An R Lecture from Practice: Part II

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Contents

Preparation

- Download the dataset "Rlecture_Diamonds.csv"

Our Goals

- Learn data operations simplified by data.table
- Learn how to summarize information of variables for cleaning
- Learn to design steps for data cleaning in data table
- Learn how to use function/for/if and other structures in R working procedure

Contents

Data Table: A Poweful Extension of Data Frame

- Install by install.packages("data.table")

```
library("data.table")
data = fread("Rlecture_Diamonds.csv")
str(data)

## Classes 'data.table' and 'data.frame':^^I53940 obs. of  11 variables:
##  $ n      : int  1 2 3 4 5 6 7 8 9 10 ...
##  $ carat  : num  0.23 0.21 0.23 0.29 0.31 0.24 0.24 0.26 0.22 0.23 ...
##  $ cut    : chr  "Ideal" "Premium" "Good" "Premium" ...
##  $ color  : chr  "E" "E" "E" "I" ...
##  $ clarity: chr  "SI2" "SI1" "VS1" "VS2" ...
##  $ depth  : num  61.5 59.8 56.9 62.4 63.3 62.8 62.3 61.9 65.1 59.4 ...
##  $ table  : num  55 61 65 58 58 57 57 55 61 61 ...
##  $ price  : int  NA 326 NA 334 335 NA NA 337 337 338 ...
##  $ x      : num  3.95 3.89 4.05 4.2 4.34 3.94 3.95 4.07 3.87 4 ...
##  $ y      : num  3.98 3.84 4.07 4.23 4.35 3.96 3.98 4.11 3.78 4.05 ...
##  $ z      : num  2.43 2.31 2.31 2.63 2.75 2.48 2.47 2.53 2.49 2.39 ...
##  - attr(*, ".internal.selfref")=<externalptr>

summary(data)

##        n             carat            cut               color
##  Min.   :    1   Min.   :0.20   Length:53940       Length:53940
##  1st Qu.:13486   1st Qu.:0.40   Class :character   Class :character
##  Median :26970   Median :0.70   Mode  :character   Mode  :character
##  Mean   :26970   Mean   :0.80
##  3rd Qu.:40455   3rd Qu.:1.04
##  Max.   :53940   Max.   :5.01
##
##    clarity             depth          table           price
##  Length:53940       Min.   :43.0   Min.   :43.0   Min.   :  326
```

Take Subset from Data Table

- Take subset like data.frame, but using list to contain variables

```
data[2:4, list(n, carat, price)] # select row 2 to 4 and column (n, carat, x)

##    n carat price
## 1: 2  0.21   326
## 2: 3  0.23    NA
## 3: 4  0.29   334
```

- Use .N as the length of data, and operations in columns

```
data[5:.N, list(n, unit_price = price/carat)]

##            n unit_price
##     1:     5       1081
##     2:     6         NA
##     3:     7         NA
##     4:     8       1296
##     5:     9       1532
##    ---
## 53932: 53936       3829
## 53933: 53937       3829
## 53934: 53938         NA
## 53935: 53939       3206
## 53936: 53940         NA
```

Introduction of Data Table

- data.table has the form: data[i, j, by = ...] like SQL

```
data[i = price > 1000, j = list(count = .N, carat = mean(carat)), by = list(cut)]

##          cut count carat
## 1:      Fair  1114 1.081
## 2:     Ideal 10814 0.876
## 3: Very Good  6507 0.978
## 4:      Good  2795 0.997
## 5:   Premium  7794 1.061
```

R (data.table)	i	j	by
SQL	WHERE	SELECT	GROUP BY

- data.table is faster than R default, especially with big data

```
system.time(read.csv("Rlecture_Diamonds.csv")) # timing (second): read csv with R default

##    user  system elapsed
##    0.33    0.00    0.33

system.time(fread("Rlecture_Diamonds.csv")) # timing (second): read csv with data.table

##    user  system elapsed
##    0.21    0.00    0.20
```

