vtreat: A Package for Automating Variable Treatment in R

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Outline

- Typical data problems & Possible solutions
- `vtreat`: Automating variable treatment in R

Data Cleaning: Typical problems

- “Bad” numerical values (NA, NaN, sentinel values)
- Categorical variables: missing values, missing levels
- Categorical variables: too many levels
- Invalid values
  - Out of range numerical values
  - Invalid category levels

We won’t discuss the last issue

Of course, we need to get our hands in the data, but the procedure for treating the first three problems will be the same in most situations. Might as well automate it

Bad Numerical Values

MPG	
50	
Inf	Electric car/bad calculation
20	
36.4	
NaN	Non-numeric typo/bad calculation
NA	Electric car

Toy example: we created the MPG column blindly from the first 2
The “source” columns are collected from different sources, who handle situations like “unknown” or “electric car” differently. Perhaps all we see is the MPG column
Row 2 is an electric car, so is Row 7 (handled differently)
Row 5 the mileage and consumption were unknown — marked 0
Row 6 the mileage was blank – converted to NA

Whither Bad Values?

- "Faulty Sensor" — values are missing at random
  - Assume they come from the same distribution as the other values
  - The mean of the "good" values is a reasonable stand-in
- Systematically missing
  - Electric cars
  - They WILL behave differently from gas or hybrid cars
  - The mean of the good values is not a valid stand-in

The "right" fix depends on why you have bad values.

Faulty Sensor — will usually be all NAs (not NaNs, Infs)

One Possible Solution

MPG
50
Inf
20
36.4
NaN
NA

MPG	MPG_isBad
50	FALSE
35.5	TRUE
20	FALSE
36.4	FALSE
35.5	TRUE
35.5	TRUE

This solution - replace bad values with the mean of the non-bad values, use an additional column to mark the bad values

35.5 is the average mileage of the “good” values

If we have a faulty sensor, then the second column is uninformative. If we have systematic missingness, then the second column can help compensate for the poor estimate we are using (the mean). Let the machine learning algorithm figure it out.

Categorical Variables: Missing Values and Novel Levels

TrainingData

Residence
CA
NV
OR
CA
CA
NA
WA
OR
WA

NewData

Residence
NV
OR
NV
WY
CA
CA
NV
NA
OR

Novel Levels - Model Failure

```
> model = lm("premium~age+sex+residence",
data=TrainingData)

> predPremium = predict(model, newdata=NewData)

Error in model.frame.default(Terms, newdata,
na.action = na.action, xlev = object$xlevels) :
factor residence has new levels WY
```

And rows where residence=NA will get NA for a prediction

One Possible Solution

Residence
CA
NV
OR
CA
CA
NA
WA
OR
WA

Res_NA	Res_CA	Res_NV	Res_WA	Res_OR
0	1	0	0	0
0	0	1	0	0
0	0	0	0	1
0	1	0	0	0
0	1	0	0	0
1	0	0	0	0
0	0	0	1	0
0	0	0	0	1
0	0	0	1	0

Making explicit the internal representation of categorical variables.

Representing a Novel Level as a Censored Level

Training Data Proportions

NA	CA	NV	WA	OR
1/9	1/3	1/9	2/9	2/9

A novel level is weighted proportional to known levels

Residence
WY

Res_NA	Res_CA	Res_NV	Res_WA	Res_OR
1/9	1/3	1/9	2/9	2/9

If WY is a transcription error or invalid level, then this representation says we don’t know what the value of Residence is, but we assume it to be any possible known level in the correct proportions — Bayesian “no information” assumption

If it’s truly a novel error, the representation isn’t as meaningful, but at least we will get *some* answer (and won’t crash the entire scoring run).

Categorical variables: Too many levels

ZIP	SalePriceK
94127	725
94564	402
90011	386
94704	790
94127	1195
94109	903
94124	625
94124	439
94564	290

- Too many levels is a computational problem for some machine learning algorithms.

