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BANA 273 Session 5

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Agenda

- Construction of test data set
- Measuring accuracy
- Assignments posted to Canvas
- Review Assignment 1

What is Testing?

- It is important to know how the decision support system is performing in real-world situations
- "Real" testing is difficult
  - How do we test the negative decisions?
- Was it right to turn down the loan application?
- Was it correct that we did not invest in the other project?
  - Even for positive decisions, the eventual outcome may not be known
- The loan that was approved has not defaulted yet, but we do not know if it would do so in the next 28 years
- Testing
  - Use a small number of old cases to see how the system performs

Training versus Testing

- It is not advisable to use the same set of cases to train the model and then test it
  - The performance would be optimistic
- Training data would perfectly capture all the stochastic relationships across the features and the goal
- As mentioned before, we partition the dataset into two subsets
  - Training set
    - Used to build the model
  - Testing set
    - Used to validate the performance of the model

Training and testing

- Natural performance measure for classification problems: *error rate*
  - *Success*: instance's class is predicted correctly
  - *Error*: instance's class is predicted incorrectly
  - Error rate: proportion of errors made over the whole set of instances
- *Resubstitution error:* error rate obtained from training data
- Resubstitution error is (hopelessly) optimistic

Making the most of the data

- Once evaluation is complete, *all the data* can be used to build the final classifier
- Generally, the larger the training data the better the classifier (but returns diminish)
- The larger the test data the more accurate the error estimate
- *Holdout* procedure: method of splitting original data into training and test set
  - Dilemma: ideally both training set *and* test set should be large!

Holdout estimation

- What to do if the amount of data is limited?
- The *holdout* method reserves a certain amount for testing and uses the remainder for training
  - Usually: one third for testing, the rest for training
- Problem: the samples might not be representative
  - Example: class might be missing in the test data
- Advanced version uses *stratification*
  - Ensures that each class is represented with approximately equal proportions in both subsets

Repeated holdout method

- Holdout estimate can be made more reliable by repeating the process with different subsamples
  - In each iteration, a certain proportion is randomly selected for training (possibly with stratification)
  - The error rates on the different iterations are averaged to yield an overall error rate
- This is called the *repeated holdout* method
- Still not optimum: the different test sets overlap
  - Can we prevent overlapping?

Cross-validation

- *Cross-validation* avoids overlapping test sets
  - First step: split data into *k* subsets of equal size
  - Second step: use each subset in turn for testing, the remainder for training
- Called *k-fold cross-validation*
- Often the subsets are stratified before the cross-validation is performed
- The error estimates are averaged to yield an overall error estimate

More on cross-validation

- Standard method for evaluation: stratified ten-fold cross-validation
- Why ten?
  - Extensive experiments have shown that this is the best choice to get an accurate estimate
- Even better: repeated stratified cross-validation
  - E.g. ten-fold cross-validation is repeated ten times and results are averaged

Leave-One-Out cross-validation

- Leave-One-Out:
  a particular form of cross-validation:
  - Set number of folds to number of training instances
  - I.e., for *n* training instances, build classifier *n* times
- Makes best use of the data
- Very computationally expensive

Accuracy Measure

- Accuracy is the percentage of test cases where the predicted and actual goals are the same
  - The test set on the right shows 70% accuracy
- Problem
  - Does it account for a bias towards a class?
- Stratified accuracy
  - Accuracy for each class
  - Accuracy for Approve=no
    - 4 out of 6 (66.7%)
  - Accuracy for Approve = yes
    - 3 out of 4 (75%)

	Approve		
No.	Actual	Predicted	Match?
1	yes	yes	1
2	yes	no	0
3	no	no	1
4	no	no	1
5	no	yes	0
6	yes	yes	1
7	no	yes	0
8	yes	yes	1
9	no	no	1
10	no	no	1
			7

Confusion Matrix

- A confusion matrix summarizes the result of running a classification model on a *test dataset*

		Predicted class	
		Yes	No
Actual class	Yes	True positive	False negative (Type 2)
	No	False positive (Type 1)	True negative

