Lecture 5: Data Preprocessing, Imputation and Feature Engineering

Alan Lee

Department of Statistics
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Outline

Today's agenda

In this lecture we discuss the importance of selecting, transforming and imputing the features used in prediction. We will cover

- Scaling
- Transforming
- Data cleaning and imputation
- Feature selection
- Feature engineering

We will use the Boston housing data as a running example. Note: References to APM refer to *Applied Predictive Modeling*: Ch 3 of APM covers the material of this lecture.

Boston housing data

This data set contains information on 506 Boston districts. The response is the median value of owner-occupied homes in $1000's, and there are 13 explanatory variables. The data are in the MASS package.

Scaling

Some of the prediction methods we have discussed work better when the features have similar magnitudes. For example

- In Neural networks, the starting values are chosen randomly on an interval around zero. This works better if the features have similar magnitudes. Also, the regularization penalty will apply equally to all variables if they have similar magnitudes.
- In ridge regression and the lasso the same argument applies.
- In unsupervised learning, there are techniques that benefit from having features with similar magnitudes (e.g. principal components.)

It is usual to scale the continuous variables by subtracting off means and dividing by standard deviations, so that the scaled data has mean zero and variance one. Note this only applies to continuous variables! If the data set contains a mixture of continuous variables and factors we need to split it into two parts. The R function `scale` can be used to scale the continuous variables:

Scaling: R code

```
library(MASS)
data(Boston)

# make variable chas into a factor
Boston$chas = factor(Boston$chas)
numericCols = unlist(lapply(Boston, is.numeric))
BostonCont = Boston[, numericCols]
BostonFactor =Boston[, !numericCols]
names(BostonFactor) = names(Boston)[!numericCols]
BostonScaled = data.frame(as.data.frame(scale(BostonCont)),
        BostonFactor)
```

Symmetrizing

It is also advantageous to transform the variables so that they have approximately symmetric distributions. The easiest way to do this is using Box-Cox transformations: we transform a variable x to $x^{(\lambda)}$ using the equation

$$x^{(\lambda)} = \frac{x^\lambda - 1}{\lambda}.$$

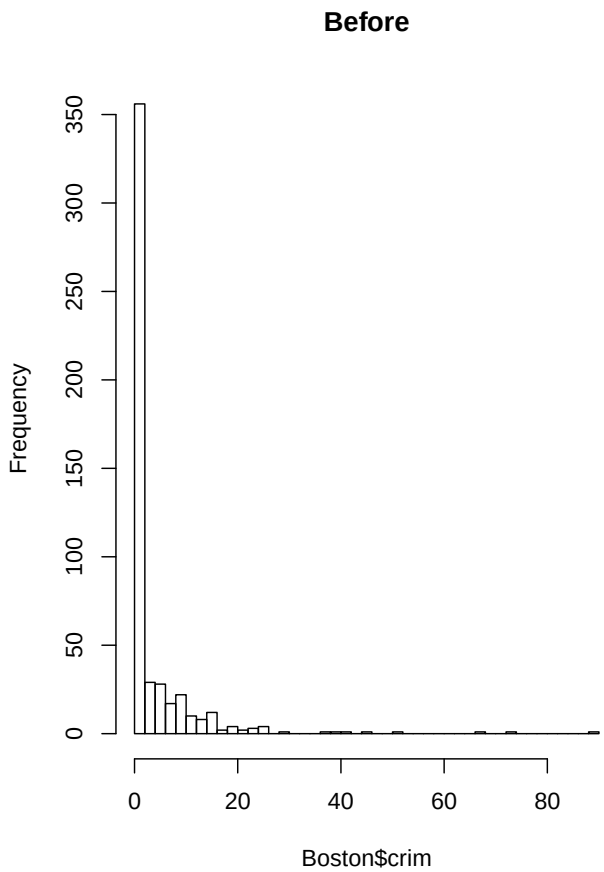
The value of λ is chosen using a maximum-likelihood argument. The R function `BoxCoxTrans` in the `caret` package can be used. (Subtracting 1 and dividing by λ makes the transformation approach a log as $\lambda \to 0$.)

