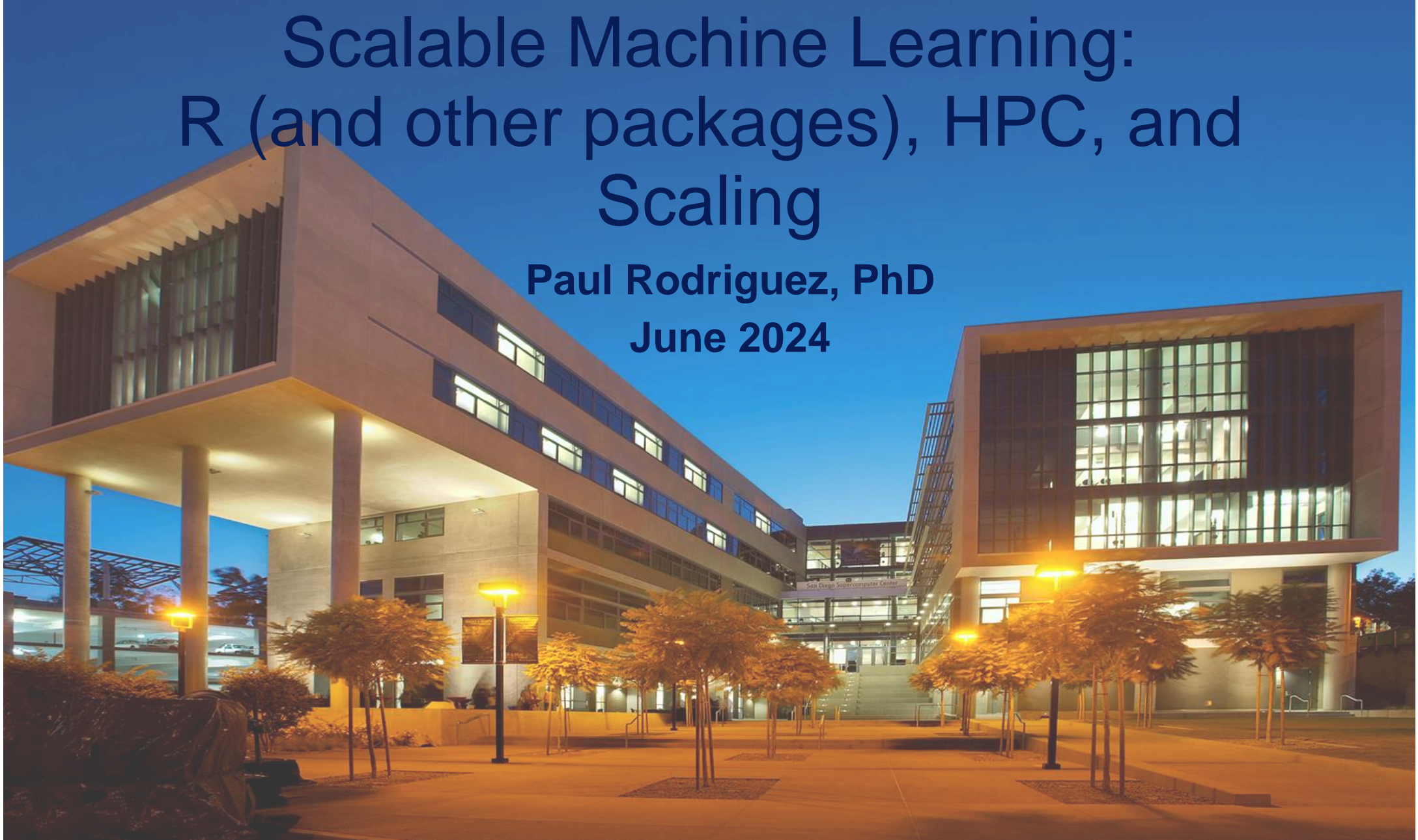


Scalable Machine Learning: R (and other packages), HPC, and Scaling

Paul Rodriguez, PhD
June 2024



Outline

- **R and Scaling**
- **Parallel R**
- **Embarrassingly Parallel R**
- **A big data exploration of R**

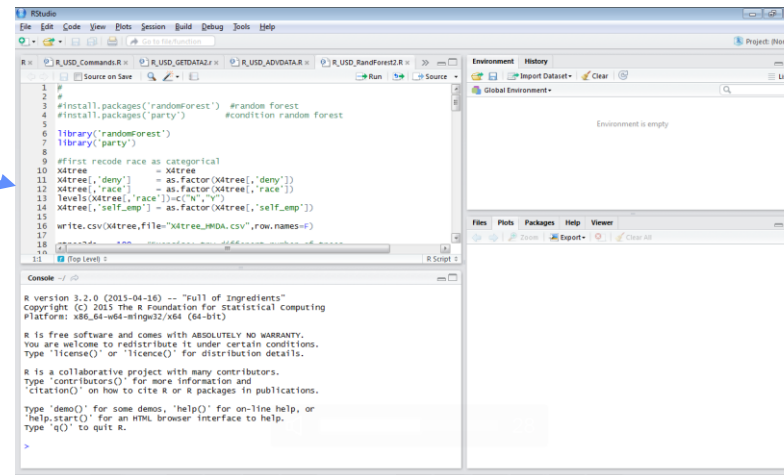
A typical R development workflow

- R studio: An Integrated development environment for R

Menu tab

*Edit window to
Build scripts*

R console



*Environment
Information on
variables and
command history*

*Plots, help
docs, package
lists*

Typical R code workflow

#READ DATA

```
X = read.csv('hmda_aer.csv', header=T, stringsAsFactors=T)
```

#SUBSET DATA

```
indices_2keep = which(X[, 's13'] %in% c(3,4,5))  
X = X[unique(indices_2keep),]
```

#CREATE/TRANSFORM VARIABLES

```
pi_rat = as.numeric(X[, 's46']/100) #debt2income ratio
```

#RUN MODEL and SHOW RESULTS

```
lm_result = lm(deny~pi_rat) #lm is 'linear model'  
summary(lm_result)
```

R strengths for HPC (IMHO)

- **Data Wrangling –**
- **Particular statistical procedure implementations -**
 - Imputation methods (for missing data)
 - Sampling methods
 - Instrument Variable (2 stage) Regression
 - Matching subjects for pairwise analysis
 - MCMC routines (but Stan is likely better package)
 - Generalized Linear Model
 - Some ML model (e.g. randomForest)

R Scaling In a nutshell

- R uses BLAS/LAPACK math libraries for operations on vectors
[Same for Matlab and Python]
- R packages provide multicore, out-of-core, multinode, or distributed data (SparkR) options
[Same for Matlab and Python]
- Some ML model implementations may be built to use parallel backends (review the available options)

R Scaling In a nutshell

- R sessionInfo() command shows math libraries

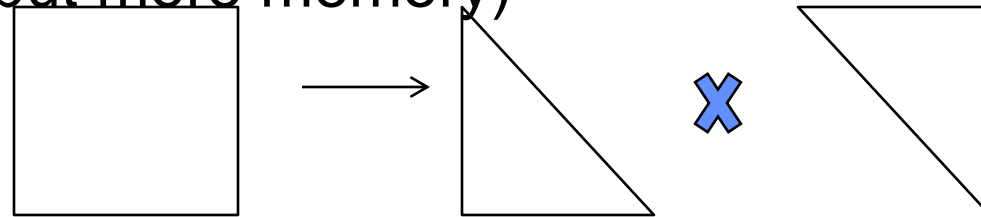
```
> sessionInfo()
R version 4.0.2 (2020-06-22)
Platform: x86_64-pc-linux-gnu (64-bit)
Running under: CentOS Linux 8 (Core)

Matrix products: default
BLAS/LAPACK: /cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen2/gcc-9.2.0/openblas
grrcfayp3br6kmcnelbgrepqmadwv43e/lib/libopenblas_zenp-r0.3.10.so

locale:
 [1] LC_CTYPE=en_US.UTF-8      LC_NUMERIC=C
 [3] LC_TIME=en_US.UTF-8      LC_COLLATE=en_US.UTF-8
 [5] LC_MONETARY=en_US.UTF-8  LC_MESSAGES=en_US.UTF-8
```

Consider Regression Computations

- **Linear Model:** $Y = X * B$
where Y =outcomes , X =data matrix
- **Algebraically, we could:**
take “inverse” of $X * Y = B$ (time consuming)
use derivatives to search for solutions (very general)
- **Or, better:**
QR decomposition of X into triangular matrices (easier to solve but more memory)



