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NPTEL ONLINE CERTIFICATION COURSE

MULTIPLE LINEAR REGRESSION-PART V
EXHAUSTIVE SEARCH

LECTURE 26

DR. GAURAV DIXIT

DEPARTMENT OF MANAGEMENT STUDIES

MULTIPLE LINEAR REGRESSION

- Steps to reduce the no. of predictors
  - Summary statistics and graphs
  - Statistical methods using computational power
    - Exhaustive search: all possible combinations
    - Partial-iterative search: algorithm based
- Exhaustive Search
  - Large no. of subsets
  - Criteria to compare models
    - Adjusted R^2

MULTIPLE LINEAR REGRESSION

- Adjusted R^2

$$R^2_{adj} = 1 - \frac{n-1}{n-p-1}(1 - R^2)$$

Where R^2 is proportion of explained variability in the model

$$R^2 = 1 - \frac{SSE}{SST} = 1 - \frac{\sum_{i=1}^{n}(yi - \hat{y}_i)}{\sum_{i=1}^{n}(yi - \bar{y})}$$

$$\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

- R^2 is called coefficient of determination

MULTIPLE LINEAR REGRESSION

- R^2 would be equal to squared correlation in a single predictor model, that is how R^2 gets its name

- Adjusted R^2 introduces a penalty on the no. of predictors to trade-off between artificial increase vs. amount of information

- High adjusted R^2 values -> low $\hat{\sigma}^2$

MULTIPLE LINEAR REGRESSION

- Exhaustive Search
  - Criteria to compare models
    - Mallow's C_p
- Mallow's C_p

$$C_p = \frac{SSR}{\widehat{\sigma_f}^2} + 2(p+1) - n$$

Where $\widehat{\sigma_f}^2$ is estimated value of σ^2 in the full model

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

MULTIPLE LINEAR REGRESSION

- Mallow's C_p
  - Assumption: full model with all predictors is unbiased
    - Predictors elimination would reduce the variability
  - Best subset model would have C_p ~ p+1 and p would be a small value
  - Requires high n value for the training partition relative to p
- Open RStudio

MULTIPLE LINEAR REGRESSION

- Partial-iterative search
  - Computationally cheaper
  - Best subset is not guaranteed
    - Potential of missing “good” sets of predictors
  - Produce close-to-best subsets
  - Preferred approach for large no. of predictors
  - For moderate no. of predictors, exhaustive search is better
- Trade-off between computation cost vs. potential of finding best subset

MULTIPLE LINEAR REGRESSION

- Partial-iterative search algorithms
  - Forward selection
    - Add predictors one by one
    - Strength as a single predictor is used
  - Backward elimination
    - Drop predictors one by one
  - Stepwise regression
    - Add predictors one by one and consider dropping insignificant ones
- Open RStudio

Key References

- Data Science and Big Data Analytics: Discovering, Analyzing, Visualizing and Presenting Data by EMC Education Services (2015)
- Data Mining for Business Intelligence: Concepts, Techniques, and Applications in Microsoft Office Excel with XLMiner by Shmueli, G., Patel, N. R., & Bruce, P. C. (2010)

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MULTIPLE LINEAR REGRESSION-PART VI
Partial Iterative Search
LECTURE 27

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MULTIPLE LINEAR REGRESSION

- Partial-iterative search
  - Computationally cheaper
  - Best subset is not guaranteed
    - Potential of missing “good” sets of predictors
  - Produce close-to-best subsets
  - Preferred approach for large no. of predictors
  - For moderate no. of predictors, exhaustive search is better
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MULTIPLE LINEAR REGRESSION

- Partial-iterative search algorithms
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    - Add predictors one by one
    - Strength as a single predictor is used
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    - Add predictors one by one and consider dropping insignificant ones
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MACHINE LEARNING TECHNIQUE
k-NEAREST NEIGHBORS (k-NN)

LECTURE 28

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k-NEAREST NEIGHBORS (k-NN)

- k-NN
  - No assumptions about the form of relationship between outcome variable and the set of predictors
  - Non-parametric method
    - No parameters from the assumed functional form to estimate
  - Useful information for modeling is extracted using the similarities between the records based on predictors' values
    - Typically, distance based similarity measures are used

k-NEAREST NEIGHBORS (k-NN)

