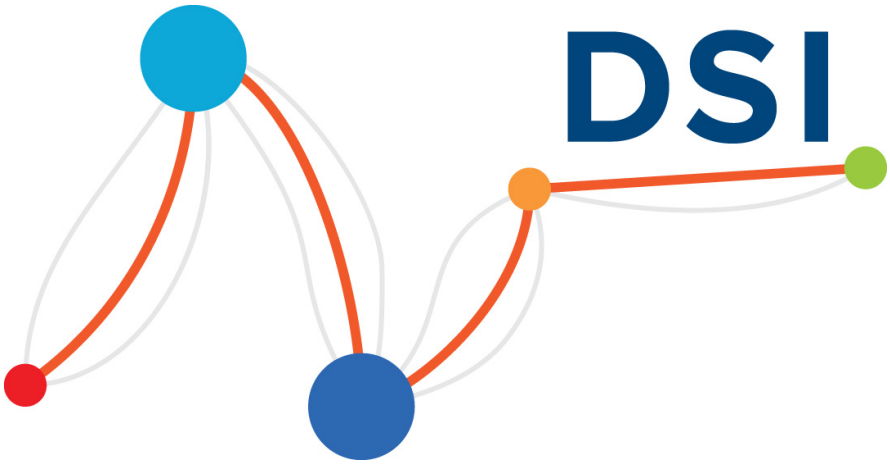


Efficiency in R

Duncan Temple Lang

Code, etc @ https://github.com/dsidavis/EfficientR

Approaches

- Find faster machine with more memory!
- Avoid unnecessary computations in functions (e.g. colClasses, adding names)
- Find function(s) in existing packages (and hope faster)
- Byte-compile the code.
- Profiling: Time code & parts of code
  - Improve the bottlenecks
- Embarrassingly parallel code
  - use parallel package & others
- Use C code, but only for the slow parts.
  - .Call(), .C(), or Rcpp
- Different data structures and algorithm/computational approach.

Find Faster Machine

- Really - this is the first thing to do
- A laptop with 16Gb of memory won't perform as fast as a compute server with 256Gb
  - You may have to share it with others which may make it less fast.
- If you can access such a machine, then run the code on it and see if it is sufficiently fast.
- Request time on research computers on campus or NSF (XCEDE), NIH, UCSD super computer, …
- Purchase time on Amazon, Azure, Google

- How much does it matter ? and to who?
- Will you or other people be running this code many times ?
- How much speedup do you need?
- Do some basic timings for different sizes of the inputs.
  - Plot the results for and see is the algorithmic complexity linear, quadratic, worse!
  - This may give you a hint as to whether you need a different approach.
  - Use system.time() or microbenchmark()

- Remove objects in your work space when you no longer need them.
  - Frees memory
  - save()/saveRDS() them to disk and reload them latter.
- Avoid computing the same thing multiple times
  - do once, pass to functions that need it.

Simple Things To Remember

- Use vectorized functions where you can
- Use lapply()/sapply() when you can rather than for() loops
- When looping, preallocate the answer to have the correct number of elements and fill them
    - Don’t concatenate to the end.

Concatenating Values to a Vector

```
N = 1e5

system.time({
    ans = integer()
    for(i in 1:N)
        ans[i] = i
})
```