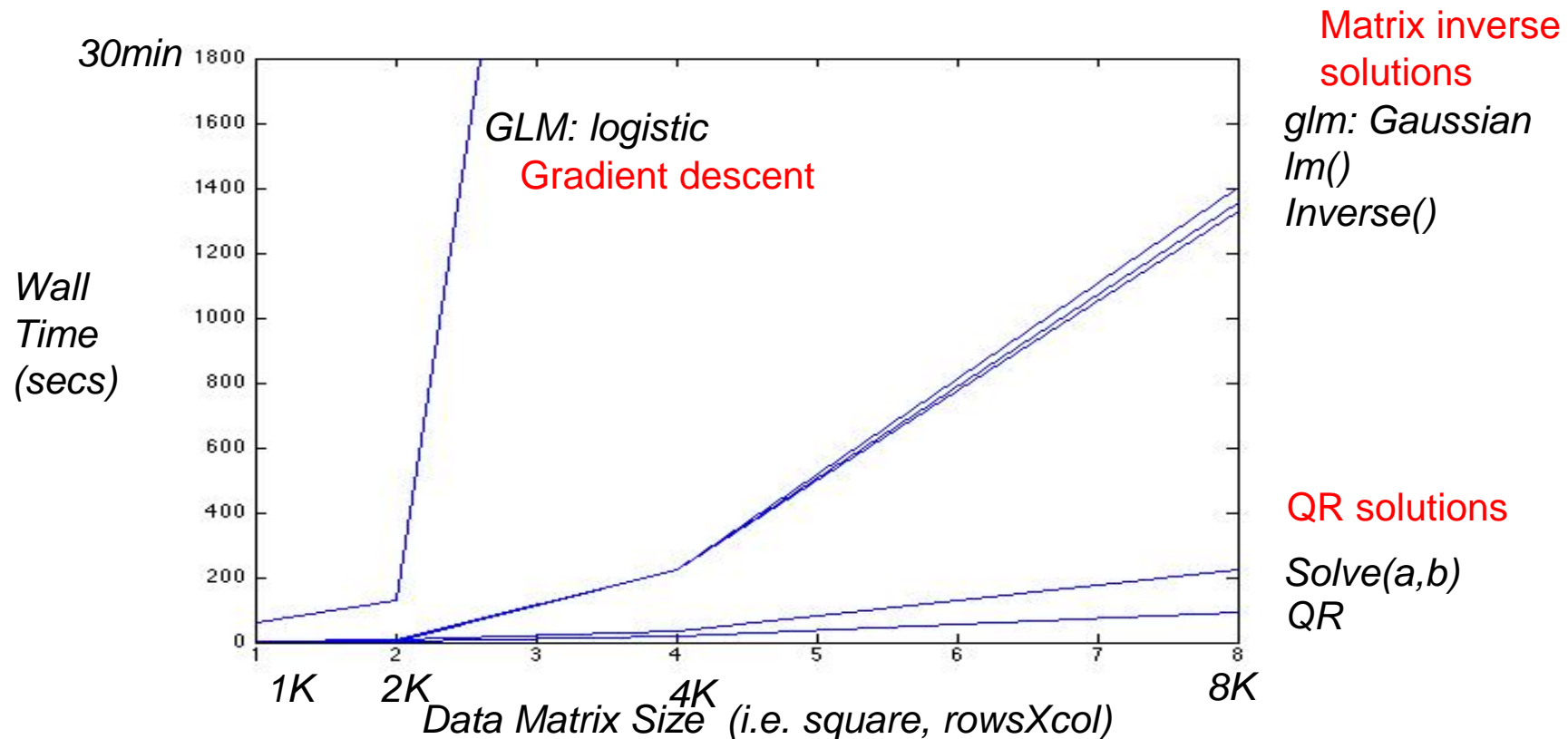
Solving Linear Systems

Performance with R, 1 compute node

R:

`glm(Y~X,family=gaussian)` #gaussn regrssn (like `lm`)

`glm(Y~X,family=binomial)` # logistic regrssn ($Y=0$ or 1)



R multicore processing

- ‘doParallel’ package – provides the back end to the ‘for each’ parallel processing command
- uses threads across cpu cores to pass data & commands
- It also works for multinode (runs on top of RMPI)

See <https://cran.r-project.org/web/packages/doParallel/vignettes/gettingstartedParallel.pdf>

R multicore coding

```
install.packages(doParallel)  
library(doParallel)  
registerDoParallel(cores=24)
```

1. allocate workers ←

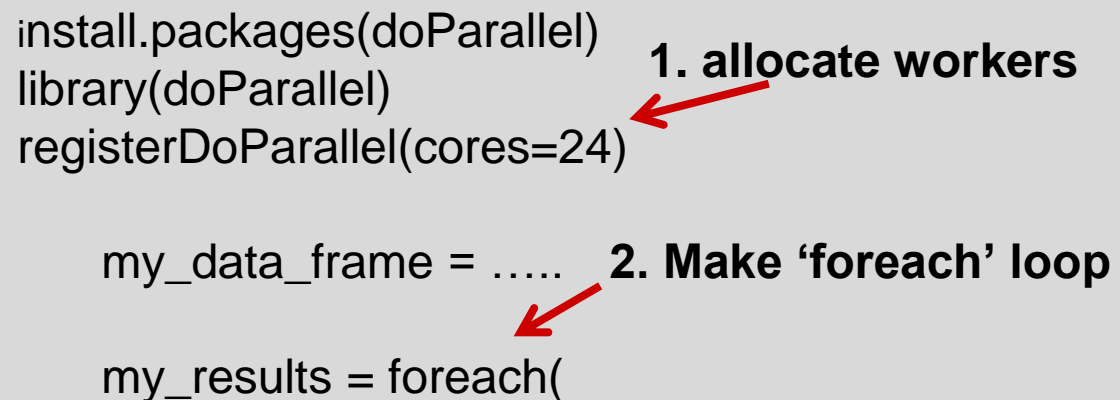
R multicore coding

```
install.packages(doParallel)  
library(doParallel)  
registerDoParallel(cores=24)
```

1. allocate workers

2. Make 'foreach' loop

```
my_data_frame = .....  
my_results = foreach(
```



R multicore coding

```
install.packages(doParallel)  
library(doParallel)  
registerDoParallel(cores=24)
```


1. allocate workers



```
my_data_frame = ..... 2. Make 'foreach' loop
```

```
my_results = foreach(i=1:24,.combine=rbind)
```

**3. specify how to
combine results**



R multicore coding

```
install.packages(doParallel)
library(doParallel)
registerDoParallel(cores=24)

my_data_frame = .....
my_results = foreach(i=1:24,.combine=rbind) %dopar%
{ ... }
```

1. allocate workers

2. Make 'foreach' loop

3. specify how to combine results

4. %dopar% runs it across cores, (%do% runs it serially)

R multicore coding

```
install.packages(doParallel)
library(doParallel)
registerDoParallel(cores=24)

my_data_frame = .....
my_results = foreach(i=1:24,.combine=rbind) %dopar%
{ ...
  your code here
  return( a variable or object )
})
```

1. allocate workers

2. Make 'foreach' loop

3. specify how to combine results

4. %dopar% runs it across cores, (%do% runs it serially)

R multicore coding

```
install.packages(doParallel)
library(doParallel)
registerDoParallel(cores=24)
```

1. allocate workers

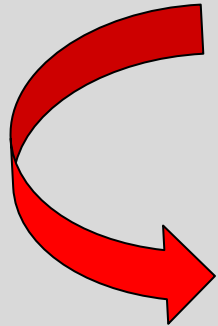
```
my_data_frame = .....
```

2. Make 'foreach' loop

```
my_results = foreach(i=1:24,.combine=rbind) %dopar%
{ ...
  your code here
  return( a variable or object )
}
```

3. specify how to combine results

4. %dopar% runs it across cores, (%do% runs it serially)



BEWARE: foreach will copy data to every core if its seems necessary

R multinode: parallel backend

```
library(doParallel)
```

```
cl <- makeCluster(48)  
registerDoParallel(cl)
```

**1. allocate cluster as
parallel backend**



R multinode: parallel backend

```
library(doParallel)
```

```
cl <- makeCluster(48)  
registerDoParallel(cl)
```


**1. allocate cluster as
parallel backend**



```
my_data_frame = .....
```

```
results = foreach(i=1:48,.combine=rbind) %dopar%  
{ ... your code here
```

**2.
%dopar% puts
loops across
cores and
nodes**



```
    return( a variable or object )  
  })  
stopCluster(cl)
```

R multinode: parallel backend

```
library(doParallel)
```

```
cl <- makeCluster(48)  
registerDoParallel(cl)
```


**1. allocate cluster as
parallel backend**



```
my_data_frame = .....
```

```
results = foreach(i=1:48,.combine=rbind) %dopar%  
{ ... your code here
```

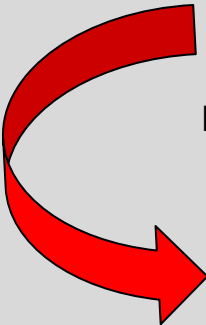
**2.
%dopar% puts
loops across
cores and
nodes**



```
return( a variable or object )
```

```
}}
```

```
stopCluster(cl)
```



BEWARE: foreach will copy data to every core in every node if it seems necessary

Speaking of R and memory...