- k-NN: distance metrics
  - Most popular metric is Euclidean distance

  For two records having values of the predictors denoted by $(x_1, x_2, \ldots, x_p)$ and $(w_1, w_2, \ldots, w_p)$

$$D_{Eu} = \sqrt{(x_1 - w_1)^2 + (x_2 - w_2)^2 + \ldots + (x_p - w_p)^2}$$

    - Low computation costs
  - Other distance metrics: statistical distance or Mahalanobis distance and Manhattan distance
  - Euclidean distance is preferred in k-NN due to many distance computations

k-NEAREST NEIGHBORS (k-NN)

- k-NN
  - Scaling of predictors: standardized values of predictors
- k-NN for Classification task
  - Main idea is to find k records in the training partition which are neighboring the new observation to be classified
  - These k neighbors are used to classify the new observation into a class
    - Predominant class among the neighbors

k-NEAREST NEIGHBORS (k-NN)

- k-NN: Finding neighbors and Classification
  - Compute the distance between the new observation and training partition records
  - Determine k nearest or closest records to the new observation
  - Find most prevalent class among k neighbors and it would be the predicted class of new observation

- Open RStudio

Key References

- Data Science and Big Data Analytics: Discovering, Analyzing, Visualizing and Presenting Data by EMC Education Services (2015)
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MACHINE LEARNING TECHNIQUE
k-NEAREST NEIGHBORS (k-NN)- Part 2

LECTURE 29

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DEPARTMENT OF MANAGEMENT STUDIES

k-NEAREST NEIGHBORS (k-NN)

- k-NN
  - Choosing appropriate value of k
  - k=1: powerful for large no. of records in training partition
  - k>1: smoothing effects (control overfitting issues)
  - Low value of k -> more likely to fit the noise
  - High value of k -> more likely to ignore the local patterns in the data
  - Trade-off between benefits from local pattern vs global effects
  - k=n: naïve rule

k-NEAREST NEIGHBORS (k-NN)

- k-NN
  - Value of k: depends on nature of the data as well
    - Low value of k for data with complex and irregular structures
  - Typical value of k: between ‘1-20’
  - Odd value of k is preferred to avoid ties in majority class decisions
- Best value of k
  - Classification performance on validation partition
- Open RStudio

Key References

- Data Science and Big Data Analytics: Discovering, Analyzing, Visualizing and Presenting Data by EMC Education Services (2015)
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MACHINE LEARNING TECHNIQUE
k-NEAREST NEIGHBORS (k-NN) PART 3

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DEPARTMENT OF MANAGEMENT STUDIES

k-NEAREST NEIGHBORS (k-NN)

- k-NN: Finding neighbors and Classification
  - Compute the distance between the new observation and training partition records
  - Determine k nearest or closest records to the new observation
  - Find most prevalent class among k neighbors and it would be the predicted class of new observation

- Open RStudio

k-NEAREST NEIGHBORS (k-NN)

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  - Odd value of k is preferred to avoid ties in majority class decisions
- Best value of k
  - Classification performance on validation partition
- Open RStudio

k-NEAREST NEIGHBORS (k-NN)

- Majority decision rule vs. cutoff probability
  - Two class scenario: majority rule ≡ cutoff value of 0.5
- k-NN for multi-class scenario
- Class of interest
  - Instead of the majority rule, compare proportion of k neighbors belonging to class of interest to a user-specified cut off value

k-NEAREST NEIGHBORS (k-NN)

- k-NN for Prediction task
  - Main idea is to find k records in the training partition which are neighboring the new observation to be predicted
  - These k neighbors are used to predict the value of new observation
    - Average value of the outcome variable among the neighbors
    - Weighted average wherein weight for a neighbor decreases as its distance from new observation increases
  - Performance metric: RMSE or some other prediction error metric

k-NEAREST NEIGHBORS (k-NN)

- k-NN: Finding neighbors and Prediction
  - Compute the distance between the new observation and training partition records
  - Determine k nearest or closest records to the new observation
  - Compute the average or weighted average of outcome variable values among k neighbors and it would be the predicted value of new observation

k-NEAREST NEIGHBORS (k-NN)

- Further Comments on k-NN algorithm
  - Computation time to find nearest neighbors for large training partition
    - Dimension reduction techniques
    - Steps to find neighbors can be optimized using efficient data structures for search operations like trees
    - Identification and pruning of redundant records from training partition which will not be included in neighbor search steps
  - Curse of dimensionality
    - Sample size requirement depends on no. of predictors
    - Leads to more computations for neighbors

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NAÏVE BAYES

LECTURE 31

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DEPARTMENT OF MANAGEMENT STUDIES