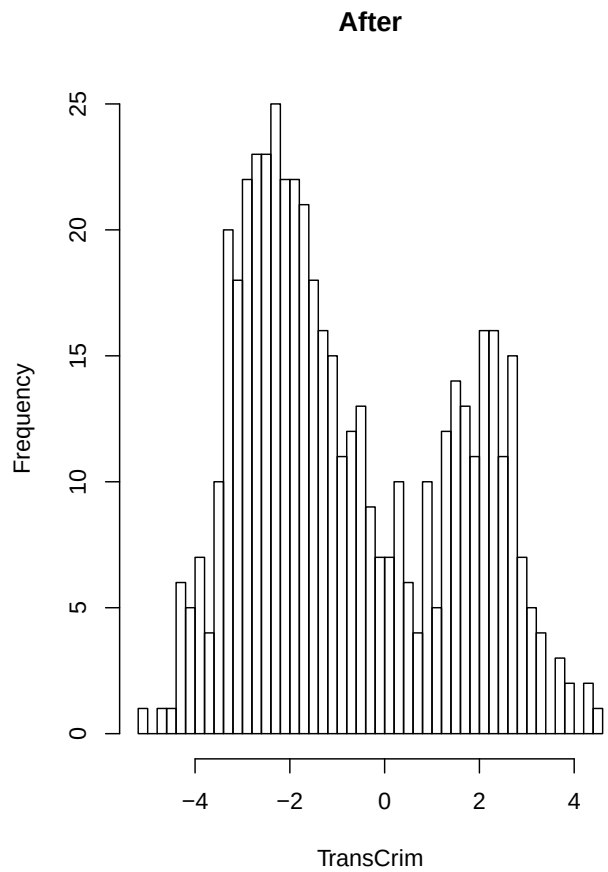
Symmetrizing: R code

```
TransCrim = predict(BoxCoxTrans(Boston$crim),
          Boston$crim)
par(mfrow=c(1,2))
hist(Boston$crim, nclass=50, main = "Before")
hist(TransCrim, nclass=50, main = "After")
```

Note the use of the predict function to perform the actual transformation.

Before and after





Putting it together

The caret function PreProcess does both symmetrizing and scaling:

```
numericCols = unlist(lapply(Boston, is.numeric))
BostonCont = Boston[, numericCols]
BostonFactor =Boston[, !numericCols]
names(BostonFactor) = names(Boston)[!numericCols]
trans = preProcess(BostonCont, method = c("BoxCox",
                    "center", "scale"))
BostonTransScaledCont = predict(trans, BostonCont)
BostonTransScaled = data.frame(BostonTransScaledCont,
                     BostonFactor)
```

Data cleaning and Imputation

- Data cleaning means correcting any mistakes in the data, which will usually correspond to impossibly large or impossibly small values. These will be revealed by range checks and plots, for example all pairs of scatterplots, or qqplots.
- However, not all outliers (large or small values) are mistakes - they may reveal interesting patterns, for example the existence of two different groups of data in the data set.
- Imputation means guessing the values of missing values. Some of our methods (or at least the software implementations) require that there be no missing values in the input data set, although others (e.g.trees) are not unduly bothered by missing values.
- Data cleaning and imputation are a very important phase of any data mining project and can be expected to absorb a big fraction of the project resources.

Data cleaning and Imputation

There are several methods for imputation:

- Complete case analysis: Delete any record that has missing values from the data set. The default in some R functions, e.g. lm.
- Nearest neighbours: to impute variable x average the value x of the k closest data points with no missing values.
- Average method: Average the value of x for the non-missing values.
- Hot deck: pick a "similar" record at random and use its value of x.
- Predictive: Fit a model to the data with variable x as the target and use it to predict the value.
- Single imputation: Draw a value at random from the conditional distribution of x given the other variables (this will have to be modeled)
- Multiple imputation: Repeatedly draw values at random from the conditional distribution of x given the other variables (this will have to be modeled), creating new data sets. Make the predictions with these now complete datasets and average the predictions.

Points to note

- Complete case analysis: This is not recommended. Unless the missingness is independent of the data, biases can result.
- Nearest neighbours: We have to decide on the definition of "close points" and the value of k.
- Average method: Easy to implement but crude.
- Hot deck: Ditto.
- Predictive: Better but understates the uncertainty in the imputation process.
- Single imputation: Again better, respects the uncertainty, but just a single value.
- Multiple imputation: generally regarded as the best method (a sample is better than a single observation.)
- We will revisit Multiple Imputation later in the lecture.