A 2x2 Confusion Matrix

```
a      b      ← classified as
905    23     | a = yes
12     323    | b = no
```

A 3x3 Confusion Matrix

```
a      b      c      ← classified as
911    24     12     | a = buy
12     374    22     | b = hold
11     14     123    | c = sell
```

Confusion Matrix

a	b	← classified as
905	23	| a = yes
12	323	| b = no

- Total number of test cases
  - 905 + 23 + 12 + 323 = 1263
- Number of correct classification
  - 905 + 323 = 1228
- Number of incorrect classification
  - 23 + 12 = 35
- Accuracy = 1228/1263 = 97.2%
- Stratified accuracy
  - Accuracy for “a” = 905/(905+23) = 97 5%
  - Accuracy for “b” = 323/(12+323) = 96.4%

The bootstrap

- CV uses sampling *without replacement*
  - The same instance, once selected, can not 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

The 0.632 bootstrap

- The *0.632 bootstrap*
  - A particular instance has a probability of $1-1/n$ of *not* being picked
  - Thus its probability of *not* ending up in the test data is:

$$\left(1-\frac{1}{n}\right)^{n} \approx e^{-1} \approx 0.368$$

  - 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 pessimistic
  - Trained on ~63% of the instances

- Therefore, combine it with the resubstitution error:

$$err = 0.632 * e_{test\_data\_set} + 0.368 * e_{training\_data\_set}$$

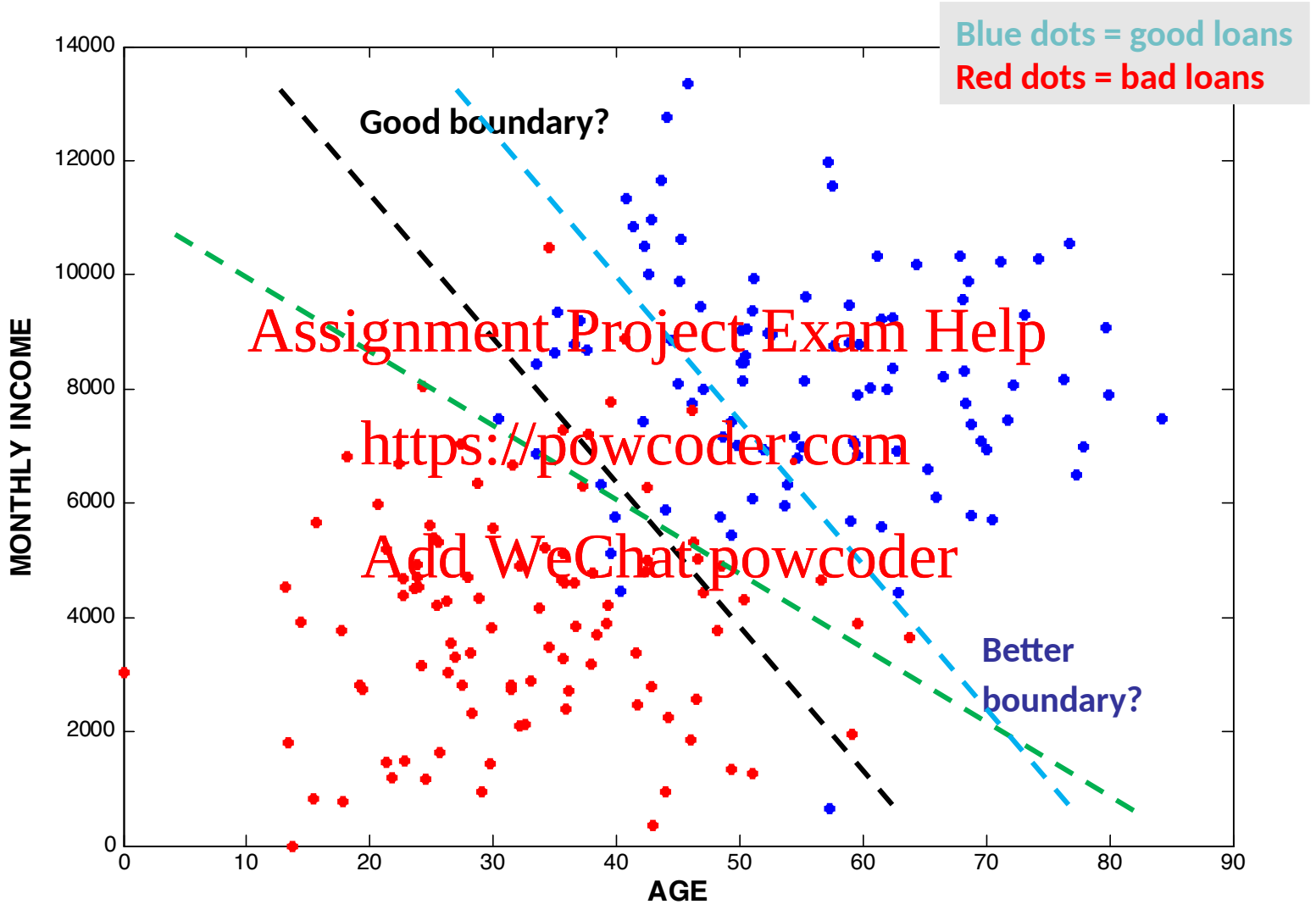
- The resubstitution error gets less weight than the error on the test data
- Repeat process several times with different replacement samples; average the results