NAÏVE BAYES

- Complete or Exact Bayes for classification
  - Search for records in training partition having same predictors' values as the new observation to be classified
  - Find the most prevalent class of the outcome variable among the records
  - Assign this class to the new observation
- Class of interest
  - User specified cut off value for the class of interest

NAÏVE BAYES

- Class of interest
  - Search for records in training partition having same predictors' values as the new observation to be classified
  - Find the probability of a record belonging to the class of interest among the records
  - If computed probability value > cut off value, assign the new observation to the class of interest

NAÏVE BAYES

- Concept of conditional probability
  - For an outcome variable with m classes $\{C_1, C_2, \ldots, C_m\}$ and p predictors $\{x_1, x_2, \ldots, x_p\}$, we are interested in the following probability value:

$$P(C_i|x_1, x_2, \ldots, x_p) = \frac{P(x_1, x_2, \ldots, xp|C_i)P(C_i)}{P(x_1, x_2, \ldots, xp|C_1)P(C_1) + \ldots + P(x_1, x_2, \ldots, xp|Cm)P(Cm)}$$

  - Assign the new observation to the class with highest probability value
  - Or, if the probability value for the class of interest > cut off value for the same, assign the new observation to the class of interest

NAÏVE BAYES

- Bayes Model for classification
  - Predictors should also be categorical
  - Numerical variables will have to be converted into categorical variables through binning
- Open Excel
- Complete or Exact Bayes Limitations
  - For a model even with small no. of predictors, many new observations to be classified might not get exact matches
  - Probability of a match might reduce significantly on adding just one variable to the set of predictors

Key References

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NAÏVE BAYES PART-2

LECTURE 32

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DEPARTMENT OF MANAGEMENT STUDIES

NAÏVE BAYES

- Bayes Model for classification
  - Predictors should also be categorical
  - Numerical variables will have to be converted into categorical variables through binning
- Open Excel
- Complete or Exact Bayes Limitations
  - For a model even with small no. of predictors, many new observations to be classified might not get exact matches
  - Probability of a match might reduce significantly on adding just one variable to the set of predictors

NAÏVE BAYES

- Instead of Complete or Exact Bayes, switch to Naïve Bayes
  - In Naïve Bayes, all the records are used instead of relying on just the matching records
- Naïve Bayes Modification
  - For class i of outcome variable, compute the probabilities (P_1, P_2, …, P_p) of belonging to class i for each predictor's value (x_1, x_2, …, x_p) taken by the new observation to be classified
  - Compute $P_1 \times P_2 \times \ldots \times P_p \times P(C_i)$
  - Execute previous two steps for all the classes

NAÏVE BAYES

- Naïve Bayes Modification
  - To compute the probability of the new observation belonging to class i, divide the value computed in step 2 by the summation of values computed in step 2 for all the classes
  - Execute previous step for all the classes
  - Classify the new observation to the class with the highest probability value

NAÏVE BAYES

- Naïve Bayes formula

$$P(C_i|x_1, x_2, \ldots, x_p) = \frac{[P(x_1|C_i)P(x_2|Ci) \ldots P(xp|Ci)]P(Ci)}{[P(x_1|C_1)P(x_2|C_1) \ldots P(xp|C_1)]P(C_1) + \ldots + [P(x_1|Cm)P(x_2|Cm) \ldots P(xp|Cm)]P(Cm)}$$

  - Naïve Bayes formula is directly derived from the exact Bayes formula after making following assumption:
  - Predictors' values $\{x_1, x_2, \ldots, xp\}$ occur independent of each other for a given class

$$P(x_1, x_2, \ldots, xp|Ci) \equiv P(x_1|Ci)P(x_2|Ci) \ldots P(xp|Ci)$$

NAÏVE BAYES

- Naïve Bayes formula
  - For classification, naïve Bayes formula works quite well
  - Since we don't require probabilities values to be accurate in absolute term, rather just a reasonably accurate rank ordering of these values
  - For the same reason, we should use the numerator only and drop the denominator which is common for all the classes
- Steps when we have a class of interest
  - User specified cut off value for the class of interest

NAÏVE BAYES

- Steps when we have a class of interest
  - Compute the probabilities (P_1, P_2, …, P_p) of belonging to class of interest for each predictor's value (x_1, x_2, …, x_p) taken by the new observation to be classified
  - Compute $P_1 \times P_2 \times \ldots \times P_p \times$ P(Class of interest)
  - Execute previous two steps for all the classes
  - To compute the probability of the new observation belonging to class of interest, divide the value computed in step 2 by the summation of values computed in step 2 for all the classes

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NAÏVE BAYES PART-3

LECTURE 33

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DEPARTMENT OF MANAGEMENT STUDIES

