Predictive Analytics Lecture 6

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Stat 422/722
at The Wharton School of the University of Pennsylvania

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Modeling Framework Refresher

Recall the general regression model:

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$\{x_1, \ldots, x_p\} \Rightarrow \{x'_1, \ldots, x'_{p'}\}$ where $p' > p$ and maybe much, much greater.

"Non-parametric" Linear Regression

Once we expand this feature set, we can now fit a larger linear model:

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Back to our problem... we can curb overfitting by ... using 3-way split oos validation but we need to select good models... how to do so? One approach is termed **subset selection methods**.

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If you choose the feature to give you the best in-sample R^2, you will eventually take all the features (until $n = p + 1$) and you will get $R^2 = 100\%$. We need a metric to tell us when we may be overfitting and halt at that moment.

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Needless to say, this is all approximate since we are assuming OLS and a whole bunch of other things (beyond scope of course).

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Stepwise Linear & Logistic Regr. Demos

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- white wine $K-$fold on AICc (why is this not a great idea?)
- telecom all 1st order interactions with oos validation on AICc
- telecom all 1st order interactions with oos validation on min logistic R^2

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Simple case where stepwise doesn't work? How about three features where x_1 is most correlated but x_2 and x_3 together are the best model but there is high collinearity between x_2 and x_3? What happens? Forward: the model enters x_1 and then x_2 but it doesn't see x_3 as a worthy addition. Backward: the model can nuke x_2 or x_3 since its p-value or F test is poor.

Conceptual Review of What We Just Did

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then we take our "raw" features and create "derived features"

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then we allowed for a large linear model:

$$Y = \beta_0 + \beta_1 x'_1 + \ldots\ldots\ldots\ldots\ldots\ldots + \beta_p x'_{p'} + \tilde{\mathcal{E}}$$

of which we took a subset by "stepping through" and reaching a local optimum:

$$Y = \beta_0 + \beta_1 x'_{(1)} + \ldots\ldots\ldots\ldots + \beta_p x'_{(p')} + \tilde{\mathcal{E}}$$

Binning

Our derived predictors

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still may not be that "flexible" as "bases" for the $\hat{f}$ (whiteboard demo).

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What if we derived predictors that split up the space of raw predictors into tiny regions. In one dimension, we can make some new derived variables:

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and assign a different β parameter (fit to be the average y) for each of these 10. This is called "binning" and allows for flexible, non-parametric fits. Why?

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Does Binning Breakdown?

In multiple dimensions, you can get nice bins by doing interactions between each dimensions' bins. For example in two dimensions, you can bin both into $B = 10$ bins. Crossing the bins makes 100 square bins. Each square gets its own β parameter (fit to be the average y).

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Better Bins?

Instead of just binning each predictor into B bins, why not try to make "custom" or "smart" bins in the regions of f that give the **most** increase in fit (i.e. higher R^2, lower SSE or $RMSE$). So you "split" the data into bins that are now "hyper-rectangle" shaped.

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Demo JMP white wine. Within each hyperrectangle ("split" or "partition"), you can split again by taking the best split, and you can keep going. Because the splits are **binary** (i.e. you split one space into two spaces), and they are hierarchical (you can trace the splits back generations), they look like "trees". JMP. How to predict? "Drop the observation down "and follow instructions all the way until the end. Does this make them interpretable?

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Decision Trees

These are known as **decision trees** since you can imagine examine when you predict, you follow the "decisions" (i.e. the **split rules**). There is some terms of anatomy to know:

- The top is the "root node"
- Nodes that split have "children" and are "inner nodes" or "split nodes".
- Nodes that do not split are called "leaves" or "terminal nodes".
- "Depth" indicates the maximum number of generations in the tree (the root has zero depth).
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Look at all possible splits ($\approx n \times p$ splits) **greedily** and take the minimum total SSE for continuous and total entropy for categorical. JMP is non-standard; it takes the maximum log worth (which is something I've never heard of) for continuous and the maximum log likelihood for categorical. My bet is the performance will be similar as it's really the same concept: get the best, most homogeneous, split!