Training, testing and validation data

- The standard for computing accuracy of a model
  - Split data into 3 parts:
    - Training data to be used for model generation
    - Validation data to be used for model selection
    - Testing data to be used for determining the accuracy of the final model

Counting the cost

- In practice, different types of classification errors often incur different costs
- Examples:
  - Loan decisions
  - Promotional mailing
  - Fault diagnosis



Classification with costs

- Default cost matrices:

		Predicted class	
		yes	*no*
Actual class	*yes*	0	1
	no	1	0

		Predicted class		
		a	*b*	*c*
Actual class	*a*	0	1	1
	b	1	0	1
	c	1	1	0

- Success rate is replaced by average cost per prediction
  - Cost is given by appropriate entry in the cost matrix

Cost-sensitive classification

Change classifier model to take account of cost of errors

- Can take costs into account when making predictions
  - Basic idea: only predict high-cost class when very confident about prediction
- Given: predicted class probabilities
  - Normally we just predict the most likely class
  - Here, we should make the prediction that minimizes the expected cost
    - Expected cost: dot product of vector of class probabilities and appropriate column in cost matrix
    - Changing the cutoff probability in Naïve Bayes

Example – Work out the cost of errors:

- Consider a classifier problem where the class variable is {Accept, Analyze, Reject}
- Suppose Naïve Bayes examines a test instance (row) and assigns the following probabilities:
  - Accept 50%, Analyze 30%, Reject 20%
- Suppose the cost matrix is

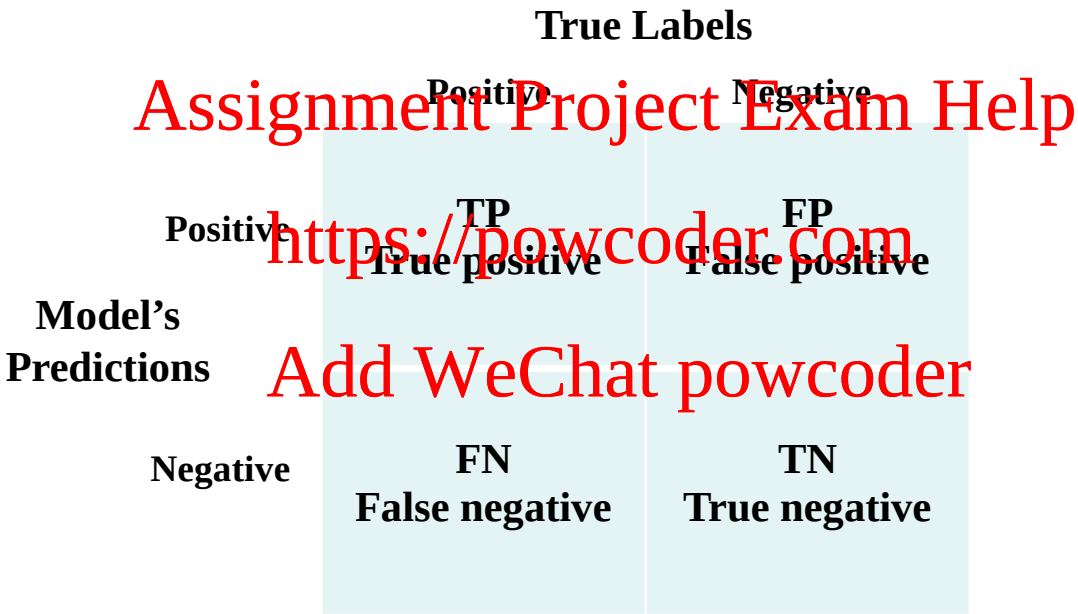
Actual↓ Predicted→	Accept	Analyze	Reject
Accept	0	1	2
Analyze	1	0	1
Reject	3	1	0