NAÏVE BAYES

- Bayes Model for classification
  - Predictors should also be categorical
  - Numerical variables will have to be converted into categorical variables through binning
- Open Excel
- Complete or Exact Bayes Limitations
  - For a model even with small no. of predictors, many new observations to be classified might not get exact matches
  - Probability of a match might reduce significantly on adding just one variable to the set of predictors

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  - Compute $P_1 \times P_2 \times \ldots \times P_p \times P(C_i)$
  - Execute previous two steps for all the classes

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  - Execute previous step for all the classes
  - Classify the new observation to the class with the highest probability value

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  - Predictors' values $\{x_1, x_2, \ldots, xp\}$ occur independent of each other for a given class

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- Steps when we have a class of interest
  - User specified cut off value for the class of interest

NAÏVE BAYES

- Steps when we have a class of interest
  - Compute the probabilities (P_1, P_2, …, P_p) of belonging to class of interest for each predictor's value (x_1, x_2, …, x_p) taken by the new observation to be classified
  - Compute $P_1 \times P_2 \times \ldots \times P_p \times$ P(Class of interest)
  - Execute previous two steps for all the classes
  - To compute the probability of the new observation belonging to class of interest, divide the value computed in step 2 by the summation of values computed in step 2 for all the classes

Key References

- Data Science and Big Data Analytics: Discovering, Analyzing, Visualizing and Presenting Data by EMC Education Services (2015)
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NAÏVE BAYES PART-4

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NAÏVE BAYES

- Naïve Bayes formula
  - For classification, naïve Bayes formula works quite well
  - Since we don't require probabilities values to be accurate in absolute term, rather just a reasonably accurate rank ordering of these values
  - For the same reason, we should use the numerator only and drop the denominator which is common for all the classes
- Steps when we have a class of interest
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NAÏVE BAYES

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  - Compute the probabilities (P_1, P_2, …, P_p) of belonging to class of interest for each predictor's value (x_1, x_2, …, x_p) taken by the new observation to be classified
  - Compute $P_1 \times P_2 \times \ldots \times P_p \times$ P(Class of interest)
  - Execute previous two steps for all the classes
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NAÏVE BAYES PART-5

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NAÏVE BAYES

- Further Comments on Naïve Bayes
  - Good performance despite assumption of independent predictors' values being far from true
  - Requires large no. of records
  - Few classes of predictors might not be represented in the training partition records
    - Zero probability is assumed
  - Good for classification but not for estimating probabilities of class membership

Key References

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- Data Mining for Business Intelligence: Concepts, Techniques, and Applications in Microsoft Office Excel with XLMiner by Shmueli, G., Patel, N. R., & Bruce, P. C. (2010)

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CLASSIFICATION & REGRESSION TREES

LECTURE 36

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DEPARTMENT OF MANAGEMENT STUDIES

CLASSIFICATION & REGRESSION TREES

- CART
  - A data-driven method
    - Based on separating observations into homogeneous subgroups by creating splits on predictors
  - Used for both prediction and classification tasks
  - Model is represented by a tree diagram
    - Easy to interpret logical rules
    - CART algorithm grows binary trees
  - Adoption across domains

CLASSIFICATION & REGRESSION TREES

- Classification Trees
  - Recursive partitioning
    - About partitioning p-dimensional space of predictors using training partition, where p is no. of predictors
  - Pruning
    - About pruning the built tree using validation data

CLASSIFICATION & REGRESSION TREES

- Recursive Partitioning
  - Partitioning p-dimensional space of predictors into non-overlapping multi-dimensional rectangles
  - The partitioning process is recursive in nature
    - Applied on the results of previous partitions
- Steps for Recursive Partitioning
  - An optimal combination of one of the predictors, x_i and its value v_i is selected to create first split of p-dimensional space into two parts
    - Part I: $x_i \leq v_i$
    - Part II: $x_i > v_i$

CLASSIFICATION & REGRESSION TREES

- Steps for Recursive Partitioning
  - Step 1 is applied again on the two parts and process continues to create more rectangular parts
  - The partitioning process continues till we reach pure homogeneous parts
    - All the observations in the part belong to just one of the classes
- Open RStudio

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CLASSIFICATION & REGRESSION TREES PART-2

LECTURE 37

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DEPARTMENT OF MANAGEMENT STUDIES

