Lecture 2: Advanced R

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Advanced R

Introduction

In this lecture, we will talk about efficient computation in R.

- R is a vector-oriented language. In most cases, vectorization speeds up computation.
- We turn to more CPUs for parallel execution to save time if there is no more room to optimize the code to improve the speed.
- Servers are accessed remotely. Communicating with a remote cluster is different from operating a local machine.

Vectorization

Despite mathematical equivalence, various ways of calculation can perform distinctively in terms of computational speed.

Does computational speed matter? For a job that takes less than a minutes, the time difference is not a big deal. But sometimes economic problems can be clumsy. For structural estimation commonly seen in industrial organization, a single estimation can take up to a week. In econometrics, other computational intensive procedures include bootstrap, simulated maximum likelihood and simulated method of moments. Even if a single execution does not take much time, repeating such a procedure for thousands of replications will consume a non-trivial duration. Moreover, machine learning methods that crunch big data usually involve tuning parameters, so the same procedure must be carried out at each point of a grid of tuning paramters. For example, the preferred algorithm in Lin et al. (2020) takes 8 hours on a 24-core remote server to find out the best combination of tuning parameters. For those problems, code optimization is essential.

Of course, optimizing code takes human time. It is a balance of human time and machine time.

Example

In OLS regression, under homoskedasticity

$$\sqrt{n}\left(\widehat{\beta}-\beta_0\right) \xrightarrow{d} N\left(0, \sigma^2\left(E\left[x_i x_i'\right]\right)^{-1}\right)$$

where the asymptotic variance can be consistently estimated by $(X'X)^{-1}\sum_{i=1}^{n}\widehat{e}^2$. However, under heteroskedasticity

$$\sqrt{n}\left(\widehat{\beta}-\beta_0\right) \xrightarrow{d} N\left(0, E\left[x_i x_i'\right]^{-1} \mathrm{var}\left(x_i e_i\right) E\left[x_i x_i'\right]^{-1}\right)$$

where var $(x_i e_i)$ can be estimated by

$$\underbrace{\frac{1}{n}\sum_{i=1}^{n} x_i x_i' \widehat{e}_i^2}_{\text{opt 1}} = \underbrace{\frac{1}{n} X' D X}_{\text{opt 2 and 3}} = \underbrace{\frac{1}{n}\left(X' D^{1/2}\right)\left(D^{1/2} X\right)}_{\text{opt 4}}$$

where D is a diagonal matrix of $\left(\widehat{e}_1^2, \widehat{e}_{2,}^2, \ldots, \widehat{e}_n^2\right)$. There are at least 4 mathematically equivalent ways to compute the "meat" of the sandwich form.

1. literally sum $\hat{e}_i^2 x_i x_i'$ over $i = 1, \ldots, n$ one by one.
2. $X'\mathrm{diag}(\hat{e}^2)X$, with a dense central matrix.
3. $X'\mathrm{diag}(\hat{e}^2)X$, with a sparse central matrix.
4. Do cross product to `X*e_hat`. It takes advantage of the element-by-element operation in R.

We first generate the data of binary response and regressors. Due to the discrete nature of the dependent variable, the error term in the linear probability model is heteroskedastic. It is necessary to use the heteroskedastic-robust variance to consistently estimate the asymptotic variance of the OLS estimator. The code chunk below estimates the coefficients and obtains the residual.

```r
# an example of robust variance matrix.
# compare the implementation via matrix, Matrix (package) and vecteroization.

# n = 5000; Rep = 10; # Matrix is quick, matrix is slow, adding is OK

source("data_example/lec2.R")

n <- 50
Rep <- 1000 # we repeat the precedure to make the time comparison easier
# because this is a very simple operation,
# a single execution takes very short time.

data.Xe <- lpm(n) # see the function in "data_example/lec2.R"
X <- data.Xe$X
e_hat <- data.Xe$e_hat

XXe2 <- matrix(0, nrow = 2, ncol = 2)
```

