Profiling & Parallelization

Lecture 20

Dr. Colin Rundel

Profiling & Benchmarking

profvis demo

```
n = 1e6

d = tibble(
  x1 = rt(n, df = 3),
  x2 = rt(n, df = 3),
  x3 = rt(n, df = 3),
  x4 = rt(n, df = 3),
  x5 = rt(n, df = 3),
) %>%
  mutate(y = -2*x1 - 1*x2 + 0*x3 + 1*x4 + 2*x5 + rnorm(n))

profvis::profvis(lm(y~., data=d))
```

Benchmarking - bench

```r
d = tibble(
  x = runif(10000),
  y = runif(10000)
)

(b = bench::mark(
  d[d$x > 0.5, ],
  d[which(d$x > 0.5), ],
  subset(d, x > 0.5),
  filter(d, x > 0.5)
))
```

```
# A tibble: 4 × 6
  expression                   min   median `itr/sec` mem_alloc `gc/sec`
  <bch:expr>              <bch:tm> <bch:tm>     <dbl> <bch:byt>    <dbl>
1 d[d$x > 0.5, ]          172.36µs 184.01µs     5392.  253.49KB     14.9
2 d[which(d$x > 0.5), ] 131.61µs  145.2µs     6832.  274.31KB     38.7
3 subset(d, x > 0.5)    241.37µs 257.11µs     3862.  289.55KB     21.5
4 filter(d, x > 0.5)      1.39ms   1.43ms      693.    2.06MB     17.2
```

Larger n

```
d = tibble(
  x = runif(1e6),
  y = runif(1e6)
)

(b = bench::mark(
  d[d$x > 0.5, ],
  d[which(d$x > 0.5), ],
  subset(d, x > 0.5),
  filter(d, x > 0.5)
))
```

```
# A tibble: 4 × 6
  expression                min   median `itr/sec` mem_alloc `gc/sec`
  <bch:expr>              <bch:tm> <bch:tm>     <dbl> <bch:byt>    <dbl>
1 d[d$x > 0.5, ]           16.9ms   17.4ms      57.0    13.4MB     49.4
2 d[which(d$x > 0.5), ]    13.3ms   13.5ms      73.7    24.8MB    156.
3 subset(d, x > 0.5)       23.4ms   23.5ms      42.5    24.8MB     92.1
4 filter(d, x > 0.5)       17.6ms   18.1ms      55.6    24.8MB     94.5
```

bench - relative results

```
summary(b, relative=TRUE)
```

```
# A tibble: 4 × 6
  expression                min median `itr/sec` mem_alloc `gc/sec`
  <bch:expr>              <dbl>  <dbl>     <dbl>     <dbl>    <dbl>
1 d[d$x > 0.5, ]           1.28   1.29      1.34      1        1
2 d[which(d$x > 0.5), ]    1      1         1.73      1.86     3.15
3 subset(d, x > 0.5)       1.76   1.74      1         1.86     1.86
4 filter(d, x > 0.5)       1.32   1.34      1.31      1.86     1.91
```

Parallelization

`parallel`

Part of the base packages in R

- tools for the forking of R processes (some functions do not work on Windows)
- Core functions:
  - `detectCores`
  - `pvec`
  - `mclapply`
  - `mcparallel` & `mccollect`

detectCores

Surprisingly, detects the number of cores of the current system.

```
1 detectCores()
2 ## [1] 16
```

pvec

Parallelization of a vectorized function call

```
system.time(pvec(1:1e7, sqrt, mc.cores = 1))
##    user  system elapsed
##   0.214   0.029   0.243

system.time(pvec(1:1e7, sqrt, mc.cores = 4))
##    user  system elapsed
##   0.442   0.185   0.631

system.time(pvec(1:1e7, sqrt, mc.cores = 8))
##    user  system elapsed
##   0.532   0.389   0.372
```

pvec - bench::system_time

```
bench::system_time(pvec(1:1e7, sqrt, mc.cores = 1))
##  process    real
##    180ms   180ms

bench::system_time(pvec(1:1e7, sqrt, mc.cores = 4))
##  process    real
##    935ms   980ms

bench::system_time(pvec(1:1e7, sqrt, mc.cores = 8))
##  process    real
##    1.01s   1.05s
```

```
bench::system_time(Sys.sleep(.5))
##  process     real
##   1.93ms 500.09ms

system.time(Sys.sleep(.5))
##    user  system elapsed
##   0.001   0.000   0.500
```

```r
cores = c(1,4,8,16)
order = 6:8
f = function(x,y) {
  system.time(
    pvec(1:(10^y), sqrt, mc.cores = x)
  )[3]
}

res = map(
  cores,
  function(x) {
     map_dbl(order, f, x = x)
  }
) %>%
  do.call(rbind, .)

rownames(res) = paste0(cores," cores")
```