CLASSIFICATION & REGRESSION TREES

- Impurity Measures
  - Gini index and Entropy measure
- Gini Index

  For an outcome variable with m classes, Gini impurity index for a rectangular part is defined as

$$gini = 1 - \sum_{k=1}^{m} {P_k}^2$$

  Where P_k is the proportion of rectangular part observations belonging to class k

CLASSIFICATION & REGRESSION TREES

- Gini Index
  - Gini values lie in the range {0, (m-1)/m} for m-class scenario and {0, 0.5} for two-class scenario
- Entropy Measure

For an outcome variable with m classes, entropy for a rectangular part is defined as

$$Entropy = -\sum_{k=1}^{m} P_k log_2(Pk)$$

CLASSIFICATION & REGRESSION TREES

- Entropy Measure
  - Entropy values lie in the range {0, $\log_2(m)$} for m-class scenario and {0, 1} for two-class scenario
- Open RStudio
- Tree diagram or tree structure
  - Each split of p-dimensional space into two parts can be depicted as a split of a node in a decision tree into two child nodes
  - First split creates branches of root node

CLASSIFICATION & REGRESSION TREES

- Two types of nodes in tree structure
  - Decision node: Depicted with a circle
  - Terminal or leaf node: Depicted with a rectangle
    - Correspond to Final rectangular parts
- Steps to classify a new observation using tree based models
  - New observation to be classified is dropped down the tree starting from root node
  - At each decision node, the appropriate branch is taken until we reach a leaf node

CLASSIFICATION & REGRESSION TREES

- Steps to classify a new observation using tree based models
  - At leaf node, majority class is assigned to the new observation
    - For class of interest scenario, proportion of records belonging to the class of interest is compared with the user specified cut off value for the same

- Open RStudio

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CLASSIFICATION & REGRESSION TREES PART-3

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CLASSIFICATION & REGRESSION TREES

- Two types of nodes in tree structure
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    - Correspond to Final rectangular parts
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  - New observation to be classified is dropped down the tree starting from root node
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CLASSIFICATION & REGRESSION TREES PART-4

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CLASSIFICATION & REGRESSION TREES

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- Classification Trees
  - Recursive partitioning
    - About partitioning p-dimensional space of predictors using training partition, where p is no. of predictors
  - Pruning
    - About pruning the built tree using validation data

CLASSIFICATION & REGRESSION TREES

- CART example has been discussed in the lecture video

CLASSIFICATION & REGRESSION TREES

- Further Comments on CART
  - Can be used as a variable selection approach
  - No variable transformation is required
  - Robust to outliers
  - Non-linear and non-parametric technique
  - Handle missing values

  - Sensitive to sample data changes
  - Predictor's strength as a single variable is modeled and not as part of a group of predictors

CLASSIFICATION & REGRESSION TREES

- Further Comments on CART
  - Might not fit linear structures or relationships between predictors
    - New predictors based on hypothesized relationships can be used
  - Require a large dataset
  - High computation time

Key References

- Data Science and Big Data Analytics: Discovering, Analyzing, Visualizing and Presenting Data by EMC Education Services (2015)
- Data Mining for Business Intelligence: Concepts, Techniques, and Applications in Microsoft Office Excel with XLMiner by Shmueli, G., Patel, N. R., & Bruce, P. C. (2010)

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CLASSIFICATION & REGRESSION TREES PART-5

LECTURE 40

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DEPARTMENT OF MANAGEMENT STUDIES

CLASSIFICATION & REGRESSION TREES

- CART example has been discussed in the lecture video

CLASSIFICATION & REGRESSION TREES

- Further Comments on CART
  - Can be used as a variable selection approach
  - No variable transformation is required
  - Robust to outliers
  - Non-linear and non-parametric technique
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  - Predictor's strength as a single variable is modeled and not as part of a group of predictors

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CLASSIFICATION & REGRESSION TREES PART-6

LECTURE 41

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DEPARTMENT OF MANAGEMENT STUDIES

CLASSIFICATION & REGRESSION TREES

- Steps to classify a new observation using tree based models
  - At leaf node, majority class is assigned to the new observation
    - For class of interest scenario, proportion of records belonging to the class of interest is compared with the user specified cut off value for the same

- Open RStudio

CLASSIFICATION & REGRESSION TREES

- Pruning
  - Avoid overfitting
    - Full grown tree leads to complete overfitting of data
    - Poor performance on new data
  - Overall error of tree models
    - Expected to decrease until the point where relationships between outcome variable and predictors are fitted
    - Then tree models start fitting to the noise and overall error starts increasing
      - Due to splits involving small number of observations