We run the 4 estimators for the same data, and compare the time.

```r
for (opt in 1:4) {
  pts0 <- Sys.time()

  for (iter in 1:Rep) {
    set.seed(iter) # to make sure that the data used
    # different estimation methods are the same

    if (opt == 1) {
      for (i in 1:n) {
        XXe2 <- XXe2 + e_hat[i]^2 * X[i, ] %*% t(X[i, ])
      }
    } else if (opt == 2) { # the vectorized version with dense matrix
      e_hat2_M <- matrix(0, nrow = n, ncol = n)
      diag(e_hat2_M) <- e_hat^2
      XXe2 <- t(X) %*% e_hat2_M %*% X
    } else if (opt == 3) { # the vectorized version with sparse matrix
      e_hat2_M <- Matrix::Matrix(0, ncol = n, nrow = n)
      diag(e_hat2_M) <- e_hat^2
      XXe2 <- t(X) %*% e_hat2_M %*% X
    } else if (opt == 4) { # the best vectorization method. No waste
      Xe <- X * e_hat
      XXe2 <- t(Xe) %*% Xe
    }

    XX_inv <- solve(t(X) %*% X)
    sig_B <- XX_inv %*% XXe2 %*% XX_inv
  }
  cat("n =", n, ", Rep =", Rep, ", opt =", opt, ", time =", Sys.time() - pts0, "\n")
}
```

```
## n = 50 , Rep = 1000 , opt = 1 , time = 0.220999
## n = 50 , Rep = 1000 , opt = 2 , time = 0.05200005
## n = 50 , Rep = 1000 , opt = 3 , time = 1.368996
## n = 50 , Rep = 1000 , opt = 4 , time = 0.02400208
```

We clearly see the difference in running time, though the 4 methods are mathematically the same. When n is small, `matrix` is fast and `Matrix` is slow; the vectorized version is the fastest. When n is big, `matrix` is slow and `Matrix` is fast; the vectorized version is still the fastest.

Efficient Loop

R was the heir of S, an old language. R evolves with packages that are designed to adapt to new big data environement. Many examples can be found in Wickham and Grolemund (2016). Here we introduce `plyr`.

In standard `for` loops, we have to do a lot of housekeeping work. Hadley Wickham's `plyr` simplifies the job and facilitates parallelization.

Example

Here we calculate the empirical coverage probability of a Poisson distribution of degrees of freedom 2. We first write a user-defined function `CI` for confidence interval, which was used in the last lecture.

This is a standard `for` loop.

```
Rep <- 100000
sample_size <- 1000
mu <- 2

source("data_example/lec2.R")
# append a new outcome after each loop
pts0 <- Sys.time() # check time
```

```r
for (i in 1:Rep) {
  x <- rpois(sample_size, mu)
  bounds <- CI(x)
  out_i <- ((bounds$lower <= mu) & (mu <= bounds$upper))
  if (i == 1) {
    out <- out_i
  } else {
    out <- c(out, out_i)
  }
}

pts1 <- Sys.time() - pts0 # check time elapse
cat("loop without pre-definition takes", pts1, "seconds\n")
```

```
## loop without pre-definition takes 12.266 seconds
```

```r
# pre-define a container
out <- rep(0, Rep)
pts0 <- Sys.time() # check time
for (i in 1:Rep) {
  x <- rpois(sample_size, mu)
  bounds <- CI(x)
  out[i] <- ((bounds$lower <= mu) & (mu <= bounds$upper))
}

pts1 <- Sys.time() - pts0 # check time elapse
cat("loop with pre-definition takes", pts1, "seconds\n")
```

```
## loop with pre-definition takes 4.971001 seconds
```

Pay attention to the line `out = rep(0, Rep)`. It *pre-defines* a vector `out` to be filled by `out[i] = ( ( bounds$lower <= mu  ) & (mu <= bounds$upper) )`. The computer opens a continuous patch of memory for the vector `out`. When new result comes in, the old element is replaced. If we do not pre-define `out` but append one more element in each loop, the length of `out` will change in each replication and every time a new patch of memory will be assigned to store it. The latter approach will spend much more time just to locate the vector in the memory.

`out` is the result container. In a `for` loop, we pre-define a container, and replace the elements of the container in each loop by explicitly calling the index.

In contrast, a `plyr` loop saves the house keeping chores, and makes it easier to parallelize. In the example below, we encapsulate the chunk in the `for` loop as a new function `capture`, and run the replication via `__ply`. `__ply` is a family of functions. `ldply` here means that the input is a list (`l`) and the output is a data frame (`d`) .

```r
library(plyr)

capture <- function(i) {
  x <- rpois(sample_size, mu)
  bounds <- CI(x)
  return((bounds$lower <= mu) & (mu <= bounds$upper))
}

pts0 <- Sys.time() # check time
out <- ldply(.data = 1:Rep, .fun = capture)

pts1 <- Sys.time() - pts0 # check time elapse
cat("plyr loop takes", pts1, "seconds\n")
```

```
## plyr loop takes 5.391003 seconds
```

This example is so simple that the advantage of `plyr` is not dramatic. The difference in coding will be noticeable in complex problems with big data frames. In terms of speed, `plyr` does not run much faster than a `for` loop. They are of similar performance. Parallel computing will be our next topic. It is quite easy to implement parallel execution with `plyr`—we just need to change one argument in the function.