Sort Data Table

- Sort data by setkey()

```
setkey(data, cut)
data[,list(n,cut)]

##             n       cut
##     1:      9      Fair
##     2:     92      Fair
##     3:     98      Fair
##     4:    124      Fair
##     5:    125      Fair
##    ---
## 53936: 53922 Very Good
## 53937: 53923 Very Good
## 53938: 53933 Very Good
## 53939: 53934 Very Good
## 53940: 53938 Very Good
```

- Select rows by key value directly

```
data["Good", .N]

## [1] 4906

data["Good", mult = "first"]

##    n carat  cut color clarity depth table price    x    y    z
## 1: 3  0.23 Good     E     VS1  56.9    65    NA 4.05 4.07 2.31
```

Column Apply in Data Table

- Apply functions into each column with lapply and .SD

```
class(data[, price])

## [1] "integer"

data[,lapply(.SD, class)]

##          n   carat       cut     color   clarity   depth   table   price
## 1: integer numeric character character character numeric numeric integer
##          x       y       z
## 1: numeric numeric numeric
```

- Take a subset of columns with .SDcols

```
data[,lapply(.SD, class), .SDcols = -c(2:5)]

##          n   depth   table   price       x       y       z
## 1: integer numeric numeric integer numeric numeric numeric
```

Contents

Data Summarization

Goal: Summarize the characters of many variables of big data

- Amount of Information vs. Readability
- Various Variable Types vs. General Method/Representation
- Elaboration vs. Quickness/Easiness

Our Solution: Use data.table to convert each variable into key statistics, and create a new summarized data.table

Summarize Variables (1): Type and Size

- First identify the type of each variable

```
data[,lapply(.SD, class)]

##            n   carat       cut     color   clarity   depth   table   price
## 1: integer numeric character character character numeric numeric integer
##            x       y       z
## 1: numeric numeric numeric
```

- count NA values of each variable

```
x = data[,price]
nonNA = function(x){
  return(sum(!is.na(x)))
}
nonNA(data[,price])

## [1] 39708

data[,lapply(.SD, nonNA)] # count of non-NA values of variables

##          n carat   cut color clarity depth table price     x     y     z
## 1: 53940 53940 53940 53940   53940 53940 53940 39708 53940 53940 53940
```

Summarize Variables (2): Numeric Statistics

- Convert numeric variable into numeric statistics

```
summary_num = function(x){
  if(class(x) == "character")
    return(NA)
  else
    x_trans = c(mean(x, na.rm = T), sd(x, na.rm = T), quantile(x, na.rm = T))
  return(x_trans)
}
summary_num(data[,price])

##                  0%   25%   50%   75%  100%
##   3928  3993   326   949  2397  5302 18818

data[,lapply(.SD, summary_num)]

##          n carat cut color clarity depth table price     x     y      z
## 1: 26971 0.798  NA    NA      NA 61.75 57.46  3928  5.73  5.73  3.539
## 2: 15571 0.474  NA    NA      NA  1.43  2.23  3993  1.12  1.14  0.706
## 3:     1 0.200  NA    NA      NA 43.00 43.00   326  0.00  0.00  0.000
## 4: 13486 0.400  NA    NA      NA 61.00 56.00   949  4.71  4.72  2.910
## 5: 26971 0.700  NA    NA      NA 61.80 57.00  2397  5.70  5.71  3.530
## 6: 40455 1.040  NA    NA      NA 62.50 59.00  5302  6.54  6.54  4.040
## 7: 53940 5.010  NA    NA      NA 79.00 95.00 18818 10.74 58.90 31.800
```

Summarize Variables (3): Frequency Table

- We create a function to get the most 5 frequent values

```
summary_value = function(x){
  freq = sort(table(x), decreasing = TRUE)
  return(names(freq)[1:5])
}
data[,lapply(.SD, summary_value)]

##    n carat       cut color clarity depth table price    x    y    z
## 1: 1   0.3     Ideal     G     SI1    62    56   605 4.37 4.34  2.7
## 2: 2  0.31   Premium     E     VS2  61.9    57   828 4.34 4.37 2.69
## 3: 3  1.01 Very Good     F     SI2  61.8    58   776 4.33 4.35 2.71
## 4: 4   0.7      Good     H     VS1  62.2    59   789 4.38 4.33 2.68
## 5: 5  0.32      Fair     D    VVS2  62.1    55   666 4.32 4.32 2.72
```