Cost-sensitive learning

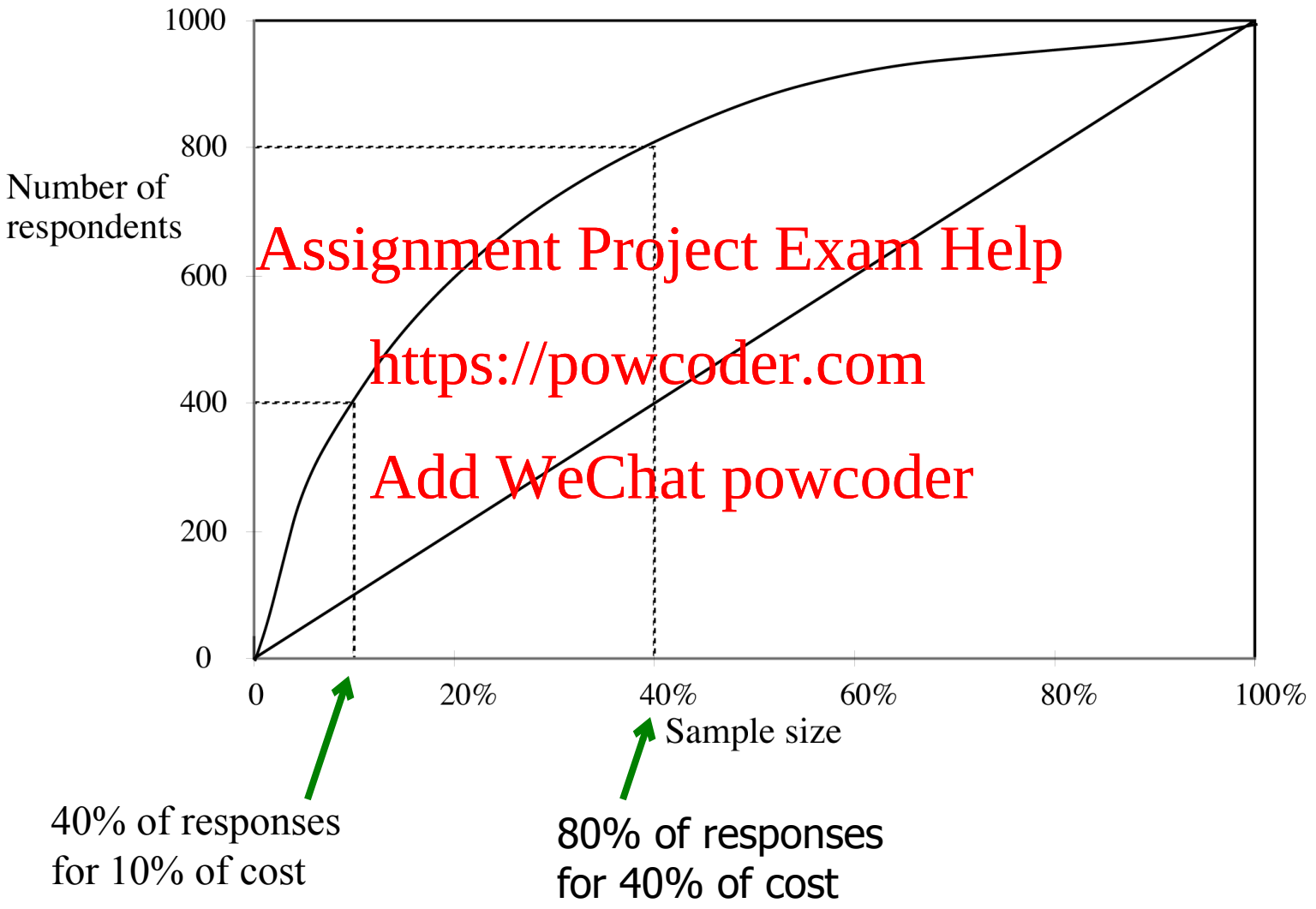
- So far we haven't taken costs into account at training time
- Most learning schemes do not perform cost-sensitive learning
  - They generate the same classifier no matter what costs are assigned to the different classes