- You will inevitably have a novel level

Problems:
1) too many levels is a computational problem for some machine learning algorithms: linear/logistic regression; randomForest (in R)
2) You will inevitably run into the “novel level” problem

Solution: “Impact Coding”

ZIP	avgPriceK	ZIP_impact
90011	386	-253.4
94109	903	263.6
94124	532	-107.4
94127	960	320.6
94564	346	-293.4
94704	790	150.6
globalAvg	639.4	0

Impact coding is transforming the original categorical variable by a single variable Bayesian model for the change from the mean output (the “impact” of the variable on the output). The transformed numerical variable has a more concise representation for modeling, assuming we are trying to predict sales prices of homes.

Here’s the data we need to create the impact coding for our example.

Information on impact coding:

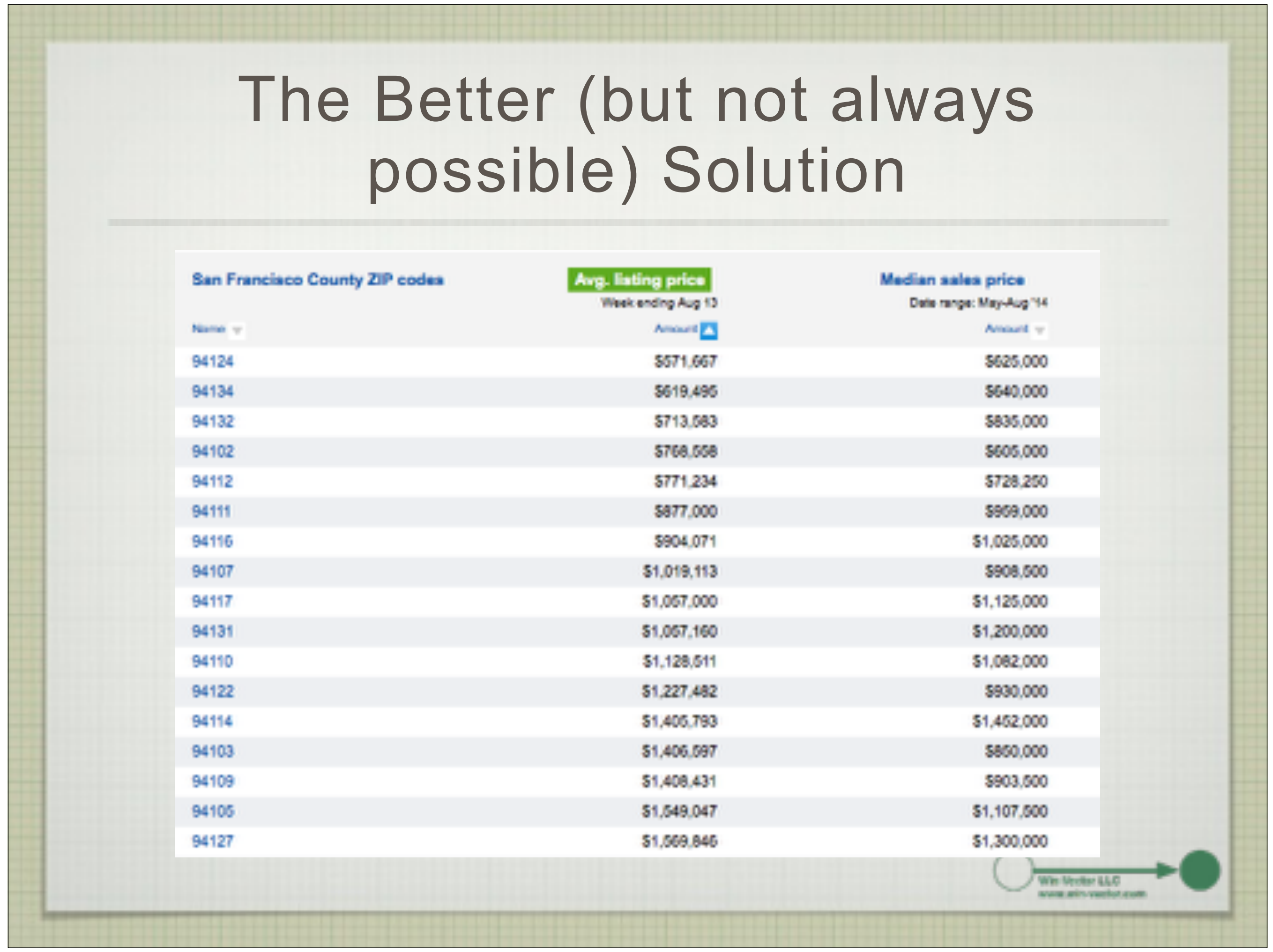
http://www.win-vector.com/blog/2012/07/modeling-trick-impact-coding-of-categorical-variables-with-many-levels/

http://www.win-vector.com/blog/2012/08/a-bit-more-on-impact-coding/

Impact-coding the ZIP variable

ZIP	ZIP_impact
94127	320.6
94564	-293.4
90011	-253.4
94704	150.6
94127	320.6
94109	263.6
94124	-107.4
94124	-107.4
93401	0