Key References

- Data Science and Big Data Analytics: Discovering, Analyzing, Visualizing and Presenting Data by EMC Education Services (2015)
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Pruning Process

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CLASSIFICATION & REGRESSION TREES

- Pruning
  - Avoid overfitting
    - Full grown tree leads to complete overfitting of data
    - Poor performance on new data
  - Overall error of tree models
    - Expected to decrease until the point where relationships between outcome variable and predictors are fitted
    - Then tree models start fitting to the noise and overall error starts increasing
      - Due to splits involving small number of observations

CLASSIFICATION & REGRESSION TREES

- Pruning
  - Stop tree growth before it starts overfitting data or fitting noise
    - No. of splits or tree depth level
    - No. of observations in a node to attempt the split
    - Accepted level of reduction in impurity
    - Difficulties in determining the stopping point for such rules
  - Prune the full grown tree back to a level where it doesn't overfit data or fit noise
    - Use validation partition to prune the tree modeled with training partition
    - Idea is to remove the tree branches which don't reduce the error rate further

CLASSIFICATION & REGRESSION TREES

- Pruning
  - Prune the full grown tree back to a level where it doesn't overfit data or fit noise
    - Find the point where error rate on validation partition starts to increase
    - Cost complexity parameter or complexity parameter (CP) in CART algorithm

$$CP = Err + PF * TL$$

Where Err is misclassification error, PF is penalty factor for tree length (TL)

  - Minimum error tree
    - Tree with minimum misclassification error on validation partition

CLASSIFICATION & REGRESSION TREES

- Pruning
  - Best pruned tree
    - Adjustment for sampling error on minimum error tree
    - Smallest tree in the pruning sequence which lies within one std. err. (of error rate) of minimum error tree
- Open RStudio
- Classification Rules
  - Each terminal node in a tree model is equivalent to a classification rule
  - Simplify and remove redundant rules

Key References

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Pruning Process Part-2

LECTURE-43

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DEPARTMENT OF MANAGEMENT STUDIES

CLASSIFICATION & REGRESSION TREES

- Pruning
  - Avoid overfitting
    - Full grown tree leads to complete overfitting of data
    - Poor performance on new data
  - Overall error of tree models
    - Expected to decrease until the point where relationships between outcome variable and predictors are fitted
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Pruning Process Part-3

LECTURE-44

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DEPARTMENT OF MANAGEMENT STUDIES

CLASSIFICATION & REGRESSION TREES

- Pruning
  - Avoid overfitting
    - Full grown tree leads to complete overfitting of data
    - Poor performance on new data
  - Overall error of tree models
    - Expected to decrease until the point where relationships between outcome variable and predictors are fitted
    - Then tree models start fitting to the noise and overall error starts increasing
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REGRESSION TREES

LECTURE 45

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DEPARTMENT OF MANAGEMENT STUDIES

CLASSIFICATION & REGRESSION TREES

- Regression Trees
  - Outcome variable should be numerical
  - Steps to build tree model are similar to that of classification trees
  - Prediction step, impurity measures and performance metrics are different
- Prediction step
  - Value of a leaf node is predicted value for a new observation that fell in that leaf node
  - Value of a leaf node is computed by taking average of training partition records constituting that leaf node

CLASSIFICATION & REGRESSION TREES

- Impurity Measures
  - Sum of squared deviations from mean of leaf node
    - Equivalent to squared errors since mean value of leaf node is predicted value
  - Lowest impurity is zero when all the observations that fell in a leaf node have same actual value of outcome variable

CLASSIFICATION & REGRESSION TREES

- Further Comments on CART
  - Can be used as a variable selection approach
  - No variable transformation is required
  - Robust to outliers
  - Non-linear and non-parametric technique
  - Handle missing values

  - Sensitive to sample data changes
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LOGISTIC REGRESSION

LECTURE 46

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DEPARTMENT OF MANAGEMENT STUDIES

LOGISTIC REGRESSION

- Equivalent of linear regression for categorical outcome variable
  - Predictors can be categorical or continuous
- Applied in following tasks
  - Classification task
    - Predicting the class of a new observation
  - Profiling
    - Understanding similarities and differences among groups

LOGISTIC REGRESSION

- Steps for logistic regression
  - Estimate probabilities of class memberships
  - Classify observations using probabilities values
    - Most probable class method: assign the observation to the class with highest probability value
      - Equivalently, for a two-class case, cutoff value of 0.5 can be used
    - Class of interest: user specified cutoff value
      - For a two-class case, typically a value greater than average probability value for class of interest, but less than 0.5 can be used

