Regression Analysis

DSE 220

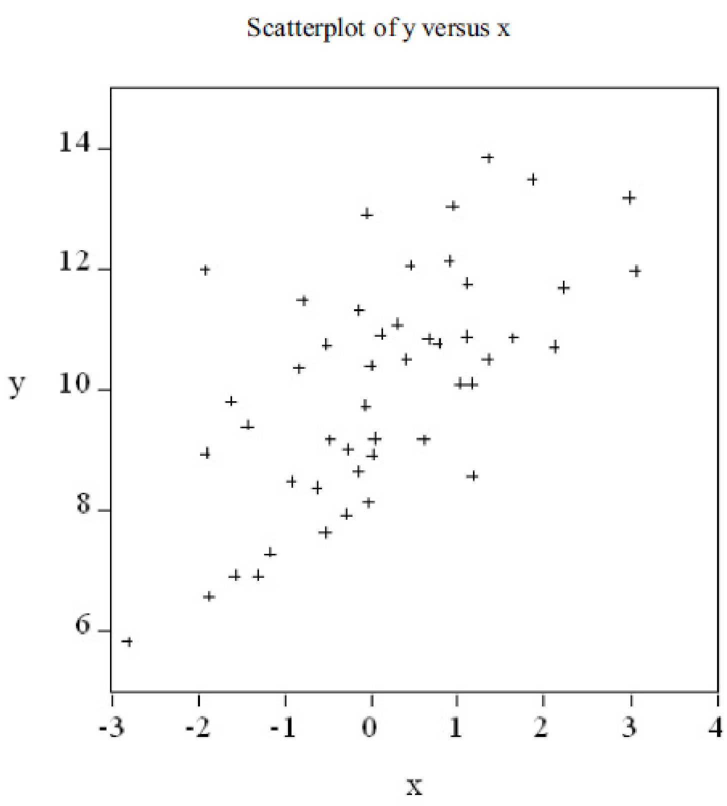
Outline

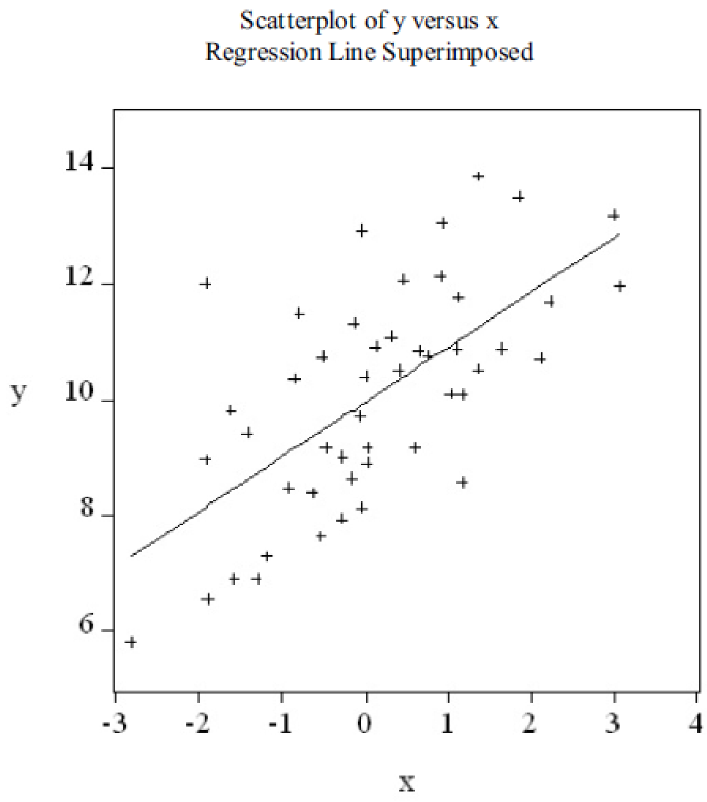
- Nonparametric Methods
  - kNN
  - ***Hands-On***
  - ***Self – practice***
- Parametric Methods
  - Generative Models
    - Naïve Bayes
    - Gaussian Generative Model
    - Fisher Linear Discriminant Analysis
    - ***Hands-On***
    - ***Self – practice***
- Regression Analysis
  - ***Hands-On***
  - ***Self – practice***
- Evaluation Metrics
  - Accuracy, Recall, Precision, Sensitivity, Specificity,…
  - ROC Curves
  - ***Hands-On***
  - ***Self – practice***

Regression Analysis

- One of the basic tools for forecasting
- A statistical technique to describe relationships among variables
- Consider two variables y and x
  - Describe y using x
  - y: dependent variable
  - x: independent variable (explanatory, exogenous)