ZIP codes that we observed in training are coded to their expected conditional impact (as shown in the previous slide). Novel ZIP codes are coded to 0 (which is the same as assuming that new ZIP codes behave like the average. 0 is also the weighted sum of the impacts from all known ZIPs (similar to the novel level encoding for categorical variables).

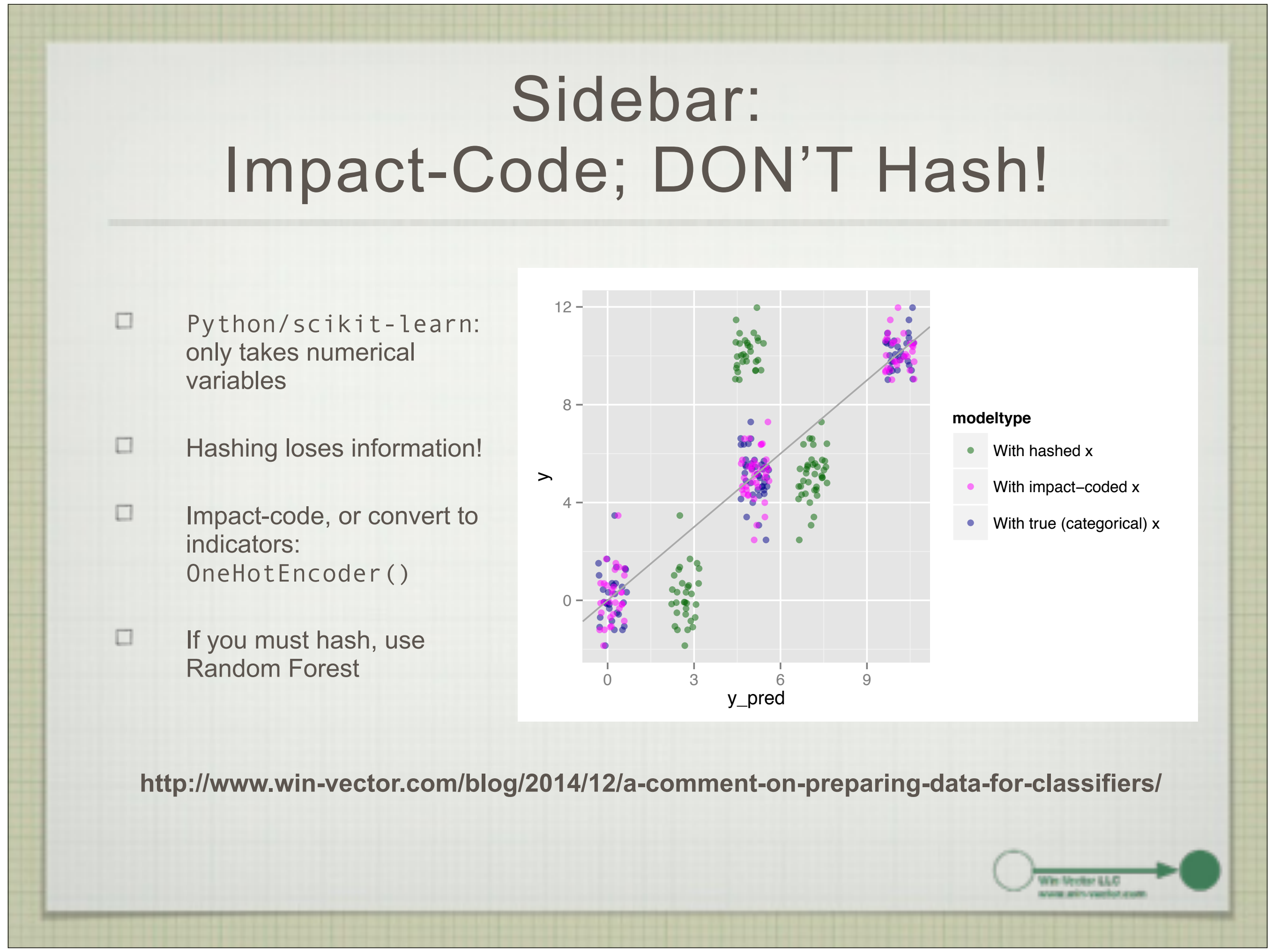


The Better (but not always possible) Solution

San Francisco County ZIP codes Name	Avg. listing price Week ending Aug 13 Amount	Median sales price Date range: May-Aug '14 Amount
94124	$571,667	$625,000
94134	$619,495	$640,000
94132	$713,083	$835,000
94102	$768,558	$605,000
94112	$771,234	$728,250
94111	$877,000	$969,000
94116	$904,071	$1,025,000
94107	$1,019,113	$908,500
94117	$1,057,000	$1,125,000
94131	$1,057,160	$1,200,000
94110	$1,128,511	$1,082,000
94122	$1,227,482	$930,000
94114	$1,405,793	$1,452,000
94103	$1,406,097	$850,000
94109	$1,408,431	$903,500
94105	$1,549,047	$1,107,500
94127	$1,569,846	$1,300,000

Of course, in many cases, categoricals with many possible levels are simply proxies for some other useful quantity (or many useful quantities — a single ZIP column could expand to many demographic facts); in this instance, if we had data for the average or median house price by location (ZIP), it would be better to use that data directly. However, impact-coding is a useful technique for inferring desired quantities, when a source for the true data is not available.

http://www.trulia.com/home_prices/California/San_Francisco_County-heat_map/



Slight digression: some machine learning algorithms (for example, the implementations in Python's scikit-learn) only take numerical input variables. We have seen clients try to get around this by hashing or memoizing the categorical values to numerical ones. The authors of the (excellent) paper "Do We Need Hundreds of Classifiers to Solve Real-World Classification Problems?" also hashed their categorical variables.

Hashing lose important structural information about the problem, and only some modeling algorithms can recover the categories from the hashing (maybe!).

Linear and logistic regression and SVMs cannot. K-Nearest Neighbors probably cannot. Random Forests often can, and GAM maybe (if there are only a few categorical levels). Even if you use an algorithm that can possible recover the category information, you are wasting the algorithm's "degrees of freedom" (expressive power) recovering known information, rather than discovering new information.

If you are using machine learning implementations like scikit-learn, which do not natively take categorical values, then you should either convert those values to indicator variables yourself (in Python: preprocessing.OneHotEncoder()) or impact-code them.

For a more detailed explanation of this issue, see:
http://www.win-vector.com/blog/2014/12/a-comment-on-preparing-data-for-classifiers/

