Writing Efficient Programs in R (and Beyond)

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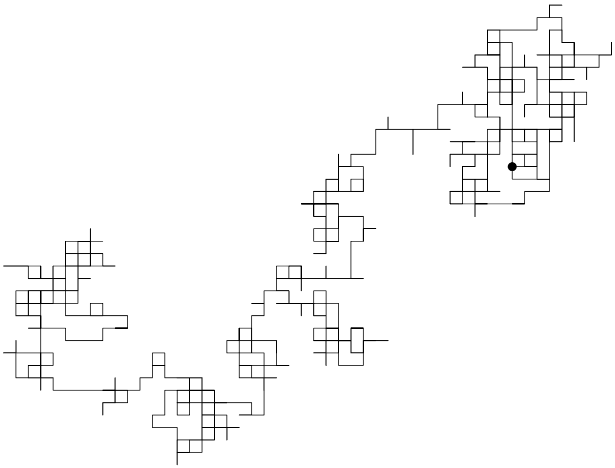

Example: Generating a 2d Simple Random Walk

A two dimensional (discrete) random walk can be defined as follows:

> *Start at the point* $(0, 0)$.
>
> *For* $i = 1, 2, 3, \ldots$ *take a unit step in a randomly chosen direction; N, S, E, W.*

It is possible to theory to study such a random walk, but it is also useful to use simulation to study the properties of random walks.

The `sample` Function

A virtual lotto ticket line.

```
> sample(1:40, 7)
[1] 34 15  3 32  4 39 37
```

Sampling with replacement.

```
> sample(1:40, 7, replace = TRUE)
[1] 13 21 23 39 23  6 38
```

Sample random directions and step sizes.

```
> sample(c(TRUE, FALSE), 1)
[1] TRUE
> sample(c(-1, 1), 1)
[1] -1
```

Version One: Naive Implementation

In this version we'll write the program the way a C, C++ or Java programmer might.

This means running a loop and generating the values one a time.

At the heart of the program we have to choose a direction (x or y) to step in and an step-size (either $+1$ or -1).

These random choices are made using the `sample` function.

Version One: R Code

```
> rw2d1 =
    function(n) {
      xpos = ypos = numeric(n)
      xdir = c(TRUE, FALSE)
      pm1 = c(1, -1)
      for(i in 2:n)
        if (sample(xdir, 1)) {
          xpos[i] = xpos[i-1] + sample(pm1, 1)
          ypos[i] = ypos[i-1]
        }
        else {
          xpos[i] = xpos[i-1]
          ypos[i] = ypos[i-1] + sample(pm1, 1)
        }
      list(x = xpos, y = ypos)
    }
```

Performance

We can time the performance of this algorithm using the `system.time` function.

```
> system.time(rw2d1(100000))
   user  system elapsed
  2.587   0.002   2.591
```

We'll use this figure as a baseline for comparison with other methods we'll develop later.

Version Two: Vectorisation

Rather than computing the position element by element, this version computes the vectors of position changes and then uses `cumsum` to compute the positions.

To compute n positions we need $n - 1$ position changes.

The step sizes can be computed as

```
steps = sample(c(-1, 1), n - 1, replace = TRUE)
```

and whether or not to step in the x direction can be determined as

```
xdir = sample(c(TRUE, FALSE), n - 1,
              replace = TRUE)
```

Version Two: R Code

```
> rw2d2 =
    function(n) {
      steps = sample(c(-1, 1), n - 1,
                     replace = TRUE)
      xdir = sample(c(TRUE, FALSE), n - 1,
                    replace = TRUE)
      xpos = c(0, cumsum(ifelse(xdir, steps, 0)))
      ypos = c(0, cumsum(ifelse(xdir, 0, steps)))
      list(x = xpos, y = ypos)
  }
```

Version Two: R Code

```
> rw2d2 =
    function(n) {
      steps = sample(c(-1, 1), n - 1,
                     replace = TRUE)
      xdir = sample(c(TRUE, FALSE), n - 1,
                    replace = TRUE)
      xpos = c(0, cumsum(ifelse(xdir, steps, 0)))
      ypos = c(0, cumsum(ifelse(xdir, 0, steps)))
      list(x = xpos, y = ypos)
  }
> system.time(rw2d2(100000))
   user  system elapsed
  0.103   0.011   0.114
```

This is 1/23 the elapsed time taken by the baseline version.