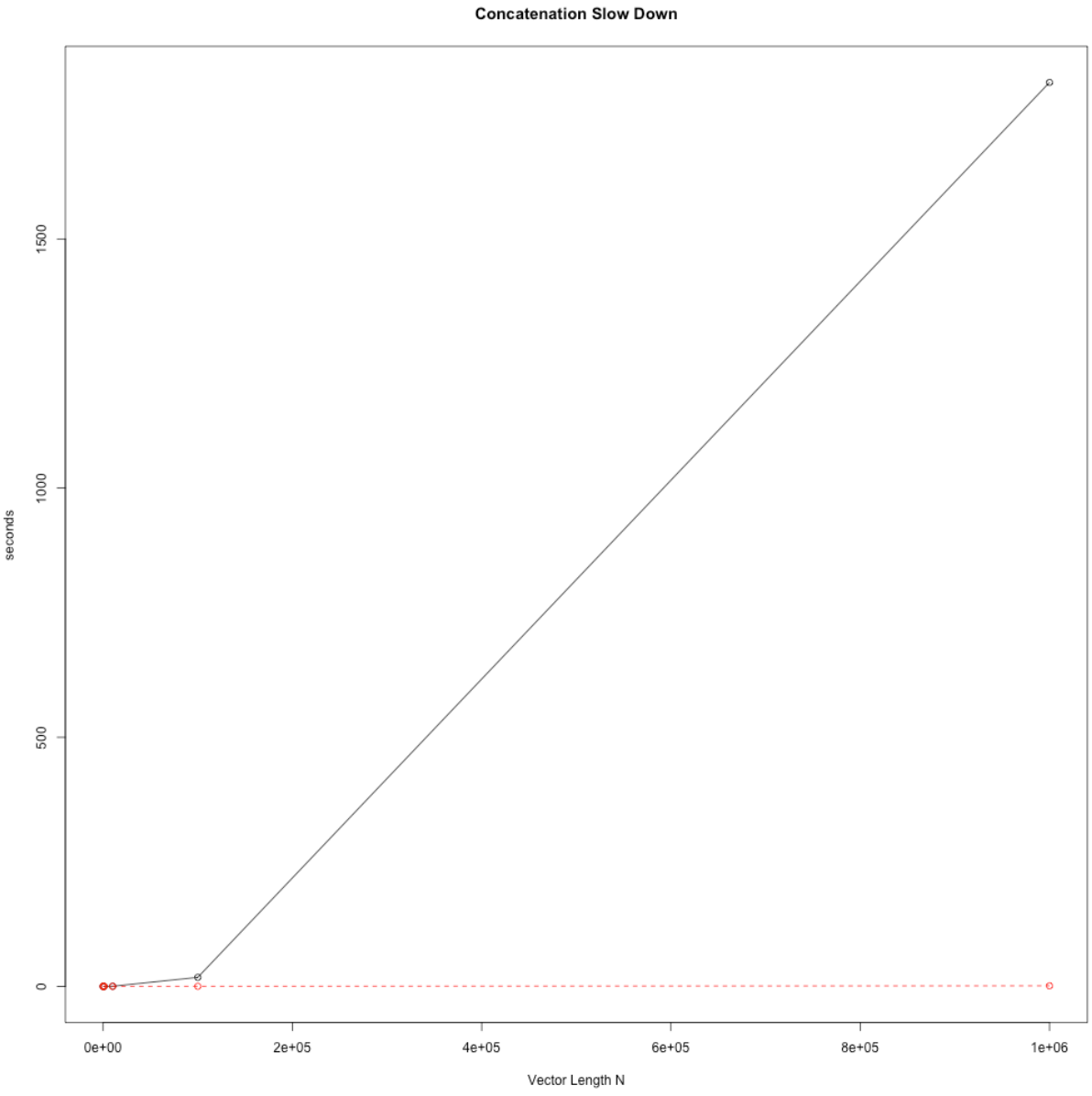
19.774 seconds

N = 1e6 1814.2

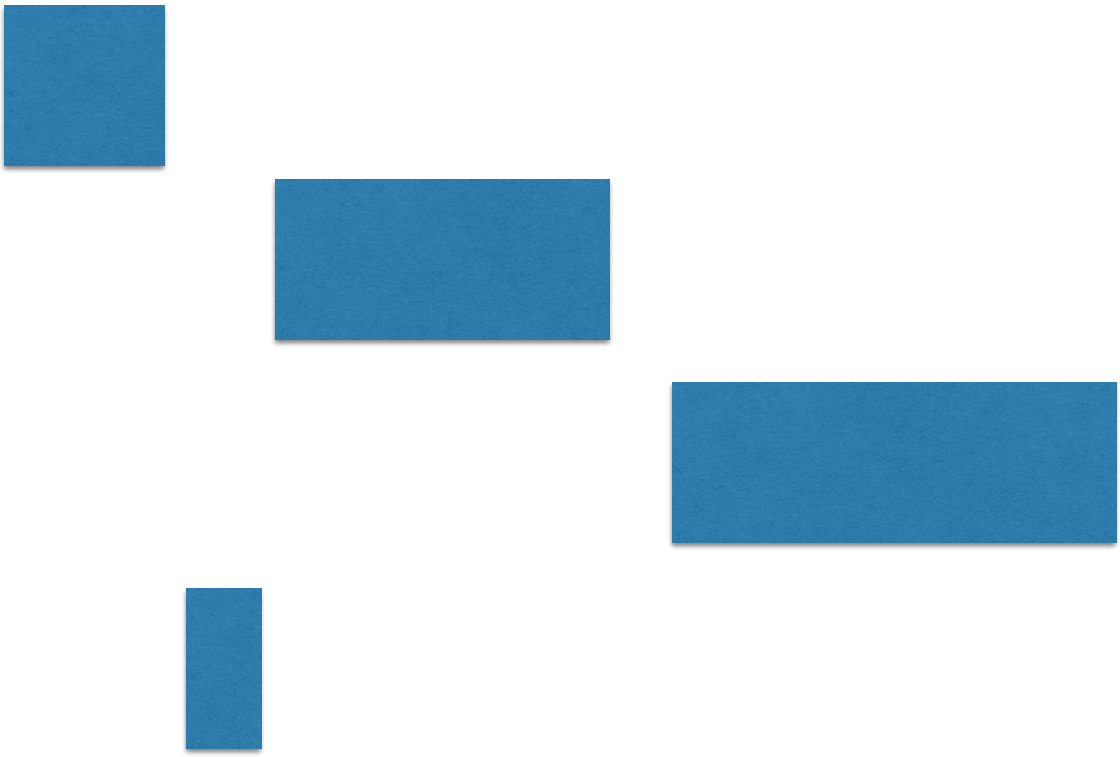
```
N = 1e5

system.time({
    ans = integer(N)
    for(i in 1:N)
        ans[i] = i
})
```

0.170 seconds

N = 1e6 1.1


Concatenation Slow Down
seconds
0
500
1000
1500
0e+00
2e+05
4e+05
6e+05
8e+05
1e+06
Vector Length N

- Also leads to memory fragmentation.



Why Concatenation is So Slow

- Think about the each iteration, e.g., 500th
- We add one element to the end of the 499-element vector
- R has to
  - allocate a new 500-element vector,
  - copy the 499 elements from the previous to the new vector
  - insert 500th value.
- Does this for each iteration.
- When we pre-allocate, just insert value. No allocation & copy.

Premature Optimization

- “Premature optimization is the root of all evil” - Don Knuth.
- Get the wrong answer faster - Jon Bentley
- Write the obvious approach, and only try to get smarter after that.
  - You have a correct version against which you can verify the results from the smarter version.
  - You can focus on the parts that are slowest.

Fibonacci Sequence

- Simple recurrence relationship
  F(n) = F(n-1) + F(n-2)

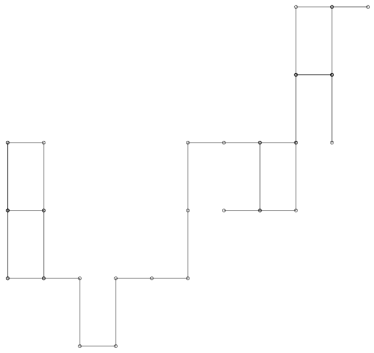
```
fib =
function(n)
{
  if(n < 2)