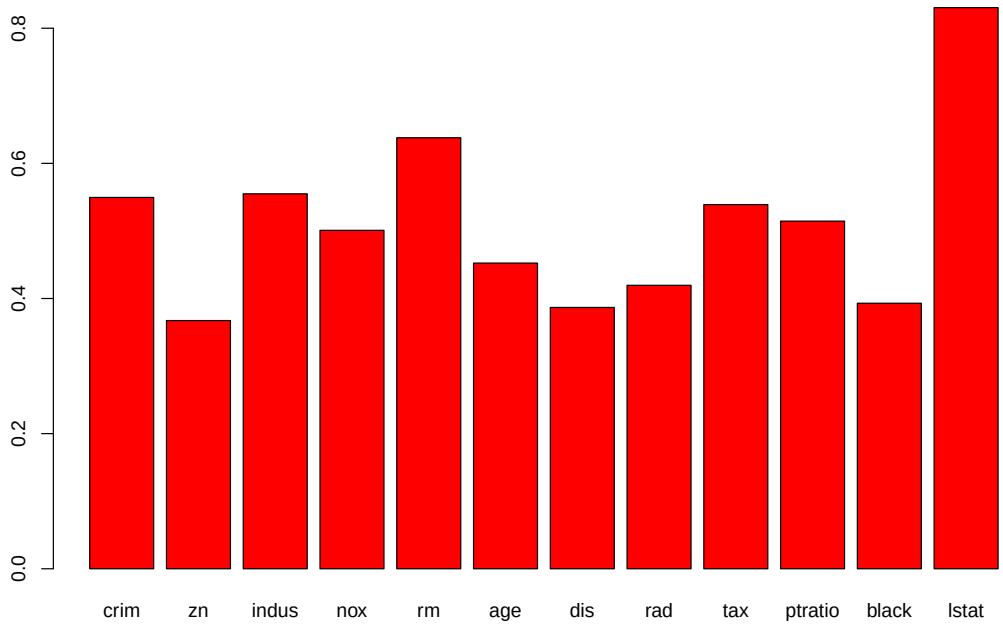
Feature selection

Features that are unrelated to the target are unlikely to improve the prediction, and will merely add to the computational burden. Thus, we can screen out variables that are unrelated, judged on the basis of correlations for continuous features, and anova tests for factors.

```
cors = cor(BostonScaled[,1:13])[1:12,13]
barplot(abs(cors), col="red")
cors = cor(BostonTransScaled[,1:13])[1:12,13]
barplot(abs(cors), col="red")
anova.fit = lm(medv~chas, data=BostonTransScaled)
anova(anova.fit)[1,5]
> anova(anova.fit)[1,5]
[1] 0.0002382315
```

This is the p-value for the F-test that there is no difference in the response between the factor levels. Just use it as an index: keep features with small p-values (say less than 0.1)

