

gputools: an R package for GPU computing

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Outline

- Contents of gptools
- Usage
- Performance
- Other R packages for the GPU

CONTENTS OF gputools

A handful of selected R functions implemented with CUDA C for use on a GPU:

- Choose your device:

gputools function	CPU analog	Same usage?
chooseGpu()	none	NA
getGpuId()	none	NA

- Linear algebra:

gputools function	CPU analog	Same usage?
gpuDist()	dist()	no
gpuMatMult()	%*% operator	no
gpuCrossprod()	crossprod()	yes
gpuTcrossprod()	tcrossprod()	yes
gpuQr()	qr()	almost
gpuSolve()	solve()	no
gpuSvd()	svd()	almost

- Simple model fitting:

gputools function	CPU analog	Same exact usage?
gpuLm()	lm()	yes
gpuLsfit()	lsfit()	yes
gpuGlm()	glm()	yes
gpuGlm.fit()	glm.fit()	yes

- Hypothesis testing:

gputools function	CPU analog	Same exact usage?
gpuTtest()	t.test()	no
getAucEstimate()	???	???

- Other routines:

gputools function	CPU analog	Same exact usage?
gpuHclust()	hclust()	no
gpuDistClust()	hclust(dist())	no
gpuFastICA()	fastICA() (fastICA package)	yes
gpuGranger()	grangertest() (lmtest package)	no
gpuMi()	???	???
gpuSvmPredict()	See www.jstatsoft.org/v15/i09/paper	no
gpuSvmTrain()	See www.jstatsoft.org/v15/i09/paper	no

getAucEstimate()

Estimates the area under a receiver operating characteristic (ROC) curve.

Used to evaluate the performance of a hypothesis test in a multiple testing scenario.

Reference:

Hand, David J. and Till, Robert J. (2001). A simple generalisation of the area under the ROC curve for multiple class classification problems. Machine Learning. 45, 171-186.

gpuHclust()

Performs hierarchical clustering on a set of points.

The distances among the points must be given in an object of class "dist".

gpuDistClust()

Given a set of points, computes all pairwise distances and then performs hierarchical clustering on the points.

Both steps are done on the GPU.

gpuFastICA

Performs Independent Component Analysis (ICA) and Projection Pursuit.

ICA, like principle component analysis, is a linear decomposition of a design matrix.

The authors of fastICA claim that, unlike PCA, ICA “unmixes” the underlying sources of variability in the data by assuming a non-Gaussian structure.

This function is exactly like the ICA implementation in the **fastICA** package except that the **gpuTools** version uses **gpuSvd()** instead of **svd()**.

References:

A. Hyvarinen and E. Oja (2000) Independent Component Analysis: Algorithms and Applications, *Neural Networks*, 13(4-5):411-430. <http://www.cis.hut.fi/aapo/>

A. Hyvarinen. Independent Component Analysis: Recent Advances. *Philosophical Transactions of the Royal Society A*, in press. <http://www.cs.helsinki.fi/u/ahyvarin/papers/PTRSA12.pdf>.

gpuGranger()

Performs the Granger Causality Test, which tests how well one time series forecasts another.

Reference:

Hacker R.S. and Hatemi-J A. (2006) "Tests for causality between integrated variables using asymptotic and bootstrap distributions: theory and application", Applied Economics, Vol. 38(13), pp. 1489-1500.

gpuMi()

Estimates the mutual information for pairs of vectors using a B spline approach.

Reference:

Carten O. Daub, Ralf Steuer, Joachim Selbig, and Sebastian Kloska. 2004. Estimating mutual information using B-spline functions - an improved similarity measure for analysing gene expression data. BMC Bioinformatics. 5:118. Available from <http://www.biomedcentral.com/1471-2105/5/118>

gpuSvmPredict()

Classifies points in a data set using a support vector machine.

In machine learning, support vector machine (SVM) is a learning model used for classification and regression.

Reference:

Carpenter, Austin. cuSVM: a cuda implementation of support vector classification and regression.

<http://patternsonascreen.net/cuSVM.html>

gpuSvmTrain()

Trains a support vector machine.

