

09/04/16

DATA ANALYTICS

NOTES

What is data mining?

- Exploration and analysis by automatic or semi-automatic means of large quantities of data in order to discover meaningful patterns and rules
- "A tool for extracting the jewel of truth from the slum of data"
- "All models are wrong but some are useful" - George Box
- "We live in a data rich world, most of us stand on the shore of a vast sea of available data, sorted up with the latest diving gear and equipped with the slickest tool and gadget, but with hardly a clue what to do."
- Need to sort data and build predictive models

Steps in problem solving process

- Recognise the problem or question
- Review previous findings
- Model the solution
- Collect the data
- Analyse the data
- Present and act on results

Time

- Time horizon for prediction
- Time window of relevant behaviour
- Time base of the population

Questions to ask:

- Source of your data?
- How well does sample data represent population?

- Why did you decide on that particular approach?
- What alternatives did you consider?
- How likely do the independent variables cause the dependent variable?

Stakeholders

- Who has stake interest of your project?
- Have they been briefed on problem and outlined for solutions?
- Resources and change?
- Review and result model
- "Data mining on its own will not provide the best models; these will be created by the interplay between the knowledge extracted from the data and the experience & specialist staff"
- Only an aid to decision making, not the decision itself
- Neither sophisticated software nor statistical techniques can overcome the inherent limitations of the raw data that goes into them
- GARBAGE IN \Rightarrow GARBAGE OUT
- Do we have enough data both cases and variables?
- Is it legal and available for use?
- How easy is it to collect and process?

Quality of Data

Accurate? complete? current? consistent?

Categorical, ordinal, quantitative

First Steps

Explore data graphically and produce descriptive stats

One variable - dot plot etc

Two vars - Scatterplot

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Many var - Scatterplot matrix

One quan, One cat: Piechart, box plot

Two cat: Frequency distribution, table

PROBLEMS WITH DATA

Outliers

- How are we sure it is an outlier?

- do nothing, ignore the case of variable, replace the values, transform the data

Missing Data

- May reduce number of cases included (reduced data size)

- Remove row of case or the variable?

- Usually coded as NA

- Look at % of each var that is missing

- % of each case that is missing

- if one missing, likely to miss another? - look for patterns

- Visualisation of Missing Values

- Assume missing data is at random

What can we do?

- nothing

- List wise deletion - only included if it has data for all cases

- Pair wise deletion - data included if the case contains certain variables like AC or D, F

- Omit variable or cases with high % (10%+) of missing data

- Weighting for non response

- Imputation - Substitution of data

- Create new variable

- Models are unique in dealing with missing data

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Imputation

- Method for substitution of missing data:
 - regression model
 - copy from left
 - bootstrap
 - mean \rightarrow sd, median, shape of distribution
 - Midrange
 - Distribution-based replacement calculated on percentiles of variable's dist.
 - Hot deck - divide sample into groups and select value at random within group
 - Most frequently occurring variable
- Disadvantage:
 - Alters relationship between variables
 - May increase biases in survey estimates.
 - Researchers may falsely treat data as a complete dataset
 - Imputed values should be flagged

Multiple imputation - Create M datasets with imputed values (complete datasets)
- Combine result which should reflect missing data uncertainty.

09/04/16 DA Classification & REGRESSION TREES

- Supervised learning with a target variable
- Categorical for classification trees, continuous for regression trees
- Need observations on other variables
- Goal: predict or classify an outcome
 - ↳ construct a rule to apply in the future
 - ↳ To see what variables are important / related to target variable

Heart attack example

- 215 cases, 37 died, 100 variables screened

Classification tree

- Upside down tree, root node - all patients
- Two branches defined by a question - Terminal nodes \Rightarrow classification

Outcome Variable definition

- Situation dependent or blindly chosen
- Consensus, prescribed, empirical, time frame