- Get the frequency of most 5 frequent values, tail and NA

```
summary_freq = function(x){
  freq = sort(table(x), decreasing = TRUE)
  return(c(freq[1:5], sum(freq[-(1:5)]), sum(is.na(x))))
}
data[,lapply(.SD, summary_freq)]

##        n carat   cut color clarity depth table price     x     y     z
## 1:     1  2604 21551 11292   13065  2239  9881   103   448   437   767
## 2:     1  2249 13791  9797   12258  2163  9724    96   437   435   748
## 3:     1  2242 12082  9542    9194  2077  8369    95   429   425   738
## 4:     1  1981  4906  8304    8171  2039  6572    91   428   421   730
## 5:     1  1840  1610  6775    5066  2020  6268    88   425   414   697
## 6: 53935 43024     0  8230    6186 43402 13126 39235 51773 51808 50260
## 7:     0     0     0     0       0     0     0 14232     0     0     0
```

Summarize Variables (4): Merge

- Use a list to collect these summaries, each reorganized by variable names as index

```
fL = list(class, nonNA, summary_num, summary_value, summary_freq)
summaryL = list()
for(i in 1:length(fL)){
  summaryL[[i]] = data[,lapply(.SD, fL[[i]])]
  summaryL[[i]] = data.table(t(summaryL[[i]]), keep.rownames=TRUE)
  setkey(summaryL[[i]], rn)
}
```

- Merge a list of data.tables into one data.table with Reduce()

```
summary_data = Reduce(function(X,Y){X[Y]}, summaryL)
colnames(summary_data) = c("variable", "type", "N",
                           "mean", "sd", "min", "Q1", "median", "Q3", "max",
                           paste("value", 1:5), paste("freq", c(1:5, "others", "NA")))
write.csv(summary_data, "Rlecture_Diamonds_summary.csv", row.names = FALSE, na = "")
```

Contents

Why Data Cleaning

- A key step to prepare big data for machine learning
- Standardize raw data for statistical models:
  - In programming: convert data to numeric matrices for general-model use (beyond linear models in R)
  - In mathematics: solve problems in data, such as NA, sparsity, outliers, ...
- Difficulty: the size and complexity of data

How to do Data Cleaning?

1. Convert all non-numeric variables into numeric variables
   - variables with prior information $\rightarrow$ values from information
   - variables without prior information $\rightarrow$ 0-1 dummy variables
2. Delete sparse varaibles (the ratio of NAs and the most frequent value near 1)
3. Delete collinear variables (strictly lower triangular correlation matrix near ± 1)
4. Fill NAs
5. Normalized Centeralization

Data Cleaning (1a): Map between Two Sets of Values

Our Goal: Convert all non-numeric variables into numeric varibles

- if we know prior information of categories (such as ordinal), then build a key-value map with data.table

```
x = data[,cut]
mapDT = data.table(c("Fair", "Good", "Very Good", "Premium", "Ideal"), 1:5, key = "V1")
mapDT
```

- Map categories into numeric values using data.table

```
map = function(x, mapDT){
  op = data.table(x, key = "x")
  op = op[mapDT]
  return(op[,V2])
}
data[, cut := map(cut, mapDT)]
data
```

Data Cleaning (1b): Dummy Variables

- Then convert all other non-numeric variables into 0-1 dummy variables

```
char_to_dummy = function(x){
  if(class(x) == "character"){
      op = data.table(model.matrix(~ factor(x)))
  } else
    op = data.table(x)
  return(op)
}
```

