6. High-throughput Work, and Writing Loops

Ken Rice
Thomas Lumley

Universities of Washington and Auckland

Seattle, June 2011

Writing loops in R

We saw that `apply()`, `sapply()` are R's preferred way of **looping** (doing the same thing many times)

Even for expert useRs, their use requires some careful thought; debugging code may be complex.

In this session we'll talk about some alternatives, and their application to **genome-wide** studies.

`for` loops

Your first computer program?

```
for(i in 1:100){
   print("Hello world!")
   print(i*i)
}
```

- Everything inside the curly brackets {...} is done 100 times
- Looped commands can depend on `i` (or whatever you called the counter)
- R creates a vector `i` with `1:100` in it. You could use **any vector that's convenient**

`for` loops

`for()` loops are very intuitive, but have some drawbacks;

- They can be **slow**;
  - 'growing' the dataset is a Very Bad idea;
    `mydata <- cbind(mydata, rnorm(1000, mean=i))`
  - set up blank output **first**, then 'fill it in'
- `apply()` is interpreted slightly faster than `for()` – but typically this **will not matter**, *contrary to those urban myths*
- `for()` loops require more typing than `apply()`! For tasks which will be repeated, writing a function really is the Right Thing to do, in the long run.

Using `for(i in 1:N)` sets up a vector (`i`) of length `N`. Do you really need this?

`for` loops

Two alternatives; (see `?Control` for details)

```
i <- 1; my.mat <- matrix(NA, N, 3)
while(i <= N){
  z <- work.on.gene(i)
  my.mat[i,] <- summary(z)
  i <- i+1
  }
```

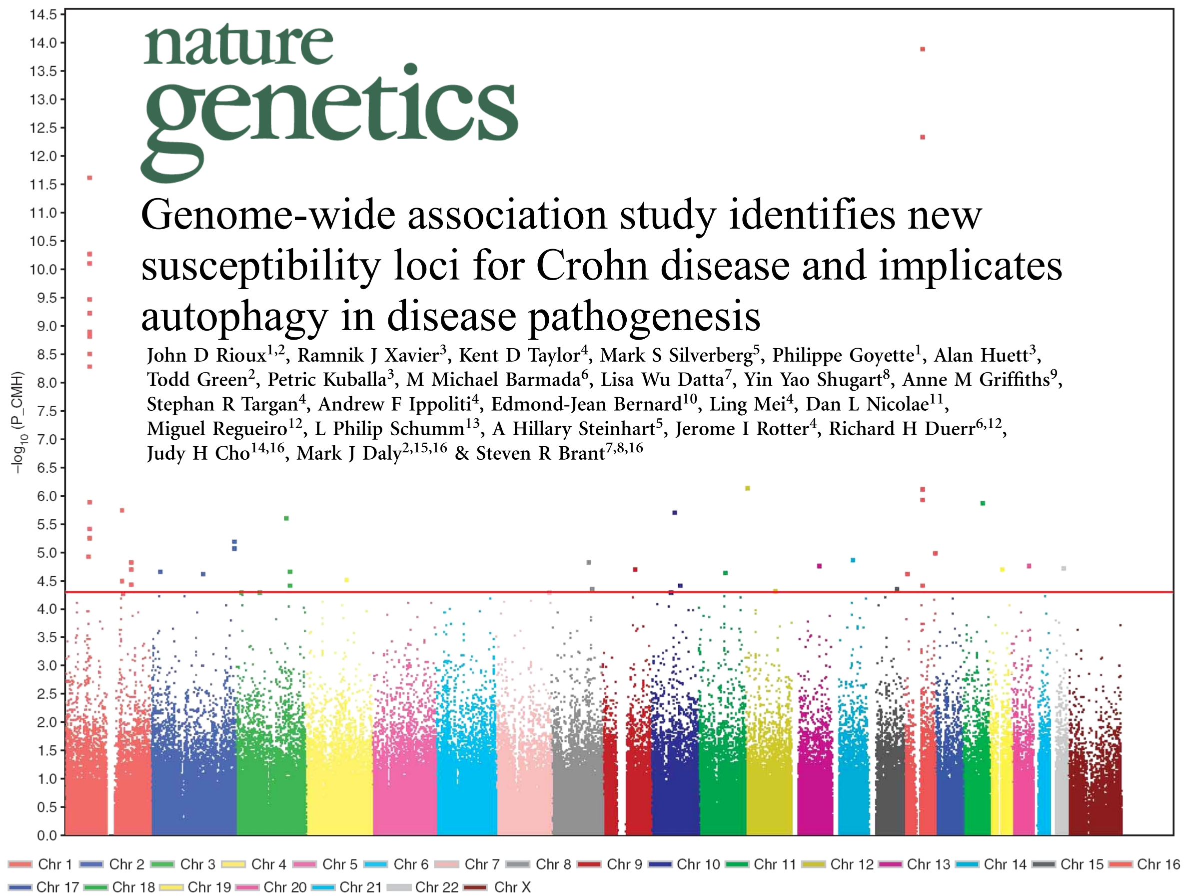
– note that we avoided 'growing' the output

```
i <- 1; my.mat <- matrix(NA, N, 3)
repeat{
  z <- work.on.gene(i)
  my.mat[i,] <- summary(z)
  i <- i+1
  if(i>=N) break()
  }
```