- coding: focus on two category outcome variable Yes/No dead/Alive

Splits for continuous variables

- At each node independently:
 - Examines all possible splits
 - Look at each value for each variable
 - Is it a good split? Which is best split?
- Importance of screening
- Outliers? \rightarrow do not affect outcome

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Splits for categorical data
- Consider all possible splits A B, C ABC etc n -values $\rightarrow 2^n$ splits

Evaluating Splits

- Will have a high class % i.e. 5 dead 300 alive etc

- Impurity Function

\rightarrow node which contains only one class is perfectly pure

\rightarrow Equal proportion of each class is least pure

\uparrow need a measure to distinguish these 2 cases

Prior probabilities

- Chance that a case will be presented to a tree

- Expert knowledge

- Data

- Assume prior

- Rare cases

N_j - Number of in class j overall

$N(t)$ - total number of cases in node t .

$N_j(t)$ # of ~~cases~~ class j cases in node t .

Proportion of class j cases in node $t = N_j(t) / N(t)$

$\pi(j)$ = prior probability $\sum_j \pi(j) = 1$

Probability that a case will be born in class j and fall into node t

$$p(j, t) = (\pi_j N_j(t)) / (N_j)$$

P of a case falling into class j given that a case is in node t

$$p(j|t) = \frac{p(j, t)}{p(t)}$$

7/04/16 DA CLASSIFICATION & R TREE

P that any case falls into Node $t = p(t) = \sum_j p(j|t)$

Common Impurity Functions

$C = \#$ categories in target variable

$$\text{Entropy} = - \sum_{j=1}^C p(j|t) \log_2(p(j|t))$$

$$\text{Gini} = \sum_{j=1}^C \sum_{k=1}^C p(j|t) p(k|t) = 1 - \sum_{j=1}^C p^2(j|t)$$

When $C=2$ $\text{Gini} = 2 * p(1|t) p(2|t)$

Smaller the better \rightarrow means probability are one big, one small

How to use this to choose split

- look at impurity of parent node $t: i(t)$
- Each split at any node gives us 2 children t_L and t_R
- We measure the impurity of the two children

$$i(t) = p_L * i(t_L) + p_R * i(t_R)$$

p_L = probability going left p_R = Prob going right

Choosing nodes

- $\Delta(t,s) = i(t) - p_L * i(t_L) - p_R * i(t_R)$
- Smaller values for $i(t_L)$ and $i(t_R)$ are better (higher classification rate)

$$p_L + p_R = 1$$

- could be 5000+ splits at each node \rightarrow evaluate for each one:

- $i(t)$ will be the same for all

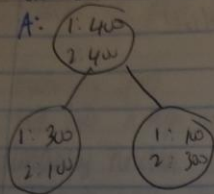
- choose split with largest $\Delta(t,s)$

- R calls this improvement.

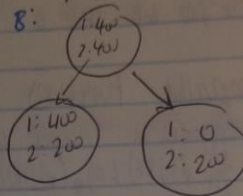
- R multiplies $\Delta(t,s)$ by N - total no. of cases

Use GINI to calculate decrease in impurity for each split

A:



B:



$$\text{Improvement: } \Delta(t_s) = i(t) - p_L i(t_L) - p_R i(t_R)$$

$$i(t) = 2 * \frac{p(1,t)}{p(t)} \frac{p(2,t)}{p(t)}$$

$$= 2 * \frac{p(1,t)}{p(t)} \frac{p(2,t)}{p(t)}$$

A. $i(t) = 2 * 0.5 * 0.5 = 0.5$

$$p_L i(t_L) = \frac{400}{800} * 2 * 0.75 * 0.25 = 0.19$$

$$p_R i(t_R) = \frac{400}{800} * 2 * 0.25 * 0.75 = 0.19$$

$$\Delta(t_s) = 0.5 - 0.19 - 0.19 = 0.12$$

B. $i(t) = 2 * 0.5 * 0.5 = 0.5$

$$p_L i(t_L) = \frac{6}{8} * 2 * \frac{2}{3} * \frac{1}{3} = 0.33$$

$$p_R i(t_R) = \frac{6}{8} * 2 * 0 * \frac{1}{4} = 0$$

$$\Delta(t_s) = 0.5 - 0.33 - 0 = 0.17$$

A has lower impurity/improvement value for the split

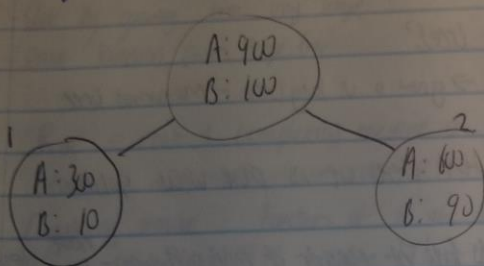
Class Assignment Rule

- Assign a class to every terminal node
- Calculate $p(i|t)$ for each class i
- Let j^* be max of $p(i|t)$
- Assign the node to class j^*
- Can assign a class or output a probability of being assigned to the node.

09/04/16 (10)/rdm & R Tree!

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Priors
- usually we equal prior 0.5, 0.5



$p(1|1)$, $p(1|2)$, $p(1)$ using equal priors and data as prior

Equal prior

$$P(A_i|1) = \frac{\pi_i N_i(1)}{N_i}$$

$$0.5 \times \frac{300}{900} = 0.17$$

$$P(A_2|1) = 0.5 \times \frac{600}{900} = 0.33$$

$$P(B_1|1) = 0.5 \times \frac{10}{100} = 0.05$$

$$P(B_2|1) = 0.5 \times \frac{90}{100} = 0.45$$

$$P(1) = 0.17 + 0.05 = 0.22$$

$$P(2) = 0.33 + 0.45 = 0.78$$

$$P(A_1|1) = \frac{P(A_1|1)}{P(1)} \times \frac{0.17}{0.22} = 0.77$$

$$P(B_1|1) = \frac{0.05}{0.22} = 0.23$$

$$P(A_2|1) = \frac{0.33}{0.22} = 1.5$$

$$P(B_2|1) = \frac{0.45}{0.22} = 2.05$$

Assign all cases in node 1 to A, all in node 2 to B.

Data 0) priors

$$\pi_A = \frac{900}{1000} = 0.9$$

$$\pi_B = \frac{100}{1000} = 0.1$$

$$P(A_1|1) = \frac{\pi_A N_1(1)}{N_1} = 0.9 \times \frac{300}{900} = 0.3$$

$$P(A_2|1) = 0.9 \times \frac{600}{900} = 0.6$$

$$P(B_1|1) = 0.1 \times \frac{10}{100} = 0.01$$

$$P(B_2|1) = 0.1 \times \frac{90}{100} = 0.09$$

$$P(1) = 0.3 + 0.01 = 0.31$$

$$P(2) = 0.6 + 0.09 = 0.69$$

$$P(A|1) = \frac{.31}{.31 + .03} = .97$$

$$P(B|1) = \frac{.03}{.31 + .03} = 0.03$$

Assign both nodes to A

$$P(A|2) = \frac{.06}{.06 + .13} = .87$$

$$P(B|2) = \frac{.09}{.06 + .13} = .13$$

When to stop growing trees?

Bottom up - classical CART \rightarrow grow a v. big tree - maximal tree
- Prune branches

Top down - Stop growing when there are no more useful splits

Classical CART approach - need to look at concept of misclassification - node level

Confusion matrix \rightarrow misclassification rate

		predicted	
	y		
observed	N		

Node Misclassification

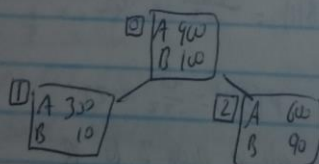
Define $r(t)$ p of misclassification at node $t = 1 - \max(p(i|t))$

$$R(t) = r(t) * p(t)$$

For the tree we can write:

$$R(\tilde{T}) = \sum_{\tilde{T}} r(t)p(t) \text{ where } \tilde{T} \text{ is all terminal nodes}$$