LOGISTIC REGRESSION

- Logistic Regression Model
  - Used typically in cases when structured model is preferred over data-driven models for classification tasks
  - Categorical outcome variable cannot be directly modeled as a linear function of predictors
    - Inability to apply various mathematical operators
    - Variable type mismatches
    - Range reasonability issues
      - LHS range={0, …, m-1}
      - RHS range=(-∞, ∞)

LOGISTIC REGRESSION

- Logistic Regression Model
  - Instead of using outcome variable (Y) in the model, a function of Y, called *logit* is used
- Logit
  - Think about modeling probability value as a linear function of predictors, specifically in a two-class case

If P is the probability of class 1 membership

$$P = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p$$

Where p is the no. of predictors

LOGISTIC REGRESSION

- Logit
  - LHS range improves from {0, 1} to [0, 1], however still cannot match RHS
  - Can we bring RHS range to [0,1]?
    - Nonlinear approach
  - Typically, a nonlinear function of the following form is used to perform the required transformation

$$P = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p)}}$$

This function is called *logistic response function*

LOGISTIC REGRESSION

- Logit
  - Rearrange the previous equation as below:

$$\frac{P}{1-P} = e^{\beta_0+\beta_1 x_1+\beta_2 x_2+\cdots+\beta_p x_p}$$

LHS is expression for *odds*, another measure of class membership

$$odds = \frac{P}{1-P}$$

  - Odds of belonging to a class is defined as ratio of probability of class 1 membership to probability of class 0 membership
    - This metric is popular in sports, horse racing, gambling, and many other areas

LOGISTIC REGRESSION

- Logit
  - Previous equation can be rewritten as

$$odds = e^{\beta_0+\beta_1 x_1+\beta_2 x_2+\cdots+\beta_p x_p}$$

    - Range is now (0, ∞)
  - Take log on both sides of previous equation

$$\log(odds) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p$$

    - Standard logistic model
    - Now, LHS and RHS both have same range (-∞, ∞)
  - Log(odds) is called logit
    - Logit is used as the outcome variable in the model instead of categorical Y

LOGISTIC REGRESSION

- Odds and logit can be written as a function of probability of class 1 membership
  - Open RStudio

- In logistic regression model, we predict the logit values and therefore corresponding probability of a categorical outcome
  - Predicted probabilities values become the basis for classification
  - A prediction model for classification task

Key References

- Data Science and Big Data Analytics: Discovering, Analyzing, Visualizing and Presenting Data by EMC Education Services (2015)
- Data Mining for Business Intelligence: Concepts, Techniques, and Applications in Microsoft Office Excel with XLMiner by Shmueli, G., Patel, N. R., & Bruce, P. C. (2010)

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LOGISTIC REGRESSION- PART 2

LECTURE 47

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DEPARTMENT OF MANAGEMENT STUDIES

LOGISTIC REGRESSION

- Logit
  - LHS range improves from {0, 1} to [0, 1], however still cannot match RHS
  - Can we bring RHS range to [0,1]?
    - Nonlinear approach
  - Typically, a nonlinear function of the following form is used to perform the required transformation

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    - Standard logistic model
    - Now, LHS and RHS both have same range (-∞, ∞)
  - Log(odds) is called logit
    - Logit is used as the outcome variable in the model instead of categorical Y

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  - Open RStudio

- In logistic regression model, we predict the logit values and therefore corresponding probability of a categorical outcome
  - Predicted probabilities values become the basis for classification
  - A prediction model for classification task

LOGISTIC REGRESSION

- Estimation Technique
  - Least squares method used in multiple linear regression cannot be used
    - Non-linear formulation of logistic regression
  - Maximum likelihood method is used
    - Estimates are optimized in order to maximize the likelihood of obtaining the observations used in training the model
    - Less robust than estimation techniques used in linear regression
    - Reliability of estimates
      - Outcome variable categories should have adequate proportion
      - Adequate sample size w.r.t no. of estimates

LOGISTIC REGRESSION

- Estimation Technique
  - Maximum likelihood method is used
    - Collinearity issues similar to linear regression
- Interpretation of Results
  - Logit model
    - Additive factor (β)
      - If $\beta < 0$, increase in x => decrease in logit values
      - If $\beta > 0$, increase in x => increase in logit values
    - For any value of x, interpretative statements of results are same

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LOGISTIC REGRESSION PART-3

LECTURE 48

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LOGISTIC REGRESSION

- Odds and odds ratios
  - Odds is a ratio of two probability values (prob. of class 1/prob. Of Class 0)
  - Odds ratio is ratio of two odds (odds of class m1/odds of class m2)
    - Odds ratio > 1 => odds of class m1 are higher than class m2