      n
  else
      fib(n - 1) + fib(n - 2)
}
```

Byte Compile

- Speed up the R implementation with the byte code compiler.
- fib = compiler::cmpfun(fib)
  - Note reassigning to fib since fib calls fib
- system.time(fib(30)) 1.878 seconds
- Almost 50% speedup on laptop, 23% on Linux server.

Vectorization

Different Computational Approach



- Consider a 2-D random walk
- Naive Approach
  At each step,
  - Toss a coin for Horizontal or Vertical
  - Then for which direction (left/right or up/down)
  - Update current position
  - Repeat

```
w2d1 = function(n) {
   xpos = ypos = numeric(n)
   truefalse = c(TRUE, FALSE)
   plusminus1 = c(1, -1)
   for(i in 2:n)
        # Decide whether we are moving horizontally
        # or vertically.
    if (sample(truefalse, 1)) {
      xpos[i] = xpos[i-1] + sample(plusminus1, 1)
      ypos[i] = ypos[i-1]
    }
    else {
      xpos[i] = xpos[i-1]
      ypos[i] = ypos[i-1] + sample(plusminus1, 1)
    }
   list(x = xpos, y = ypos)
 }
```

- N = 1e6 steps
- Naive version: 26.5 seconds.
- Heavily vectorized version: .096 seconds
- Speedup Factor: 276
- On Linux machine, speedup x 88

- 4 possible directions at each step.
  (1, 0), (-1, 0), (0, 1), (0, -1)

- Sample all N steps at once, i.e. in one call.