Using tree:



and data as priors

$$\text{Node 0: } r(t) = 1 - 0.9 = 0.1$$

$$R(t_0) = r(t_0) * p(t_0) = 0.1 * .1 = 0.1$$

$$\text{Node 1: } r(t) = 1 - .97 = .03$$

$$R(t_1) = r(t_1) * p(t_1) = 0.03 * \frac{340}{1000} = 0.0093$$

$$\text{Node 2: } r(t) = 1 - \frac{80}{90} = .13$$

$$R(t_2) = r(t_2) * p(t_2) = .13 * \frac{890}{1000} = 0.0897$$

$$R(\tilde{T}) = 0.0093 + 0.0897 = 0.099$$

09/04/16 (Co)lab + R Tree

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Cost Complexity Pruning

- 2 Stage 1: Develop a node sequence for evolution
- 2: Choose final tree

- Start by growing tree very large
- Prune branches from large tree

$R_{\alpha} =$ cost + complexity measure of the tree T

Define cost as misclassification rate $R(T)$

Complexity measure: function of # of terminal nodes

$$R_{\alpha} = R(T) + \alpha \cdot |T| \quad \text{Where } |T| = \# \text{ of terminal nodes}$$

α = penalty placed on complexity

- For a single node: $t: R(t)\alpha + \alpha$
- For a subtree $T_t: R(T_t)\alpha = R(T_t) + \alpha |T_t|$
- When α increases both $R(t)\alpha$ and $R(T_t)\alpha$ increase but $R(T_t)\alpha$ increases faster
- Value of $R(t)\alpha = R(T_t)\alpha$
- Price paid for complexity - adding on to tree

$$\alpha = \frac{R(t) - R(T_t)}{|T_t| - 1}$$

- Bigger value for α implies it is a better branch
- Smaller \rightarrow weaker

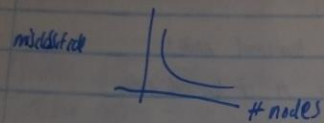
Some example tree

$$\text{For 2 node tree } R(T_t)\alpha = R(T_t) + 2\alpha$$

$$\alpha = \frac{R(t) - R(T_t)}{|T_t| - 1} = \frac{.1 - 0.099}{2 - 1} = .001$$

- calculate α at each node
- Prune tree with lowest α - weakest link
- Recalculate again

In R α is called complexity parameter
 (calculated same way but is divided by the risk) - misclassification of the node
 - keep deleting branches and re-calculating



- Can set a stopping rule for CP
- Choose tree with min misclassification or cross validation
- Use training and test data \rightarrow see where they cross over \rightarrow choose the CP value here.
- Gives a rule and J-E when you use multiple test sets

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CART vs Logistic Regression

- CART excels in detection of local structure
- Each half of tree is analysed separately
- Discovery of patterns becomes progressively more local
- Information from different nodes is not pooled or combined
- The fit at one node is never adjusted to take into account fit at other nodes
- Good at interaction
- Automatic separation of relevant from irrelevant predictors - only ones are which define "good" splits - screen data
- Does not require transform like log etc
- Automatic interaction detection - variables don't need to be deleted in advance
- Impervious to outliers
- Has methods for dealing with missing values
- Requires only moderate supervision by analyst
- First time model is often as good as a neural net by an expert
- Non parametric - doesn't require specification of any functional form

Disadvantage of CART

- May have unstable decision tree - insignificant modification or leaving sample such as eliminating observations could lead to radical changes in the decision tree
- CART splits only by one variable - all splits are perpendicular to axis i.e. when splitting all data into boxes, all boxes are rectangles - if data has more complex structure, CART may not catch correct structure & does