Automating Variable Treatment in R: `vtreat`

Two-step Process

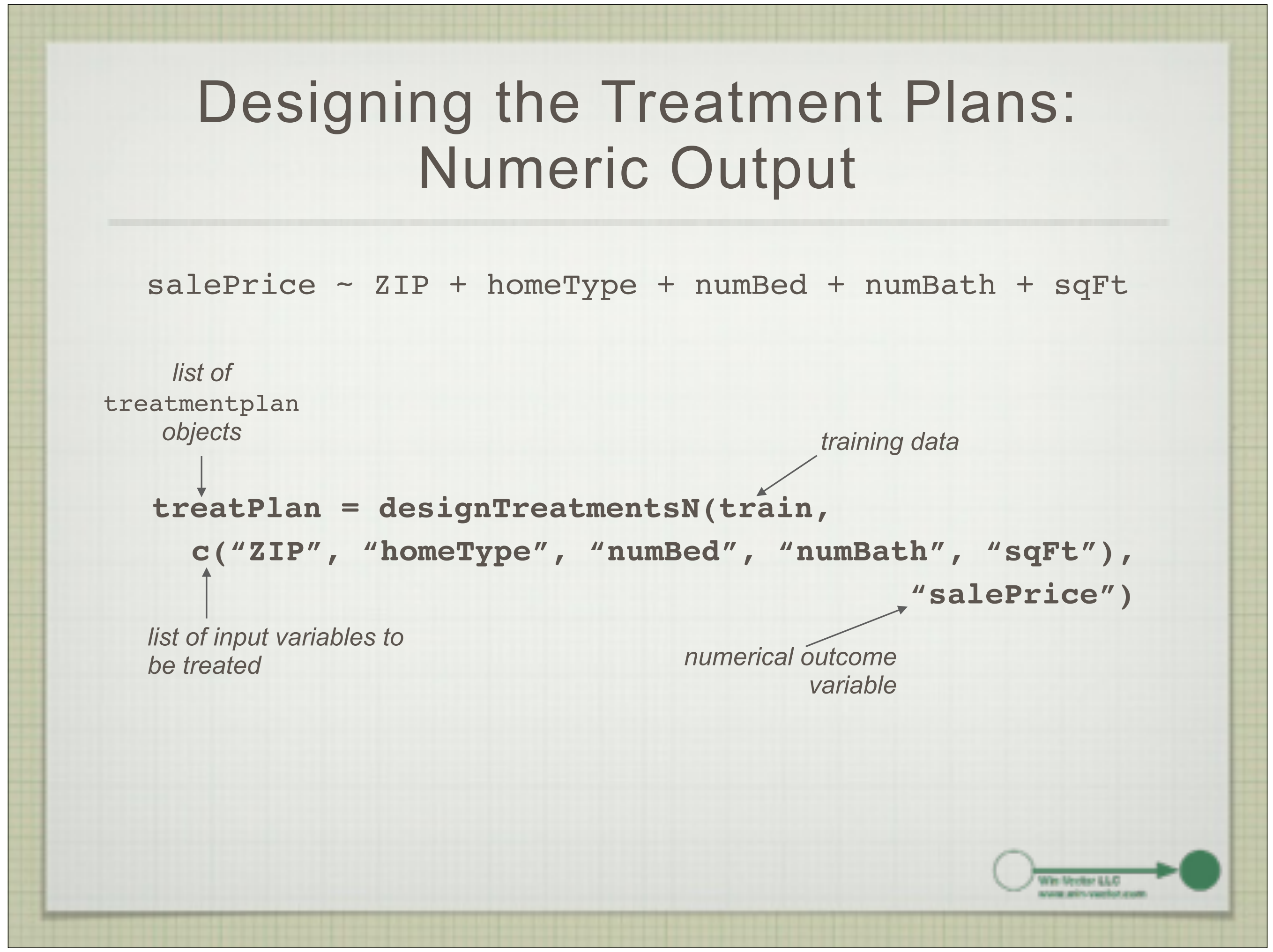
- Design the data treatment plans
  - Numeric outcome:

    ```
    tPln = designTreatmentsN(train, xv, y)
    ```

  - Binary class outcome

    ```
    tPln = designTreatmentsC(train, xv, y, target)
    ```

- Prepare the data sets
  - `train.treat = prepare(tPln, train)`
  - `test.treat = prepare(tPln, test)`



Predicting home sale price
ZIP : large categorical
homeType: small categorical (say, “single-family”, “condo”, “townhouse”, “flat”)
numBed, numBath, sqFt: numerical

Example Input

```
    ZIP  homeType numBed numBath sqFt salePrice
  94499     condo      4       4 1025    815678
  94403     condo      2       3 1082    600635
  94361 townhouse      1       3  751    444609
  94115     condo      2       3 1093    349433
  94217      <NA>     NA       3  914    692468
```

many-level categorical

categorical

numeric

```
treatPlan = designTreatmentsN(train,
   c("ZIP", "homeType", "numBed", "numBath", "sqFt"),
                                          "salePrice")
```

Using the treatment plan to prepare data

```
df.treat = prepare(treatPlan, df)
```