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More on interpretation: AND rules? Overall effect of y on x? No ... not so clear. Categorical variable splitting? Very nice interpretation.

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- You no longer need to worry about transformations such as logs since the split variables will take care of optimal splits.

Disadvantages of Decision Trees

- Non-parametric modeling does not give us inference. Can we ask how important alcohol is in determining wine quality? It looks important since it's the root, but we can't get a reassurance that it will stand up to sampling error formally as a p-value.

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The Tree's History and Improving the Tree

Trees were conceived in 1963 and were made rigorous in the mid-1980's with the book "Classification and Regression Trees". The 1990's saw a few huge advances:

1. Bagging (bootstrap aggregation) in 1994 (Breiman).
2. Boosting (finding errors and reweighting to fix them) in 1995 (Freund and Shapire).
3. Sampling predictors in 1997 (Amit and Geman).

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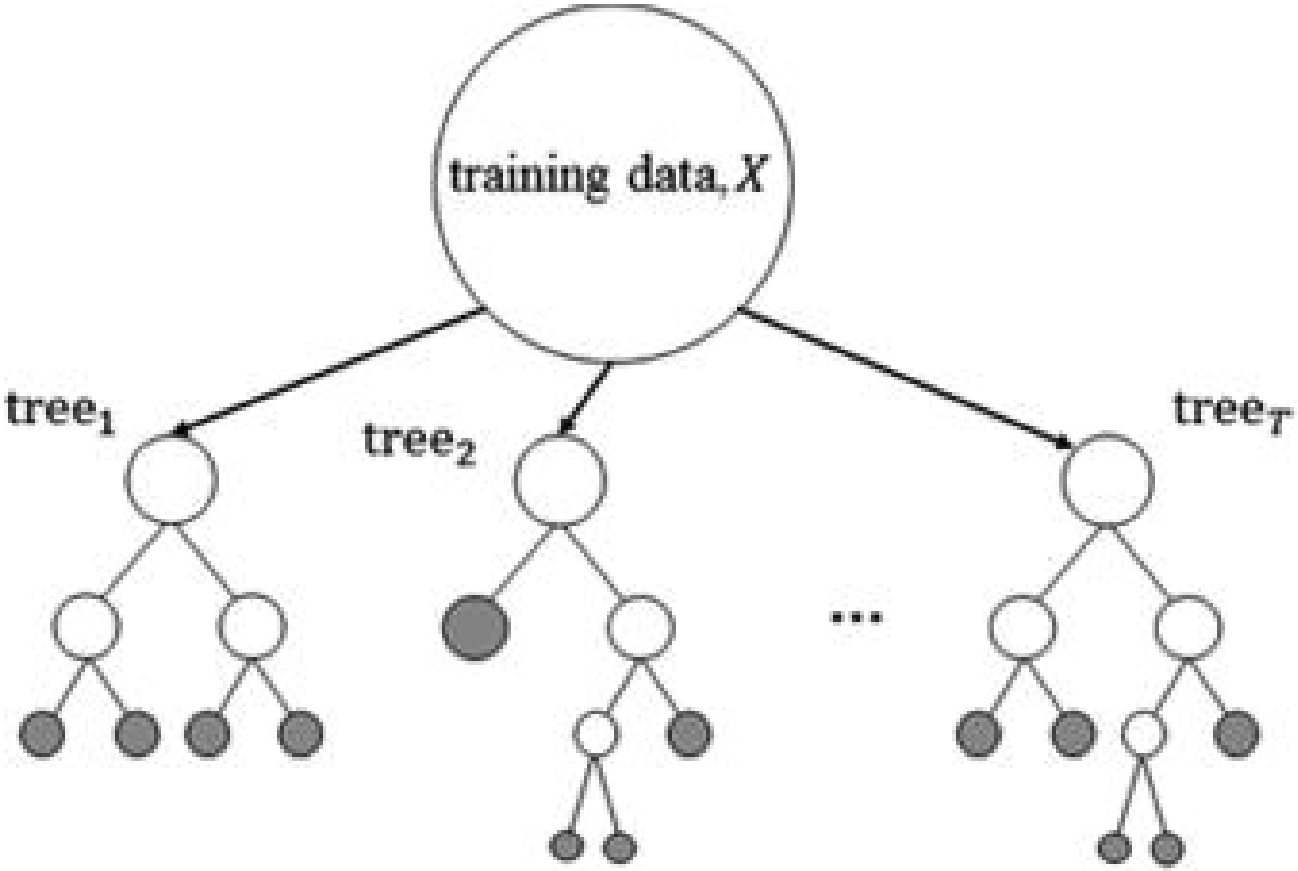
Many, Many Trees Together