Logistic Regression

- Provides a smooth continuous predicted probability of class membership
- Effective capture of global features of the data
- Main effect model refers show probability related to predictor & over entire range of x
- Some flexibility allowed with transformation, polynomial and interaction
- Provides standard errors of coefficients
- Independent variables don't have to be normally distributed
- Handles non-linear effects
- You derive model by Selecting
- No homogeneity of variance assumption

Disadvantage

- Need larger sample of data
- Have to identify correct independent variable
- Limited out variables
- Independent observations required
- Over fitting model
- Numerical approximation - does not always converge towards an optimal solution
- Does not handle missing values of continuous variable
- Sensitive to extreme values

- Requires expert

- CART bad at detecting linear structure, recognizes it but can't represent it effectively
- With many variables, linear model may not be chosen from CART model
- Can produce a very large tree in an attempt to represent very simple relationship
- Logistic Regression - good for linear relationship
- LR may not linear structure can still be reasonably approximated with a model
- If an incorrectly specified logistic regression can perform well

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Combine CART and Logistic Regression?

- No information left in terminal nodes to support further analysis
- In a well developed CART tree, no other model should be applicable in the nodes
- Run a shallow tree
- Assign every case a terminal node
- Terminal node assignment represented by categorical variable with as many levels as terminal nodes
- Feed this categorical variable in the form of terminal node dummies to LR model

CART only with terminal node

$$y = \beta_0 + \beta_1 N_1 + \dots + \beta_{J-1} N_{J-1}$$

N_{j-1} = dummy variable

CART-Logistic Regression Hybrid model

$$y = \beta_0 + \beta_1 N_1 + \dots + \beta_{J-1} N_{J-1} + \alpha_1 Z_1 + \dots + \alpha_r Z_r$$

Z_i = extra variable

= CART node Dummy + Hybrid Logistic

Surrogates

- A variable with possibly equivalent information
- A surrogate is a splitter that splits in a fashion similar to the primary splitter
- Reveals structure of the info in the variable at a particular node in the tree
- If the primary is expensive or difficult to gather - use surrogate instead
- Use surrogate split if data is missing
- Carel with data for both splits
- For any node t , primary splitter s sends t_L cases to left and t_R to right
- For any other split s^* of the node t into t_L^* and t_R^*
- $N_{j(LL)}$ number of cases in t that both s and s^* send left for class j .
- $N_{j(RR)}$ # cases in t that both s and s^* send right for class j .

- Surrogates are node dependent - calculated at the local level
- Surrogates measure competition
- Useful for examining what node is trying to do
- Can choose how many you calculate at each node

Variable Importance

- Assess the relative importance of the variables in a tree
- Measured by impurity improvement
- Look at primary Splitter for each node and all the surrogate splitters tested on rpart for every node
- Can control the number of Surrogates
- Calculated over tree
- Calculated as a %

Calculation of $p(S, S^*)$

For this example $j=2$

$NN_{1L} = 50$	$NN_{2L} = 100$	$NN_{LL} = 800$ ← from confusion matrix
$NN_{1L}^* = 400$	$NN_{2L}^* = 150$	$NN_2(LL) = 100$
$NN_{1R} = 100$	$NN_{2R} = 300$	$NN_1(KR) = 50$
$NN_{1R}^* = 150$	$NN_{2R}^* = 250$	$NN_2(KR) = 250$

Calculating Similarity

- Split S and surrogate split S^* , for node t .
- j : no. of classes and π_j is prior probability of class j .
- Probability S correctly predicts $S^* = p(S, S^*)$

$$p(S, S^*) = P_{RR}(S, S^*) + P_{LL}(S, S^*)$$

$$P_{LL}(S, S^*) = \frac{P(t_L, t_L^*)}{P(t)} = \sum_j \frac{\pi_j N_j(LL)}{N_j} / p(t)$$

e.g. for $P_{RR}(S, S^*)$

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$$p(t) = \sum_j p(s, t) = \sum_j \frac{\pi_s N_j(t)}{N_j}$$

