

Writing better, faster code in R

Julia Wrobel

Overview

Today, we cover:

- Resampling methods
 - Permutation tests
- Improving code speed:
 - Benchmarking
 - Vectorization
 - Parallelization

Announcements:

- HW1 grades are up
- HW2 posted and due 2/11 at 10:00AM
- No class tomorrow (Thursday, January 29) but still have Office Hours

Permutation tests

Typically bootstrap is used for CI rather than hypothesis testing. For hypothesis testing and p-values, we can use a **permutation test**.

- Idea: use resampling to generate a **null distribution** for a test statistic, then compare it to the one you observe in the real data
- **Null distribution**: the distribution of a quantity of interest (i.e. $\hat{\beta}$) if the null hypothesis H_0 is true
- The null distribution is available theoretically in some cases. For example, assume $Y_i \sim N(\mu, \sigma^2), i = 1, \dots, n$.
 - Under $H_0 : \mu = 0$, we have $\bar{Y} \sim N(0, \sigma^2/n)$
 - Test H_0 by comparing \bar{Y} with $N(0, \sigma^2/n)$
- Use **permutation test** when null distribution cannot be obtained theoretically

Permutation tests

The basic procedure of permutation test for H_0 :

- Permute data under H_0 B times. Each time recompute the test statistics. The test statistics obtained from the permuted data form the null distribution.
- Compare the observed test statistics with the null distribution to obtain statistical significance.

Permutation test example: difference in means

Assume there are two sets of independent normal r.v.'s with the same known variance and different means:

- $X_i \sim N(\mu_1, \sigma^2)$
- $Y_i \sim N(\mu_2, \sigma^2)$

Our goal is to test $H_0 : \mu_1 = \mu_2$. Define test statistic: $t = \bar{X} - \bar{Y}$. Permutation test steps:

1. Randomly shuffle labels of X and Y
2. Compute $t^* = \bar{X}^* - \bar{Y}^*$
3. Repeat n_{perm} times. Resulting t^* values form the **empirical null distribution** of t .
4. To compute p-values calculate $Pr(|t^*| > |t|)$

Permutation test example: difference in means

```
set.seed(111)
x = rnorm(30, 2, 2)
y = rnorm(30, 0.5, 1.5)
mean_diff = mean(x) - mean(y)

nperm = 10000
perm_mean_diff = rep(NA, nperm)
for(perm in 1:nperm){
  combined_data = c(x, y)
  x_index = sample(1:length(combined_data), size = length(x), replace = FALSE)
  x_perm = combined_data[x_index]
  y_perm = combined_data[-x_index]

  perm_mean_diff[perm] = mean(x_perm) - mean(y_perm)
}

p = sum(abs(perm_mean_diff) >= abs(mean_diff))/nperm
p
```

```
[1] 0.0437
```

Permutation test example: regression coefficient

$$Y_i = \beta_0 + \beta_{treatment} X_{i1} + \mathbf{Z}_i^T \gamma + \epsilon_i$$

- Our goal is to test $H_0 : \beta_{treatment} = 0$ and we observe $\hat{\beta}_{treatment} = 1.2$.

How will we perform the permutations?

Permutation test example: classification accuracy

We used a random forest model to build a binary classifier for disease detection and achieved accuracy of 78%.

- Goal is to test if this is significantly different than random guessing (50%)

How will we perform the permutations?

Choosing the number of permutations

- Monte Carlo error: If the true p-value is p , then

$$\hat{p} \sim \text{Binomial}(nperm, p)/nperm$$

and

$$SE(\hat{p}) = \sqrt{\frac{p(1-p)}{nperm}}$$

Choosing the number of permutations

```
p_true = 0.05  
nperm = c(10, 100, 10000)  
  
# standard error  
sqrt(p_true*(1-p_true)/nperm)
```

```
[1] 0.068920244 0.021794495 0.002179449
```

Lab: resampling methods

We will spend the next 20-30 minutes going through this lab.