mclapply

Parallelized version of `lapply`

```
system.time(rnorm(1e6))
##    user  system elapsed
##   0.101   0.007   0.107

system.time(unlist(mclapply(1:10, function(x) rnorm(1e5), mc.cores = 2)))
##    user  system elapsed
##   0.148   0.136   0.106

system.time(unlist(mclapply(1:10, function(x) rnorm(1e5), mc.cores = 4)))
##    user  system elapsed
##   0.242   0.061   0.052
```

```r
system.time(unlist(mclapply(1:10, function(x) rnorm(1e5), mc.cores = 4)))
##    user  system elapsed
##   0.097   0.047   0.079

system.time(unlist(mclapply(1:10, function(x) rnorm(1e5), mc.cores = 8)))
##    user  system elapsed
##   0.193   0.076   0.040

system.time(unlist(mclapply(1:10, function(x) rnorm(1e5), mc.cores = 10)))
##    user  system elapsed
##   0.162   0.083   0.041

system.time(unlist(mclapply(1:10, function(x) rnorm(1e5), mc.cores = 12)))
##    user  system elapsed
##   0.098   0.065   0.037
```

mcparallel

Asynchronously evaluation of an R expression in a separate process

```
1 m = mcparallel(rnorm(1e6))
2 n = mcparallel(rbeta(1e6,1,1))
3 o = mcparallel(rgamma(1e6,1,1))
4
5 str(m)
```

```
List of 2
 $ pid: int 44778
 $ fd : int [1:2] 4 7
 - attr(*, "class")= chr [1:3] "parallelJob" "childProcess" "process"
```

```
1 str(n)
```

```
List of 2
 $ pid: int 44779
 $ fd : int [1:2] 5 9
 - attr(*, "class")= chr [1:3] "parallelJob" "childProcess" "process"
```

mccollect

Checks `mcparallel` objects for completion

```
1  str(mccollect(list(m,n,o)))
```

```
List of 3
 $ 44778: num [1:1000000] 0.743 0.377 -0.121 -1.024 -0.299 ...
 $ 44779: num [1:1000000] 0.1747 0.4037 0.0611 0.3125 0.6287 ...
 $ 44780: num [1:1000000] 0.601 0.479 2.154 0.136 1.499 ...
```

mccollect - waiting

```
1 p = mcparallel(mean(rnorm(1e5)))
2 mccollect(p, wait = FALSE, 10) # will retrieve the result (since it's fast)
```

```
$`44781`
[1] -0.001510259
```

```
1 mccollect(p, wait = FALSE)     # will signal the job as terminating
```

```
NULL
```

```
1 mccollect(p, wait = FALSE)     # there is no longer such a job
```

```
NULL
```

doMC & foreach

doMC & foreach

Packages by Revolution Analytics that provides the `foreach` function which is a parallelizable `for` loop (and then some).

- Core functions:
  - `registerDoMC`
  - `foreach`, `%dopar%`, `%do%`

registerDoMC

Primarily used to set the number of cores used by `foreach`, by default uses `options("cores")` or half the number of cores found by `detectCores` from the parallel package.

```
options("cores")
## $cores
## NULL

detectCores()
## [1] 16

getDoParWorkers()
## [1] 1

registerDoMC(4)
getDoParWorkers()
## [1] 4
```

foreach

A slightly more powerful version of base `for` loops (think `for` with an `lapply` flavor). Combined with `%do%` or `%dopar%` for single or multicore execution.

```
1  for(i in 1:10) {
2    sqrt(i)
3  }
4
5  foreach(i = 1:5) %do% {
6    sqrt(i)
7  }
```

```
[[1]]
[1] 1

[[2]]
[1] 1.414214

[[3]]
[1] 1.732051
```

```
[[4]]
[1] 2
```

`foreach` - iterators

`foreach` can iterate across more than one value, but it doesn't do length coercion

```
1 foreach(i = 1:5, j = 1:5) %do% {
2   sqrt(i^2+j^2)
3 }
```

```
[[1]]
[1] 1.414214

[[2]]
[1] 2.828427

[[3]]
[1] 4.242641

[[4]]
[1] 5.656854

[[5]]
```

```
1 foreach(i = 1:5, j = 1:2) %do% {
2   sqrt(i^2+j^2)
3 }
```

```
[[1]]
[1] 1.414214

[[2]]
[1] 2.828427
```