Parallel Computing

Parallel computing becomes essential when the data size is beyond the storage of a single computer, for example Li et al. (2018). Here we explore the speed gain of parallel computing on a multicore machine.

Here we introduce how to cooridate multiple cores on a single computer. The packages `foreach` and `doParallel` are useful for parallel computing. Below is the basic structure. `registerDoParallel(number)` prepares a few CPU cores to accept incoming jobs.

```r
library(plyr); library(foreach); library(doParallel)

registerDoParallel(a_number) # opens specified number of CPUs

out <- foreach(icount(Rep), .combine = option) %dopar% {
  my_expressions
}
```

If we have two CPUs running simultaneously, in theory we can cut the time to a half of that on a single CPU. Is that what happening in practice?

Example

Compare the speed of a parallel loop and a single-core sequential loop.

```r
library(foreach)
library(doParallel)

registerDoParallel(2) # open 2 CPUs

pts0 <- Sys.time() # check time

out <- foreach(1:Rep, .combine = c) %dopar% {
  capture(i)
}

pts1 <- Sys.time() - pts0 # check time elapse
cat("parallel loop takes", pts1, "seconds\n")
```

```
## parallel loop takes 28.02403 seconds
```

Surprisingly, the above code block of parallel computing runs even more slowly. It is because the task in each loop can be done in very short time. In contrast, the code chunk below will tell a different story. There the time in each loop is non-trivial, and then parallelism dominates the overhead of the CPU communication. The only difference between the two implementations below is that the first uses `%dopar%` and the latter uses `%do%`.

```r
Rep <- 200
sample_size <- 2000000

registerDoParallel(8) # change the number of open CPUs according to
# the specification of your computer

pts0 <- Sys.time() # check time
out <- foreach(icount(Rep), .combine = c) %dopar% {
  capture()
}

cat("8-core parallel loop takes", Sys.time() - pts0 , "seconds\n")
```

```
## 8-core parallel loop takes 2.463002 seconds
```

```r
pts0 <- Sys.time()
out <- foreach(icount(Rep), .combine = c) %do% {
  capture()
}

cat("single-core loop takes", Sys.time() - pts0 , "seconds\n")
```

```
## single-core loop takes 15.79703 seconds
```

Remote Computing

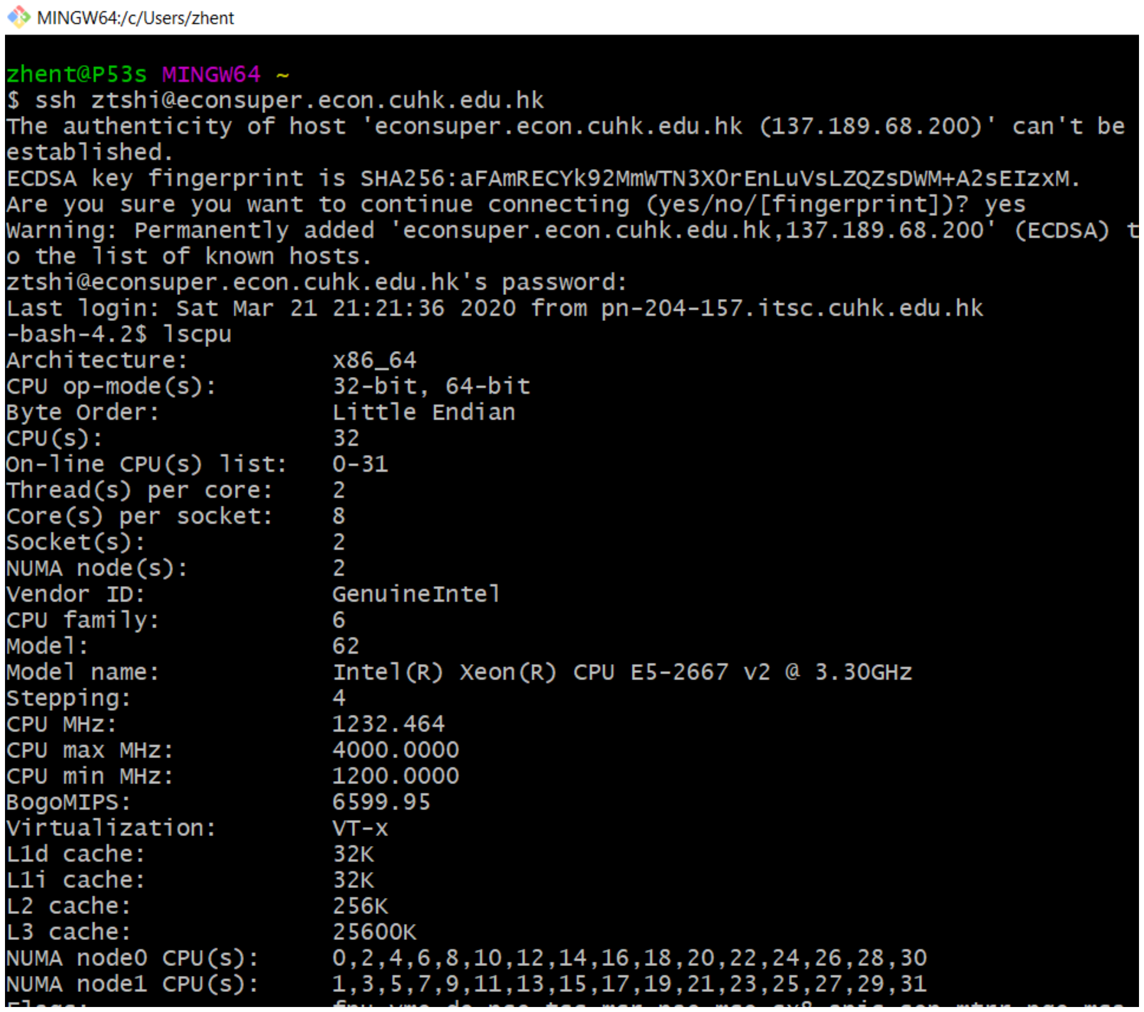
Investing money from our own pocket to an extremely powerful laptop to conduct heavy-lifting computational work is unnecessary. (i) We do not run these long jobs every day, it is more cost efficient to share a workhorse. (ii) We cannot keep our laptop always on when we move it around. The right solution is remote computing on a server.