Improving speed

Two ways to find bottlenecks in code:

- Benchmarking
- Profiling

Comparing R code for speed

- R package `microbenchmark` is well-suited for comparing small chunks of code
- Your code can often be significantly improved

```
library(microbenchmark)
x <- 120
microbenchmark(
  sqrt(x),
  x^(0.5)
)
```

Unit: nanoseconds

	expr	min	lq	mean	median	uq	max	neval
	<code>sqrt(x)</code>	0	0	8.61	0.0	0	615	100
	<code>x^(0.5)</code>	41	41	132.84	61.5	82	7093	100

Comparing R code for speed

```
p <- 1000
x <- runif(p, min = 100, max = 120)
microbenchmark(
  sqrt(x),
  x^(0.5)
)
```

Unit: nanoseconds

expr	min	lq	mean	median	uq	max	neval
sqrt(x)	861	902	1373.09	984	1701.5	8528	100
x^(0.5)	8364	8446	8924.47	8569	9389.0	12956	100

Comparing R code for speed

```
p <- 100000
x <- runif(p, min = 100, max = 120)
microbenchmark(
  sqrt(x),
  x^(0.5)
)
```

Unit: microseconds

expr	min	lq	mean	median	uq	max	neval
sqrt(x)	89.339	126.1570	131.4530	130.0110	136.3455	173.635	100
x^(0.5)	838.696	876.8055	952.6649	885.2925	920.7985	2917.396	100

Comparing R code for speed

- Take advantage of **crossprod** and **tcrossprod** functions. Suppose we want to calculate $x^T A x$

```
p <- 3000
x <- rnorm(p)
A <- matrix(rnorm(p^2), p, p)
microbenchmark(
  t(x) %*% A %*% x,
  crossprod(x, A %*% x)
)
```

Unit: milliseconds

	expr	min	lq	mean	median	uq	max
	t(x) %*% A %*% x	2.965571	3.023402	3.153676	3.133999	3.217926	4.069045
	crossprod(x, A %*% x)	6.250163	6.336960	6.417527	6.423039	6.486692	6.661475
neval							
100							

Example: R Loops

R is very bad at resizing objects since it copies to resize

- Do not grow an object inside of a loop!
- Instead, make an empty object first and then fill elements.

```
bad = function (x){  
  obj = c()  
  for(i in 1:x){  
    obj = c(obj, i)  
  }  
  return(obj)  
}
```

```
better = function (x){  
  obj = rep(NA, x)  
  for (i in 1:x){  
    obj[i] = i  
  }  
  return(obj)  
}
```

Example: R Loops

```
microbenchmark(bad (100), better (100))
```

Unit: microseconds

expr	min	lq	mean	median	uq	max	neval
bad(100)	15.252	16.113	27.34864	16.523	17.220	1046.484	100
better(100)	2.419	2.501	14.42626	2.542	2.624	1184.367	100

Measuring speed in simulations

If you are interested in measuring computation time in a simulation study, say, to compare how fast different methods are, I **would not** recommend `microbenchmark`. Instead, do the following:

```
library(tictoc)

tic()
## do some stuff
large_vector <- rnorm(1e7) # Create a vector of 10 million random numbers
sum_large_vector <- sum(large_vector)
time_stamp = toc(quiet = TRUE) # stop the timer and print the time elapsed

time_stamp$toc - time_stamp$tic # human time in seconds
```

```
elapsed
0.249
```

Vectorization

R is **vectorized**, meaning it efficiently performs operations on entire vectors or arrays in a single step, avoiding explicit loops and leveraging optimized low-level code for speed and simplicity.

- Often, there is more than one way to do something in R
- Take advantage of vectorization!
 - Often it is more concise and significantly faster

Vectorization

```
# non vectorized squaring operation
x <- c(1, 2, 3, 4, 5)
result <- numeric(length(x))
for (i in seq_along(x)) {
  result[i] <- x[i]^2
}
```

```
# same operation, vectorized
x <- c(1, 2, 3, 4, 5)
result <- x^2
```

Why vectorization?

Another example- which is the vectorized version?

```
x <- matrix(rnorm(30), 10, 3)
```

```
colMeans(x)
```

```
[1] -0.0324887 -0.2387936 -0.2873906
```

```
apply(x, 2, mean)
```

```
[1] -0.0324887 -0.2387936 -0.2873906
```

Why vectorization?

- **colSums**, **colMeans** and corresponding row functions are vectorized

```
n <- 100
p <- 3000
A <- matrix(rnorm(n * p), n, p)
microbenchmark(
  colMeans(A),
  apply(A, 2, mean)
)
```

Unit: microseconds

	expr	min	lq	mean	median	uq	max
	colMeans(A)	98.933	99.466	102.1909	100.368	103.4635	118.326
	apply(A, 2, mean)	6696.038	6925.597	7878.1475	7023.771	7148.2885	14615.557
	neval						23
	100						

Parallel computing

A modern CPU (Central Processing Unit) is at the heart of every computer. While traditional computers had a single CPU, modern computers can ship with multiple processors, which in turn can each contain multiple cores. These processors and cores are available to perform computations.