`foreach` - combining results

```
1 foreach(i = 1:5, .combine='c') %do% {
2   sqrt(i)
3 }
```

```
[1] 1.000000 1.414214 1.732051 2.000000 2.236068
```

```
1 foreach(i = 1:5, .combine='cbind') %do% {
2   sqrt(i)
3 }
```

```
     result.1 result.2 result.3 result.4 result.5
[1,]        1 1.414214 1.732051        2 2.236068
```

```
1 foreach(i = 1:5, .combine='+') %do% {
2   sqrt(i)
3 }
```

```
[1] 8.382332
```

`foreach` - parallelization

Swapping out `%do%` for `%dopar%` will use the parallel backend.

```
registerDoMC(4)
```

```
system.time(foreach(i = 1:10) %dopar% mean(rnorm(1e6)))
```

```
   user  system elapsed
  0.276   0.024   0.093
```

```
registerDoMC(8)
system.time(foreach(i = 1:10) %dopar% mean(rnorm(1e6)))
```

```
   user  system elapsed
  0.283   0.032   0.065
```

```
registerDoMC(12)
system.time(foreach(i = 1:10) %dopar% mean(rnorm(1e6)))
```

```
   user  system elapsed
  0.309   0.045   0.054
```

furrr / future

```
system.time( purrr::map(c(2,2,2), Sys.sleep) )
##  user  system elapsed
##  0.032   0.024   6.004

system.time( furrr::future_map(c(2,2,2), Sys.sleep) )
##   user  system elapsed
##  0.110   0.028   6.066

future::plan(future::multisession) # See also future::multicore
system.time( furrr::future_map(c(2,2,2), Sys.sleep) )
##   user  system elapsed
##  0.075   0.010   2.395
```