- Simple methods for cost-sensitive learning:
  - Thresholding: Adjust probability threshold for setting class labels
  - Rebalancing: Resampling of instances according to costs

Terminology



A hypothetical lift chart



Generating a lift chart

- Sort instances according to predicted probability of being positive:

	Predicted probability	Actual class
1	0.95	Yes
2	0.93	Yes
3	0.93	No
4	0.88	Yes
…	…	…

- Lift Chart
  - x axis is sample size
    y axis is number of true positives

Binary Classification: Lift Curves

Sort test examples by their predicted score

For a particular threshold compute

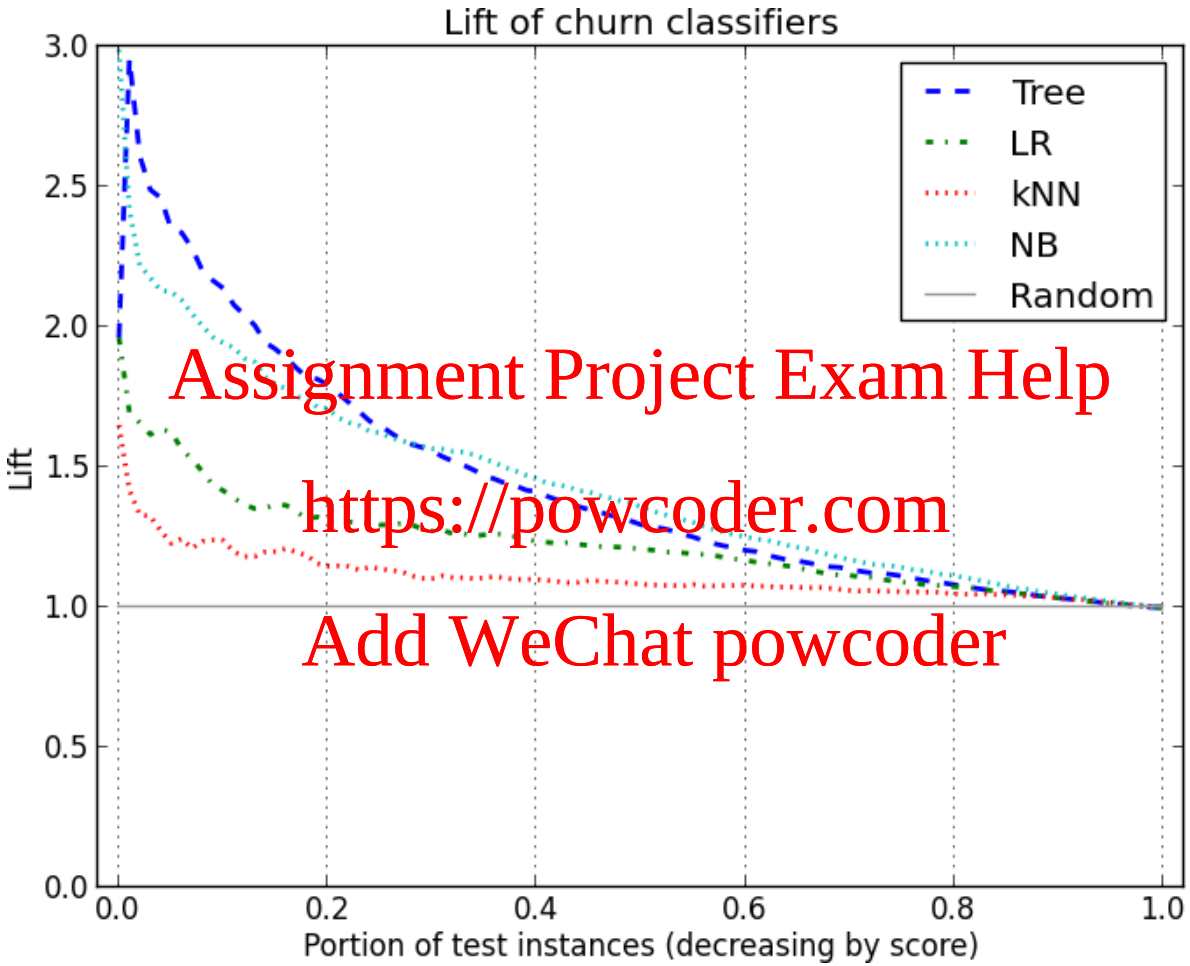
(1) NTP = number of true positive examples detected by the model