Recall the other day
Marty noticed, someone
was running R (using
\$top)

Several R processing
going, and only 16Gb
free memory left!

```
top - 16:27:58 up 35 days, 22:29, 234 users, load average: 211.08, 147.10, 87.3
Threads: 7388 total, 25 running, 7118 sleeping, 242 stopped, 3 zombie
%Cpu(s):  5.8 us,  7.5 sy,  0.0 ni, 67.4 id, 19.0 wa,  0.1 hi,  0.1 si,  0.0 st
MiB Mem : 127842.9 total, 15550.3 free, 61423.8 used, 50868.8 buff/cache
MiB Swap: 12288.0 total, 244.0 free, 12044.0 used. 64421.1 avail Mem
```

PID	USER	PR	NI	VIRT	RES	SHR	S	%CPU	%MEM	TIME+	COMMAND
8170165	mrincon	20	0	7016	3448	1540	R	99.9	0.0	14:48.71	gzip
8430379	keyajos+	20	0	529984	26628	13900	R	99.7	0.0	21:05.47	cpptraj
8503080	keyajos+	20	0	528032	26388	14052	R	99.7	0.0	8:13.02	cpptraj
3563	root	20	0	9881.4m	138724	135408	S	43.8	0.1	17638:46	in:imjo+
2979421	jis038	20	0	7968716	31444	11536	R	41.0	0.0	34:23.16	R
2979433	jis038	20	0	7968716	31444	11536	R	41.0	0.0	34:21.34	R
2979432	jis038	20	0	7968716	31444	11536	R	40.3	0.0	34:21.18	R
2979435	jis038	20	0	7968716	31444	11536	R	40.3	0.0	34:25.71	R
2979431	jis038	20	0	7968716	31444	11536	R	40.0	0.0	34:22.04	R
8531483	sgolzari	20	0	2437332	1.6g	17492	R	12.7	1.2	0:37.56	conda
1965101	sgolzari	20	0	7928092	27712	5752	R	11.7	0.0	31:53.05	R
397946	sgolzari	20	0	7909624	26136	4788	R	11.1	0.0	60:16.22	R
1965093	sgolzari	20	0	7928092	27712	5752	R	11.1	0.0	31:49.91	R
397945	sgolzari	20	0	7909624	26136	4788	R	10.8	0.0	60:17.28	R
397947	sgolzari	20	0	7909624	26136	4788	R	10.8	0.0	60:18.83	R
827069	sgolzari	20	0	7909628	26468	5360	R	10.8	0.0	51:36.85	R

1/1 [=====]

Testing/Evaluating R parallel command line

- Exercise: 'TestdoParallel' R script

1. Log into expanse portal
2. \$ srun-compute
3. \$ cd ciml..institute../4.2_r_on_HPC folder
4. \$ Rscript --vanilla TestDoParallel_v1.R
(this might first install DoParallel R package and ask for confirmation and repo site – choose a US site)

```
[train113@exp-1-24 4.2.RandHPC]$ Rscript --vanilla ./TestDoParallel_v1.R
Loading required package: doParallel
Loading required package: foreach
Loading required package: iterators
Loading required package: parallel
[1] "starting dopar test"
[1] "Using N rows= 10000 P cols= 200"
[1] "X size is: 15.3 Mb"
item selected 6.43 MB
```

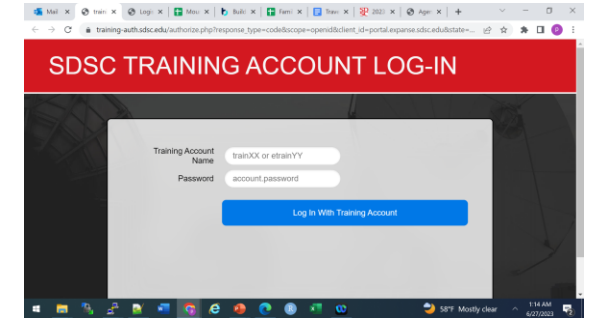
Also start a 2nd terminal and ssh into that compute node and run top -u \$USER - how memory usage?

Testing/Evaluating R parallel

- Exercise: 'TestdoParallel' R script

1. Log into expanse portal and start R studio

goto URL: *<https://portal.expanse.sdsc.edu/training>*



2. Also log into expanse command line and ssh to compute node

3. run 'top -u username' to see performance

- look for tradeoffs in memory vs execution as matrix size varies (see next slides)

The screenshot shows the SDSC Expanse Portal interface. The 'Interactive Apps' dropdown menu is open, highlighting 'RSTUDIO'. Below, the 'batch_connect/sys/rstudio/session_contexts/new' page is shown, where the 'Partition' is set to 'compute' and the 'Number of hours' is left blank.

1 Open portal ->
Interactive Apps ->
Rstudio

Enter

Node: "compute"

Cores: "64"

Memory: 124 Gb

(other fields defaults ok)

2 Also login to Expanse terminal
window

```
-----
Last login: Fri Jun  4 15:01:29 2021 from 71.128.8.73
[p4rodrig@login02 ~]$ squeue -u p4rodrig
          JOBID PARTITION    NAME             USER  ST       TIME  NODES NODELIST(REAS
SON)
          3246260      compute sys/dash p4rodrig    R       0:27      1 exp-2-15
[p4rodrig@login02 ~]$ ssh exp-2-15
Last login: Sat Jun  5 13:09:04 2021
[p4rodrig@exp-2-15 ~]$ top -u $USER
```

\$ squeue -u \$USER

\$ ssh exp-##-##

\$ top -u \$USER

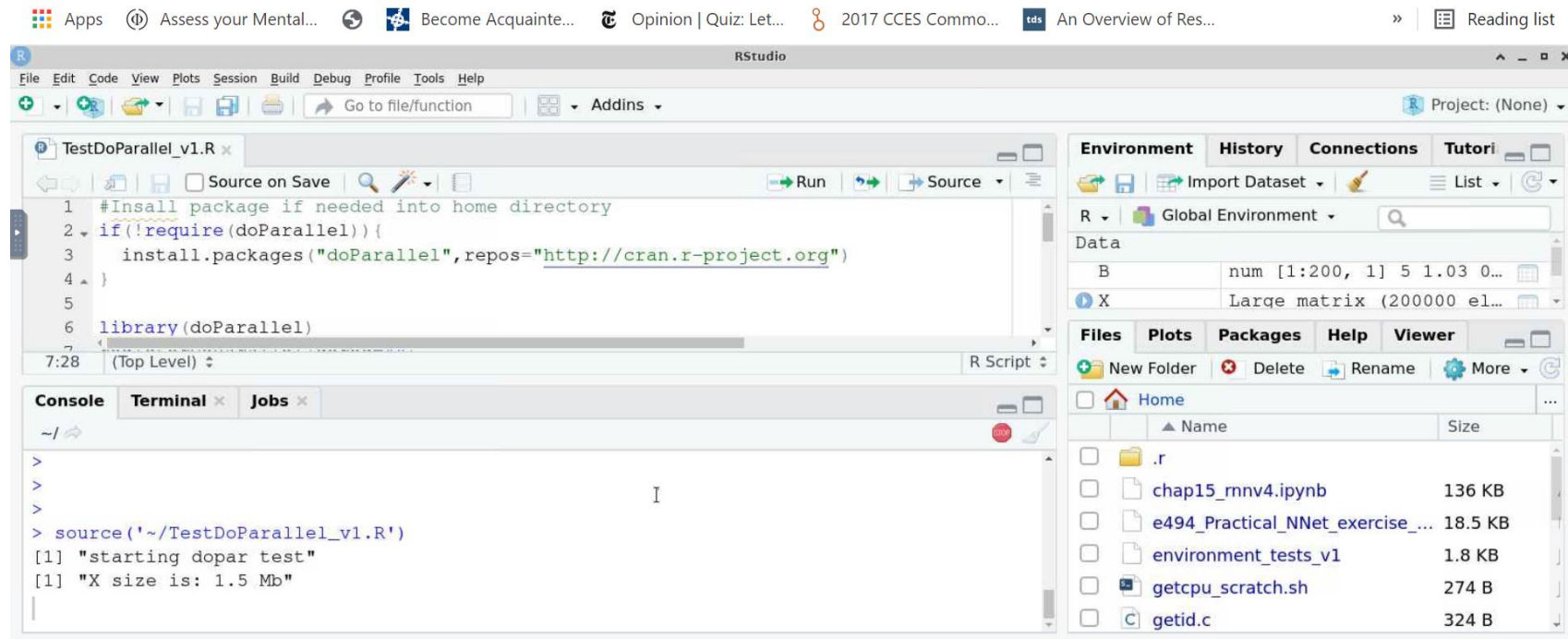
'H' will toggle threads

'f', downarrow to P, space, esc.