Use `apply()`, `sapply()` to avoid the 'setup' stage

Application to whole-genome study

Whole genome studies look **very intimidating** ...



Application to whole-genome study

... however, each p-value on that picture comes from a **single** logistic regression.

There may be 304,413 tests in total; if each one takes 1/10 sec, the analysis is **done** in under an hour;

Time per test	Total time
0.01 sec	51 mins
0.1 sec	8 hours 27 mins
1 sec	3 days 12.5 hrs
5 sec	17 days 15 hrs (!)
5 mins	3 yrs 11 months (!!!)

Cutting time per test from 1 sec $\rightarrow$ 0.1 sec is **clearly worthwhile**

Proposing analyses where each test takes $>$ 5 secs is **silly**.

Making code run faster, part 1

Some easy 'streamlining' ideas;

- Write a function to do **just the analysis you want**
  `> my.output <- apply(my.data, 1, my.function)`

- Pre-process/'clean' your data before analysis; e.g. `sum(x)/length(x)` doesn't error-check like `mean(x)`

- Similarly, you can streamline `glm` to just `glm.fit` [see examples]

- Use vectorized operations, where possible

- Store data as matrices, not data.frames

Making code run faster, part 2

Streamlining, for 'experts-only'

- Write **small but important** pieces of code in `C`, and call these from `R`

- **Batch mode** processing lets you break down e.g. the whole genome into 23 chromosomes – great if you have 23 processors to use.
  - Save your analysis in 23 output files
  - read in the answers
  - **finally** produce e.g. multi-color pictures

Timing

"Premature optimization is the root of all evil"

Donald Knuth

Do you need to optimize your code? Running 2 or 3 times faster may **not be worth the time spent coding/debugging!**

But going an **order of magnitude** faster is A Good Thing, in any high-throughput setting.

After you have code that works, you may need to speed it up. Experienced useRs may be able to 'eyeball' the problem; measurement is an **easier and more reliable** approach

Timing

- `proc.time()` returns the current time. Save it before a task and subtract from the value after a task.

- `system.time()` times the evaluation of expression

- R has a **profiler**; this records which functions are being run, many times per second. `Rprof(filename)` turns on the profiler, `Rprof(NULL)` turns it off. `summaryRprof(filename)` reports how much time was spent in each function.

Remember that a 1000-fold speedup in a function used 10% of the time is **less helpful** than a 30% speedup in a function used 50% of the time.

High-throughput code – caveats

We saw before that ‘weird’ datasets can crash your code. These **will appear** in genome-wide studies, and a crash at SNP 2,499,999 will be **very frustrating**.

- Some ‘weirdness’ is easy to spot;
  - Everyone is homozygous
  - All cases missing
  - No variation in outcome ...
- In more complex models, it’s easier to ‘try it and see’. Use `tryCatch()` – see Session 5.
- When ‘weirdness’ is found, high-throughput code should;
  - Produce sensible output (`NA`, `-999` etc)
  - Handle these appropriately in summary outputfo