Reference:

Carpenter, Austin. cuSVM: a cuda implementation of support vector classification and regression.
<http://patternsonascreen.net/cuSVM.html>

USAGE

- gptools is already installed on impact1.stat.iastate.edu, ready to load with `library(gptools)` in R.
- For other GPU systems, download gptools from CRAN with a simple `install.packages("gptools")` in R.
 - **WARNING:** installation will fail on non-GPU systems since the CUDA C compiler doesn't exist
- Documentation:
 - <http://brainarray.mbnl.med.umich.edu/Brainarray/Rgpgpu/>
 - <http://cran.r-project.org/web/packages/gptools/index.html>
 - <http://cran.r-project.org/web/packages/gptools/gptools.pdf>
- Requirements:
 - R (\geq version 2.8.0)
 - Nvidia's CUDA toolkit (\geq version 2.3)

MANAGING YOUR DEVICES: chooseGpu() AND getGpuId()

Impact1 has four GPUs, each with a unique index from 0 to 3. To see this for yourself, log into impact1 and run the following:

```
[landau@impact1 ~]$ cd /usr/local/NVIDIA_GPU_Computing_SDK/C/bin/linux/release  
[landau@impact1 release]$ ./deviceQuery
```

Here are some pieces of the (quite verbose) output of
`./deviceQuery`:

```
[deviceQuery] starting...
```

```
./deviceQuery Starting...
```

```
CUDA Device Query (Runtime API) version (CUDART static linking)
```

```
Found 4 CUDA Capable device(s)
```

```
Device 0: "Tesla M2070"
```

CUDA Driver Version / Runtime Version	4.1 / 4.1
CUDA Capability Major/Minor version number:	2.0
Total amount of global memory:	5375 MBytes (5636554752 bytes)
(14) Multiprocessors x (32) CUDA Cores/MP:	448 CUDA Cores
GPU Clock Speed:	1.15 GHz
Memory Clock rate:	1566.00 Mhz
Memory Bus Width:	384-bit
L2 Cache Size:	786432 bytes

Device 1: "Tesla M2070"

CUDA Driver Version / Runtime Version	4.1 / 4.1
CUDA Capability Major/Minor version number:	2.0
Total amount of global memory:	5375 MBytes (5636554752 bytes)
(14) Multiprocessors x (32) CUDA Cores/MP:	448 CUDA Cores
GPU Clock Speed:	1.15 GHz
Memory Clock rate:	1566.00 Mhz
Memory Bus Width:	384-bit
L2 Cache Size:	786432 bytes

Device 2: "Tesla M2070"

CUDA Driver Version / Runtime Version	4.1 / 4.1
CUDA Capability Major/Minor version number:	2.0
Total amount of global memory:	5375 MBytes (5636554752 bytes)
(14) Multiprocessors x (32) CUDA Cores/MP:	448 CUDA Cores
GPU Clock Speed:	1.15 GHz
Memory Clock rate:	1566.00 Mhz
Memory Bus Width:	384-bit
L2 Cache Size:	786432 bytes

Device 3: "Tesla M2070"	
CUDA Driver Version / Runtime Version	4.1 / 4.1
CUDA Capability Major/Minor version number:	2.0
Total amount of global memory:	5375 MBytes (5636554752 bytes)
(14) Multiprocessors x (32) CUDA Cores/MP:	448 CUDA Cores
GPU Clock Speed:	1.15 GHz
Memory Clock rate:	1566.00 Mhz
Memory Bus Width:	384-bit
L2 Cache Size:	786432 bytes

Things to note:

- Device 3 is a GPU
- “Tesla M2070” is the name of the model of the GPU.
- Device 3 contains multiple cores, or “sub-processors”. From the output, it has 448 CUDA-capable cores.

EXAMPLE: MATRIX MULTIPLICATION

Now, suppose I want to do a giant matrix multiplication on Device 3. I'm automatically set to Device 0:

```
> getGpuId()
[1] 0
```

So I change to Device 3:

```
> chooseGpu(3)
[[1]]
[1] 3
```

and then if I want, I can verify the change:

```
> getGpuId()
[1] 3
```

Now, I define the matrices that I want to multiply on Device 3:

```
> A <- matrix(runif(1e+7), nrow = 1e+4)
> B <- matrix(runif(1e+7), ncol = 1e+4)
```

Then, I tell the device to multiply A and B using the GPU hardware:

```
> ptm <- proc.time(); C <- gpuMatMult(A, B); proc.time() - ptm  
    user  system elapsed  
2.959   2.190   5.159
```