Each of the above combines many decision trees together (T trees instead of one tree). Predictions are generated by the average leaf $\hat{y}$ (during regression) or the modal class (during classification).



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Bagging beats single trees... but once we bag, no interpretability anymore! Complete black box due to that function $\hat{f}$ being so complicated!!

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- Number of trees — we want a lot to reduce variance (default is 500 in R)
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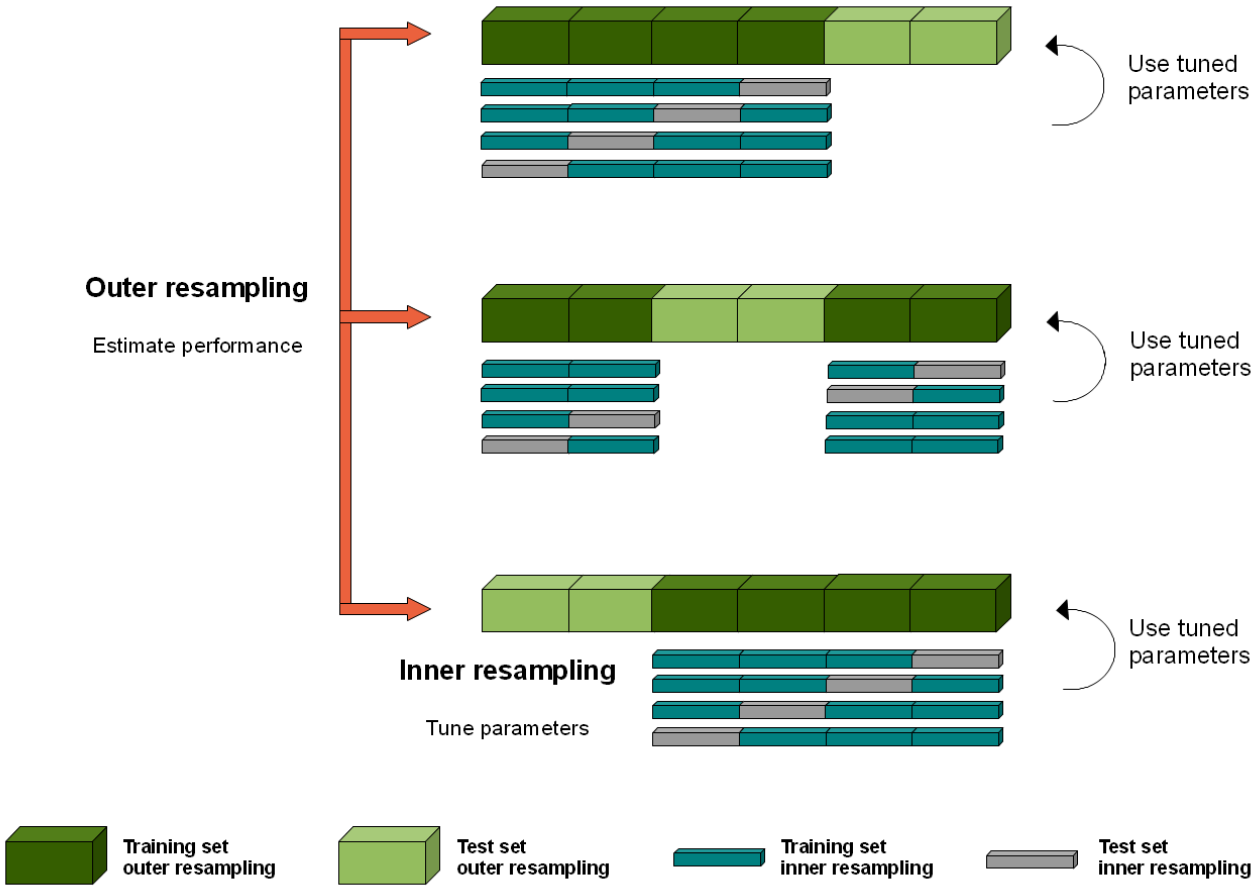
The amazing thing is ... the defaults work so well, you hardly ever need to change them!! **RF in my opinion is the best predictive model out-of-the-box.**