Example - Bootstraping

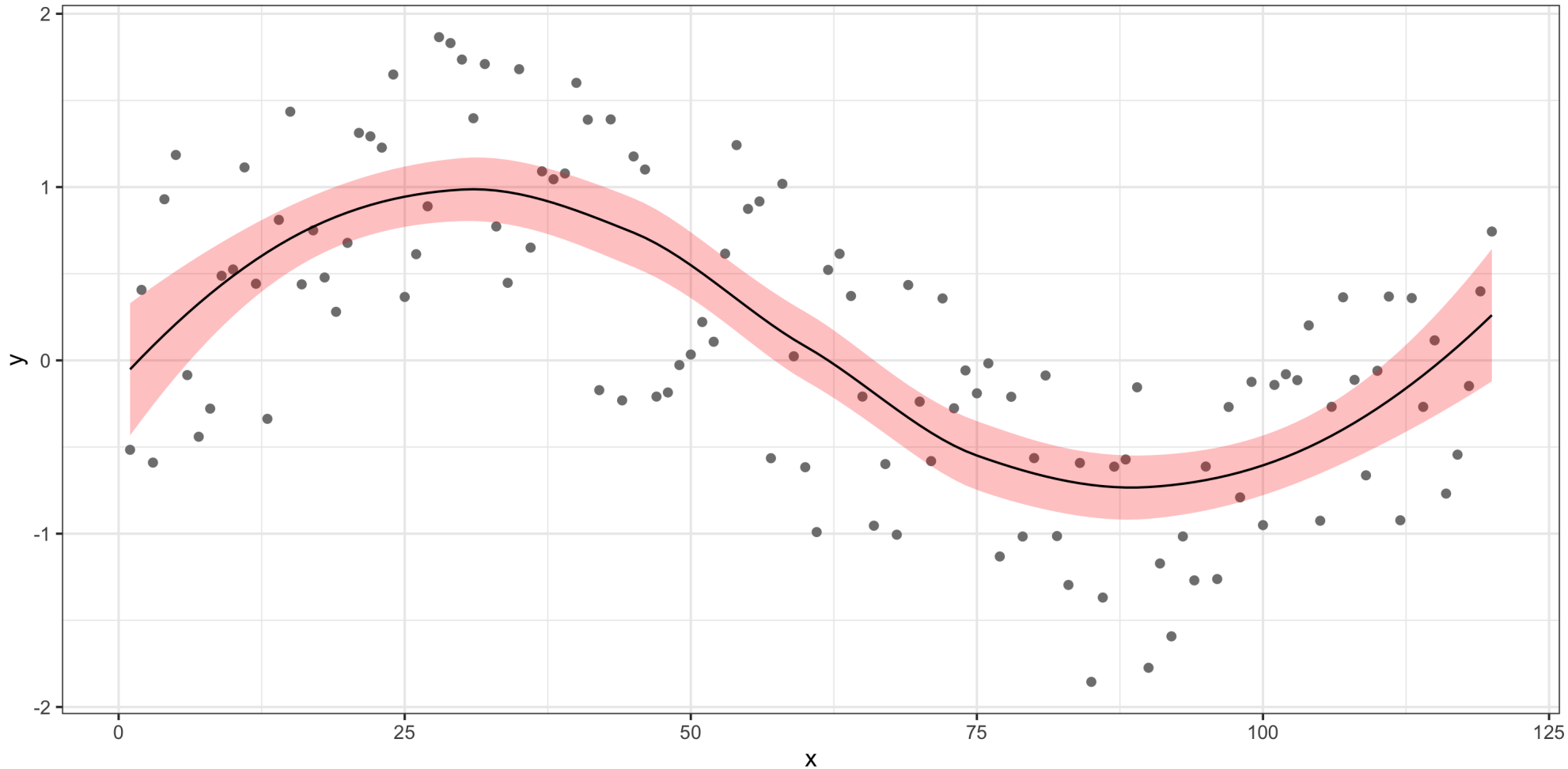
Bootstrapping is a resampling scheme where the original data is repeatedly reconstructed by taking a samples of size *n* (with replacement) from the original data, and using that to repeat an analysis procedure of interest. Below is an example of fitting a local regression (`loess`) to some synthetic data, we will construct a bootstrap prediction interval for this model.

```r
set.seed(3212016)
d = data.frame(x = 1:120) %>%
    mutate(y = sin(2*pi*x/120) + runif(length(x),-1,1))

l = loess(y ~ x, data=d)
p = predict(l, se=TRUE)

d = d %>% mutate(
  pred_y = p$fit,
  pred_y_se = p$se.fit
)
```

```r
ggplot(d, aes(x,y)) +
  geom_point(color="gray50") +
  geom_ribbon(
    aes(ymin = pred_y - 1.96 * pred_y_se,
        ymax = pred_y + 1.96 * pred_y_se),
    fill="red", alpha=0.25
  ) +
  geom_line(aes(y=pred_y)) +
  theme_bw()
```


2
1
0
-1
-2
y
0
25
50
75
100
125
x

What to use when?

Optimal use of multiple cores is hard, there isn't one best solution

- Don't underestimate the overhead cost
- Experimentation is key
- Measure it or it didn't happen
- Be aware of the trade off between developer time and run time

BLAS and LAPACK

Statistics and Linear Algebra

An awful lot of statistics is at its core linear algebra.

For example:

- Linear regession models, find

$$\hat{\beta} = (X^T X)^{-1} X^T y$$

- Principle component analysis
  - Find $T = XW$ where W is a matrix whose columns are the eigenvectors of $X^T X$.
  - Often solved via SVD - Let $X = U\Sigma W^T$ then $T = U\Sigma$.

Numerical Linear Algebra

Not unique to Statistics, these are the type of problems that come up across all areas of numerical computing.

- Numerical linear algebra $\neq$ mathematical linear algebra
- Efficiency and stability of numerical algorithms matter
  - Designing and implementing these algorithms is hard
- Don't reinvent the wheel - common core linear algebra tools (well defined API)

BLAS and LAPACK

Low level algorithms for common linear algebra operations

BLAS

- **B**asic **L**inear **A**lgebra **S**ubprograms
- Copying, scaling, multiplying vectors and matrices
- Origins go back to 1979, written in Fortran

LAPACK

- **L**inear **A**lgebra **Pack**age
- Higher level functionality building on BLAS.
- Linear solvers, eigenvalues, and matrix decompositions
- Origins go back to 1992, mostly Fortran (expanded on LINPACK, EISPACK)

Modern variants?