Regression Analysis





Regression Analysis

- How to find the line that fits best?
  - Line: $y = \beta_0 + \beta_1 X$
  - How to find β_0 and β_1?
- Example

Regression Analysis

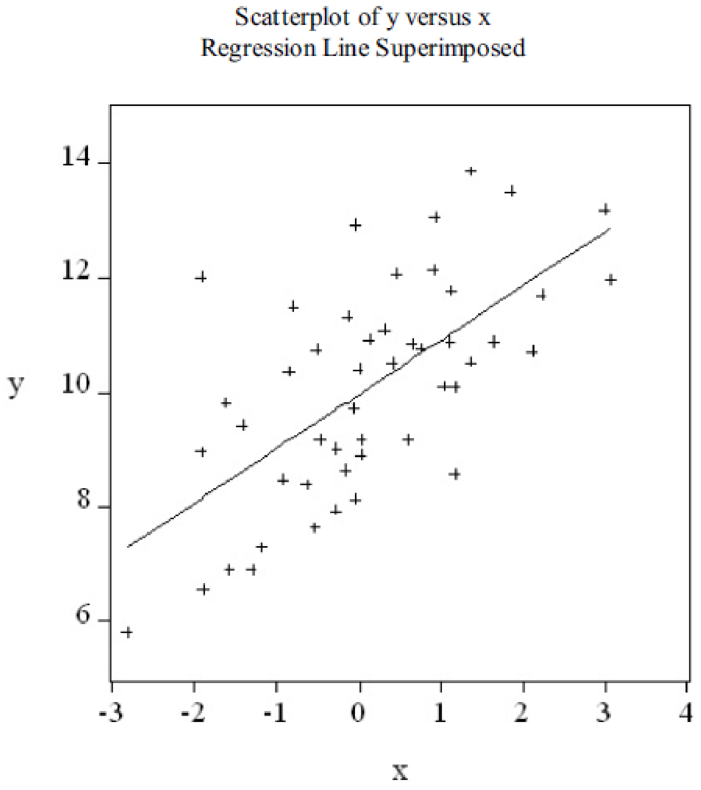
- Probabilistic Model
  - $y_t = \beta_0 + \beta_1 x_t + \varepsilon_t$
  - $\varepsilon_t \overset{iid}{\rightarrow} N(0, \sigma^2)$
  - Model parameters: $\beta_0, \beta_1, \sigma^2$
- If this model is correct:
  - Expected value of y conditional on $x = x^*$
    - $E(y|x^*) = \beta_0 + \beta_1 x^*$

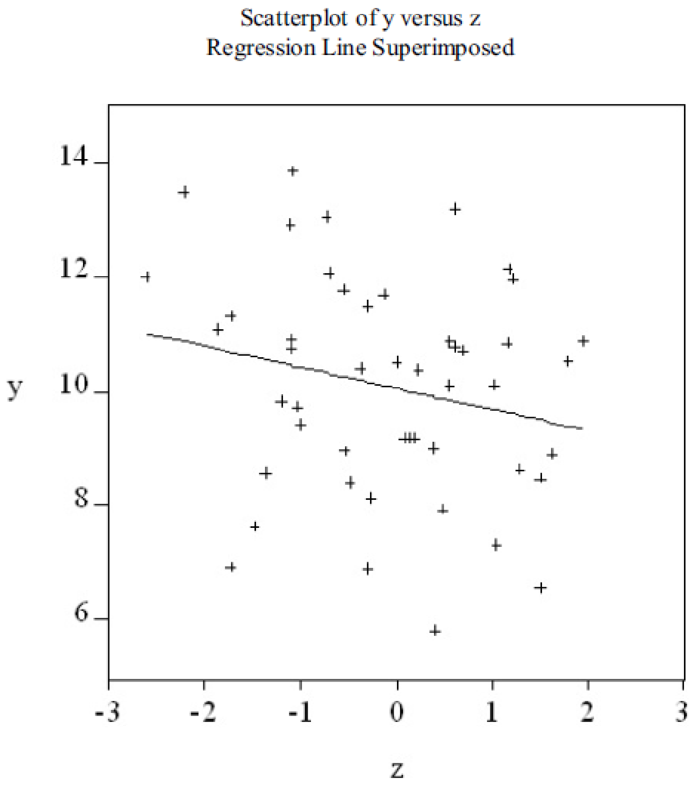
Regression Analysis

- Fitted values
  - $\hat{y}_t = \hat{\beta}_0 + \hat{\beta}_1 x_t$
- Minimize residuals
  - Residuals = in-sample forecast errors
  - $e_t = y_t - \hat{y}_t$
- Least-squares estimation
    - $\sum_{t=1}^{T} (y_t - \hat{y}_t)^2$