(2) NTPR = number of true positive examples that would be detected by random ordering

Lift = NTP/NTPR

Lift curve = Lift as a function of number of examples above the threshold, as the threshold is varied

Expect that good models will start with high lift (and will eventually decay to 1)



From Chapter 8: Visualizing Model Performance, in Data Science for Business (O Reilly, 2013),

Computing Profits using Lift charts

- Example: promotional mailing to 1,000,000 households @ $0.50 each. Company earns on average, $600 from each response
  - Mail to all; 0.1% respond (1000).
  - Total Profit = 600,000 – 500,000 = $100,000

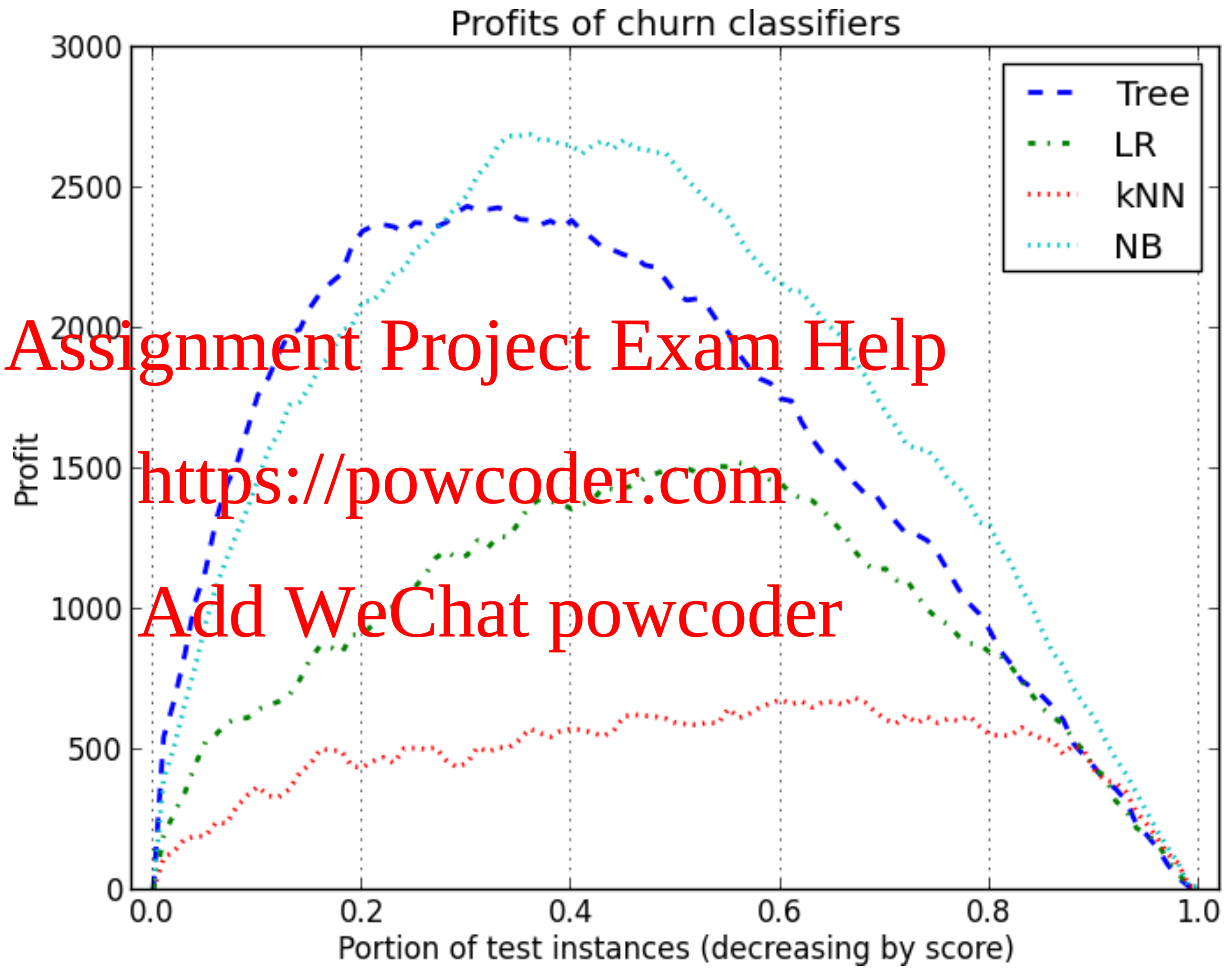
- Data mining tool identifies subset of 100,000 most promising, 0.4% of these respond (400)
  - Lift Ratio = 0.4 / 0.1 = 4
  - Total profit =

- Identify subset of 400,000 most promising, 0.2% respond (800)
  - Lift Ratio = 0.2 / 0.1 = 2
  - Total profit =

- A *lift chart* allows a visual comparison

Example of an Empirical “Profit Curve”

12:1 benefit/cost ratio
(more lucrative)



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ROC curves

- ROC curves are similar to lift charts
  - Stands for "receiver operating characteristic"
  - Used in signal detection to show tradeoff between hit rate and false alarm rate over noisy channel
- Differences to lift chart:
  - y axis shows percentage of true positives in sample *rather than absolute number*
  - x axis shows percentage of false positives in sample *rather than sample size*

ROC Plots

		True Labels: Positive	True Labels: Negative
Model's Predictions	Positive	TP True positive	FP False positive
	Negative	FN False negative	TN True negative

TPR = True Positive Rate = TP / (TP + FN)

= ratio of correct positives predicted to actual number of positives

(same as recall, sensitivity, hit rate)