Compare the run time to that of the analogous CPU run on impact1:

```
> ptm <- proc.time(); D <- A %*% B; proc.time() - ptm  
    user  system elapsed  
116.389   0.166 116.503
```

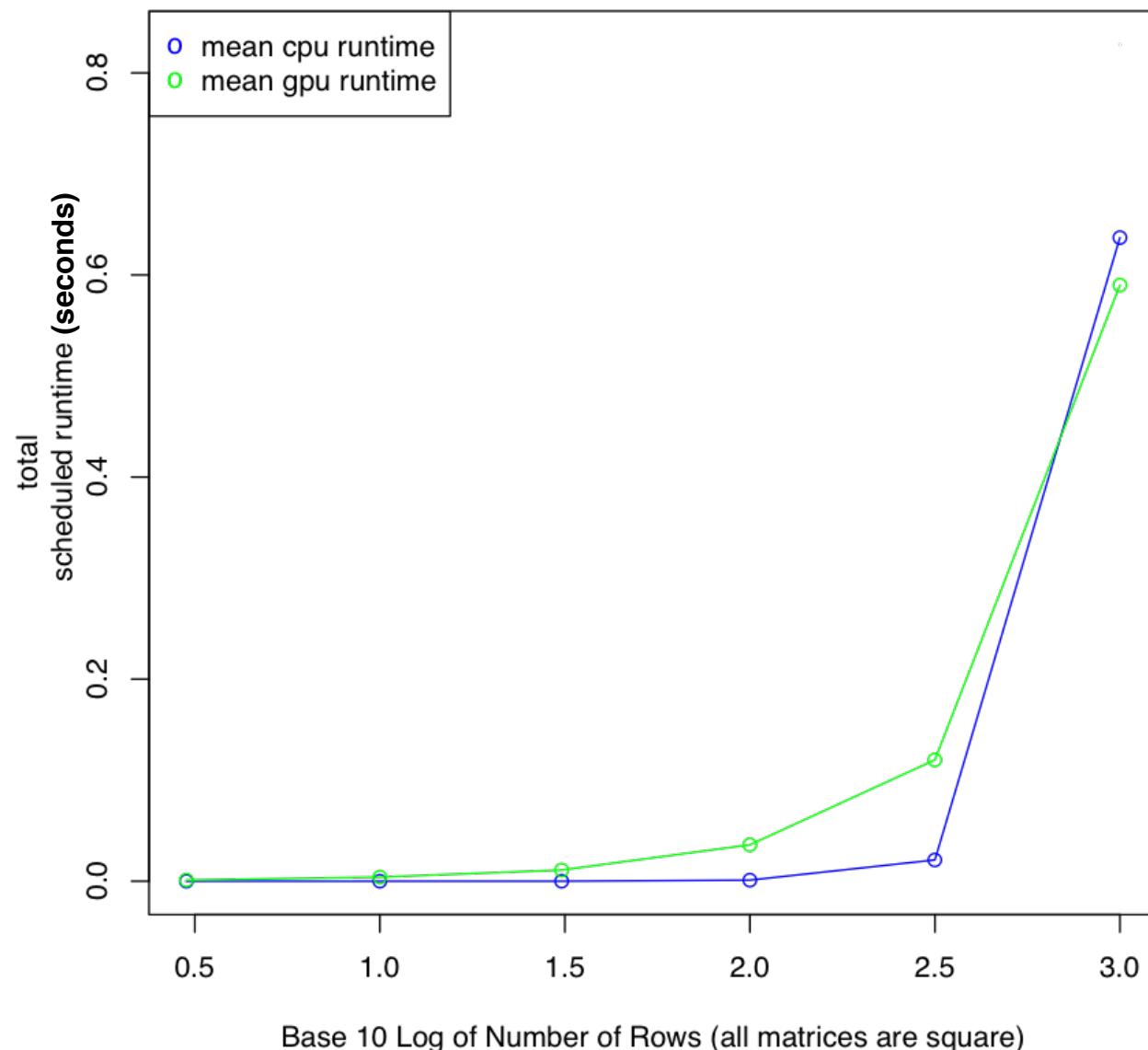
PERFORMANCE