Correlation plot



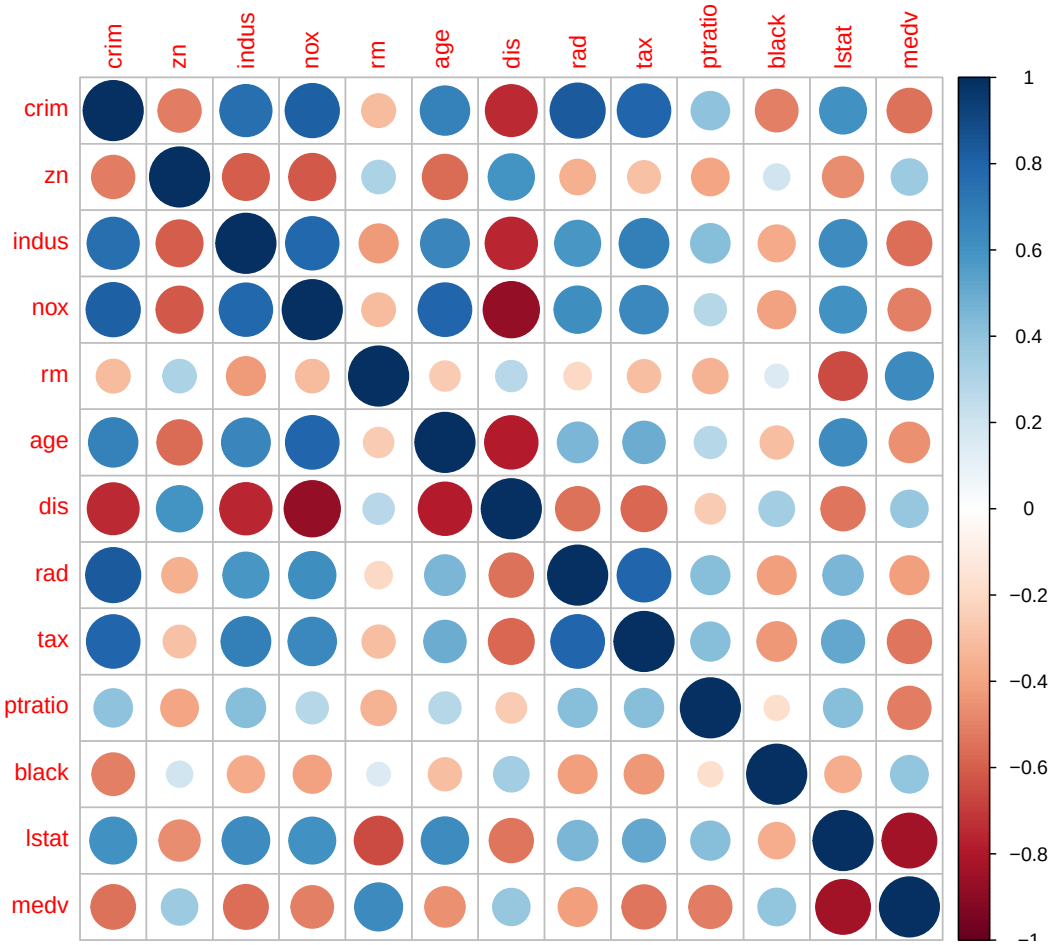
All seem to have some relationship to the target (recall that the best linear model included all the features)

Correlation between features

If two features are very highly correlated, it may not be necessary to include them both in the predictor (as in collinearity in linear regression). A correlation plot can be useful in identifying groups of highly correlated predictors.

```
library(corrplot)
correlations = cor(BostonTransScaled[,1:13])
corrplot(correlations)
```

Correlation plot



Correlation matrix

```
> round(correlations,2)
         crim    zn indus   nox    rm   age   dis   rad   tax ptratio black lstat  medv
crim     1.00 -0.52  0.75  0.81 -0.32  0.67 -0.74  0.84  0.79    0.41 -0.50  0.61 -0.55
zn      -0.52  1.00 -0.61 -0.61  0.31 -0.57  0.59 -0.35 -0.30   -0.39  0.19 -0.47  0.37
indus    0.75 -0.61  1.00  0.79 -0.42  0.66 -0.76  0.59  0.68    0.43 -0.38  0.63 -0.55
nox      0.81 -0.61  0.79  1.00 -0.31  0.80 -0.88  0.62  0.65    0.29 -0.40  0.61 -0.50
rm      -0.32  0.31 -0.42 -0.31  1.00 -0.25  0.27 -0.21 -0.30   -0.35  0.16 -0.65  0.64
age      0.67 -0.57  0.66  0.80 -0.25  1.00 -0.79  0.46  0.50    0.29 -0.31  0.62 -0.45
dis     -0.74  0.59 -0.76 -0.88  0.27 -0.79  1.00 -0.54 -0.58   -0.26  0.35 -0.54  0.39
rad      0.84 -0.35  0.59  0.62 -0.21  0.46 -0.54  1.00  0.80    0.42 -0.42  0.45 -0.42
tax      0.79 -0.30  0.68  0.65 -0.30  0.50 -0.58  0.80  1.00    0.42 -0.43  0.51 -0.54
ptratio  0.41 -0.39  0.43  0.29 -0.35  0.29 -0.26  0.42  0.42    1.00 -0.17  0.42 -0.51
black   -0.50  0.19 -0.38 -0.40  0.16 -0.31  0.35 -0.42 -0.43   -0.17  1.00 -0.37  0.39
lstat    0.61 -0.47  0.63  0.61 -0.65  0.62 -0.54  0.45  0.51    0.42 -0.37  1.00 -0.83
medv    -0.55  0.37 -0.55 -0.50  0.64 -0.45  0.39 -0.42 -0.54   -0.51  0.39 -0.83  1.00
```

See the R function `findCorrelation` in the `caret` package to see if any features should be removed.