- Use cbind() for combine matrix/data by columns

```
data_clean = 0
for(i in colnames(data)){
  data_sub = char_to_dummy(data[,get(i)])
  split_name = as.data.table(strsplit(colnames(data_sub), ")"))
  if(dim(split_name)[2] > 1)
    colnames(data_sub) = paste0(i, "_", split_name[2])
  else
    colnames(data_sub) = i
  data_clean = cbind(data_clean, data_sub)
}
dim(data_clean)

## [1] 53940    25
```

Data Cleaning (2): Delete Sparse Variables

- Check the number of NAs and most frequent values of each variable, define it as sparity

```
# data_clean[,lapply(.SD, summary_freq)]
sparsity = function(x){
  x_freq = summary_freq(x)
  return(sum(x_freq[c(1,7)]/length(x)))
}
(sparse = data_clean[ , lapply(.SD, sparsity)])

##    data_clean        n  carat cut color_(Intercept color_E color_F color_G
## 1:          1 1.85e-05 0.0483 0.4                1   0.818   0.823   0.791
##    color_H color_I color_J clarity_(Intercept clarity_IF clarity_SI1
## 1:   0.846   0.899   0.948                  1      0.967       0.758
##    clarity_SI2 clarity_VS1 clarity_VS2 clarity_VVS1 clarity_VVS2  depth
## 1:        0.83       0.849       0.773        0.932        0.906 0.0415
##    table price       x      y      z
## 1: 0.183 0.266 0.00831 0.0081 0.0142
```

- Delete all variables with sparsity higher than 99.99%

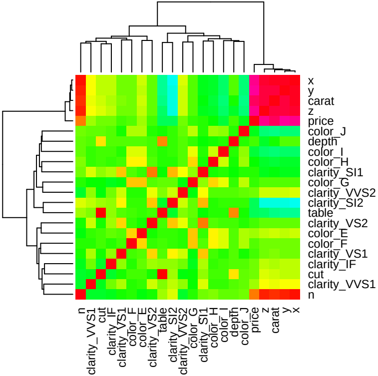
```
data_clean = data_clean[, (names(sparse)[sparse < 0.9999]), with = FALSE]
dim(data_clean)

## [1] 53940    22
```

Correlation Matrix and Visualization

- Use correlation matrix to detect collinearity

```r
cm = cor(data_clean, use = "pairwise.complete.obs")
heatmap(cm, col = rainbow(100), scale = "none")
write.csv(cm, "Rlecture_Diamonds_cm.csv")
## Then open "Rlecture_Diamonds_cm.csv" in Microsoft Excel (2010+):
## Ctrl+A -> tag: Home -> Conditional Formatting -> Color Scales
```



Data Cleaning (3): Delete Collinear Variables

- Delete collinear variables with lower triangular of correlation matrix

```
(collinear = apply(lower.tri(cm) & (abs(cm) > 0.95), 1, any))

##            n        carat          cut      color_E      color_F
##        FALSE        FALSE        FALSE        FALSE        FALSE
##      color_G      color_H      color_I      color_J   clarity_IF
##        FALSE        FALSE        FALSE        FALSE        FALSE
##   clarity_SI1  clarity_SI2  clarity_VS1  clarity_VS2 clarity_VVS1
##        FALSE        FALSE        FALSE        FALSE        FALSE
## clarity_VVS2        depth        table        price            x
##        FALSE        FALSE        FALSE        FALSE         TRUE
##            y            z
##         TRUE         TRUE

data_clean = data_clean[, (names(collinear)[!collinear]), with = FALSE]
dim(data_clean)

## [1] 53940    19
```

Data Cleaning (4): Fill NAs

- Check NA values

```
data_clean[, lapply(.SD, function(x){sum(is.na(x))})]

##    n carat cut color_E color_F color_G color_H color_I color_J clarity_IF
## 1: 0     0   0       0       0       0       0       0       0          0
##    clarity_SI1 clarity_SI2 clarity_VS1 clarity_VS2 clarity_VVS1
## 1:           0           0           0           0            0
##    clarity_VVS2 depth table price
## 1:            0     0     0 14232
```