- Use a separate cumulative sum of the X and Y coordinates.

Vectorized 2-D Walk

```
rw2d5 =
    # Sample from 4 directions, not horizontally and vertically
    # then left/right or up/down.
function(n = 100000) {
    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)
}
```

Profiling

- What can you do to speed up your code?
- Profile it to identify how long each function takes.
- Count how many times those functions are called.
- Rprof(), summaryRprof(), trace(), untrace()
- Rprof("nameOfOutputFile")
  # run code
  Rprof(NULL)
- summaryRprof("nameOfOutputFile")$by.self

Output from summaryRprof()$by.self

	self.time	self.pct	total.time	total.pct
"match"	11.88	48.77	14.16	58.13
"%in%"	2.48	10.18	16.52	67.82
"FUN"	2.16	8.87	24.36	100.00
"rbinom"	1.62	6.65	1.62	6.65
"$"	1.20	4.93	6.44	26.44
"[[.data.frame"	1.18	4.84	4.08	16.75
"<Anonymous>"	1.00	4.11	1.74	7.14
"$.data.frame"	0.76	3.12	5.24	21.51
"[["	0.40	1.64	4.48	18.39
"sys.call"	0.32	1.31	0.32	1.31
"lapply"	0.30	1.23	24.36	100.00
"nargs"	0.18	0.74	0.18	0.74
"all"	0.14	0.57	0.14	0.57
"cat"	0.12	0.49	0.12	0.49
"is.matrix"	0.12	0.49	0.12	0.49

- Used named matching, not ids %in% names(obj)

- Use vectorized versions of rnorm, rbinom, etc.
  Vectorized in the parameters.

- Use sapply() or better vapply() when function returns scalars.
  do.call(rbind(, lapply()))

Infection Simulation

- See sim.R (after initializing different inputs to the simulation)

How Many Calls ?

- Profiling indicates functions R spends more time in.
- But these may not be slow - just called a lot more times.
- So we want to know the number of calls to our bottleneck functions.
- Use trace() to monitor all calls to a function.
- k = genCallCollector()
  trace(rnorm, quote(k("rnorm")), print = FALSE)

C/C++ Code

- Look for C/C++ code to do what you need or write it yourself.
- Translate only very small elements of the R code,
  mostly for() loops where the iterations depend on each other.
- Makes entire code a little more complicated
  - Need compiler installed, etc.
  - Can compile C code and manually load it into R session
  - R CMD SHLIB foo.c bar.c
  - dyn.load("foo.so") # or foo.dll on Windows.

Fibonacci Sequence

- Simple recurrence relationship
  F(n) = F(n-1) + F(n-2)

```
fib =
function(n)
{
  if(n < 2)
      n
  else
      fib(n - 1) + fib(n - 2)
}
```

Fibonacci Sequence

```
int fib(int n) {
    if(n < 2)
        return(n);
    else
        return(fib(n - 1) + fib(n - 2));
}
```

C code
can find online

```
void
R_fib(int *rn, int *ans)
{
    *ans = fib( *rn );
}
```

R wrapper routine
call via .C() in R

- R CMD SHLIB fib.c
- dyn.load(“fib.so”)
- .C(“R_fib”, 30L, ans = 0L)$ans
- fib(30) times
  R function : 2.791
  C code: 0.006
  Speedup factor: 465

Use an R Package

- For simplicity, with C code, create an R package
  - Put R code in R/ directory, C/C++ code in src/
  - Add NAMESPACE file with
    useDynLib(packageName)
  - Copy and edit a DESCRIPTION file
  - R CMD INSTALL myPackage

- Long discussion of an example of writing code in R, C, data structures in Data Science in R: A Case Studies Approach http://rdatasciencecases.org/ BML cars chapter.

Appeal for Mutual Help

- You have to adapt your code to make it run faster.
- What if we could analyze your code before it is run and translate it to faster code!
- Nick, Clark and I are working on this.
  - E.g. we can take the naive 2-D random walk function as-is compiled it automatically to machine code.
  - Speedup of factor of 2 over best vectorized version.

Appeal for Mutual Help

- We'd love to get your R code that is slow & that you care about as examples for our research.