Almost-zero-variance-features

If a feature has all values constant, it contributes nothing to the prediction. If almost all values are constant (e.g. a binary feature with very few 1's) then there may be problems with resampling, and the few 1's may have an undue influence on the predictor. Such features are best not included in the modeling. However, tree-based models are not affected by such features, as they won't be included in any split. Linear models will have problems if presented with zero-variance predictors if the software is not smart enough to exclude them (as `lm` does). The `caret` package has a function `nearZeroVar` that identifies almost-zero-variance features (see APM p 55)

```
> library(caret)
> nearZeroVar(BostonTransScaled)
integer(0)
# Returns column numbers of the
# near-zero-variance features
```

Dummy variables

You will recall that factors are handled in statistical modelling by turning them into dummy variables. Most of the modeling software does this automatically, but sometimes it is necessary to do this explicitly. There is a function (see APM p 56) `dummyVars` in the `caret` package that will do the job:

```
> dummy = dummyVars(~chas, data=BostonTransScaled)
> dummy.df = predict(dummy, newdata=BostonTransScaled)
> head(dummy.df)
  chas.0 chas.1
1      1      0
2      1      0
3      1      0
4      1      0
5      1      0
6      1      0
```

Feature engineering

Sometimes we want to make new variables our of old ones: a process known as feature engineering. Which new variables to make will be guided by subject matter knowledge. For example

1. Geographical coordinates could be turned into distances
2. Stock prices could be turned into log of the daily changes (returns)
3. Absolute numbers can be turned into rates
4. Several fertures can be combined into principal components .

Imputation: MCAR, MAR and NMAR

MCAR : data is completely missing at random: "missingness" is independent of the data values. In this situation using only the complete data (cases having no missing values) will give an unbiased result, but with a smaller sample size than if no data was missing. Can result in ignoring a large proportion of the data.

MCAR : data is missing at random: "missingness" depends only on the non-missing data (and thus in principle the missing values can be predicted from them).

NMAR : not missing at random - "missingness" depends on the missing and non-missing data. Not much can be done in this situation.

Basic idea of multiple imputation

- For each variable in turn, impute a missing value by drawing from the conditional distribution of the variable, given the rest of the data.
- This amounts to predicting the missing value, and adding small amount of noise to the prediction.
- Use the imputed data to construct a predictor.
- Repeat this several times to obtain multiple predictors.
- Average or "majority vote" to get a final predictor.

Another idea

- Start with a guess for the missing values, using one of the simple imputation methods. Or, alternatively, keep the missing values - the RF's can handle them.
- For each variable in turn, predict the missing values using a random forest with the other variables as targets. Fill in the missing values.
- Iterate this until no change.
- Use the imputed data to construct a predictor.

Advantages and disadvantages

- Works for any data set. Modeling the conditional distributions can be tricky for mixed data sets, since the conditional distribution needs to be estimated.
- Doesn't take account of the uncertainly in the imputation process.
- No method of adjusting the PE to account for the imputation.

How trees cope with missing values

- When considering splits, we only consider splits of the form $X < c$ where c is one of then non-missing values of X.
- We evaluate the splitting criterion ignoring the missing values.
- For each split, we identify "surrogate splits" - splits using different variables that result in similar partitions of the feature space.
- We use these if a case has a missing value in the primary split, when assigning cases to regions.
- When calculating the value of the tree in a region, we ignore missing values in the target.

Since trees cope, so do random forests.

R packages

- The package `missForest` implements the program on the last few slides.
- The packages `mice` and `mi` use a variety of prediction methods.
- See the tutorial at
  https://www.analyticsvidhya.com/blog/2016/03/tutorial-powerful-packages-imputing-missing-values/
  for more information on other packages.

Summarizing patterns of missing data

This is best done visually.

- Use barcharts of missing value proportions.
- Use the `image` function to show where the missing values are in the data set.
- Use the `md.pattern` in the `mice` package for a text summary of the missing value patterns.