FPR = False Positive Rate

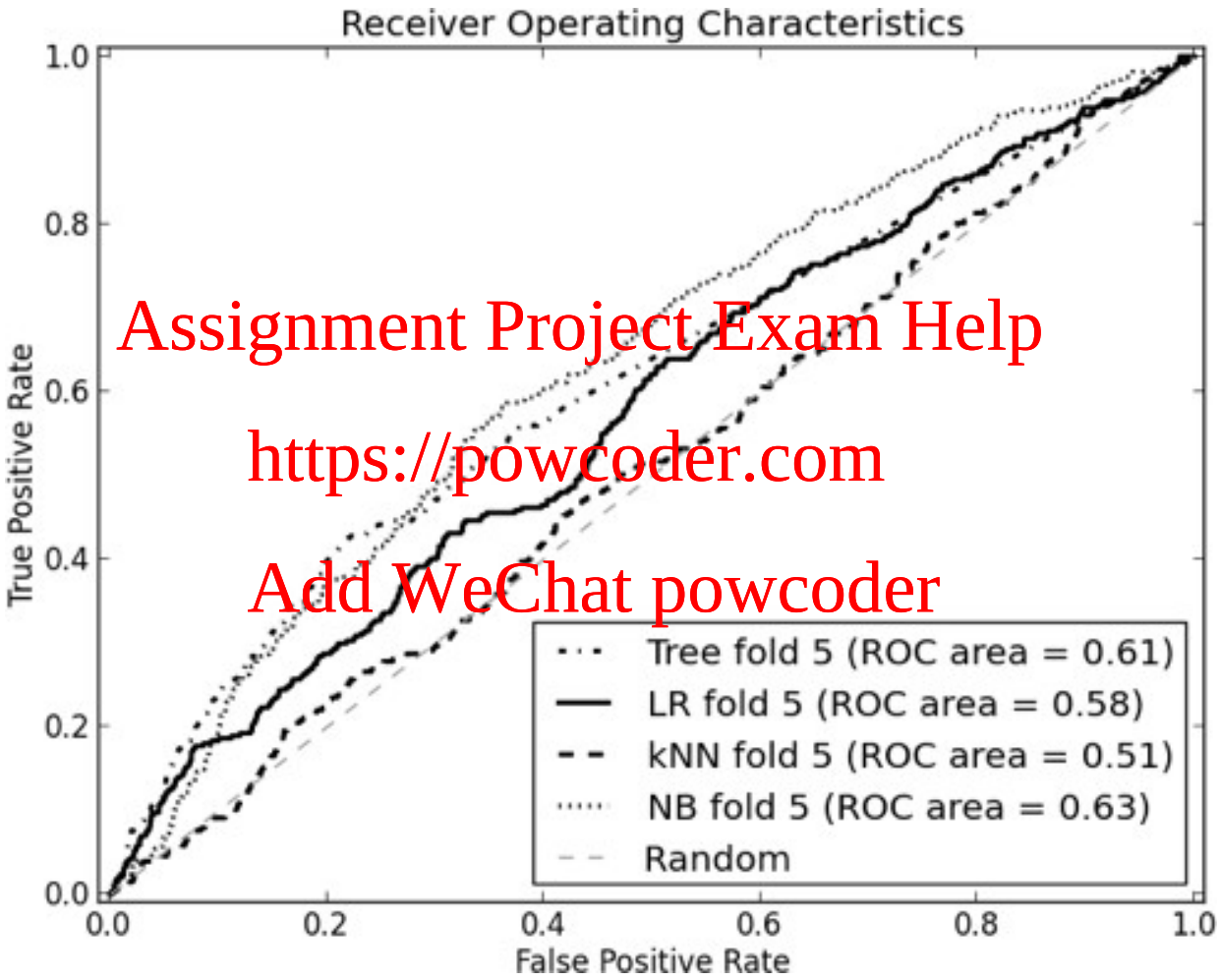
= FP / (FP + TN) = ratio of incorrect negatives predicted to actual number of negatives

(same as false alarm rate)

Receiver Operating Characteristic: plots TPR versus FPR as threshold varies

As we decrease our threshold, both the TPR and FPR will increase, both ending at [1, 1]

Example of an Actual ROC



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In the following confusion matrix, the number of errors is

A 3x3 Confusion Matrix

a	b	c	← classified as
911	24	12	| a = buy
12	374	22	| b = hold
11	14	123	| c = sell

A: 123

B: 374

C: 99

D: 911

E: None of the above

A lift chart is useful for

A: Calculating Bayesian lift

B: Calculating the difference function

C: Calculating the optimal number of promotional mailings

D: Calculating the accuracy of Naïve Bayes

E: None of the above

Review Assignment 1

Weka Example – Classification using Naïve Bayes

- Download file from EEE (session 9):
  - 4bank-data-8.arff
- Switch tab to “classify”
- Select method: NaiveBayes
- Verify class variable set to “pep”
- Use 10 fold cross validation
- Run classifier
- Examine confusion matrix

Next Session

- Decision Tree based classification