Regression Analysis

- Multiple linear regression
  - y is described by more than one explanatory variable





Regression Analysis

- Multiple linear regression model
  - $y_t = \beta_0 + \beta_1 x_t + \beta_2 z_t + \varepsilon_t$
  - $\varepsilon_t \overset{iid}{\longrightarrow} N(0, \sigma^2)$
- Fitted values
  - $\hat{y}_t = \hat{\beta}_0 + \hat{\beta}_1 x_t + \hat{\beta}_2\, z_t$
- Residuals
  - $e_t = y_t - \hat{y}_t$
- Least-squares estimation
  - $\sum_{t=1}^{T} (y_t - \hat{y}_t)^2$

Goodness-of-fit Statistics

- Sum squared residuals (errors):
  - Objective of the least-squares estimation
  - Sum of squared residuals
  - Not of much value in isolation
  - Input to other diagnostics
  - Useful for comparing models and testing hypotheses

$$SSE = \sum_{t=1}^{T} e_t^2 \xrightarrow{\text{similar}} \text{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

Goodness-of-fit Statistics

- the residual sum of squares (sum of squared estimate of errors):

$$SSE = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

- the regression sum of squares is:

$$SSR = \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2$$

- total sum of squares is:

$$SST = \sum_{i=1}^{n}(y_i - \bar{y})^2$$

Goodness-of-fit Statistics

- the residual sum of squares (sum of squared estimate of errors):

$$SSE = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

- the regression sum of squares is:

$$SSR = \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2$$

- total sum of squares is:

$$SST = \sum_{i=1}^{n}(y_i - \bar{y})^2$$

$$SST = SSE + SSR$$

Goodness-of-fit Statistics

- R-squared (R^2)
  - Indicates how much of var(y) can be explained by the variables included in the regression
  - Intuition: $\frac{var(y|x)}{var(y)}$
  - Measurement of in-sample success of the regression equation
  - If intercept is included, $0 < R^2 < 1$

$$R^2 = 1 - \frac{\frac{1}{T}\sum_{t=1}^{T} e_t^2}{\frac{1}{T}\sum_{t=1}^{T} (y_t - \bar{y}_t)^2} = \frac{SSR}{SST} = 1 - \frac{SSE}{SST}$$

Goodness-of-fit Statistics

- Adjusted R-squared $(\bar{R}^2)$
  - Same interpretation as R^2 but formula is slightly different
  - Adjusted for degrees of freedom used in fitting the model
  - Adjustment: penalize the amount of right-hand-side variables

$$\bar{R}^2 = 1 - \frac{\frac{1}{T-k}\sum_{t=1}^{T} e_t^2}{\frac{1}{T-1}\sum_{t=1}^{T}(y_t - \bar{y}_t)^2}$$

Goodness-of-fit Statistics

- Akaike info criterion (AIC)
  - Estimate of the out-of-sample forecast error variance
  - Similar to s^2 but penalizes degrees of freedom more harshly
  - Used to compare forecasting models

$$\mathrm{AIC} = e^{\left(\frac{2k}{T}\right)} \frac{\sum_{t=1}^{T} e_t^2}{T}$$

Goodness-of-fit Statistics

- Schwarz criterion (SIC)
  - Alternative to AIC
  - Harsher penalty for degrees-of-freedom
  - Used to compare forecasting models

$$SIC = T^{\left(\frac{k}{T}\right)} \frac{\sum_{t=1}^{T} e_t^2}{T}$$

Goodness-of-fit Statistics

- Durbin-Watson stat. (DW)
  - Errors from a good forecasting model should be unforecastable
    - Forcastable error -> room for improvement in the model
    - Correlation among errors -> forecastable information
    - DW tests if the regression disturbances over time are serially correlated.

- $y_t = \beta_0 + \beta_1 x_t + \varepsilon_t$, where $\varepsilon_t = \varphi \varepsilon_{t-1} + v_t$

$$v_t \overset{iid}{\longrightarrow} N(0, \sigma^2)$$

    - ε_t is serially correlated when $\varphi \neq 0$.
    - Ideal case $\varphi = 0$