Tuning RF — Nested Resampling

Remember this from last class? Here's where it's used... But I do not recommend doing this!



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However, RF does overfit in-sample. How? 2/3 of the T trees, it overfits and 1/3 of the T trees is OOB for every observation. Thus it is mostly overfit! Never trust in-sample R^2 from an RF! Only look at OOB!

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Note: there is a PhD student right now in this department exploring when this works and how much you can trust it! Bleeding edge of stats...

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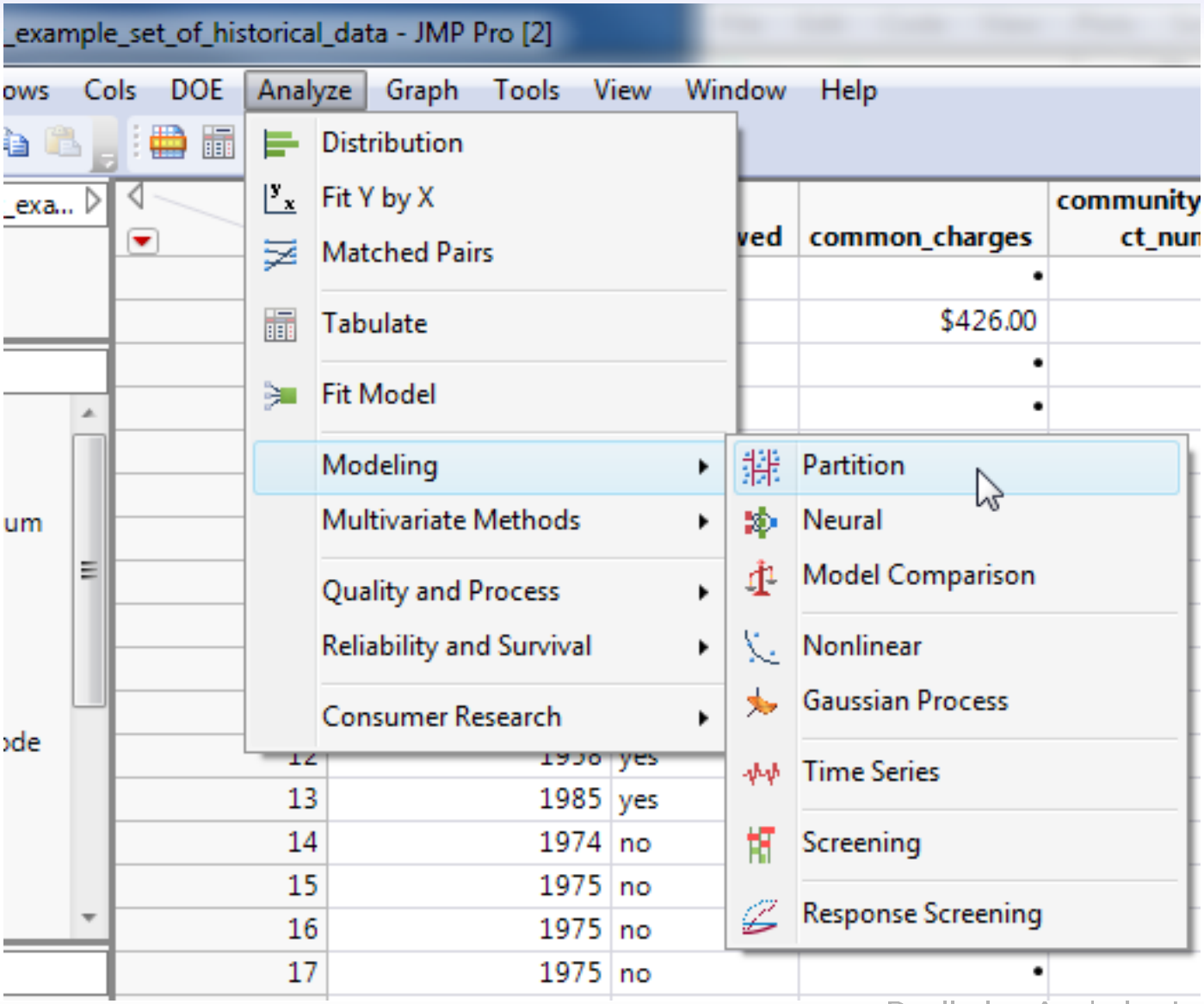
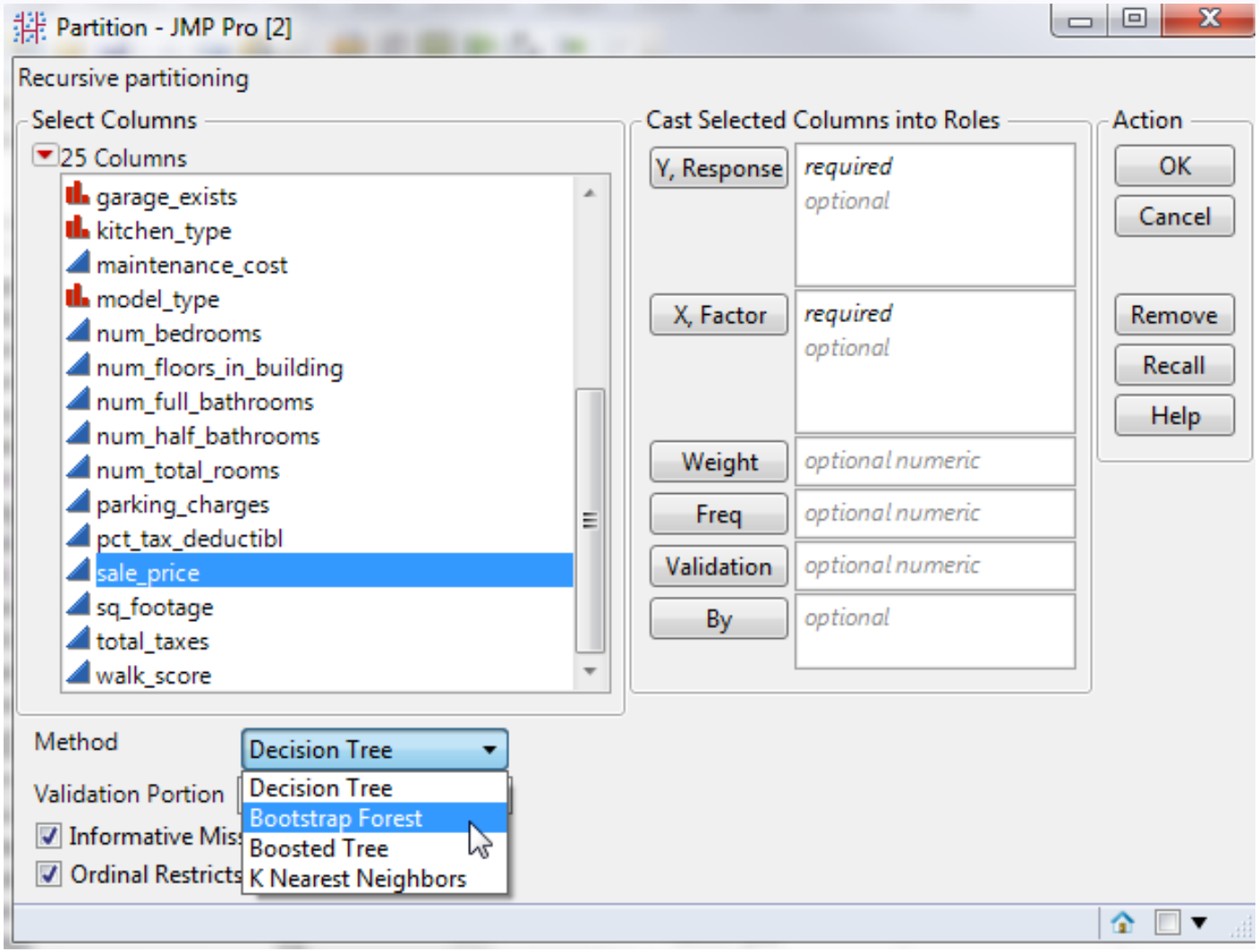
- When there are not "too many" features. $p > n$ is a problem for everyone. RF can find what it believes to be a nice predictor, but it's really fake and only idiosyncratically related to the response.
- When you need interpretation, RF cannot give you what you want! Note: many people working on this... it was actually part of my thesis! See package `ICEBox` in R.

