td>
<td>50</td>
<td>25</td>
<td>25</td>
<td>0</td>
<td>75%</td>
</tr>
<tr>
<td>C</td>
<td>25</td>
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<td>0</td>
<td>25</td>
<td>75%</td>
</tr>
<tr>
<td>D</td>
<td>37</td>
<td>37</td>
<td>13</td>
<td>13</td>
<td>74%</td>
</tr>
</tbody>
</table>

- 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)

<table>
<thead>
<tr>
<th>classifier</th>
<th>TP</th>
<th>TN</th>
<th>FP</th>
<th>FN</th>
<th>Accuracy</th>
</tr>
</thead>
<tbody>
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<td>25</td>
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<td>75</td>
<td>25</td>
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</tr>
<tr>
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<td>0</td>
<td>50</td>
<td>75%</td>
</tr>
<tr>
<td>C</td>
<td>50</td>
<td>0</td>
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<td>0</td>
<td>25%</td>
</tr>
<tr>
<td>D</td>
<td>30</td>
<td>100</td>
<td>50</td>
<td>20</td>
<td>65%</td>
</tr>
</tbody>
</table>

- 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)?

Sensitivity wrt positives = \( \frac{\text{No. of correct positive predictions}}{\text{No. of positives}} \)

\[
\text{Sensitivity, wrt positives} = \frac{TP}{TP + FN}
\]

Sometimes sensitivity wrt negatives is termed specificity.

Exercise: Write down the formula for specificity.
What is precision?

<table>
<thead>
<tr>
<th></th>
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<th>predicted as negative</th>
</tr>
</thead>
<tbody>
<tr>
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<td>FN</td>
</tr>
<tr>
<td>negative</td>
<td>FP</td>
<td>TN</td>
</tr>
</tbody>
</table>

Precision = $\frac{\text{No. of correct positive predictions}}{\text{No. of positives predictions}}$ = $\frac{\text{TP}}{\text{TP} + \text{FP}}$
Unbalanced population revisited

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

<table>
<thead>
<tr>
<th>classifier</th>
<th>TP</th>
<th>TN</th>
<th>FP</th>
<th>FN</th>
<th>Accuracy</th>
<th>Sensitivity</th>
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<td>50%</td>
<td>25%</td>
</tr>
<tr>
<td>B</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
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<td>0</td>
<td>150</td>
<td>0</td>
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<td></td>
<td></td>
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<tr>
<td>D</td>
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<td>100</td>
<td>50</td>
<td>20</td>
<td>65%</td>
<td>60%</td>
<td>38%</td>
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</tbody>
</table>
Abstract model of a classifier

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

$t$ is the decision threshold of the classifier

changing $t$ affects the recall and precision, and hence accuracy, of the classifier
Recall that …

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

<table>
<thead>
<tr>
<th>S</th>
<th>P(S)</th>
<th>N(S)</th>
<th>Actual Class</th>
<th>Predicted Class ( @ t = 3 )</th>
<th>Predicted Class ( @ t = 2 )</th>
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<tr>
<td>2</td>
<td>0.961252</td>
<td>0.038748</td>
<td>P</td>
<td>P</td>
<td>P</td>
</tr>
<tr>
<td>3</td>
<td>0.435302</td>
<td>0.564698</td>
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<td>N</td>
<td>N</td>
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<tr>
<td>6</td>
<td>0.691596</td>
<td>0.308404</td>
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<td>N</td>
<td>P</td>
</tr>
<tr>
<td>7</td>
<td>0.180885</td>
<td>0.819115</td>
<td>N</td>
<td>N</td>
<td>N</td>
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<td>8</td>
<td>0.814909</td>
<td>0.185091</td>
<td>P</td>
<td>P</td>
<td>P</td>
</tr>
<tr>
<td>10</td>
<td>0.887220</td>
<td>0.112780</td>
<td>P</td>
<td></td>
<td>P</td>
</tr>
</tbody>
</table>

|          |         |          |             | accuracy: 5/6 | recall: 3/4 |
|          |         |          |             |               | precision: 3/3 |
|          |         |          |             |               |               |

|          |         |          |             | accuracy: 6/6 | recall: 4/4 |
|          |         |          |             |               | precision: 4/4 |

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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

\[
F = \frac{2 \times \text{recall} \times \text{precision}}{\text{recall} + \text{precision}} \quad \text{(wrt positives)}
\]

<table>
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<td>50%</td>
<td>33%</td>
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<tr>
<td>C</td>
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<td>0</td>
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<td>40%</td>
</tr>
<tr>
<td>D</td>
<td>30</td>
<td>100</td>
<td>50</td>
<td>20</td>
<td>65%</td>
<td>46%</td>
</tr>
</tbody>
</table>

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

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

where \alpha + \beta = 1

typically, \alpha = \beta = 0.5

<table>
<thead>
<tr>
<th>classifier</th>
<th>TP</th>
<th>TN</th>
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<th>Adj Accuracy</th>
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<tbody>
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<td>50</td>
<td>20</td>
<td>65%</td>
<td>63%</td>
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</table>
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. \( (1 - \text{specificity}) \).
- 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?
Construction of a classifier

Training samples → Build Classifier → Classifier

Test instance → Apply Classifier → Prediction
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 $p(S) / n(S) \geq t$

$t$ 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

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

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)

Neighborhood

5 of class

3 of class

= 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

- 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 $k$. 

### Graph

Accuracy vs. Size of training set.
Food for thought

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

• What / whose accuracy does it really estimate?
Curse of dimensionality
Recall kNN …

Neighborhood

5 of class
3 of class

=  

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!
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?
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 with low intra-class distance
- Choose a feature with high inter-class distance
Signal selection (e.g., t-statistics)

The t-stats of a signal is defined as

\[ t = \frac{|\mu_1 - \mu_2|}{\sqrt{\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}}} \]

where \( \sigma_i^2 \) is the variance of that signal in class \( i \), \( \mu_i \) 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?
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
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?
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


• Trevor Hastie et al., *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*, Springer, 2001. Chapters 1, 7

• Lance D. Miller et al., Optimal gene expression analysis by microarrays, *Cancer Cell* 2:353--361, 2002

• David Hand et al., *Principles of Data Mining*, MIT Press, 2001

• Jinyan Li et al., Data mining techniques for the practical bioinformatician, *The Practical Bioinformatician*, Chapter 3, pages 35—70, WSPC, 2004