A COMPARISON OF `gpuQr()` AND `qr()`

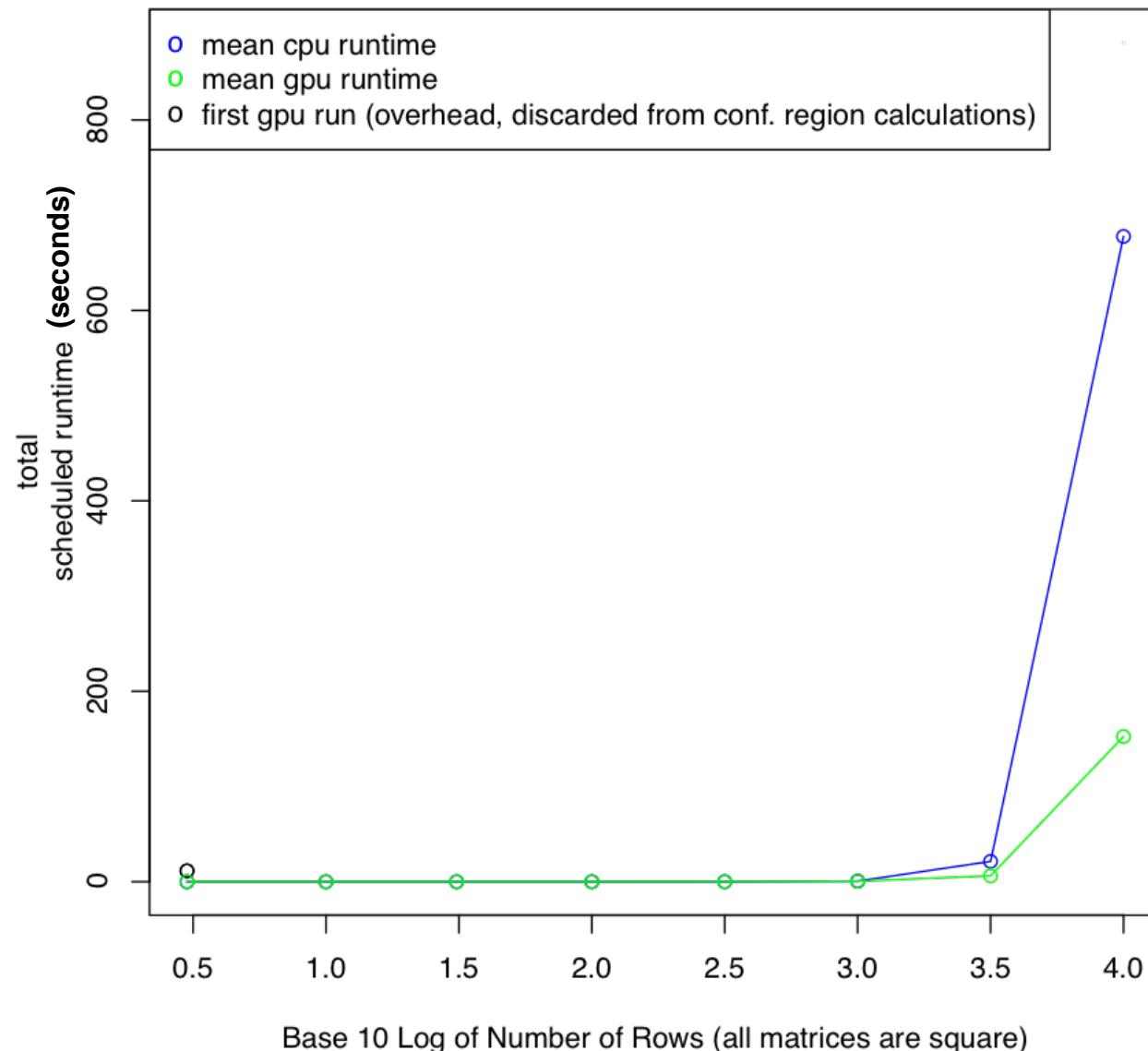
The R script, `gpuQr.r`, compares the performance of `gpuQr(arg)` and `qr(arg)` for square matrices `arg` of varying sizes.

See the results on the next few slides.