3 Open the 'Test_doParallel' Rscript

Select 'source' to run the whole script, it will install 'doParallel' package (if the R installation doesn't have it already)

look for # <<< ----- comments to change data parameters



The screenshot shows the RStudio interface with the following components:

- Script Editor:** Contains the R script 'TestDoParallel_v1.R' with the following code:

```
1 #Install package if needed into home directory
2 if(!require(doParallel)){
3   install.packages("doParallel",repos="http://cran.r-project.org")
4 }
5
6 library(doParallel)
```
- Console:** Shows the output of running the script:

```
> source('~/.TestDoParallel_v1.R')
[1] "starting dopar test"
[1] "X size is: 1.5 Mb"
```
- Environment:** Shows the Global Environment with variables 'B' (a numeric vector) and 'X' (a large matrix).
- Files:** Shows a file explorer view of the home directory with files like '.r', 'chap15_mnv4.ipynb', 'e494_Practical_NNet_exercise...', 'environment_tests_v1', 'getcpu_scratch.sh', and 'getid.c'.

Review the top output

```
p4rodrig@exp-9-27:~$ top
top - 15:35:51 up 87 days, 21:07, 1 user, load average: 20.97, 5.76, 4.37
Tasks: 1788 total, 41 running, 1747 sleeping, 0 stopped, 0 zombie
%Cpu(s): 32.6 us, 0.1 sy, 0.0 ni, 67.0 id, 0.0 wa, 0.2 hi, 0.1 si, 0.0 st
MiB Mem : 257517.8 total, 210968.9 free, 42132.2 used, 4416.7 buff/cache
MiB Swap: 0.0 total, 0.0 free, 0.0 used, 210846.5 avail Mem

  PID USER      PR  NI    VIRT    RES    SHR S  %CPU  %MEM    TIME+   COMMAND
 54587 p4rodrig  20   0   17.5g   896016  4196 R 100.0   0.3   0:37.27 rsession
 54562 p4rodrig  20   0   17.5g   896016  4196 R  99.7   0.3   0:37.48 rsession
 54568 p4rodrig  20   0   17.5g   896016  4196 R  99.7   0.3   0:37.46 rsession
 54571 p4rodrig  20   0   17.5g   896016  4196 R  99.7   0.3   0:37.35 rsession
 54572 p4rodrig  20   0   17.5g   896016  4196 R  99.7   0.3   0:37.33 rsession
 54574 p4rodrig  20   0   17.5g   896016  4196 R  99.7   0.3   0:37.38 rsession
 54579 p4rodrig  20   0   17.5g   896016  4196 R  99.7   0.3   0:37.33 rsession
 54591 p4rodrig  20   0   17.5g   896016  4196 R  99.7   0.3   0:37.24 rsession
```

Notice the elapsed time and memory size

Change the NxP matrix size and rerun

(start with N=10K, P=2K)

```
7:28 (Top Level)
Console Terminal x Jobs x
~/
>
> source('~/TestDoParallel_v1.R')
[1] "starting dopar test"
[1] "X size is: 1.5 Mb"
      user system elapsed
1.176   1.969  30.620
>
```

```
10 # Make up some random data and lis
11 N=100000;      #N rows start with
12 P=2000;        #P columns 200 for
13
14 #make random data with 1 column ar
15 X =matrix(rnorm(N*P),N,P)
16 X[,1] =X[,1]+1
17
16:28 (Top Level)
Console Terminal x Jobs x
~/
Loading required package: foreach
Loading required package: iterators
Loading required package: parallel
[1] "starting dopar test"
[1] "X size is: 1.5 Gb"
```

Try this at home:

Let $N=100K$, $P=2000$

Notice the memory used is close to 124Gb we asked for

```
p4rodrig@exp-9-27:~  
top - 15:38:40 up 87 days, 21:10, 1 user, load average: 10.77, 6.29, 4.76  
Tasks: 1749 total, 19 running, 1730 sleeping, 0 stopped, 0 zombie  
%Cpu(s): 14.0 us, 0.0 sy, 0.0 ni, 85.8 id, 0.0 wa, 0.0 hi, 0.0 si, 0.0 st  
MiB Mem : 257517.8 total, 130239.0 free, 123199.7 used, 4079.0 buff/cache  
MiB Swap: 0.0 total, 0.0 free, 0.0 used, 129947.3 avail Mem
```

PID	USER	PR	NI	VIRT	RES	SHR	S	%CPU	%MEM	TIME+	COMMAND	P
55219	p4rodrig	20	0	24.2g	7.6g	2696	R	100.0	3.0	0:24.52	rsession	68
55227	p4rodrig	20	0	24.2g	7.6g	3064	R	100.0	3.0	0:24.55	rsession	88
55235	p4rodrig	20	0	24.2g	7.6g	2696	R	100.0	3.0	0:24.56	rsession	80
55236	p4rodrig	20	0	24.2g	7.6g	2696	R	100.0	3.0	0:24.70	rsession	100
55237	p4rodrig	20	0	24.2g	7.6g	2696	R	100.0	3.0	0:24.50	rsession	47
55242	p4rodrig	20	0	24.2g	7.6g	2696	R	100.0	3.0	0:24.36	rsession	32
55253	p4rodrig	20	0	24.2g	7.6g	2696	R	100.0	3.0	0:24.69	rsession	126
55259	p4rodrig	20	0	24.2g	7.6g	2696	R	100.0	3.0	0:24.00	rsession	16
55261	p4rodrig	20	0	24.2g	7.6g	2696	R	100.0	3.0	0:24.25	rsession	24
55265	p4rodrig	20	0	24.2g	7.6g	2696	R	100.0	3.0	0:23.96	rsession	6
55239	p4rodrig	20	0	24.2g	7.6g	2696	R	99.7	3.0	0:24.61	rsession	20
55241	p4rodrig	20	0	24.2g	7.6g	2696	R	99.7	3.0	0:24.43	rsession	8
55243	p4rodrig	20	0	24.2g	7.6g	2836	R	99.7	3.0	0:24.53	rsession	104

If you ask for 248Gb will it run?

What if you use only 24 cores?

Parallezing for loops

(pseudo code)

R with doParallel

makecluster
registercluster

foreach with dopar,

combine results

Matlab with parallel toolbox

parcluster('local')
parpool()

parfor
or
'spmd' with
distributed arrays

gather array

Python with dask.distributed

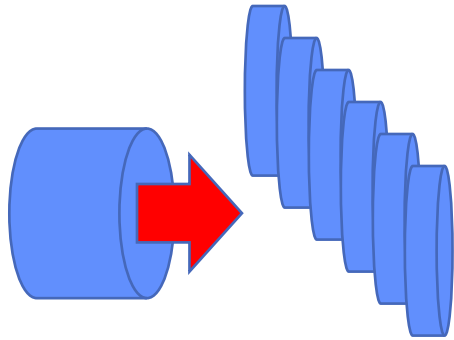
Import delayed, Client
Client(numwkr)

for i in range(numwkr):
 A=delayed(my_func)(i)
 Acombine.append(A)

Acombined.compute()

An option for (embarrassingly) Parallel R

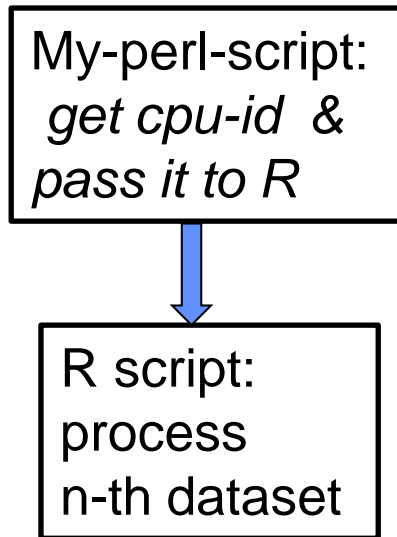
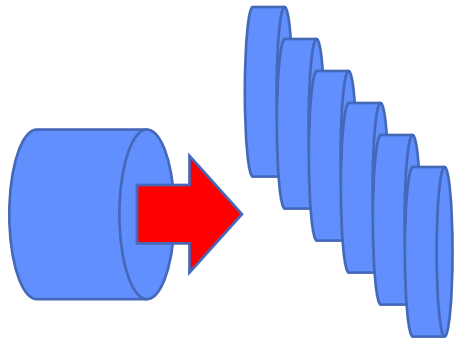
1. Split up data into N parts