Demo time...

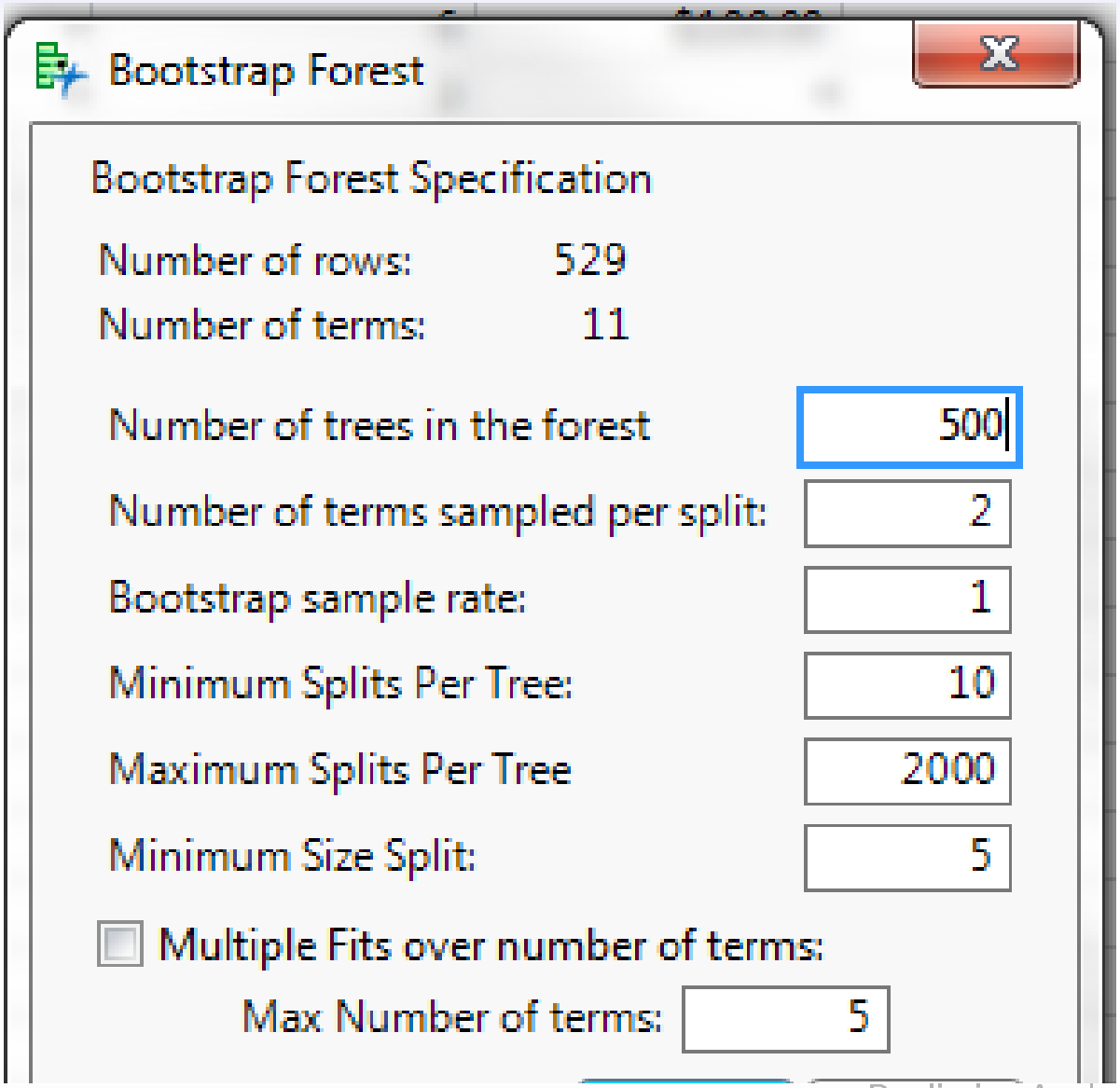
JMP 1/4


_example_set_of_historical_data - JMP Pro [2]
ows Cols DOE Analyze Graph Tools View Window Help
Distribution
Fit Y by X
Matched Pairs
Tabulate
Fit Model
Modeling
Multivariate Methods
Quality and Process
Reliability and Survival
Consumer Research
Partition
Neural
Model Comparison
Nonlinear
Gaussian Process
Time Series
Screening
Response Screening
common_charges
community ct_nun
$426.00
13 1985 yes
14 1974 no
15 1975 no
16 1975 no
17 1975 no

JMP 2/4


Partition - JMP Pro [2]
Recursive partitioning
Select Columns
25 Columns
garage_exists
kitchen_type
maintenance_cost
model_type
num_bedrooms
num_floors_in_building
num_full_bathrooms
num_half_bathrooms
num_total_rooms
parking_charges
pct_tax_deductibl
sale_price
sq_footage
total_taxes
walk_score
Cast Selected Columns into Roles
Y, Response
required
optional
X, Factor
required
optional
Weight
optional numeric
Freq
optional numeric
Validation
optional numeric
By
optional
Action
OK
Cancel
Remove
Recall
Help
Method
Decision Tree
Validation Portion
Informative Miss
Ordinal Restricts
Decision Tree
Bootstrap Forest
Boosted Tree
K Nearest Neighbors

JMP 3/4


Bootstrap Forest
Bootstrap Forest Specification
Number of rows: 529
Number of terms: 11
Number of trees in the forest 500
Number of terms sampled per split: 2
Bootstrap sample rate: 1
Minimum Splits Per Tree: 10
Maximum Splits Per Tree 2000
Minimum Size Split: 5
Multiple Fits over number of terms:
Max Number of terms: 5