- A computer with one processor may still have 4 cores (quad-core), allowing 4 computations to be executed at the same time.
- **Parallel computing** is the simultaneous use of multiple processors or computers to solve a problem by dividing it into smaller, independent tasks, i.e. operating **in parallel**.

Parallel computing

You can check how many **cores** your computer has to see how many tasks can be run at once.

```
# Load the parallel package
library(parallel)

# Get the number of cores
detectCores()

# 12
```

When to parallelize

- Using 2 cores does not mean your code will be $2\times$ faster
- Not all tasks can be parallelized
- Loops and repetitive tasks are great candidates
 - What are some computations we have looked at already that might be good candidates for parallelization?

Example : foreach and doParallel

```
library(doParallel)
library(foreach)

# Set up parallel backend with 10 cores
num_cores = detectCores() - 2
cl = makeCluster(num_cores)
registerDoParallel(cl)

# define Monte Carlo function to estimate Pi
monte_carlo_pi <- function(n) {
  inside_circle <- sum(runif(n, -1, 1)^2 + runif(n, -1, 1)^2 <= 1)
  return((inside_circle / n) * 4)
}

nsim = 100
```

Example : foreach and doParallel

```
pi_estimates = foreach(i = 1:nsim, .combine = c) %dopar% {  
  n = 1000  
  monte_carlo_pi(n)  
}
```

```
# overall estimate of pi  
mean(pi_estimates)
```

Example : foreach and doParallel

Useful arguments include multiple iterators, error catching, combine

```
foreach(  
  ...,  
  .combine,  
  .init,  
  .final = NULL,  
  .inorder = TRUE,  
  .multicombine = FALSE,  
  .maxcombine = if (.multicombine) 100 else 2,  
  .errorhandling = c("stop", "remove", "pass"),  
  .packages = NULL,  
  .export = NULL,  
  .noexport = NULL,  
  .verbose = FALSE  
)
```

Resources

- Advanced R: chapters 22-24
- foreach vignette
- furrr package for tidyverse parallelization

Profiling your code

Some good references on profiling to learn more (a lot of overlap):

- Advanced R
- profvis R package
- Rstudio guide
- proftools R package

There has been some changes on how profiling works from R v.3 to v.4 which (sometimes) makes profiler output confusing

Profiling in R

- `profvis` is built on R's built-in profiler tool, `Rprof`
- `Rprof` is a statistical profiler that uses sampling
- When you run `profvis`, it stops the R interpreter every 10ms (default interval) and records which function is currently executing, as well as the entire call stack (i.e., which function called that function)
 - The results are not deterministic

Profiling in R

From R programming for Data Science

“Rprof() keeps track of the function call stack at regularly sampled intervals and tabulates how much time is spent inside each function. By default, the profiler samples the function call stack every 0.02 seconds. This means that if your code runs very quickly (say, under 0.02 seconds), the profiler is not useful. But if your code runs that fast, you probably don't need the profiler.”

Profiling: return to Ex. 2 (powers of a matrix)

Rprof() function gives a report of (approximately) how much time each function/operation within your code takes. To see the effect of memory allocation, enable tracking of **garbage collection** (GC)

```
Rprof(gc.profiling = TRUE) # start monitoring  
invisible(powers1(x, 8)) # suppress function output  
Rprof(NULL) # stop monitoring  
summaryRprof() # see the report
```

Rprof()

- **by.total** divides the time spend in each function by the total run time
- **by.self** first subtracts out time spent in functions above the current function in the call stack (**more useful typically**)

Garbage collection (GC)

Garbage collection - freeing the memory from objects that are no longer in use (more in Section 2.6 of Advanced R)

If significant time of your program is spend in GC

- you may be doing a lot of dynamic memory allocation (the case of powers1)
- you may be storing a lot of temporary objects
- you may be consistently changing objects of large sizes

Profiling: return to Ex. 3 (powers of a matrix)

```
powers3 <- function(x, dg){  
  # allocate memory in advance  
  pw <- matrix(x, length(x), dg)  
  prod <- x # current product  
  for (i in 2:dg){  
    prod <- prod * x  
    pw[ , i] <- prod # no cbind  
  }  
  return(pw)  
}
```