An option for (embarrassingly) Parallel R

1. Split up
data into N
parts

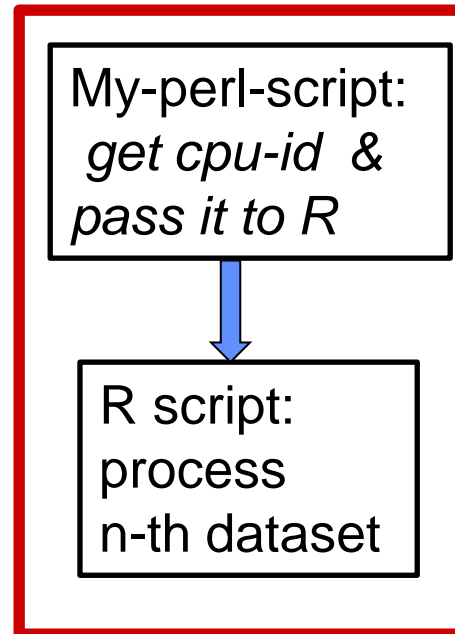
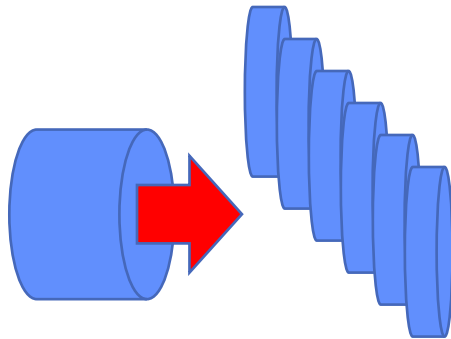
2. In slurm batch script:
`mpirun ... my-perl-script`



An option for (embarrassingly) Parallel R

1. Split up
data into N
parts

2. In slurm batch script:
`mpirun ... my-perl-script`



*This gets
distributed
across nodes
and cores by
slurm & mpi
parameters*

Slurm parameters: one R instance per core across all nodes

Normal
batch
job info

```
...  
#SBATCH --partition=compute  
#SBATCH --nodes=2  
#SBATCH --ntasks-per-node=128  
#SBATCH --cpus-per-task=1
```

2 x 128 = 256 mpi ranks

```
module load slurm  
module load cpu  
module load gcc  
module load intel-mpi
```

256 perl script/R instances
1 core each

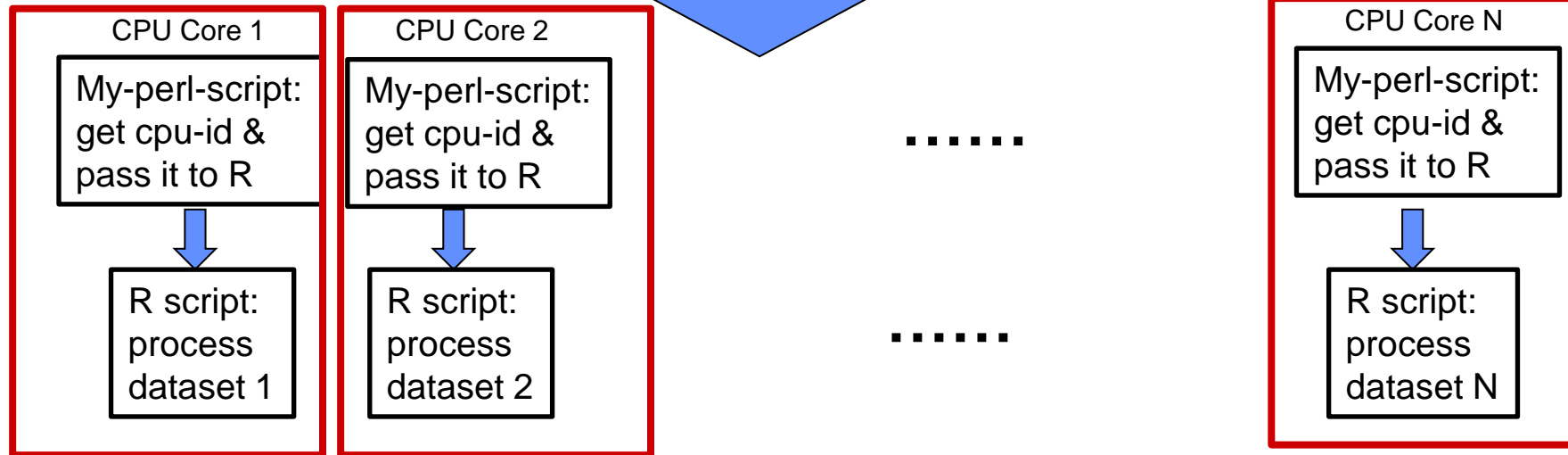
```
mpirun -genv I_MPI_PIN_DOMAIN=omp:compact ./get_mpirank_runcmd.pl
```

(based on /cm/shared/examples/sdsc/mpi-openmp-hybrid/hybrid-slurm.sb)

one R instance per core across all nodes

1. Split up
data into N
parts

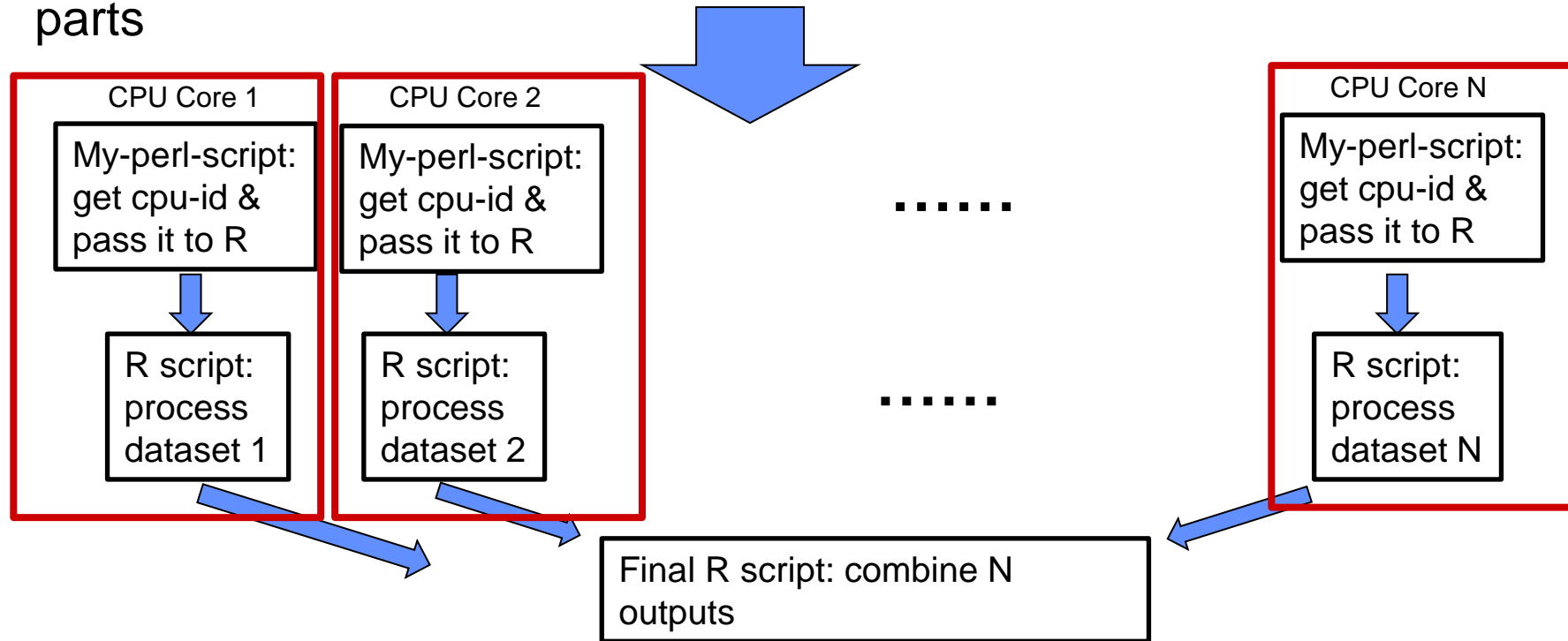
2. In slurm batch script:
`mpirun ... my-perl-script`



one R instance per core across all nodes

1. Split up data into N parts

2. In slurm batch script:
mpirun ... my-perl-script



More programming but perhaps more useful

Slurm parameters: one R instance per node with 128 cores per R instance

Normal
batch
job info

```
...  
#SBATCH --partition=compute  
#SBATCH --nodes=2  
#SBATCH --ntasks-per-node=1  
#SBATCH --cpus-per-task=128  
  
module load slurm  
module load cpu  
module load gcc  
module load intel-mpi  
  
module load r  
  
mpirun -genv I_MPI_PIN_DOMAIN=omp:compact ./get_mpirank_runcmd.pl
```