Goodness-of-fit Statistics

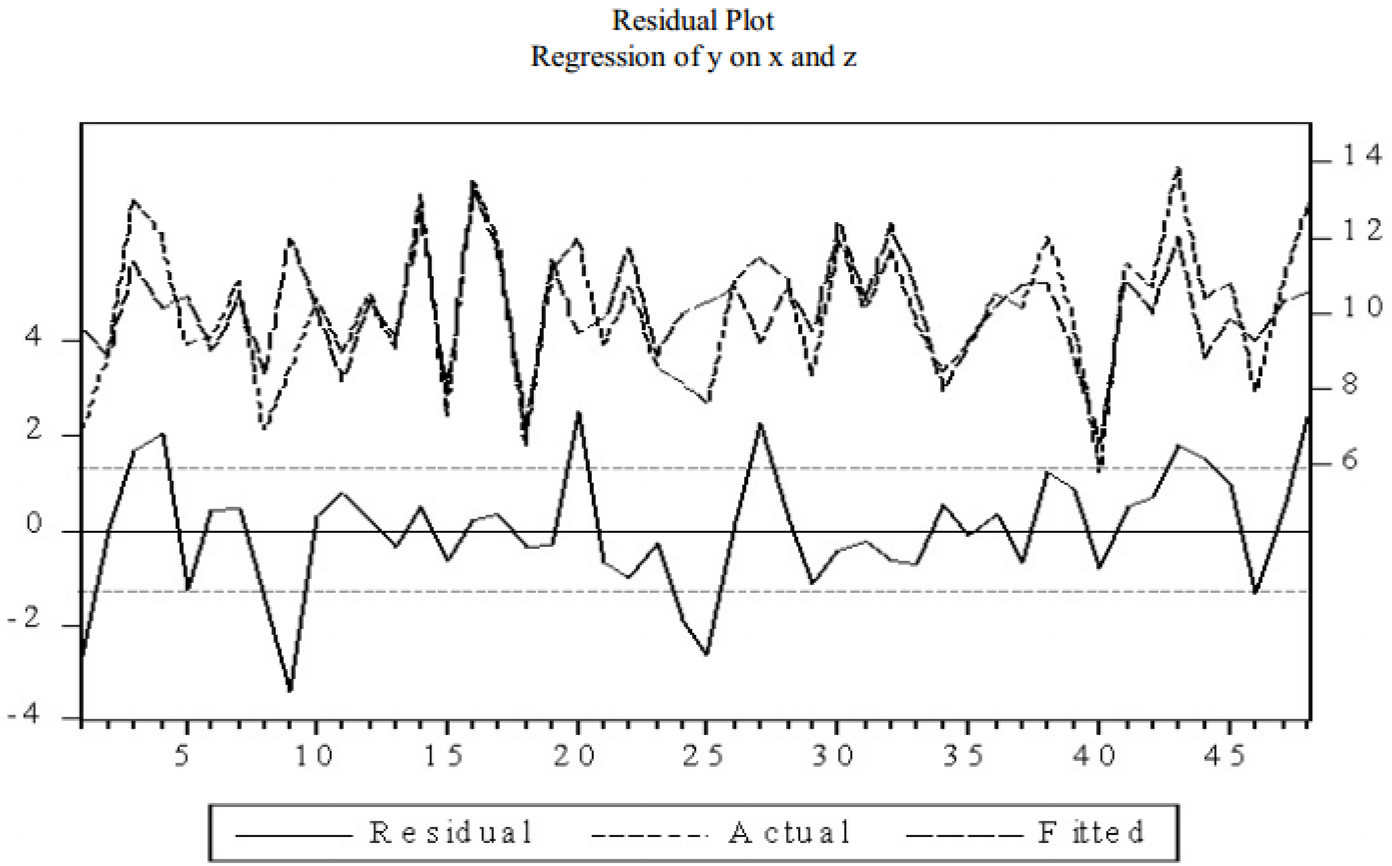
- Durbin-Watson stat. (DW)
  - $H_0: \varphi = 0$
  - $0 \leq DW \leq 4$
    - **OK:** $DW \sim 2$
    - **Alarm:** $DW < 1.5$
      - Consult DW tables for significance level for rejecting the null hypothesis

$$DW = \frac{\sum_{t=2}^{T} (e_t - e_{t-1})^2}{\sum_{t=1}^{T} e_t^2}$$

Goodness-of-fit Statistics

- Residual plot
  - Examine :
    - Actual data (y_t)
    - Fitted values ($\hat{y}_t$)
    - Residuals (e_t)

Goodness-of-fit Statistics



Evaluation Metrics

Evaluation Metrics

- Up to now: measure a model's performance by some simple metric
  - classifier error rate, accuracy, …
- Simple example: accuracy

$$accuracy = \frac{\text{Number of correct decisions made}}{\text{Total number of decisions made}}$$

- Classification accuracy is popular, but usually **too simplistic** for applications of data mining to real business problems
- **Decompose** and count the different types of correct and incorrect decisions made by a classifier