No fundamental difference lies between local and remote computing. We prepare the data and code, open a shell for communication, run the code, and collect the results. One potential obstacle is dealing with a command-line-based operation system. Such command line tools is the norm of life two or three decades ago, but today we mostly work in a graphic operating system like Windows or OSX. For Windows users (I am one of them), I recommend `Git Bash` as a shell, and `WinSCP`, a graphic interface for input and output.

Most servers run Unix/Linux operation system. Here are a few commands for basic operations.

- `mkdir`: make directory
- `cd`: change directory
- `copy`: copy files
- `top`: check login status
- `screen`: a separated screen for isolation
- `ssh`: user@address
- start a program

Our department's computation infrastructure has been improving. A server dedicated to professors is a 32-core machine. Students also have access to a powerful multi-core computer.



MINGW64:/c/Users/zhent

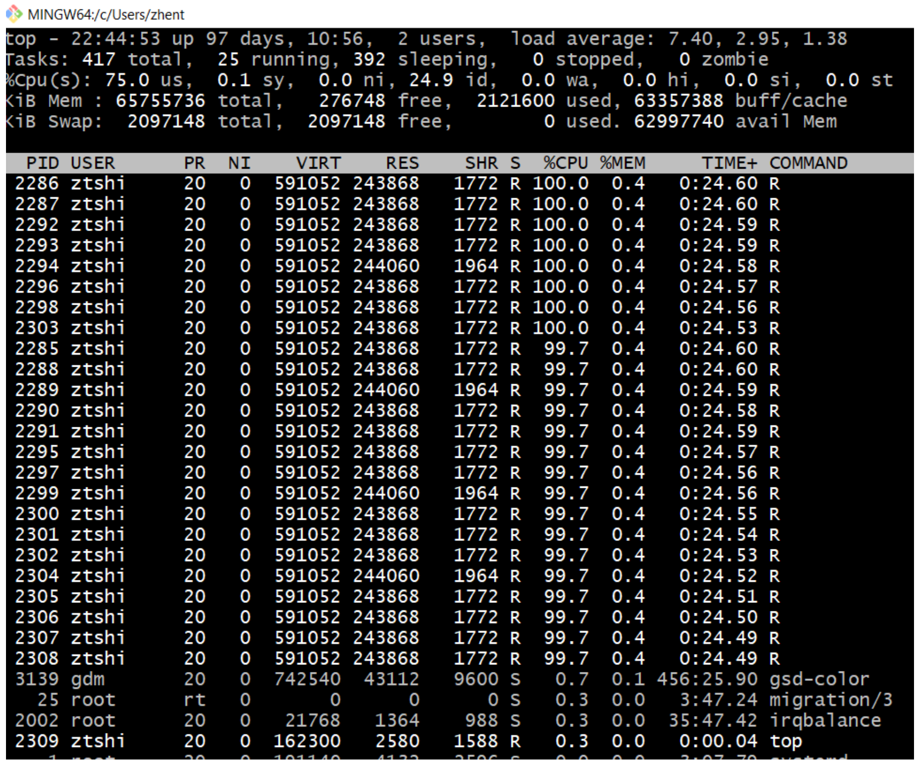
```
zhent@P53s MINGW64 ~
$ ssh ztshi@econsuper.econ.cuhk.edu.hk
The authenticity of host 'econsuper.econ.cuhk.edu.hk (137.189.68.200)' can't be
established.
ECDSA key fingerprint is SHA256:aFAmRECYk92MmWTN3XOrEnLuVsLZQZsDWM+A2sEIzxM.
Are you sure you want to continue connecting (yes/no/[fingerprint])? yes
Warning: Permanently added 'econsuper.econ.cuhk.edu.hk,137.189.68.200' (ECDSA) t
o the list of known hosts.
ztshi@econsuper.econ.cuhk.edu.hk's password:
Last login: Sat Mar 21 21:21:36 2020 from pn-204-157.itsc.cuhk.edu.hk
-bash-4.2$ lscpu
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Byte Order:            Little Endian
CPU(s):                32
On-line CPU(s) list:   0-31
Thread(s) per core:    2
Core(s) per socket:    8
Socket(s):             2
NUMA node(s):          2
Vendor ID:             GenuineIntel
CPU family:            6
Model:                 62
Model name:            Intel(R) Xeon(R) CPU E5-2667 v2 @ 3.30GHz
Stepping:              4
CPU MHz:               1232.464
CPU max MHz:           4000.0000
CPU min MHz:           1200.0000
BogoMIPS:              6599.95
Virtualization:        VT-x
L1d cache:             32K
L1i cache:             32K
L2 cache:              256K
L3 cache:              25600K
NUMA node0 CPU(s):     0,2,4,6,8,10,12,14,16,18,20,22,24,26,28,30
NUMA node1 CPU(s):     1,3,5,7,9,11,13,15,17,19,21,23,25,27,29,31
```

Figure 1: Log into `econsuper` and check CPU with `lscpu`

1. Log in `econsuper.econ.cuhk.edu.hk`;
2. Upload R scripts and data to the server;
3. In a shell, run `R --vanilla <file_name.R> result_file_name.out`;
4. To run a command in the background, add `&` at the end of the above command.