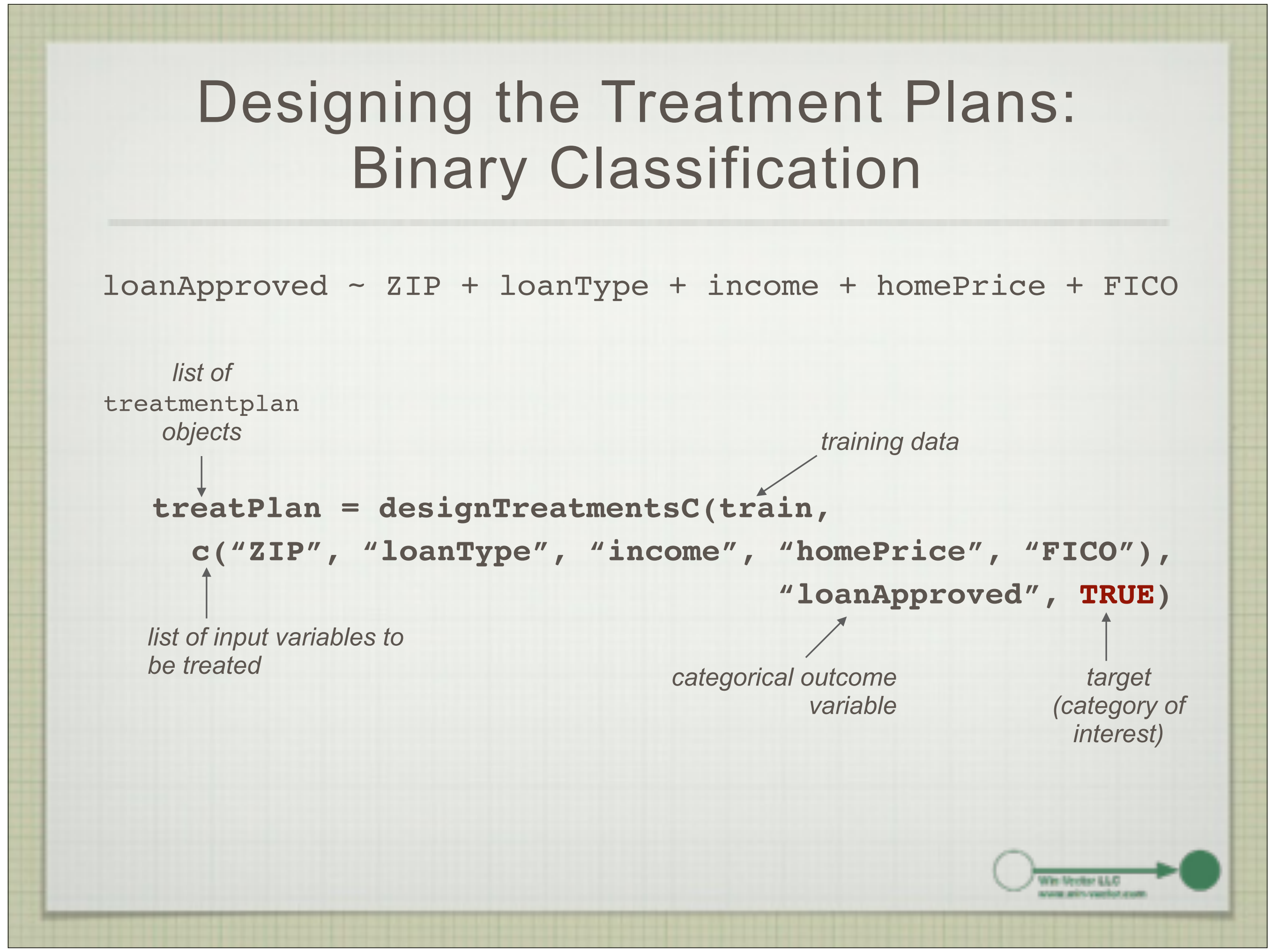
`df` is any frame of appropriate format (training or test)

```
  ZIP_catN homeType_lev_NA homeType_lev_x.condo homeType_lev_x.loft
190033.174               0                    1                   0
 -5320.826               0                    1                   0
 35596.174               0                    0                   0
-119202.826              0                    1                   0
 -94775.326              1                    0                   0

homeType_lev_x.single.family homeType_lev_x.townhouse numBed_clean numBed_isBAD
                           0                        0     4.000000            0
                           0                        0     2.000000            0
                           0                        1     1.000000            0
                           0                        0     2.000000            0
                           0                        0     2.456325            1

numBath_clean numBath_isBAD sqFt_clean salePrice
     4.000000             0       1025    815678
     3.000000             0       1082    600635
     3.000000             0        751    444609
     3.000000             0       1093    349433
     3.000000             0        914    692468
```

vtreat determines automatically whether a categorical variable should be impact coded, based on whether or not there are too many “rare levels” — too many levels that are off most of the time. By default “off too much” = on less than 2% of the time, and “too many rare levels” = the number of rare levels combined represent more than 4% of the data. These thresholds can be changed using the minFraction and maxMissing arguments to designTreatmentsN() and designTreatmentsC()