- Fill NA values with the median/mean/... of the column (Not necessary for predicted variable Y)

```
fillNA = function(x){
  a = median(x, na.rm = TRUE)
  x[is.na(x) == TRUE] = a
  return(x)
}
data_clean = data_clean[, lapply(.SD, fillNA)]
data_clean[, lapply(.SD, function(x){sum(is.na(x))})]

##    n carat cut color_E color_F color_G color_H color_I color_J clarity_IF
## 1: 0     0   0       0       0       0       0       0       0          0
##    clarity_SI1 clarity_SI2 clarity_VS1 clarity_VS2 clarity_VVS1
## 1:           0           0           0           0            0
##    clarity_VVS2 depth table price
## 1:            0     0     0     0
```

Data Cleaning (5): Normalized Centeralization

- For homework: Standardize all variables with mean 0 and standard deviation 1

Contents

Preparation

- Download the dataset "Rlecture_Diamonds.csv"

Our Goals

- Learn to clean data for machine learning models
- Learn to divide training/validation sets and cross-validation
- Choose and train models
- Evaluate results of models

Contents

A Machine Learning Question

- If we want to evaluate the unknown price of diamonds as precisely as possible
- We can use the information of the sample with known price

What is Machine Learning?

- Machine learning explores the study and construction of algorithms that can learn from and make predictions on data. (Wikipedia)
- Model: $Y_{n\times q} = f(X_{n\times p}) + \varepsilon_{n\times q}$
- Objective: find best $\hat{f}$ to minimize $||Y, \hat{f}(X)||$
  - $||Y, \hat{f}(X)||$: the distance between Y and $\hat{f}(X)$
  - Y is also called label of data
- Example: for linear regression, $q = 1$, $f(X) = \beta_0 + X\beta$ and $||Y, f(X)|| = \sum_{i=1}^{n}(y_i - f(X)_i)^2$
- In our case,
  - $Y_{n\times 1}$: price of diamonds
  - $X_{n\times p}$: other variables
  - $f()$: the model we want to choose
  - $||Y, f(X)||$: the distance criteria we want to choose

How to Choose the Distance?

- Here are some examples of distance

Distance	Expression	Use
L^2 (Euclidean)	$\sum_{i=1}^{n}(y_i - f(X)_i)^2$	Regression
L^1 (Absolute)	$\sum_{i=1}^{n}\lvert y_i - f(X)_i\rvert$	Regression
L^0 (0-1)	$\sum_{i=1}^{n} 1(y_i - f(X)_i \neq 0)$	Classification
Cross Entropy	$\sum_{i=1}^{n} \log(f(X)_i{}^{y_i}(1 - f(X)_i)^{1-y_i})$	Classification

- In mathematics, L^p distance is denoted by $d^p = ||Z||_p^p = \sum_{i=1}^{n} |z_i|^p$
- As a regression problem, we can choose L^2 distance (also called SSE) as our criteria of evaluating precision
- Since the price varies in magnitude, we use log(price) as Y

```
data[,price := log(price)]
summary(data[,price])

##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.    NA's
##       6       7       8       8       9      10   14232
```

Create a Distance Function in R

- We create an average L^p distance (use mean instead of sum)

```
Lp_dist = function(y, y_hat, p = 2){
  return(mean(abs(y - y_hat)^p))
}
```

- We examine it by a weather forecast example

```
rain_forecast = c(0.9, 0.2, 0.3, 0.6, 0.1) # the probability of rain forecasted
rain = c(1, 0, 1, 0, 0) # the true weather
Lp_dist(rain, rain_forecast) # default: L2 distance (MSE)

## [1] 0.182

Lp_dist(rain, rain_forecast, p = 1) # L1 distance (MAE)

## [1] 0.34

Lp_dist(rain, rain_forecast, p = 1e-10) # L0 distance (Error Rate)

## [1] 1

Lp_dist(rain, rain_forecast > 0.5, p = 1e-10) # L0 distance with discretizing classification

## [1] 0.4
```