This example comes from Lin et al. (2020). As a demonstration, we only use 15% of the data and a sparse grid of tuning parameters. It makes about 9 minutes with 24 cores.

```
ssh ztshi@econsuper.econ.cuhk.edu.hk
cd data_example
R --vanilla <Beijing_housing_gbm.R> GBM_BJ.out &
```



```
top - 22:44:53 up 97 days, 10:56,  2 users,  load average: 7.40, 2.95, 1.38
Tasks: 417 total,  25 running, 392 sleeping,   0 stopped,   0 zombie
%Cpu(s): 75.0 us,  0.1 sy,  0.0 ni, 24.9 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
KiB Mem : 65755736 total,   276748 free,  2121600 used, 63357388 buff/cache
KiB Swap:  2097148 total,  2097148 free,        0 used. 62997740 avail Mem

  PID USER      PR  NI    VIRT    RES    SHR S  %CPU %MEM     TIME+ COMMAND
 2286 ztshi     20   0  591052 243868   1772 R 100.0  0.4   0:24.60 R
 2287 ztshi     20   0  591052 243868   1772 R 100.0  0.4   0:24.60 R
 2292 ztshi     20   0  591052 243868   1772 R 100.0  0.4   0:24.59 R
 2293 ztshi     20   0  591052 243868   1772 R 100.0  0.4   0:24.59 R
 2294 ztshi     20   0  591052 244060   1964 R 100.0  0.4   0:24.58 R
 2296 ztshi     20   0  591052 243868   1772 R 100.0  0.4   0:24.57 R
 2298 ztshi     20   0  591052 243868   1772 R 100.0  0.4   0:24.56 R
 2303 ztshi     20   0  591052 243868   1772 R 100.0  0.4   0:24.53 R
 2285 ztshi     20   0  591052 243868   1772 R  99.7  0.4   0:24.60 R
 2288 ztshi     20   0  591052 243868   1772 R  99.7  0.4   0:24.60 R
 2289 ztshi     20   0  591052 244060   1964 R  99.7  0.4   0:24.59 R
 2290 ztshi     20   0  591052 243868   1772 R  99.7  0.4   0:24.58 R
 2291 ztshi     20   0  591052 243868   1772 R  99.7  0.4   0:24.59 R
 2295 ztshi     20   0  591052 243868   1772 R  99.7  0.4   0:24.57 R
 2297 ztshi     20   0  591052 243868   1772 R  99.7  0.4   0:24.56 R
 2299 ztshi     20   0  591052 244060   1964 R  99.7  0.4   0:24.56 R
 2300 ztshi     20   0  591052 243868   1772 R  99.7  0.4   0:24.55 R
 2301 ztshi     20   0  591052 243868   1772 R  99.7  0.4   0:24.54 R
 2302 ztshi     20   0  591052 243868   1772 R  99.7  0.4   0:24.53 R
 2304 ztshi     20   0  591052 244060   1964 R  99.7  0.4   0:24.52 R
 2305 ztshi     20   0  591052 243868   1772 R  99.7  0.4   0:24.51 R
 2306 ztshi     20   0  591052 243868   1772 R  99.7  0.4   0:24.50 R
 2307 ztshi     20   0  591052 243868   1772 R  99.7  0.4   0:24.49 R
 2308 ztshi     20   0  591052 243868   1772 R  99.7  0.4   0:24.49 R
 3139 gdm       20   0  742540  43112   9600 S   0.7  0.1 456:25.90 gsd-color
   25 root      rt   0       0      0      0 S   0.3  0.0   3:47.24 migration/3
 2002 root      20   0   21768   1364    988 S   0.3  0.0  35:47.42 irqbalance
 2309 ztshi     20   0  162300   2580   1588 R   0.3  0.0   0:00.04 top
```