Vectorisation clearly makes a huge difference to run times.

Version Three: Heavy Vectorisation

A potential problem with the previous version is the use of the `ifelse` function to deal with the x and y directions separately.

As a final improvement let's deal with the four step directions separately and simply choose one of the four directions at random.

The directions can be chosen via

```
dirs = sample(1:4, n - 1, replace = TRUE)
```

and this can then be used to select the appropriate increments in the x and y directions from precomputed vectors.

Version Three: R Code

```
> rw2d3 =
    function(n) {
      xsteps = c(-1,  1,  0,  0)
      ysteps = c( 0,  0, -1,  1)
      dir = sample(1:4, n - 1, replace = TRUE)
      xpos = c(0, cumsum(xsteps[dir]))
      ypos = c(0, cumsum(ysteps[dir]))
      list(x = xpos, y = ypos)
  }
```

Version Three: R Code

```
> rw2d3 =
    function(n) {
      xsteps = c(-1,  1,  0,  0)
      ysteps = c( 0,  0, -1,  1)
      dir = sample(1:4, n - 1, replace = TRUE)
      xpos = c(0, cumsum(xsteps[dir]))
      ypos = c(0, cumsum(ysteps[dir]))
      list(x = xpos, y = ypos)
  }

> system.time(rw2d3(100000))
   user  system elapsed
  0.011   0.001   0.013
```

This has cut the running time to about 1/9 of the previous version and 1/200 of the baseline version.

Profiling

Profiling is a useful tool which can be used to find out how much time is being spent inside each function when some R code is run.

When profiling is turned on, R gathers information on where the program is at regularly spaced time points (20 millisecond separation by default) and stores the information in a file.

After profiling is turned off the information stored in the file can be analysed to produce a summary of how much time is spent in each function.

It can be quite surprising to find out just where R is spending its time and this can help to find ways to make programs run faster.

Profiling Example

The following code will enable use to find out where R is spending its time when running the `rw2d2` function.

Because the process is statistical we'll run the function a number of times to ensure that enough data is being gathered.

```
> Rprof()
> for(i in 1:100)
      pos = rw2d2(100000)
> Rprof(NULL)
```

Profiling Analysis

```
> prof = summaryRprof()
> prof$by.self[1:5,]
         self.time self.pct total.time total.pct
"ifelse"      5.08     52.2       7.94      81.5
"&"           1.30     13.3       1.30      13.3
"sample"      1.10     11.3       1.10      11.3
"!"           1.08     11.1       1.08      11.1
"cumsum"      0.34      3.5       0.34       3.5
```

81.5% of the time is being spent in the `ifelse` function (and calls made to other R functions from inside the `ifelse` function).

This explains why removing the `ifelse` calls has such a big effect.

Lessons

- Producing efficient programs in R requires thought and experimentation.
- In general, vectorisation is a big win and converting loops into vectorised alternatives almost always pays off.
- Code profiling can give a way to locate those parts of a program which will benefit most from optimisation.
- Unfortunately, it is not always possible to produce efficient programs using vectorisation.

Directions for New Research

- There are new high-level languages which which produce very efficient code by using careful code analysis and transformation.
  - SaC — Single assignment C (University of Kiel)
  - CT — C for Throughput Computing (Intel)
- These languages are not interactive.
- Whether it is possible to bring the techniques used by these languages to an interactive languages is an open question.

- The other alternative is to try to make naively written programs run fast.
- How to do this in an interactive language is an open question.

A Quick Progress Report

- We believe that it is possible to make naively specified programs in a language not unlike R run much faster than R (up to 600 times faster for some problems).

- Integrating this with method-dispatch in object-oriented languages is tricky, but looks possible.

- This is not going to be enough to take advantage of the potential offered by the parallel processing architectures now becoming available.

- To harness that potential, the techniques used in languages like Sac and CT must be used.

- It is not clear whether this is possible in interactive languages.