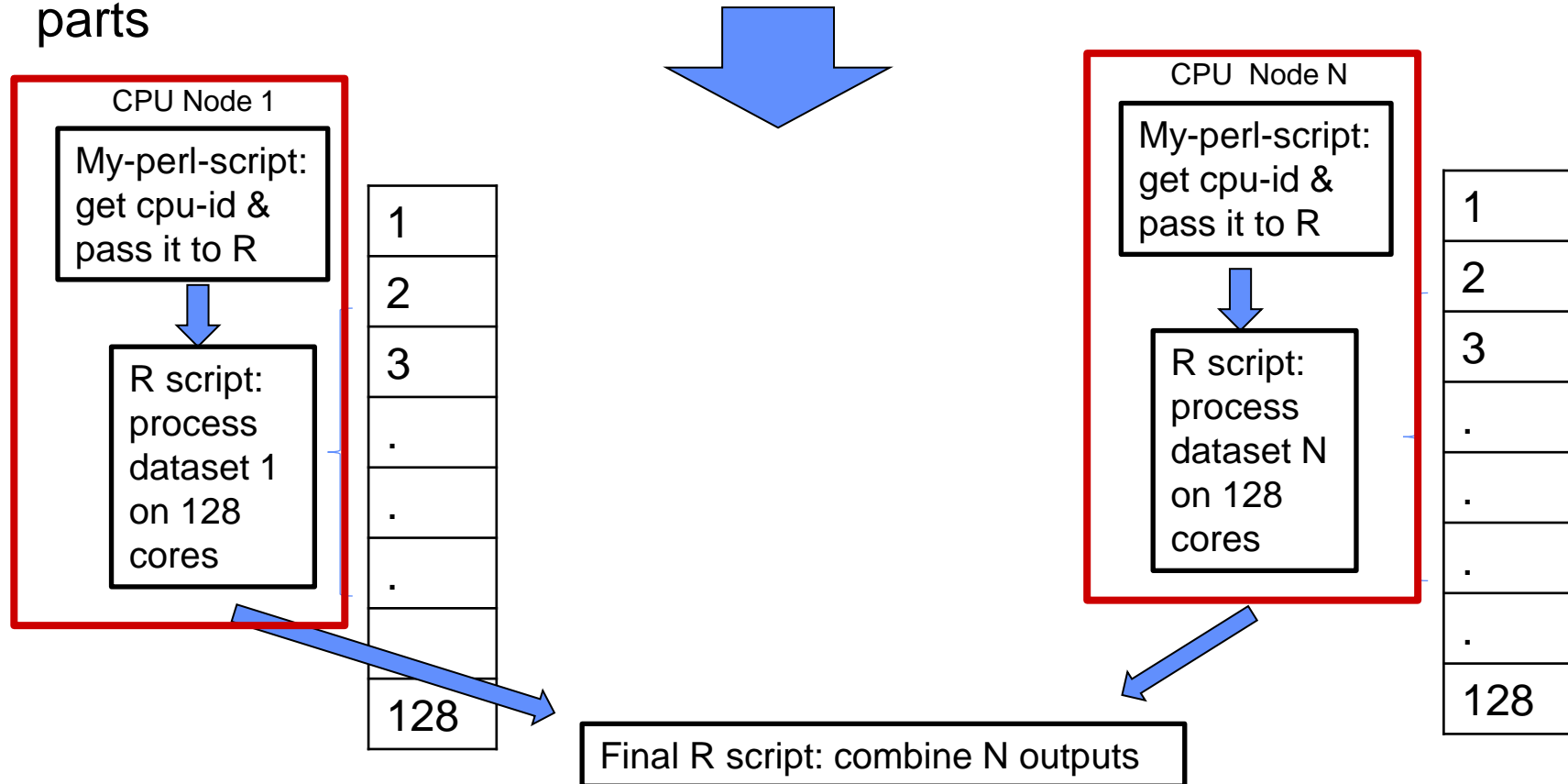
2 x 1 = 2 mpi ranks

2 perl script/R instances
128 cores each
(doParallel can use them)

Example: One R instance per node, doParallel across all cores in each node

1. Split up
data into N
parts

2. In slurm batch script:
mpirun ... my-perl-script



Big Data exploration

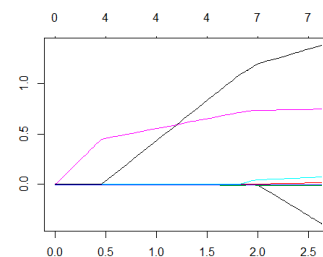
- Run R 'biglasso' with a dataset too big for RAM
- Create large CSV file (117Gb) of X data matrix and Y outcomes:
 $Y = X * B + \text{noise}$ (where X is 100K x 50K)
- Explore other packages with out-of-core dataset functions:
Matlab, Dask-ML, Spark, Keras
- Beware: lasso implementations can differ;
also, Y, X, B should be 'nice'

Lasso Regression

- Penalized Loss function $L = MSE + \lambda \sum |b_i|$
- Recall: using penalty term is the same as using a constraint (constrained optimization)

find min MSE such that $\sum |b_i| < S$

- Different implementations may:
 - use different fit methods (ie forward stepwise, coordinate descent, gradient descent,...)
 - might parallelize by splitting up data, computations, or vectorizing
 - read/load data more or less efficiently



Considerations

- All packages have special functions to handle out of core dataset
- Sometimes better to have Y,X together; sometimes two files are better
- All were run as Expanse batch jobs, not through notebook/portal
- All were set up run on 1 compute node (248Gb RAM) and use scratch (ssd) space. (Large memory nodes are available on Expanse, but not tested)
- Mostly default parameters used; Little optimization performed; Not a benchmark study!

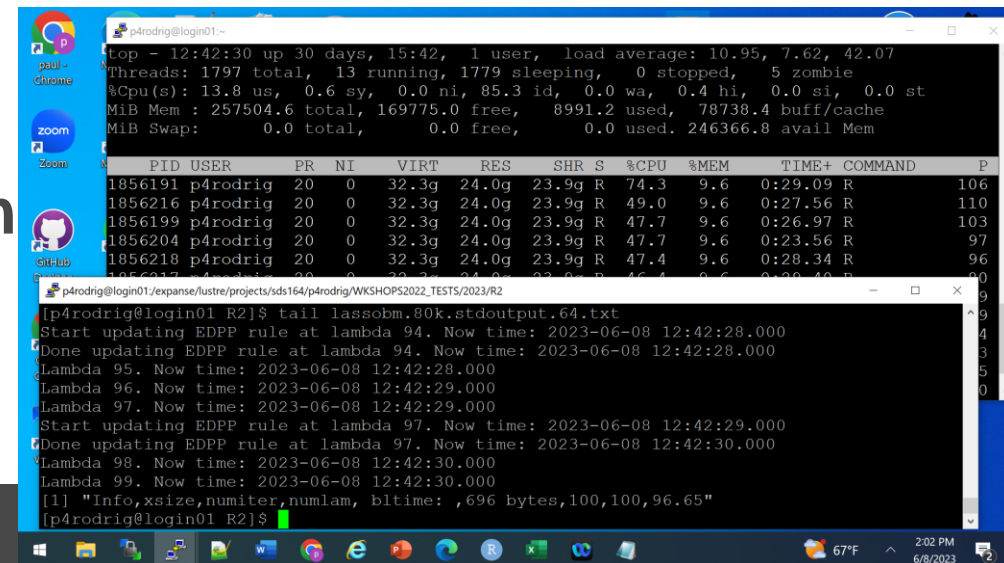
R

- R – biglasso (bigmatrix) package to set up file backed dataframe

<https://cran.rstudio.com/web/packages/biglasso/>

Issue: the file backend for the big data object path option was hard to get right – ended up just running out of scratch SSD as working directory;