Figure 2: Running 24 cores on ‘econsuper‘

Graphics

An English cliche says “One picture is worth ten thousand words”. John Tukey, a renowned mathematical statistician, was one of the pioneers of statistical graphs in the computer era. Nowadays, powerful software is able to produce dazzling statistical graphs, sometimes web-based and interactive. Outside of academia, journalism hooks a wide readership with professional data-based graphs. New York Times and The Economists are first-rate examples; South China Morning Post sometimes also does a respectable job. A well designed statistical graph can deliver an intuitive and powerful message. I consider graph prior to table when writing a research report or an academic paper. Graph is lively and engaging. Table is tedious and boring.

We have seen an example of R graph in the OLS regression linear example in Lecture 1. `plot` is a generic command for graphs, and is the default R graphic engine. It is capable of producing preliminary statistical graphs.

Over the years, developers all over the world have had many proposals for more sophisticated statistical graphs. Hadley Wickham’s `ggplot2` is among the most successful.

`ggplot2` is an advanced graphic system that generates high-quality statistical graphs. It is not possible to cover it in a lecture. Fortunately, the author wrote a comprehensive reference **ggplot2**

book, which can be downloaded via the CUHK campus network (VPN needed).

`ggplot2` accommodates data frames of a particular format. `reshape2` is a package that helps prepare the data frames for `ggplot2`.

The workflow of ggplot is to add the elements in a graph one by one, and then print out the graph all together. In contrast, `plot` draws the main graph at first, and then adds the supplementary elements later.

`ggplot2` is particularly good at drawing multiple graphs, either of the same pattern or of different patterns. Multiple subgraphs convey rich information and easy comparison.

Example

Plot the density of two estimators under three different data generating processes. This is an example to generate subgraphs of the same pattern.

```
load("data_example/big150.Rdata")
library(ggplot2)
library(reshape2)

big150_1 <- big150[, c("typb", "b1", "b1_c")]
print(head(big150_1))
```