Using data of prices we can show $p(t) = \frac{\sum_j N_j(t)}{\sum_j N_j}$

$$\pi_1 = \frac{N_1}{N_1 + N_2} = 0.6 \quad \pi_2 = 0.4$$

- In this case, since we are at the row node, $p(t) = 1$

$$- p_{LL}(s^*, s) = 0.6 \left(\frac{400}{600} \right) + 0.4 \left(\frac{100}{400} \right) = 0.5$$

$$- p_{RR}(s^*, s) = 0.6 \left(\frac{20}{600} \right) + 0.4 \left(\frac{20}{400} \right) = 0.3$$

$$p(s, s^*) = p_{LL}(s, s^*) + p_{RR}(s, s^*) = 0.5 + 0.3 = 0.8$$

$$\text{Error} = 1 - 0.8 = 0.2$$

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Derived Variables

- Define new variables to make data more useful and informative
- Creative part of the process
- Improve quality of data
- Well chosen derived variables enhance the ability of models to be understood and interpreted
- Change over time
- Allows analysts incorporate human insights and background knowledge into modelling process
- Important skill to come up with "right" variable - what works in one model may not work in another
- Depends on country, setting/context
- Replace categorical variable with quantitative when many categories
- Use point values of target variable or census data
- Be careful with time

More

- What information to use? # opps? # phase calls? meta? model?
- Sometimes variables are too hard to use

Single Variable Transform

- Standardized numeric variables
- Centered variables - can increase interpretability
- Rescale \Rightarrow allow comparison between variables
- Turn number values into percentiles works with any distribution
- Useful when you are interested in relative position then absolute value
- Turn counts into rates

- Replace categorical variables with numeric - do not do so arbitrarily
- Create indicator variables, would work with few categories
- Capture important information
- Place - latitude and longitude
- Use previous data from target data make sure it is going to be possible in the future
- Bin numerical data - equal intervals or quantiles
 ↳ may not be good with some techniques

Combination of Variables

- BMI
- Price earnings ratio
- Highly correlated variable - draw scatter plot before correlation calculation
- Nearly synonymous variables
- When two variables are equal, most of the time few placed where the difference may be informative
- Depends on DM technique used Multicollinearity bad for regression

Correlated Variables

- Get rid of one - the one with less variance
- Talk to people with background knowledge as they may have more info or will understand the model
- Try to derive a variable with high variance which is independent of its constituent variables
- Ratio of the variables

Netflix example

- Ratings on scale 1-5, 480M users, 17770 movies
- individual ratings
- total number of ratings
- number in first month

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Derived Variable

- Proportion in first month
- Rating 1 per month
- Proportion of 1 ratings etc
- Average Rating
- Average Rating for next month
- Ratio of 1 to 5 ratings
- Date from release to rating
- Comparison of rated to population
- Population average - rate average per month

- Reduce variable : PCA, FA, cluster membership

KAPPA STATISTIC

- Cohen's Kappa Statistic
- Agreement between raters originally
- Level of agreement taking into account the accuracy that would be generated by chance

$$Kappa = \frac{(\text{Observed accuracy} - \text{accuracy expected by chance})}{(1 - \text{accuracy expected by chance})} = \frac{(O-E)}{(1-E)}$$

- Value range from -1 to 1
- 0 value means no agreement
- Measures relative improvement over random predictor.