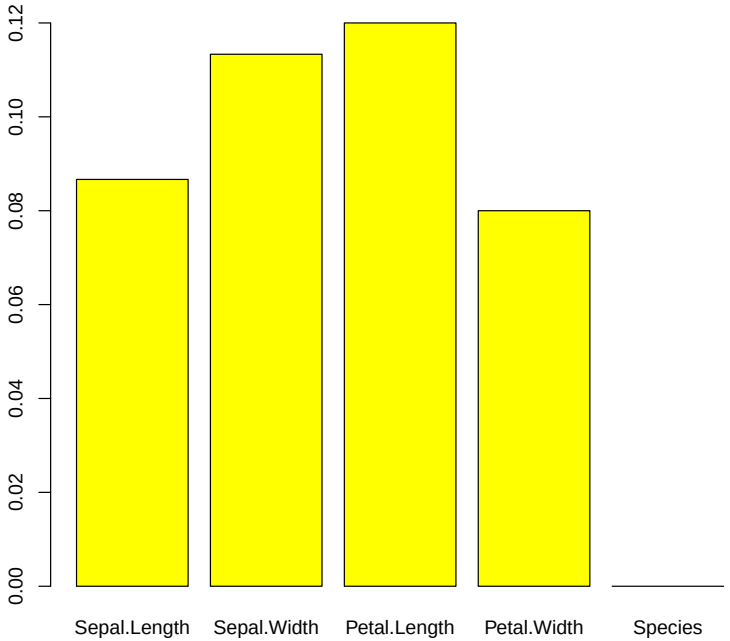
Example: the iris data

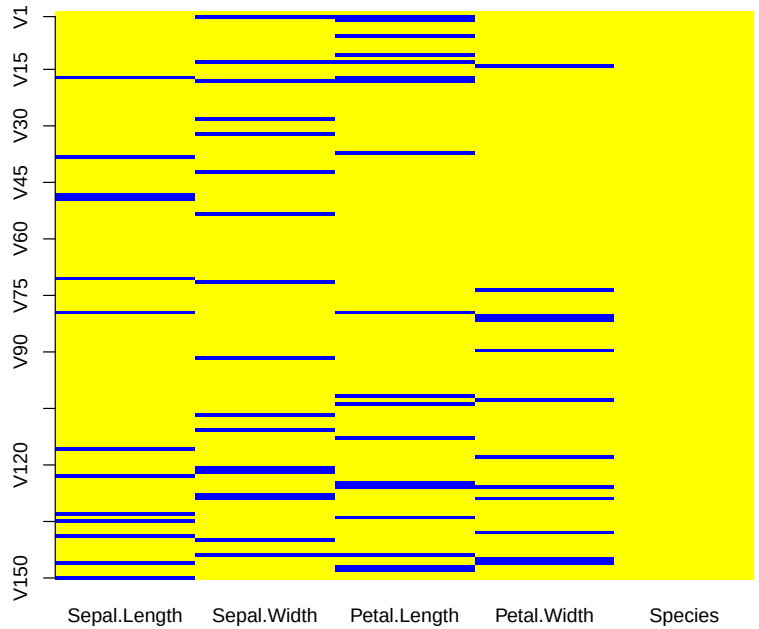
For the setosa data, we made data values go missing (replaced with NA's) in 10% of the size data. Similarly, for versicolor and virginica, 5% and 15% were set to NA. This we have a dataset that is MAR, none of the species values are missing.

Example: missingness patterns

```
> library(mice)
> md.pattern(iris.miss)
    Species Sepal.Length Sepal.Width Petal.Width Petal.Length
102       1            1           1           1            1  0
  7       1            0           1           1            1  1
  7       1            1           0           1            1  1
 21       1            1           1           1            0  1
  8       1            1           1           0            1  1
  2       1            1           0           1            0  2
  2       1            0           1           0            1  2
  1       1            0           0           1            0  3
          0           10          10          10           24 54
```

Example: the iris data





Example: Code

```
# plot of missings
par(mfrow=c(1,2))
k = dim(iris.miss)[2]
freq = numeric(k)
for(i in 1:k) freq = apply(iris.miss, 2,
     function(x)mean(is.na(x)))
barplot(freq, col="yellow")
```

Example: Code, pt 2

```
NAvec = as.vector(is.na(iris.miss))*1
reverseRows = function(A) A[rev(row(A)[,1]),]
image(t(reverseRows(NAmat)), col=my.col, axes=FALSE)
axis(1, at = seq(0,1, length=k), labels = colnames(NAmat),
    tick=FALSE)
vars = seq(0,150, by=15)
vars[1]=1
ticks = 1-vars/150
axis(2, at = ticks, labels = paste("V",vars, sep=""),
    tick=TRUE)
```

Or, use the functions in the VIM package.