Outcome: R copies everything into binary file and descriptor file and got results in about 2hours



```
p4rodrig@login01:~$ top - 12:42:30 up 30 days, 15:42, 1 user, load average: 10.95, 7.62, 42.07
Threads: 1797 total, 13 running, 1779 sleeping, 0 stopped, 5 zombie
%Cpu(s): 13.8 us, 0.6 sy, 0.0 ni, 85.3 id, 0.0 wa, 0.4 hi, 0.0 si, 0.0 st
MiB Mem : 257504.6 total, 169775.0 free, 8991.2 used, 78738.4 buff/cache
MiB Swap: 0.0 total, 0.0 free, 0.0 used, 246366.8 avail Mem

  PID USER      PR  NI   VIRT   RES   SHR  S  %CPU  %MEM     TIME+ COMMAND      P
1856191 p4rodrig  20   0  32.3g  24.0g  23.9g  R   74.3    9.6   0:29.09 R        106
1856216 p4rodrig  20   0  32.3g  24.0g  23.9g  R   49.0    9.6   0:27.56 R        110
1856199 p4rodrig  20   0  32.3g  24.0g  23.9g  R   47.7    9.6   0:26.97 R        103
1856204 p4rodrig  20   0  32.3g  24.0g  23.9g  R   47.7    9.6   0:23.56 R         97
1856218 p4rodrig  20   0  32.3g  24.0g  23.9g  R   47.4    9.6   0:28.34 R         96
1856217 p4rodrig  20   0  32.3g  24.0g  23.9g  R   46.4    9.6   0:28.48 R         90
```

```
p4rodrig@login01:~/expansion/lucre/projects/sds164/p4rodrig/WKSHOP2022_TESTS/2023/R2
[p4rodrig@login01 R2]$ tail lassobm.80k.stdout.64.txt
Start updating EDPP rule at lambda 94. Now time: 2023-06-08 12:42:28.000
Done updating EDPP rule at lambda 94. Now time: 2023-06-08 12:42:28.000
Lambda 95. Now time: 2023-06-08 12:42:28.000
Lambda 96. Now time: 2023-06-08 12:42:29.000
Lambda 97. Now time: 2023-06-08 12:42:29.000
Start updating EDPP rule at lambda 97. Now time: 2023-06-08 12:42:29.000
Done updating EDPP rule at lambda 97. Now time: 2023-06-08 12:42:30.000
Lambda 98. Now time: 2023-06-08 12:42:30.000
Lambda 99. Now time: 2023-06-08 12:42:30.000
[1] "Info,xsize,numiter,numlam, bltime: ,696 bytes,100,100,96.65"
[p4rodrig@login01 R2]$
```

R code highlights

Use biglasso package

Y data fits in memory so just read it in

X data will be setup with file-backed memory

biglasso() arguments look like the glmnet implementation

```
library(biglasso)

....
Y.bm=read.big.matrix(inputYfile,sep = ",")
X.bm=setupX(inputXfile,sep=","
            type="double",
            backingfile  = "x.bin",
            descriptorfile = "x.desc")

....

bl_results=biglasso( X.bm, Y.bm,
                    row.idx = 1:nrow(X.bm),
                    penalty = c("lasso"),
                    family = c("gaussian"),
                    ncores = numcores, ...)
```


Batch script for R biglasso, highlights

.....

```
#SBATCH --partition=compute
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=64
#SBATCH -A account
... etc
```

```
module load slurm
module load r
...etc
```

```
#copy data to scratch
cp Xmatrix_100000_50000.csv /scratch/$USER/job_${SLURM_JOB_ID}/Xinput.csv
cp Ymatrix_100000_1.csv /scratch/$USER/job_${SLURM_JOB_ID}/Yinput.csv
```

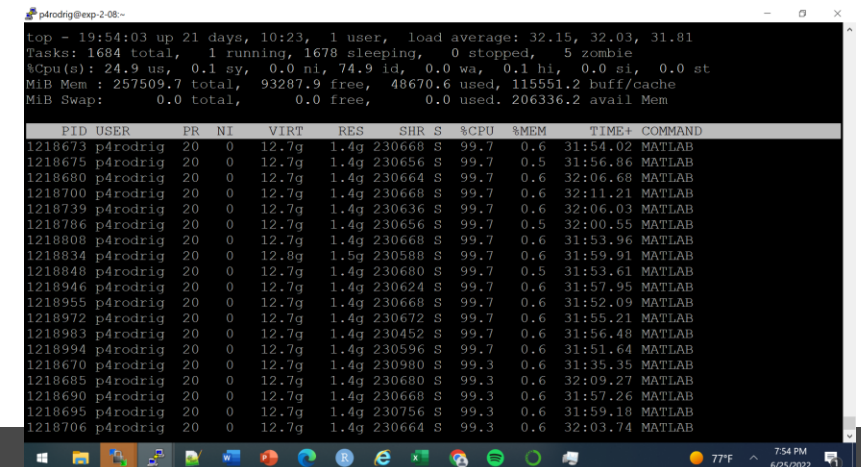
```
Rscript --vanilla path-2-your-script/rLassov2.R
    /scratch/$USER/job_${SLURM_JOB_ID}/Xinput.csv
    /scratch/$USER/job_${SLURM_JOB_ID}/Yinput.csv 64 TRUE > save_std_output.txt
```

Matlab

- Matlab – has tall table functions to read in large CSV file; but lasso needs tall array

I found a 'table2array' function that helped set up the data

But matlab tall arrays are not intended to run with too much memory, or too many columns, b/c lasso uses correlation matrix



```
p4rodrig@exp-2-08:~$ top
top - 19:54:03 up 21 days, 10:23, 1 user, load average: 32.15, 32.03, 31.81
Tasks: 1684 total, 1 running, 1678 sleeping, 0 stopped, 5 zombie
%Cpu(s): 24.9 us, 0.1 sy, 0.0 ni, 74.9 id, 0.0 wa, 0.1 hi, 0.0 si, 0.0 st
MiB Mem : 257509.7 total, 93287.9 free, 48670.6 used, 115551.2 buff/cache
MiB Swap: 0.0 total, 0.0 free, 0.0 used, 206336.2 avail Mem

  PID USER      PR  NI   VIRT   RES   SHR  S  %CPU  %MEM     TIME+ COMMAND
1218673 p4rodrig  20   0  12.7g   1.4g  230668 S   99.7   0.6   31:54.02 MATLAB
1218675 p4rodrig  20   0  12.7g   1.4g  230656 S   99.7   0.5   31:56.86 MATLAB
1218680 p4rodrig  20   0  12.7g   1.4g  230664 S   99.7   0.6   32:06.68 MATLAB
1218700 p4rodrig  20   0  12.7g   1.4g  230668 S   99.7   0.6   32:11.21 MATLAB
1218739 p4rodrig  20   0  12.7g   1.4g  230636 S   99.7   0.6   32:06.03 MATLAB
1218786 p4rodrig  20   0  12.7g   1.4g  230656 S   99.7   0.5   32:00.55 MATLAB
1218808 p4rodrig  20   0  12.7g   1.4g  230668 S   99.7   0.6   31:53.96 MATLAB
1218834 p4rodrig  20   0  12.8g   1.5g  230588 S   99.7   0.6   31:59.91 MATLAB
1218848 p4rodrig  20   0  12.7g   1.4g  230680 S   99.7   0.5   31:53.61 MATLAB
1218946 p4rodrig  20   0  12.7g   1.4g  230624 S   99.7   0.6   31:57.95 MATLAB
1218955 p4rodrig  20   0  12.7g   1.4g  230668 S   99.7   0.6   31:52.09 MATLAB
1218972 p4rodrig  20   0  12.7g   1.4g  230672 S   99.7   0.6   31:55.21 MATLAB
1218983 p4rodrig  20   0  12.7g   1.4g  230452 S   99.7   0.6   31:56.48 MATLAB
1218994 p4rodrig  20   0  12.7g   1.4g  230596 S   99.7   0.6   31:51.64 MATLAB
1218670 p4rodrig  20   0  12.7g   1.4g  230980 S   99.3   0.6   31:35.35 MATLAB
1218685 p4rodrig  20   0  12.7g   1.4g  230680 S   99.3   0.6   32:09.27 MATLAB
1218690 p4rodrig  20   0  12.7g   1.4g  230668 S   99.3   0.6   31:57.26 MATLAB
1218695 p4rodrig  20   0  12.7g   1.4g  230756 S   99.3   0.6   31:59.18 MATLAB
1218706 p4rodrig  20   0  12.7g   1.4g  230664 S   99.3   0.6   32:03.74 MATLAB
```