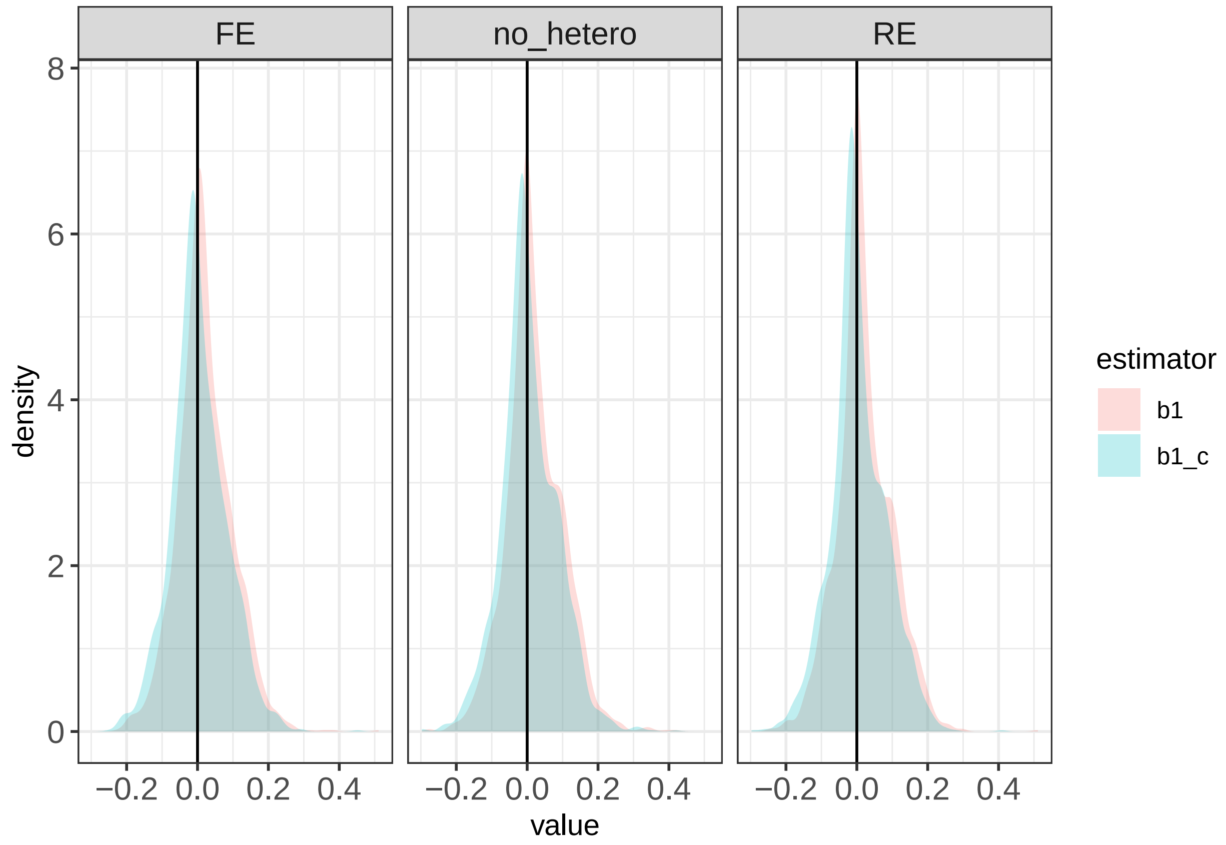
```
##       typb           b1        b1_c
## 12001   FE  0.124616242  0.11690387
## 12002   FE  0.267670157  0.25202802
## 12003   FE -0.030689329 -0.03976746
## 12004   FE  0.121169923  0.11866138
## 12005   FE  0.008300031 -0.02399673
## 12006   FE -0.026199118 -0.05231120
```

```
big150_1 <- melt(big150_1, id.vars = "typb", measure.vars = c("b1", "b1_c"))
names(big150_1)[2] <- c("estimator")
print(head(big150_1))
```

```
##   typb estimator        value
## 1   FE        b1  0.124616242
## 2   FE        b1  0.267670157
## 3   FE        b1 -0.030689329
## 4   FE        b1  0.121169923
## 5   FE        b1  0.008300031
## 6   FE        b1 -0.026199118
```

```
p1 <- ggplot(big150_1)
p1 <- p1 + geom_area(
  stat = "density", alpha = .25,
  aes(x = value, fill = estimator), position = "identity"
)
p1 <- p1 + facet_grid(. ~ typb)
p1 <- p1 + geom_vline(xintercept = 0)
p1 <- p1 + theme_bw()
```

```
p1 <- p1 + theme(
  strip.text = element_text(size = 12),
  axis.text = element_text(size = 12)
)
print(p1)
```