Unequal costs and benefits

- How much do we care about the different **errors** and correct decisions?
  - Classification accuracy makes no distinction between **false positive** and **false negative** errors
  - In real-world applications, different kinds of errors lead to different consequences!
- Examples for medical diagnosis:
  - a patient has cancer (although he does not)
    → **false positive error**, expensive, but not life threatening
  - a patient has cancer, but she is told that she has not
    → **false negative error**, more serious
- Errors should be counted separately
  - Estimate cost or benefit of each decision

Confusion Matrix

- A confusion matrix for a problem involving n classes
  - is an $n \times n$ matrix with the columns labeled with actual classes and the rows labels with predicted classes

		Predicted Classes	
		p	**n**
True Values	**1**	True Positives (TP)	False Negative (FN)
	0	False Positives (FP)	True Negatives (TN)

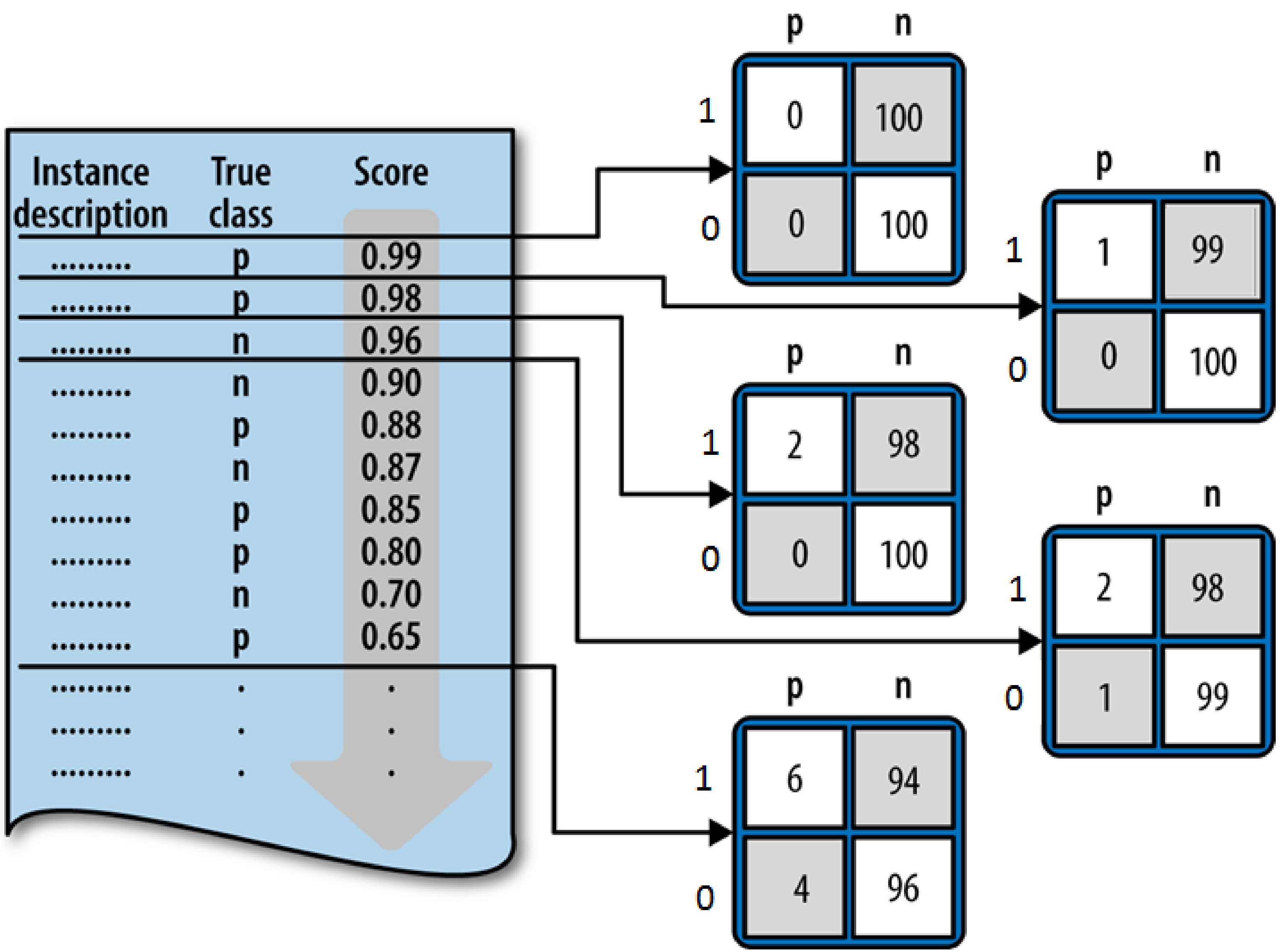
- Each example in a test set has an **actual class label** and the **class predicted** by the classifier
- The confusion matrix separates out the decisions made by the classifier
  - actual/true classes: **1** (Positive Label), **0** (Negative Label)
  - predicted classes: **p**(ositive), **n**(egative)
  - The main diagonal contains the count of correct decisions