Most default BLAS and LAPACK implementations (like R's defaults) are somewhat dated

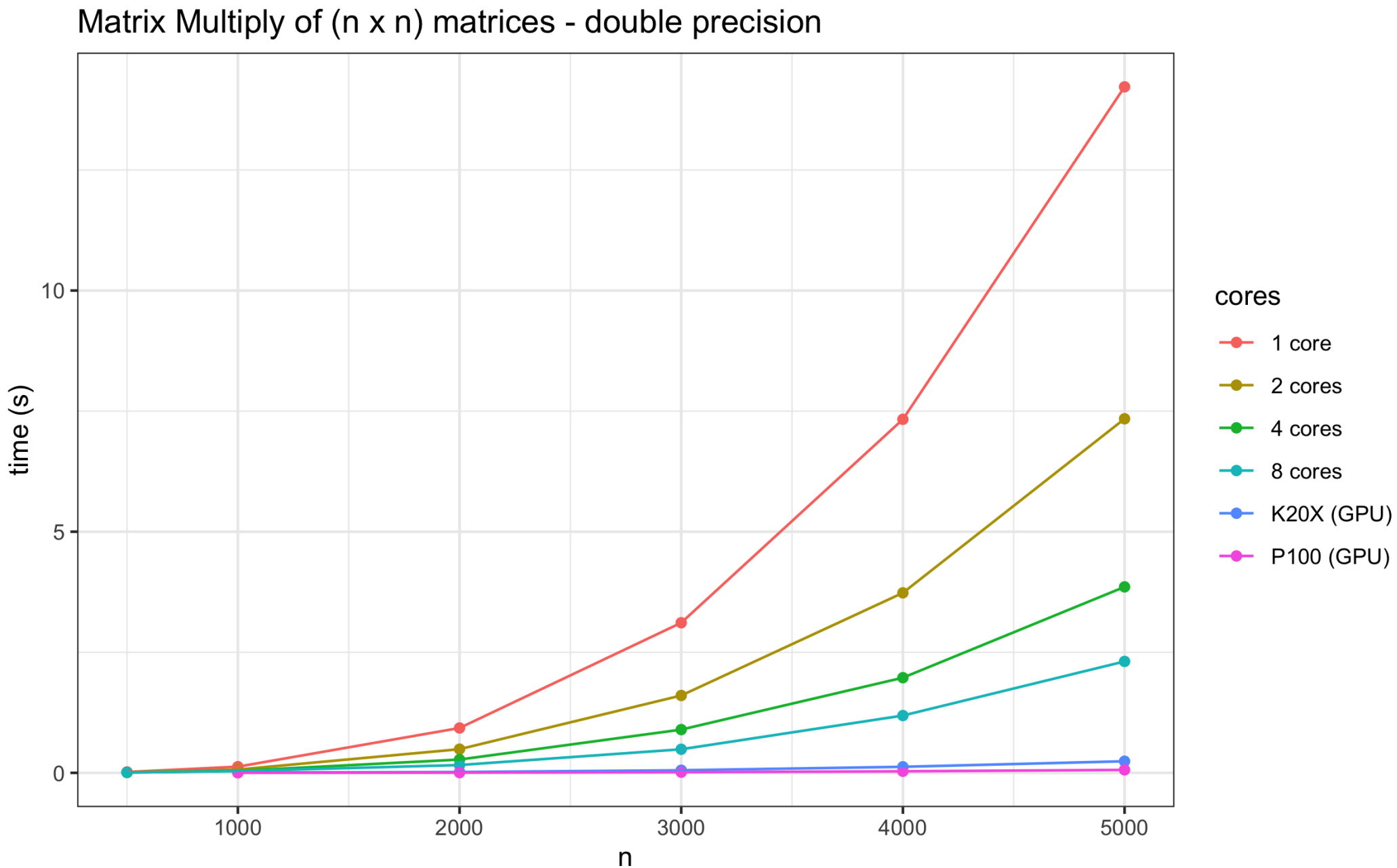
- Written in Fortran and designed for a single cpu core
- Certain (potentially non-optimal) hard coded defaults (e.g. block size).