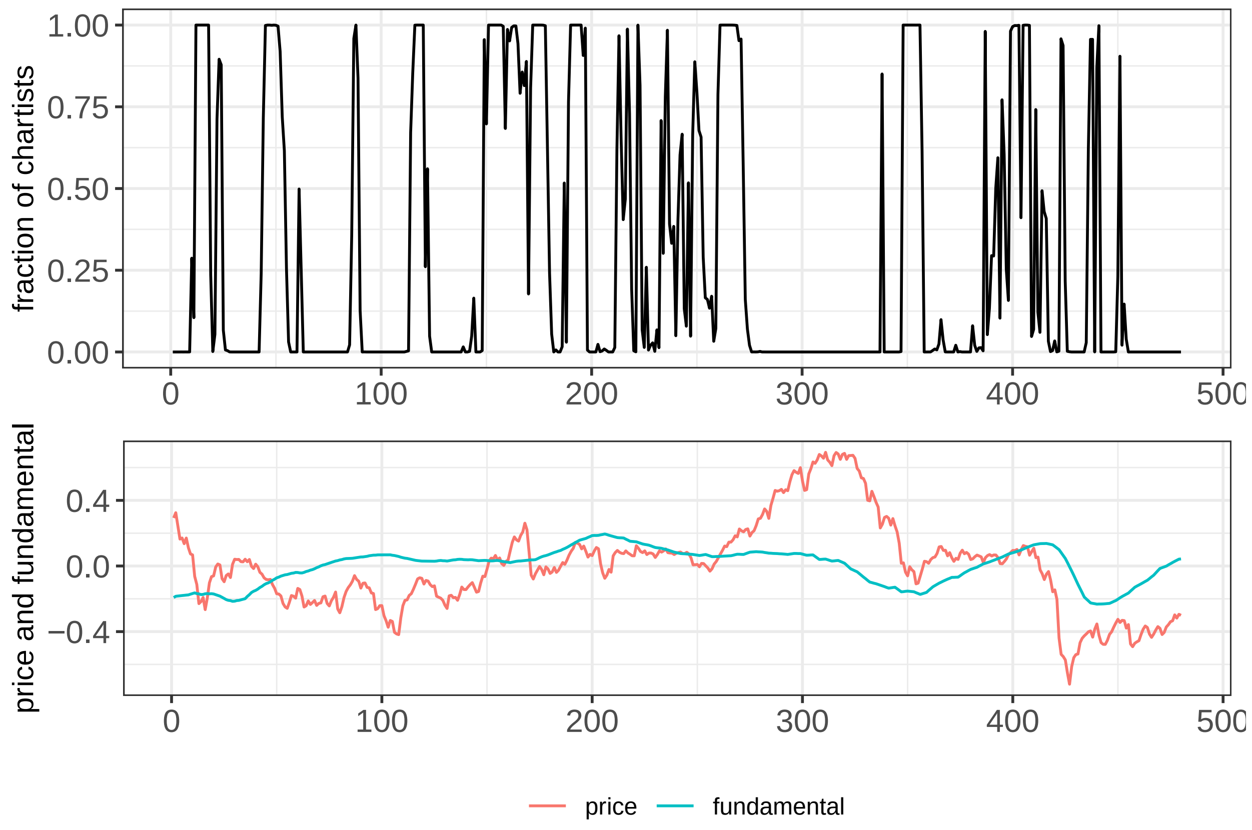
The function `ggplot` specifies which dataset to use for the graph. `geom_***` determines the shape to draw, for example scatter dots, lines, curves or areas. `theme` is to tune the supplementary elements like the background, the size and font of the axis text and so on.

Example

This example aligns two graphs of different patterns in one page.

```
# graph packages
library(lattice)
library(ggplot2)
library(reshape2)
library(gridExtra)

load("data_example/multigraph.Rdata") # load data


# unify the theme in the two graphs
theme1 <- theme_bw() + theme(
```

```r
  axis.title.x = element_blank(),
  strip.text = element_text(size = 12),
  axis.text = element_text(size = 12),
  legend.position = "bottom", legend.title = element_blank()
)

# sub-graph 1
d1 <- data.frame(month = 1:480, m = m_vec)
p1 <- qplot(x = month, y = m, data = d1, geom = "line")
p1 <- p1 + theme1 + ylab("fraction of chartists")


# sug-graph 2
d2$month <- 1:480
p2 <- ggplot(d2)
p2 <- p2 + geom_line(aes(x = month, y = value, col = variable))
p2 <- p2 + theme1 + ylab("price and fundamental")

# generate the grahp
grid.arrange(p1, p2, nrow = 2)
```



In order to unify the theme of the two distinctive subgraphs, we define an object `theme1` and apply it in both graphic objects `p1` and `p2`.

Reading

Wickham and Grolemund: Ch 3, 10, 11, 21, and 26-30

References

Li, Quefeng, Guang Cheng, Jianqing Fan, and Yuyan Wang. 2018. "Embracing the Blessing of Dimensionality in Factor Models." *Journal of the American Statistical Association* 113 (521): 380–89.

Lin, Wei, Zhentao Shi, Yishu Wang, and Ting Hin Yan. 2020. "Unfolding Beijing in a Hedonic Way." The Chinese University of Hong Kong. https://www.researchgate.net/publication/339551353_Unfolding_Beijing_in_a_Hedonic_Way.

Wickham, Hadley, and Garrett Grolemund. 2016. *R for Data Science: Import, Tidy, Transform, Visualize, and Model Data*. O'Reilly Media, Inc.