Other Evaluation Metrics

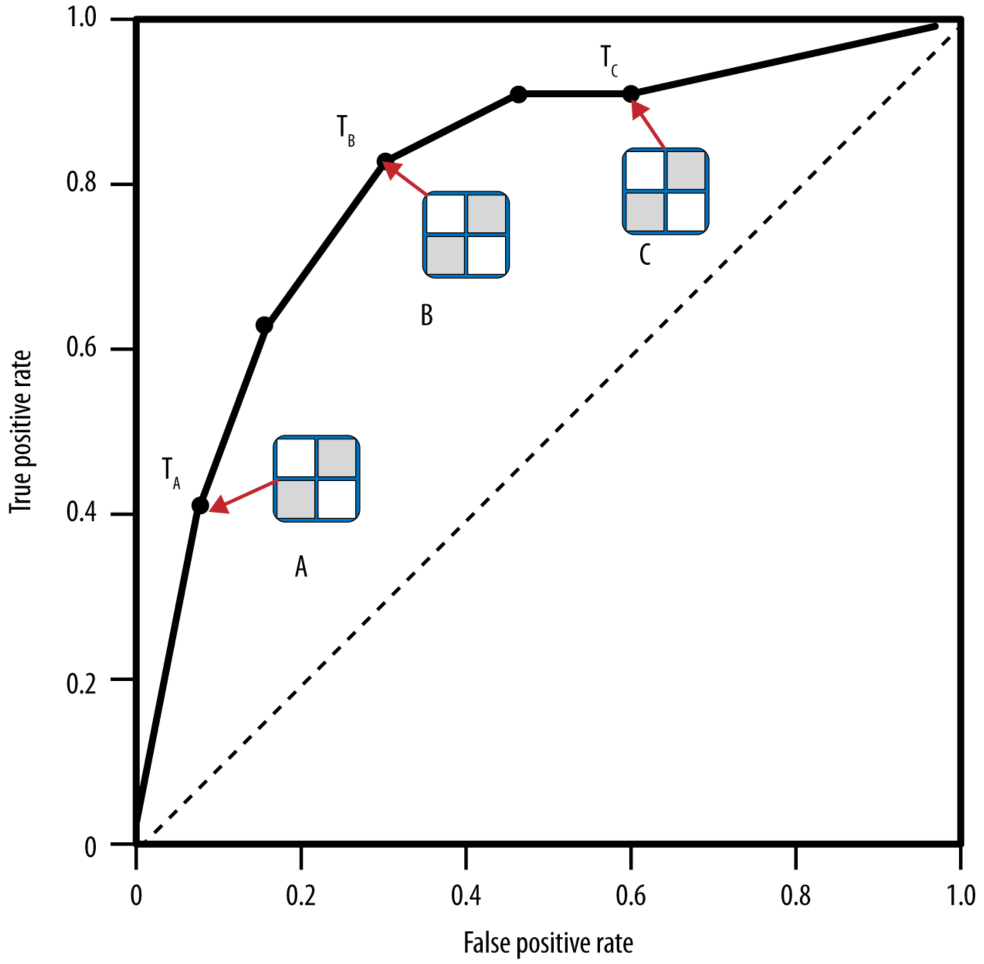
- Based on the entries of the confusion matrix, we can describe various evaluation metrics
  - True positive rate (Recall): $\frac{TP}{TP+FN}$
  - False negative rate: $\frac{FN}{TP+FN}$
  - Precision (accuracy over the cases predicted to be positive): $\frac{TP}{TP+FP}$
  - F-measure (harmonic mean): $2 \cdot \frac{precision \cdot recall}{precision + recall}$
  - Specificity: $\frac{TN}{TN+FP}$
  - Sensitivity: $\frac{TP}{TP+FN}$
  - Accuracy (count of correct decisions): $\frac{TP+TN}{P+N}$