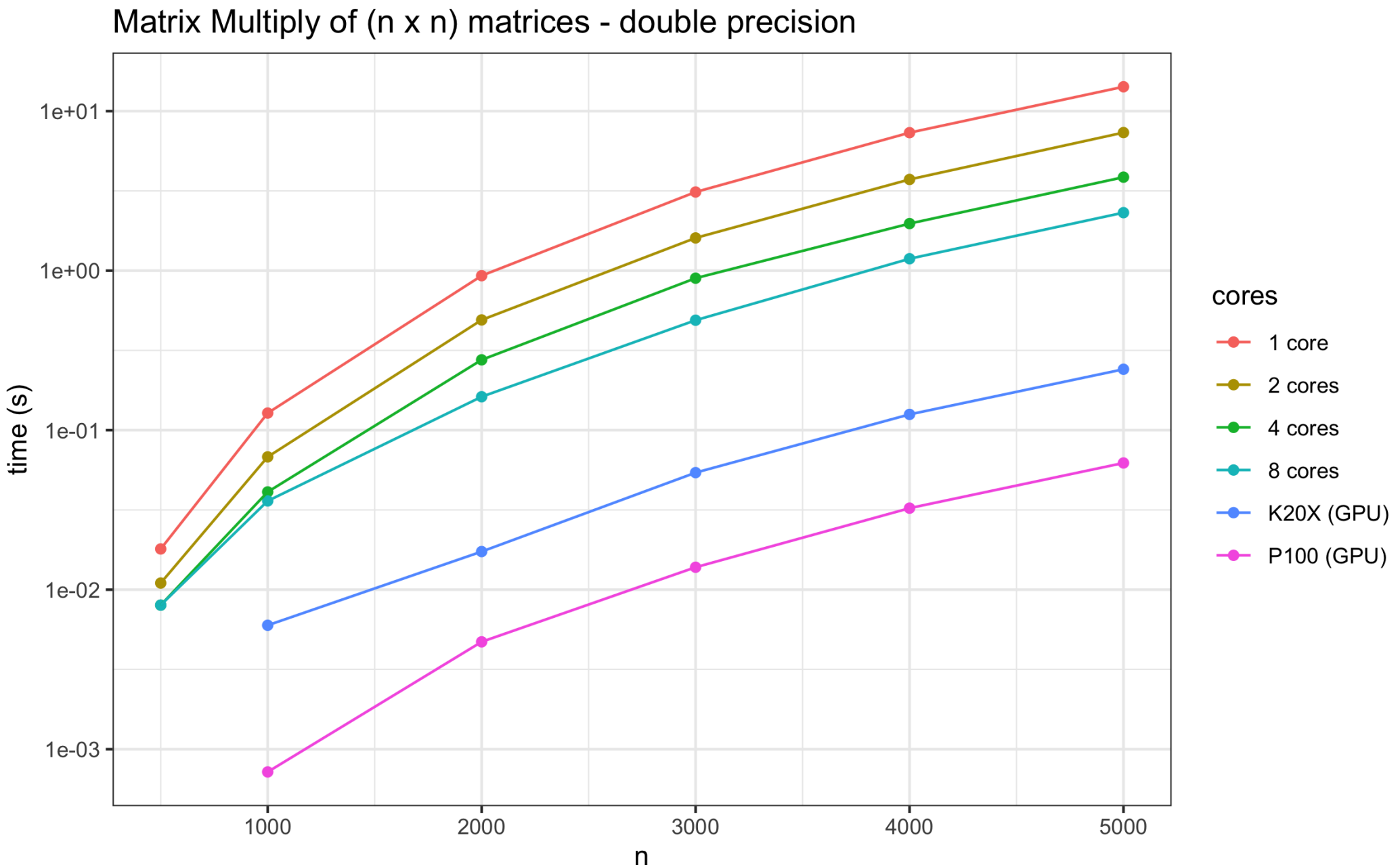
Multithreaded alternatives:

- ATLAS - Automatically Tuned Linear Algebra Software
- OpenBLAS - fork of GotoBLAS from TACC at UTexas
- Intel MKL - Math Kernel Library, part of Intel's commercial compiler tools
- cuBLAS / Magma - GPU libraries from Nvidia and UTK respectively

OpenBLAS Matrix Multiply (DGEMM) Performance

n	1 core	2 cores	4 cores	8 cores
100	0.001	0.001	0.000	0.000
500	0.018	0.011	0.008	0.008
1000	0.128	0.068	0.041	0.036
2000	0.930	0.491	0.276	0.162
3000	3.112	1.604	0.897	0.489
4000	7.330	3.732	1.973	1.188
5000	14.223	7.341	3.856	2.310


Matrix Multiply of (n x n) matrices - double precision
time (s)
10
5
0
1000
2000
3000
4000
5000
n
cores
1 core
2 cores
4 cores
8 cores
K20X (GPU)
P100 (GPU)


Matrix Multiply of (n x n) matrices - double precision
time (s)
1e+01
1e+00
1e-01
1e-02
1e-03
1000
2000
3000
4000
5000
n
cores
1 core
2 cores
4 cores
8 cores
K20X (GPU)
P100 (GPU)