JMP 4/4

Bootstrap Forest for sale_price

Specifications

Target Column:	sale_price	Training rows:	529
		Validation rows:	0
Number of trees in the forest:	500	Test rows:	0
Number of terms sampled per split:	2	Number of terms:	11
		Bootstrap samples:	529
		Minimum Splits Per Tree:	10
		Minimum Size Split:	5

Overall Statistics

Individual Trees	RMSE
In Bag	1049084
Out of Bag	1415828

RSquare	RMSE	N
0.623	110008.48	529

Per-Tree Summaries

Actual by Predicted Plot

You don't need to do oos validation on Random Forests as the "out of bag" is as good as oos.

R 1/2

```
#load the data
X = read.csv(
 "stat_422_722_project_example_set_of_historical_data.csv")
#recode sale_price as a number
X$sale_price = as.numeric(gsub('[$,]','',
  as.character(X$sale_price)))
#install and load up the RF package
install.packages("randomForest")
library(randomForest)
#run the RF
rf_mod = randomForest(sale_price ~
coop_condo + num_bedrooms +
num_full_bathrooms + walk_score, X)
rf_mod #print out its output
```

R 2/2

```
> rf_mod

Call:
 randomForest(formula = sale_price ~ coop_condo + num_bed
rooms +      num_full_bathrooms + walk_score, data = X)
               Type of random forest: regression
                     Number of trees: 500
No. of variables tried at each split: 1

          Mean of squared residuals: 10620431253
                    % Var explained: 66.96
```

We Made It! Now a Summary and Review...

A quick review of the topics (and the topics that will not be covered on the final next week).