ROC Curves

Ranking Instead of Classifying



ROC Graphs and Curves



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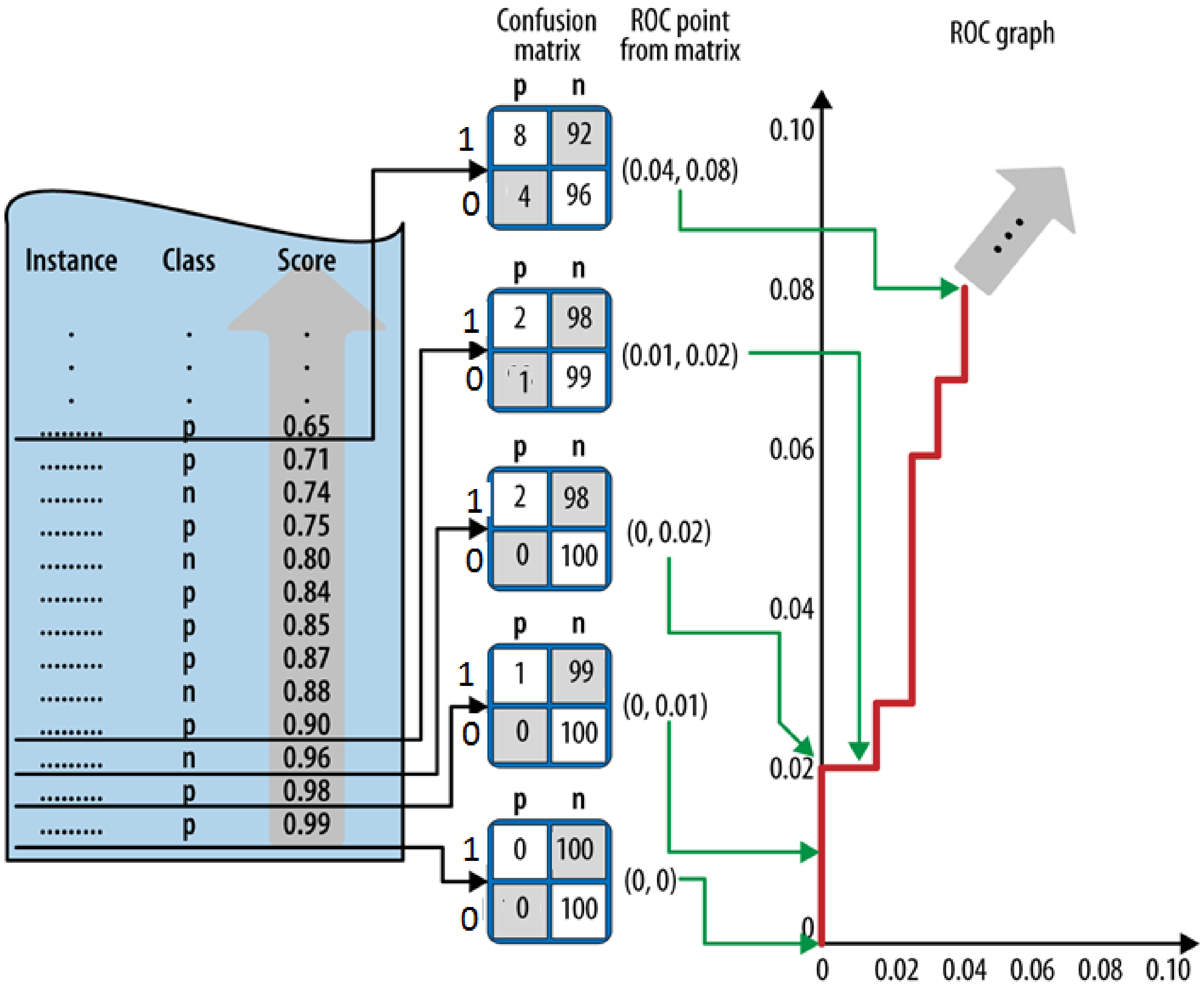


Generating ROC curve: Algorithm

- Sort the test set by the model predictions
- Start with cutoff = max (prediction)
- Decrease cutoff, after each step count the number of true positives TP (positives with prediction above the cutoff) and false positives FP (negatives above the cutoff)
- Calculate TP rate (TP/P) and FP (FP/N) rate
- Plot current number of TP/P as a function of current FP/N

Area Under the ROC Curve (AUC)

- The area under a classifier's curve expressed as a fraction of the unit square
  - Its value ranges from zero to one
- The AUC is useful when a single number is needed to summarize performance, or when nothing is known about the operating conditions
  - A ROC curve provides more information than its area
- Equivalent to the Mann-Whitney-Wilcoxon measure
  - Also equivalent to the Gini Coefficient (with a minor algebraic transformation)
  - Both are equivalent to the probability that a randomly chosen positive instance will be ranked ahead of a randomly chosen negative instance

Performance Evaluation

- Training Set:

Model	Accuracy
Classification Tree	95%
Logistic Regression	93%
k-Nearest Neighbors	100%
Naive Bayes	76%

- Test Set:

Model	Accuracy	AUC
Classification Tree	91.8%$\pm$0.0	0.614$\pm$0.014
Logistic Regression	93.0%$\pm$0.1	0.574$\pm$0.023
k-Nearest Neighbors	93.0%$\pm$0.0	0.537$\pm$0.015
Naive Bayes	76.5%$\pm$0.6	0.632$\pm$0.019