Doing the imputation

```
ntrees=100
iris.imp = missForest(iris.miss, variablewise=TRUE,
                      ntree=ntrees)
iris.imp$OOB
      MSE       MSE       MSE       MSE       PFC
0.1071421 0.0938676 0.0619656 0.0284400 0.0000000
```

The imputed data is in the data frame `iris.imp$ximp`.

Example: QDA

```
fit.qda = qda(Species~., data = iris.imp$ximp)
predClasses = predict(fit.qda)$class
qdaTable = table(predClasses, iris$Species)

predClasses  setosa versicolor virginica
  setosa         50          0         0
  versicolor      0         48         1
  virginica       0          2        49
  > mean(is.na(iris.miss))
[1] 0.08133333
```

In fact, this is the same table that results from the complete data, so we have paid no price for the 8% of missing data.

An experiment

Suppose we have data following a multivariate normal distribution with mean zero and covariance matrix Σ where

$$\Sigma_{ij} = \begin{cases} 1, & i = j \\ \rho, & i \neq j. \end{cases}$$

The data consist of $n = 200$ draws from this distribution. The target is the first variable in the data set and the remaining 19 variables are the features.

An experiment (cont)

We have four data sets:

1. A training set, as above.
2. A test set generated in the same way.
3. A "missing" data set where the values of the training set have been set to NA with probability π.
4. An "imputed" data set where the missing values have been inputed using `missForest`.

We calculate (1) the test set estimate of prediction error, using a linear predictor and the complete data, (2) the test set estimate of prediction error, using a linear predictor and the imputed data, and (3) a CV estimate of the prediction error, using the imputed data.

Results

We show these 3 quantities for different values of ρ and π.

	$\pi = 0.05$			$\pi = 0.10$		
	Comp	Imp	CV	Comp	Imp	CV
$\rho = 0.5$	0.60	0.60	0.54	0.57	0.57	0.53
$\rho = 0.6$	0.47	0.47	0.42	0.47	0.47	0.42
$\rho = 0.7$	0.35	0.36	0.30	0.34	0.35	0.31
$\rho = 0.8$	0.24	0.24	0.21	0.24	0.24	0.22
$\rho = 0.9$	0.12	0.12	0.11	0.12	0.12	0.11
	$\pi = 0.15$			$\pi = 0.20$		
	Comp	Imp	CV	Comp	Imp	CV
$\rho = 0.5$	0.59	0.60	0.53	0.57	0.58	0.52
$\rho = 0.6$	0.48	0.48	0.41	0.47	0.47	0.40
$\rho = 0.7$	0.34	0.35	0.32	0.36	0.36	0.30
$\rho = 0.8$	0.23	0.24	0.21	0.24	0.24	0.21
$\rho = 0.9$	0.12	0.12	0.11	0.12	0.12	0.11

Points to note

- The effect of the missing values is negligible: Imp error is never much more than the the Comp error.
- The CV estimate under-estimates, so while the predictions aren't much affected, the estimate of error is.
- The degree of underestimation doesn't seem to depend much on either ρ or π, and is around 85-90%.

References

1. Hastie, T., Tibshirani, R.J. and Friedman, J. (2009). *The Elements of Statistical Learning, 2nd Ed*. Springer.
2. James, G., Witten, D., Hastie. and Tibshirani, R.J. (2013). *An Introduction to Statistical Learning*. Springer.
3. Steckhoven, D.J. and Bühlman, P. (2012). MissForest - non-parametric missing value imputation for mixed-type data. `Bioinformatics`, 28, 112-118.
4. van Buuren, S. and Groothuis-Oudshoorn, K. (2011) mice: Multivariate Imputation by Chained Equations in R. `Journal of Statistical Software`, 45 (3).