okapi.math.unr.edu

24 cores 2 GPUs 384 GB RAM 20 TB HD

caprine.math.unr.edu

128 cores 2 GPUs 512 GB RAM 20 TB HD Okapi and Caprine are department servers that

- are available to all graduate students and faculty.
- can be used for small computational runs.
- provide a Linux software environment.
- help learn about HPC and statistical simulation.

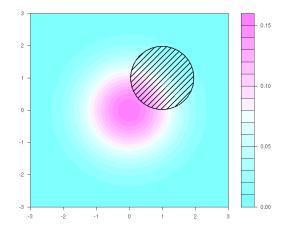
Goal:

• Learn how to use okapi.

How?

- Attend the graduate student seminar.
- Consider a simple computation.
- Watch someone run it.
- Try it yourself.

Problem: Let *P* be the standard normal probability measure on \mathbb{R}^2 and *A* be the circle of radius *r* with center *v*. Find P(A).



Problem: Let P be the standard normal probability measure on \mathbb{R}^2 and A be the circle of radius r with center v. Find P(A).

Thus

$$A = \left\{ x \in \mathbf{R}^2 : \|x - v\| < r \right\}$$

and

$$P(A) = \int_{A} e^{-\frac{1}{2} \|x\|^{2}} dx.$$

Computation: Independently sample a bunch of points in \mathbb{R}^2 and then count how many of those points lie in A.

- 1 r <- 1
- 2 V <- C(1,1)
- $3 \text{ inA} <- \text{ function}(x) \text{ sum}((x-v)^2) < r^2$
- 4 N <- 100000
- 5 X <- matrix(rnorm(2*N),N)</pre>
- 6 C <- sum(as.integer(apply(X,1,inA)))</pre>
- 7 cat(sprintf("P(A)=%g\n",C/N))

Computation: Independently sample a bunch of points in \mathbb{R}^2 and then count how many of those points lie in A.

- \$ Rscript sim.R
- P(A)=0.18022
- \$ Rscript sim.R
- P(A)=0.18151
- \$ Rscript sim.R
- P(A) = 0.17964
- \$ Rscript sim.R
- P(A)=0.18023

Each simulation took 1/2 second on my notebook, but the approximations only agree to a couple digits.

• Use a better method to approximate P(A).

Sometimes the best method still takes a long time.

- Scale up a simulation using a server.
- Many cores are available.
- Can run for days without problem.
- The laptop doesn't overheat.

Computation: Sample a bunch of points in \mathbb{R}^2 , count how many lie in A and do this a whole bunch of times.

1 r <- 1

2 V <- C(1,1)

- $3 \text{ inA} <- \text{ function}(x) \text{ sum}((x-v)^2) < r^2$
- $_4$ N <- 100000; K <- 1000; T <- 0

5 for (k in 1:K){

- 6 X <- matrix(rnorm(2*N),N)</pre>
- 7 C <- sum(as.integer(apply(X,1,inA)))</pre>

8 T <- T+C

9 }

10 cat(sprintf("P(A)=%g\n",T/N/K))

Computation: Sample a bunch of points in \mathbb{R}^2 , count how many lie in A and do this a whole bunch of times in parallel.

6 r <- 1

- 7 v <- c(1,1)
- s inA <- function(x) sum((x-v)^2)<r^2
- 9 N <- 100000; K <- 1000
- 10 C <- foreach(k=1:K,.combine='c') %dopar% {</pre>
- 11 X <- matrix(rnorm(2*N),N)
- 12 sum(as.integer(apply(X,1,inA)))

13 }

14 cat(sprintf("P(A)=%g\n",sum(C)/N/K))

Programming Details: Parallel processing in R requires some setup at the beginning and teardown at the end.

Parallel setup:

- 1 library("doParallel")
- 2 library("foreach")
- 3 cluster <- makeCluster(7)</pre>
- 4 registerDoParallel(cluster)

Parallel teardown:

16 stopCluster(cluster)

You might need install.packages to install the libraries.

Logging in to Okapi: Let's start with something simple and avoid parallel processing and those extra libraries.

Connect with ${\tt ssh}$ or Remote Desktop. For example



Submitting a Job on Okapi: Let's start with something simple and avoid parallel processing and those extra libraries.

The batch submission file looks like

1 #!/bin/bash

2 time Rscript scaled.R

Download the files

- scaled.R The non-parallel Monte Carlo code.
- scaled.slm The batch submission file.

from

https://fractal.math.unr.edu/~okapi/2023/

Running the Script: Use the sbatch command to launch the R script. Then use squeue to check if it's running.

\$ mkdir demo2023 \$ cd demo2023 \$ wget -q https://fractal.math.unr.edu/~okapi/2023/scaled.R \$ wget -q https://fractal.math.unr.edu/~okapi/2023/scaled.slm									
· · · ·	\$ ls								
scaled.R scaled.slm									
\$ sbatch scaled.slm									
Submitted batch job 263301									
squeue									
JOBID	NAME	USER	ST	TIM	E MIN	CPU	REASON	PARTITION	
263301	scaled.slm	ejolson	R	0:0	2 2G	1	None	fast	
\$		2							

The script will run for about 6 minutes.

To cancel it type scancel n where n is the JobID.

Submitting a Parallel Job on Okapi: If there's time we'll try parallel processing and installing those extra libraries.

To install the libraries start R interactively and type

```
$ R
R version 4.3.1 (2023-06-16) -- "Beagle Scouts"
Copyright (C) 2023 The R Foundation for Statistical Computing
> install.packages("doParallel")
--- Please select a CRAN mirror for use in this session ---
Selection: 72
> install.packages("foreach")
> quit()
Save workspace image? [y/n/c]: n
$
```

The rest is similar to running the non-parallel code.

Submitting a Parallel Job on Okapi: If there's time we'll try parallel processing and installing those extra libraries.

The batch file looks like

- 1 #!/bin/bash
- 2 #SBATCH -n8
- $_{\rm 3}$ time Rscript parallel.R

Note the -n8 corresponds to ${\tt makeCluster(7)}$ in the R parallel setup as follows.

• For luck the number 8 is one more than 7.

The batch file reserves 8 cores for the job; the R script uses 7 for parallel processing and reserves 1 for everything else.

Running the Parallel Script: Use the sbatch command to launch the R script. Then use squeue to check if it's running.

\$ wget -q	\$ wget -q https://fractal.math.unr.edu/~okapi/2023/parallel.R										
<pre>\$ wget -q https://fractal.math.unr.edu/~okapi/2023/parallel.slm</pre>											
\$ ls											
parallel.R parallel.slm scaled.R scaled.slm											
\$ sbatch parallel.slm											
Submitted batch job 263303											
\$ squeue											
JOBID	NAME	USER	ST	TIME	MIN	CPU	REASON	PARTITION			
263303	parallel.slm	ejolson	R	0:40	2G	8	None	fast			
\$											

The script will finish in less than a minute. Check the output:

\$ cat slurm-263303.out Loading required package: foreach Loading required package: iterators Loading required package: parallel P(A)=0.180611