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- Data collection: sampling and measurement to create a data frame

Review...

- Good machine learning (sampling and featurization) vs. bad machine learning (mindless data dumps of convenience)
- Parametric vs non-parametric worldview when modeling
- Definition of parameters
- Definition of parameter estimates (model fitting)
- Residuals and loss functions (**SSE** *, SAE)
- Measures of fit: R^2, SSE, $RMSE$ and their interpretations and their equivalence
- Empirical rule $\hat{y} \pm RMSE$

Review...

Lecture 2

- Graphical causal models with bubbles and arrows
- Definition of noise in statistical models
- Probabilistic Causation
- Three sources of noise (1) Irreducible Error (2) Model Misspecification due to a parametric assumption (3) Model Estimation Error
- The reasonable assumption of $\mathcal{E}$ distributed normally
- The four OLS assumptions and what this buys you
- What a likelihood is and what a log-likelihood is
- What maximum likelihood estimation is
- What the likelihood ratio is and when to reject (big values that exceed critical χ^2 values)

Review...

- OLS regression: Omnibus / global F-tests
- OLS regression: Partial F-test
- OLS regression: t-test
- OLS regression: how to predict ($\hat{y}$ calculations)
- Proper interpretation of $\hat{\beta}_j$
- Causation and correlation
- Lurking / confounding predictors
- Spurious (or coincidental) correlations
- Natural observation vs. manipulated measurements
- Randomized experiments can reveal additive causal effects
- Why "science is impossible"
- Why collinearity may invalidate $\hat{\beta}_j$ interpretation
- Why correlations are still useful

Review...

- Data dredging
- Multiple testing correction with Bonferroni (hedges against dredging)
- Generalizability of models

Lecture 3

- Extrapolation (a violation of generalizability)
- How different modeling strategies extrapolate differently
- Optimal design in linear models (over sample predictors' extreme values)
- Optimal design in highly non-parametric models (more towards even spacing throughout predictors' ranges)
- Odds, logistic link function and its sigmoidal shape, logit function (log odds)
- Fitting $\hat{\beta}_j$'s in logistic regression

Review...

- How to draw inference in logistic regression (likelihood ratio test)
- How to predict conditional probabilities $\hat{p}$'s in logistic regression
- How to use classification rules based on a threshold $\hat{p}_0$
- Confusion Matrices, FN, FP, TP, TN, sensitivity, specificity, FNR, FPR, FDR, FOR
- ROC Curve, ROC table and AUC metric

Lecture 4

- Asymmetric costs in classification, weighted misclassification error, minimizing this metric to find best p_0
- Survival Model — the response and why it's censored
- Interpreting $\hat{\beta}_j$ in an exponential survival model
- How to draw inference in survival regression (likelihood ratio test)
- Predictions in survival models

Review...

- Testing linearity for one covariate in linear regression
- Interpreting quadratic effects
- Interpreting interaction effects
- Overfitting and optimizing for the idiosyncratic $\mathcal{E}$ terms
- In-sample vs. oos metrics of fit (complexity-fit tradeoff curves)
- Single training-test splits for oos validation
- The test set as a lockbox that can be opened once and only once
- Tradeoffs for training-test split sizes

Lecture 5

- K-fold cross validation (CV)
- Advantage of doing K-fold CV
- Using three splits to perform model selection

Review...

- Missing data: selection models vs. pattern mixture models
- Mechanisms: MCAR, MAR, NMAR
- Why listwise deletion is nothing to write home about
- Imputation under missingness due to each of the three mechanisms
- Creating missingness features (the $\boldsymbol{m}$'s)
- Forward stepwise regression using t-test, AICc and R^2 in a oos set

Lecture 6

- Binning — advantages and disadvantages
- Better bins through greedy splitting (decision trees)
- Leaf assignment in decision trees
- Pruning / stopping the growth of decision trees
- Advantages and disadvantages of decision trees

Review...

- Model averaging over multiple trees
- Bagging (bootstrap and aggregation)
- Sampling predictors
- The 3 ideas above together = random forests (RF)
- OOB estimates as oos estimates
- When RF performs well and when it does not