- Open RStudio

Key References

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LOGISTIC REGRESSION PART-4

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DEPARTMENT OF MANAGEMENT STUDIES

LOGISTIC REGRESSION

- Odds and logit can be written as a function of probability of class 1 membership
  - Open RStudio

- In logistic regression model, we predict the logit values and therefore corresponding probability of a categorical outcome
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  - A prediction model for classification task

LOGISTIC REGRESSION

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LOGISTIC REGRESSION

- Interpretation of Results
  - Odds model
    - Multiplicative factor (e^{β})
      - If $\beta < 0$, increase in x => decrease in odds
      - If $\beta > 0$, increase in x => increase in odds
    - For any value of x, interpretative statements of results are same
  - Probability model
    - For a unit increase in a particular predictor, corresponding change in the probability value is not a constant, while holding all other predictors constant
      - Depends on the specific values of the predictor
    - Interpretative statements of results depend on specific values of x

LOGISTIC REGRESSION

- Odds and odds ratios
  - Odds is a ratio of two probability values (prob. of class 1/prob. Of Class 0)
  - Odds ratio is ratio of two odds (odds of class m1/odds of class m2)
    - Odds ratio > 1 => odds of class m1 are higher than class m2

- Open RStudio

LOGISTIC REGRESSION

- Linear Regression for a categorical outcome variable?
  - Can be done by treating the outcome variable as continuous and coding it numerically
  - However, anomalies will lead to spurious modeling
    - Predictions can take any value, not just dummy values {0,1}
    - Outcome variable or residuals don't follow normal distribution
      - binomial distribution
    - Variance of outcome variable is not constant across all records (violation of homoscedasticity)
      - np(1-p)

LOGISTIC REGRESSION

- Logistic Regression for Profiling Task
  - Apart from model performance on validation partition
  - Model's fit to data is assessed on training partition
    - However, still avoid overfitting
    - Usefulness of predictors is examined
  - Goodness of fit metrics
    - Overall fit of the model
      - Deviance (equivalent to SSE in linear regression)
      - 1 - Deviance/Null Deviance (equivalent to multiple R^2 in linear regression)
    - Single predictors

LOGISTIC REGRESSION

- Outcome variable with m classes (m>2)
  - Multinomial logistic regression
    - Separate binary logistic regression model for m-1 classes (one class is treated as reference class)
  - Ordinal logistic regression
    - Large no. of ordinal classes: treat ordinal variable as continuous variable and apply multiple linear regression

LOGISTIC REGRESSION

- Outcome variable with m classes (m>2)
  - Ordinal logistic regression
    - Small no. of ordinal classes: Proportional odds or cumulative logit method
      - Separate binary logistic regression model for m-1 cumulative probabilities

    For a three class case: C1, C2, and C3 and a single predictor x1

$$logit(C1) = \alpha_0 + \beta_1 x_1$$
$$logit(C1 or\ C2) = \beta_0 + \beta_1 x_1$$

- RStudio

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LOGISTIC REGRESSION PART-5

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DEPARTMENT OF MANAGEMENT STUDIES

LOGISTIC REGRESSION

- Interpretation of Results
  - Odds model
    - Multiplicative factor (e^{β})
      - If $\beta < 0$, increase in x => decrease in odds
      - If $\beta > 0$, increase in x => increase in odds
    - For any value of x, interpretative statements of results are same
  - Probability model
    - For a unit increase in a particular predictor, corresponding change in the probability value is not a constant, while holding all other predictors constant
      - Depends on the specific values of the predictor
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  - Model's fit to data is assessed on training partition
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    - Usefulness of predictors is examined
  - Goodness of fit metrics
    - Overall fit of the model
      - Deviance (equivalent to SSE in linear regression)
      - 1 - Deviance/Null Deviance (equivalent to multiple R^2 in linear regression)
    - Single predictors

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    - Separate binary logistic regression model for m-1 classes (one class is treated as reference class)
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LOGISTIC REGRESSION

- Outcome variable with m classes (m>2)
  - Ordinal logistic regression
    - Small no. of ordinal classes: Proportional odds or cumulative logit method
      - Separate binary logistic regression model for m-1 cumulative probabilities

For a three class case: C1, C2, and C3 and a single predictor x1

$$logit(C1) = \alpha_0 + \beta_1 x_1$$
$$logit(C1 or\ C2) = \beta_0 + \beta_1 x_1$$

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