Predicting whether a customer will bid on a house

ZIP : large categorical
loanType: small categorical (what's plausible)
income, homePrice, FICO: numerical

Variable Importance Scores

Simple Example

```
N = 1000
df=data.frame(x1=rnorm(N, mean=10),
              x2=runif(N, min=5, max=15))
df$y=with(df, 2*x1+rnorm(N)) # only x1 affects y

treatPlan = designTreatmentsN(df, c("x1","x2"), “y")
treatPlan$varScores

# $x1_clean
# [1] 0.1833111
#
# $x2_clean
# [1] 1.000069
```

varScore: Based on Press Statistic

- Press Statistic of a model: Sum of variances of all hold-one-out models (**P**redicted **R**esidual **S**um of **S**quares)
  - sum of $(y_i - f_i)^2$
  - y_i = outcome of i^{th} data point
  - f_i = prediction of model built using all data points *except* the i^{th}
  - measure of predictive power
  - http://www.win-vector.com/blog/2014/09/estimating-generalization-error-with-the-press-statistic/

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varScore: indication of variable importance

- varScore of j_{th} variable, x_j:
  - Press statistic of `lm(y~x_j)` / Press statistic of `mean(y)`
    - Smaller is better.
    - varScore ≥ 1: x_j predicts outcome no better than `mean(y)`
  - By default, `prepare()` prunes variables with varScore > 0.99

```
treatPlan$varScores
# $x1_clean
# [1] 0.1833111
#
# $x2_clean
# [1] 1.000069

df.treat = prepare(treatPlan, df)
summary(df.treat)
# x1_clean            y
# Min.   : 7.365   Min.   :13.75
# 1st Qu.: 9.372   1st Qu.:18.66
# Median : 9.992   Median :20.09
# Mean   :10.013   Mean   :20.07
# 3rd Qu.:10.694   3rd Qu.:21.48
# Max.   :13.329   Max.   :27.79

df.treat = prepare(treatPlan, df, pruneLevel=NULL)
summary(df.treat)
# x1_clean         x2_clean            y
# Min.   : 7.365   Min.   : 5.002   Min.   :13.75
# 1st Qu.: 9.372   1st Qu.: 7.145   1st Qu.:18.66
# Median : 9.992   Median : 9.586   Median :20.09
# Mean   :10.013   Mean   : 9.719   Mean   :20.07
# 3rd Qu.:10.694   3rd Qu.:12.152   3rd Qu.:21.48
# Max.   :13.329   Max.   :14.991   Max.   :27.79
```

There are other automatic variable prunings as well: for variables that don’t vary, as well as for variables that are “on” for less than a minimal fraction of the data (rare variables)

Conclusions

- There’s no substitute for getting your hands in the data
- Nonetheless, some variable treatments are reusable again and again
- We’ve presented our go-to data treatments, and an R implementation for them: `vtreat`

More references on `vtreat`

- `vtreat` blog article
  - http://www.win-vector.com/blog/2014/08/vtreat-designing-a-package-for-variable-treatment/
- vtreat code on GitHub
  - https://github.com/WinVector/vtreat

Further References

- Impact Coding
  - http://www.win-vector.com/blog/2012/07/modeling-trick-impact-coding-of-categorical-variables-with-many-levels/
  - http://www.win-vector.com/blog/2012/08/a-bit-more-on-impact-coding/
- Converting Categorical Variables to Numerical (No Hashing)
  - http://www.win-vector.com/blog/2014/12/a-comment-on-preparing-data-for-classifiers/
- PRESS statistic
  - http://www.win-vector.com/blog/2014/09/estimating-generalization-error-with-the-press-statistic/

Thank You