Dask-ml

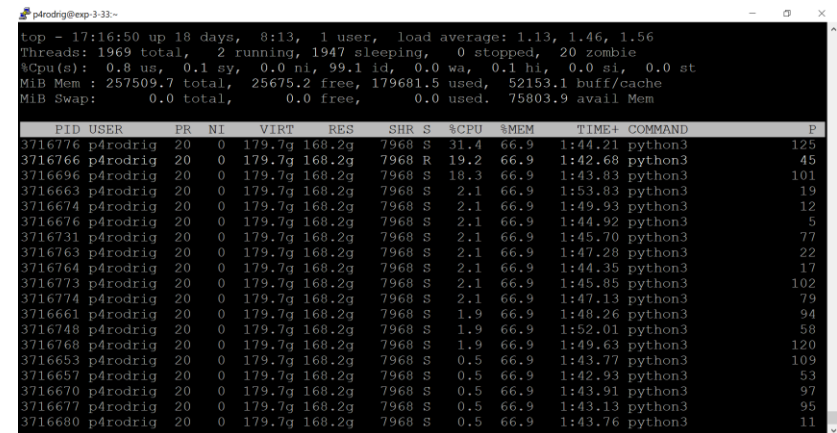
- Dask-ML – worked easily with distributed dataframe, built on top of sklearn,

`read_csv` uses a 'blocksize' parameter

repeatedly calls sklearn 'partial-fit' functions that iterate 1 time for 'batch' processing

worked better with Y&X in one dataframe

I stopped it after 4hrs, but it was running



The image shows a terminal window with the following content:

```
p4rodrig@exp-3-33:~$ top - 17:16:50 up 18 days, 8:13, 1 user, load average: 1.13, 1.46, 1.56
Threads: 1969 total, 2 running, 1947 sleeping, 0 stopped, 20 zombie
%Cpu(s): 0.8 us, 0.1 sy, 0.0 ni, 99.1 id, 0.0 wa, 0.1 hi, 0.0 si, 0.0 st
MiB Mem : 257509.7 total, 25675.2 free, 179681.5 used, 52153.1 buff/cache
MiB Swap: 0.0 total, 0.0 free, 0.0 used, 75803.9 avail Mem
```

PID	USER	PR	NI	VIRT	RES	SHR	S	%CPU	%MEM	TIME+	COMMAND	P
3716776	p4rodrig	20	0	179.7g	168.2g	7968	S	31.4	66.9	1:44.21	python3	125
3716766	p4rodrig	20	0	179.7g	168.2g	7968	R	19.2	66.9	1:42.68	python3	45
3716696	p4rodrig	20	0	179.7g	168.2g	7968	S	18.3	66.9	1:43.83	python3	101
3716663	p4rodrig	20	0	179.7g	168.2g	7968	S	2.1	66.9	1:53.83	python3	19
3716674	p4rodrig	20	0	179.7g	168.2g	7968	S	2.1	66.9	1:49.93	python3	12
3716676	p4rodrig	20	0	179.7g	168.2g	7968	S	2.1	66.9	1:44.92	python3	5
3716731	p4rodrig	20	0	179.7g	168.2g	7968	S	2.1	66.9	1:45.70	python3	77
3716763	p4rodrig	20	0	179.7g	168.2g	7968	S	2.1	66.9	1:47.28	python3	22
3716764	p4rodrig	20	0	179.7g	168.2g	7968	S	2.1	66.9	1:44.35	python3	17
3716773	p4rodrig	20	0	179.7g	168.2g	7968	S	2.1	66.9	1:45.85	python3	102
3716774	p4rodrig	20	0	179.7g	168.2g	7968	S	2.1	66.9	1:47.13	python3	79
3716661	p4rodrig	20	0	179.7g	168.2g	7968	S	1.9	66.9	1:48.26	python3	94
3716748	p4rodrig	20	0	179.7g	168.2g	7968	S	1.9	66.9	1:52.01	python3	58
3716768	p4rodrig	20	0	179.7g	168.2g	7968	S	1.9	66.9	1:49.63	python3	120
3716653	p4rodrig	20	0	179.7g	168.2g	7968	S	0.5	66.9	1:43.77	python3	109
3716657	p4rodrig	20	0	179.7g	168.2g	7968	S	0.5	66.9	1:42.93	python3	53
3716670	p4rodrig	20	0	179.7g	168.2g	7968	S	0.5	66.9	1:43.91	python3	97
3716677	p4rodrig	20	0	179.7g	168.2g	7968	S	0.5	66.9	1:43.13	python3	95
3716680	p4rodrig	20	0	179.7g	168.2g	7968	S	0.5	66.9	1:43.76	python3	11

Spark

- Spark – uses distributed dataframe with pyspark.ml.regression package

Use the vector assembler options to get Y and 'features' all in one dataframe

Got some help on spark session options:

device & executor memory, eg: local[64], 8Gb, 2Gb

I stopped it after 4 hrs; it was running

Local[64], 50 min in, 1 iteration

```
p4rodrig@exp-6-40:~$ top - 11:34:21 up 18 days, 18:18, 1 user, load average: 1.12, 4.39, 26.17
Threads: 1980 total, 2 running, 1971 sleeping, 0 stopped, 7 zombie
%Cpu(s): 1.0 us, 0.6 sy, 0.0 ni, 98.4 id, 0.0 wa, 0.0 hi, 0.0 si, 0.0 st
MiB Mem : 257509.7 total, 96845.3 free, 24911.5 used, 135752.9 buff/cache
MiB Swap: 0.0 total, 0.0 free, 0.0 used, 230237.8 avail Mem

  PID USER      PR  NI   VIRT   RES    SHR   S  %CPU  %MEM    TIME+  COMMAND      P
3307477 p4rodrig  20   0  37.3g  15.6g  31100  R   98.3   6.2  15:45.96 Thread-4      65
3307364 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:55.26 java        113
3307366 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:55.05 java        34
3307369 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:55.03 java       115
3307373 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:55.20 java        12
3307374 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:55.22 java        16
3307375 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:55.20 java        83
3307380 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:55.13 java         3
3307381 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:55.17 java        33
3307395 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:54.79 java        67
3307396 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:54.90 java        30
3307402 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:54.82 java        66
3307409 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:55.14 java        82
3307411 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:54.93 java        52
3307420 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:54.92 java       116
3307426 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:54.86 java        23
3307430 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:54.90 java        63
3307433 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:55.25 java        64
3307435 p4rodrig  20   0  37.3g  15.6g  31100  S    1.7   6.2  30:55.20 java       112
```

Keras

- Keras - set up a tensorflow dataset with data generator (to reading batches at a time from csv file); a little tricky to get shapes right;

I set up a 1 layer linear neural network with a L1 regularizer on weights

runs, 1000 epochs in 1 hour+ (on cpu)

I did not set up convergence options like other Lasso implementations

Some notes

- **Start with small data with interactive session or notebook – maybe even just use a smaller sample?**
- **All packages generally work as documented, but**
- **All packages require working through some implementation issues or environment options for the session/job/execution**

How to use R directly on Expanse

1. Get an interactive compute node:

2. Try

`$ module spider r` *(this tells you what modules you need)*

3. Enter

`$ module load cpu/0.15.4`

`$ module load gcc/9.2.0`

`$ module load r/4.0.2-openblas`

`$ R`

R version 4.0.2 (2020-06-22) -- "Taking Off Again"

Copyright (C) 2020 The R Foundation for Statistical Computing

Platform: x86_64-pc-linux-gnu (64-bit)

.....

Type 'q()' to quit R.

>

```
[p4rodrig@login02 ~]$ module spider r
```

```
-----  
r: r/4.0.2-openblas  
-----
```

```
Other possible modules matches:
```

```
AMDuProf, amber, aria2, arm-forge, berkeley-db, bism
```

```
You will need to load all module(s) on any one of the li  
"r/4.0.2-openblas" module is available to load.
```

```
cpu/0.15.4 gcc/9.2.0
```

```
Help:
```

A note on installing R Packages (into your own directories)

- In R (might help to be on interactive node):

install.packages('package-name')

(see <https://cran.r-project.org/> for package lists and reviews)

- Sometimes you have to be explicit:

*install.packages('ggmap',
 repos='http://cran.us.r-project.org',dependencies=TRUE)*

If compiling is required and you get an error, call support

Packages are put into your /home/user/R directory

Other R package possibilities:

- Rspark - R interface to Spark
- R Keras – R interface to Keras
- pdbR - distributed matrix support (better for dense matrices vs Spark)
- Rgputools – GPU support

THE END