Performance Evaluation

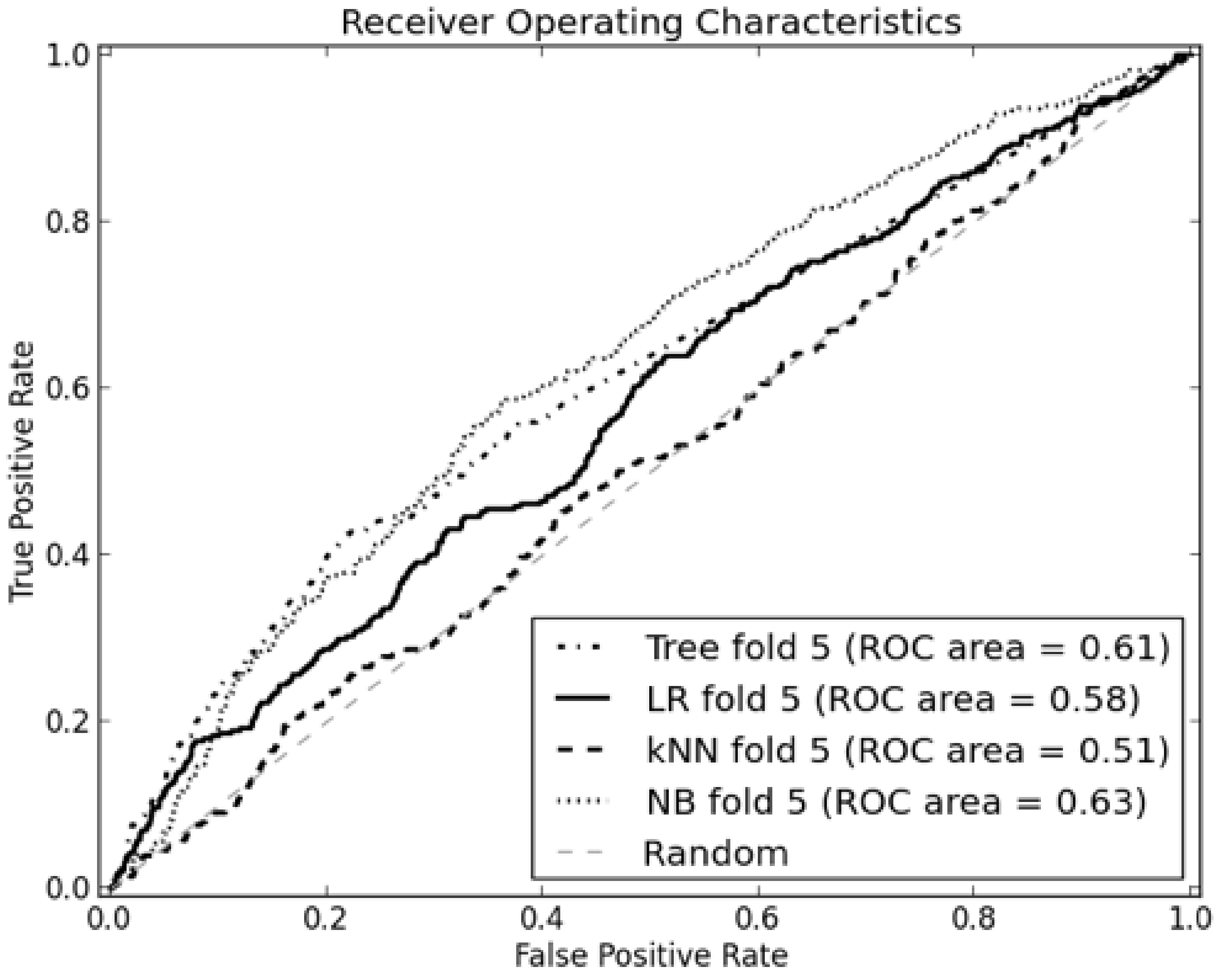
- Naive Bayes confusion matrix:

	p	n
1	127 (3%)	200 (4%)
0	848 (18%)	3518 (75%)

- k-Nearest Neighbors confusion matrix:

	p	n
1	3 (0%)	324 (7%)
0	15 (0%)	4351 (93%)

ROC Curve


Receiver Operating Characteristics
True Positive Rate
False Positive Rate
0.0
0.2
0.4
0.6
0.8
1.0
Tree fold 5 (ROC area = 0.61)
LR fold 5 (ROC area = 0.58)
kNN fold 5 (ROC area = 0.51)
NB fold 5 (ROC area = 0.63)
Random

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