Contents

Training and Validation Set

- How do we know we catch the true effect $f(X)$ by model $\hat{f}(X)$?
  - Example: we can fit $Y_{n\times 1}$ perfectly by an n-degree polynomial
- Solution: divide labeled data (X, Y) into two parts (X_T, Y_T), (X_V, Y_V)
  - (X_T, Y_T): Training set, for training model
  - (X_V, Y_V): Validation set, for validating model

Create Training/Validation Sets in R

- We can only use labeled data for training/validation sets

```
setkey(data_clean, n)
set.seed(56789)
group = data_clean[!is.na(price), list(n, igroup = rank(runif(.N)) %% 10 + 1)]
id_valid = group[igroup == 1]
id_train = group[igroup != 1]
```

- Try to train and validate with a linear model

```
model = lm(price ~ . - n, data = data_clean[id_train,])
Lp_dist(data_clean[id_train, price], model$fitted.values) # training error

## [1] 0.351

yhat = predict(model, newdata = data_clean[id_valid,])
Lp_dist(data_clean[id_valid, price], yhat) # validation error

## [1] 0.342
```

Cross Validation

- Idea: Evaluate the prediction error of a model more precisely and estimate its range
- Divide same data into multiple pairs of training/validation sets
- K-folds cross validation:
    1. Cut the index of data randomly into K groups with equal size
    2. Take one group as validation set, and others as training set to train a model
    3. Do step 2 for K times, in each choose a different validation set, and get K models
    4. Use K models to predict the unlabeled data, take the average of prediction result

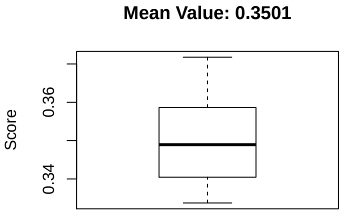
Do Cross Validation in R

- We use a list with a for-loop to build cross validation models

```
modelL = list()
score = c()
for(i in 1:max(group)){
  id_valid = group[igroup == i]
  id_train = group[igroup != i]
  modelL[[i]] = lm(formula = price ~ . - n, data = data_clean[id_train,])
  yhat = predict(modelL[[i]], newdata = data_clean[id_valid,])
  score = c(score, Lp_dist(data_clean[id_valid, price], yhat))
}
score

##  [1] 0.342 0.354 0.360 0.372 0.340 0.359 0.344 0.339 0.334 0.358

boxplot(score, ylab = "Score", main = paste("Mean Value:", round(mean(score), 4)))
```



Contents

Over-Fitting

- Idea: $\hat{f}(X) = \hat{f}_f(X) + \hat{f}_\varepsilon(X) \to Y = f(X) + \varepsilon$
- Variance:
  - $Var(Y - \hat{f}(X)) = Var((f - \hat{f}_f)(X)) \downarrow + Var(\varepsilon) + Var(\hat{f}_\varepsilon(X)) \uparrow$
- Over-fitting: $Var(\hat{f}_\varepsilon(X)) \uparrow$ at a speed faster than $Var((f - \hat{f}_f)(X)) \downarrow$
  - The model spend too much complexity on fitting random errors
- To prevent over-fitting, we often use loss and penalty functions in model structures

Loss and Penalty Functions

- Idea: Try to prevent over-fitting through controlling the complexity of model $\hat{f}$
- Loss function: $||Y, f(X)||_L$
- Penalty function: $||f||_P$
- Objective: find best $\hat{f}$ to minimize $||Y, \hat{f}(X)||_L + \lambda||\hat{f}||_P$
- $\lambda \geq 0$ is the penalty coefficient: the larger the λ become, the simpler the $\hat{f}$ will be

Models (GLM)	Loss	Penalty
Linear Regression	$\|\|Y - f(X)\|\|_2^2$	None
Stepwise Selection (AIC)	$\|\|Y - f(X)\|\|_2$	$\|\|\beta\|\|_0^0$
Ridge Regression	$\|\|Y - f(X)\|\|_2^2$	$\|\|\beta\|\|_2^2$
Lasso Regression	$\|\|Y - f(X)\|\|_2^2$	$\|\|\beta\|\|_1$
Quantile Regression	$\|\|Y - f(X)\|\|_1$	None