Actual	Obs	Predicted	
		Yes	No
Yes	10	10	20
No	30	50	80
		40	60

$$O = \frac{10+100}{1000} = 0.6 \text{ observed accuracy}$$

$$E = \left[\frac{40}{1000} \times \frac{20}{100} \right] + \left[\frac{60}{1000} \times \frac{80}{100} \right] = 0.56$$

$$Kappa = \frac{0.6 - 0.56}{1 - 0.56} = 0.09$$

0 - 0.2 inferior

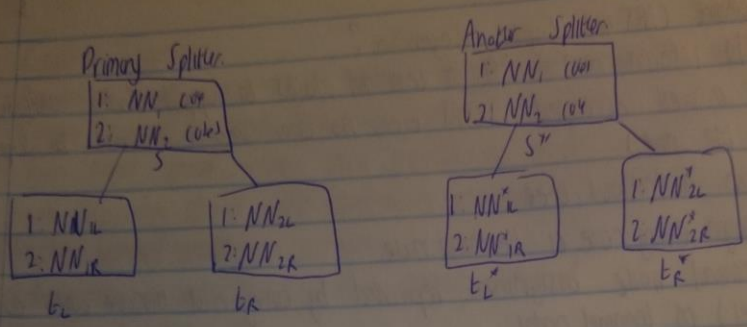
0.21 - 0.40 slight

0.41 - 0.60 sufficient

0.61 - 0.80 good

0.81 - 1.00 excellent

even with large gran of diff.

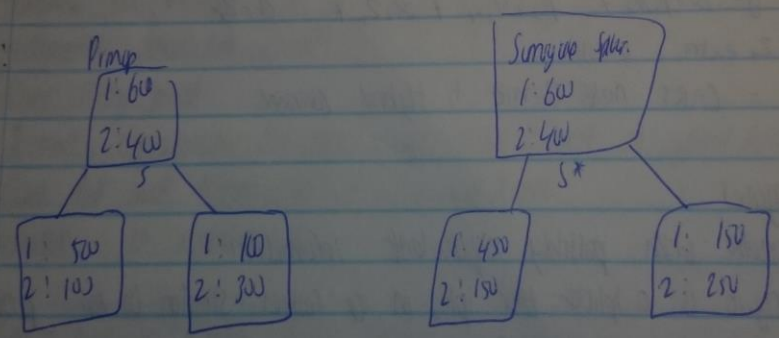


Perfect Splitter:

$$NN_{1L} = NN_{1L}^* \quad NN_{2L} = NN_{2L}^* \quad NN_{1R} = NN_{1R}^* \quad \text{or} \quad NN_{2R} = NN_{2R}^*$$

- same case - just not similar name.
- Need to calculate probability that both splitters send case in the same direction
- call this $P(S, S^*)$

EXAMPLE:



(101) 1		Primary			(101) 2		Primary		
Surf		L	R		Surf		L	R	
	L	400	50	450		L	100	50	150
	R	100	50	150		R	0	250	250
		500	100				100	300	

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How good a predictor is S^* ?

- How well can another split S^* mimic the primary splitter S ?
- How high is $p(S, S^*)$?
- Comparison or default rule
- For node t suppose that S sends cases with prob p_L and p_R right (reduces)
- New case \Rightarrow predict t_L if $p_L = \max(p_L, p_R)$ else t_R
- $r(t)$ (misclassification rate) = $\min(p_L, p_R)$

Same example

- Using the data for our priors we can compute Bex directly from the tree
- $p_L = 0.6$, $p_R = 0.4$
- Default rule \Rightarrow send everything left, error = $1 - 0.6 = 0.4$
- Compare this to Surrogate rule

Surrogate rule:

- $p(S, S^*) = 0.8 \Rightarrow$ called agreement in R
- error rate = 0.2
- \Rightarrow = the ratio $\frac{\text{class 1 LL + RR} + \text{class 2 LL + RR}}{n \text{ (total) cases}}$

Association:

$$= \frac{\min(p_L, p_R) - (1 - p(S^*, S))}{\min(p_L, p_R)}$$

$$= \frac{\text{default mismatch} - \text{surrogate mismatch}}{\text{default mismatch}}$$

$$p_L = 0.6 \quad p_R = 0.4 \quad \Rightarrow \quad \frac{0.4(1 - 0.8)}{0.4} = 0.5 \quad \text{50\% reduction}$$

Relative reduction in error obtained by using S^* to predict S instead of $\max(p_L, p_R)$ called adj in R