**total
scheduled runtime:
 $qr()$ vs $gpuQr()$**



**total
scheduled runtime:
 $qr()$ vs $gpuQr()$**

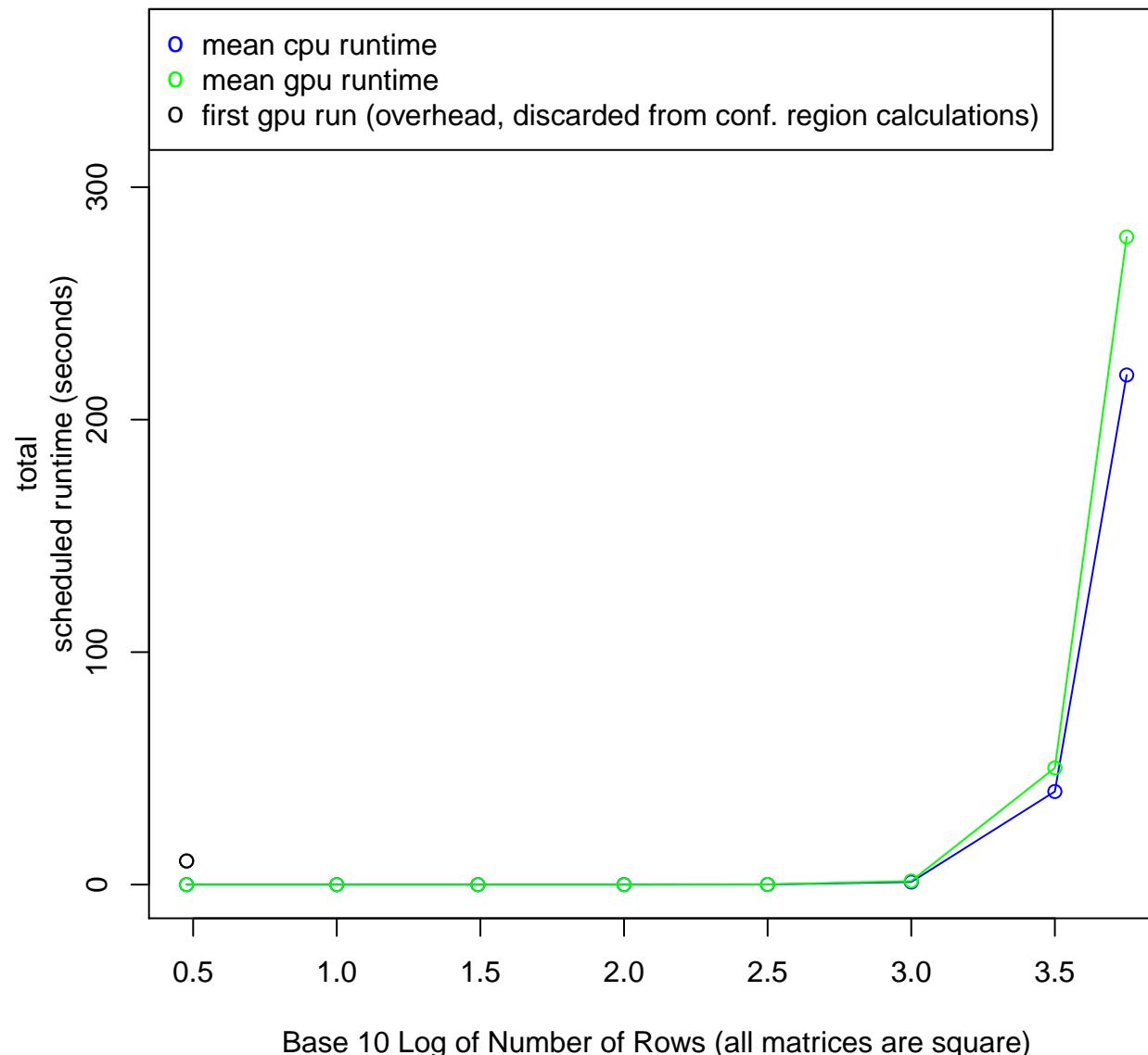


A COMPARISON OF `gpuSolve()` AND `solve()`

The R script, `gpuSolve.r`, compares the performance of `gpuSolve(arg)` and `solve(arg)` for square matrices `arg` of varying sizes.

See the results on the next slide.

**total
scheduled runtime (seconds):
solve() vs gpuSolve()**



A COMPARISON OF `gpuLm()` AND `lm()`

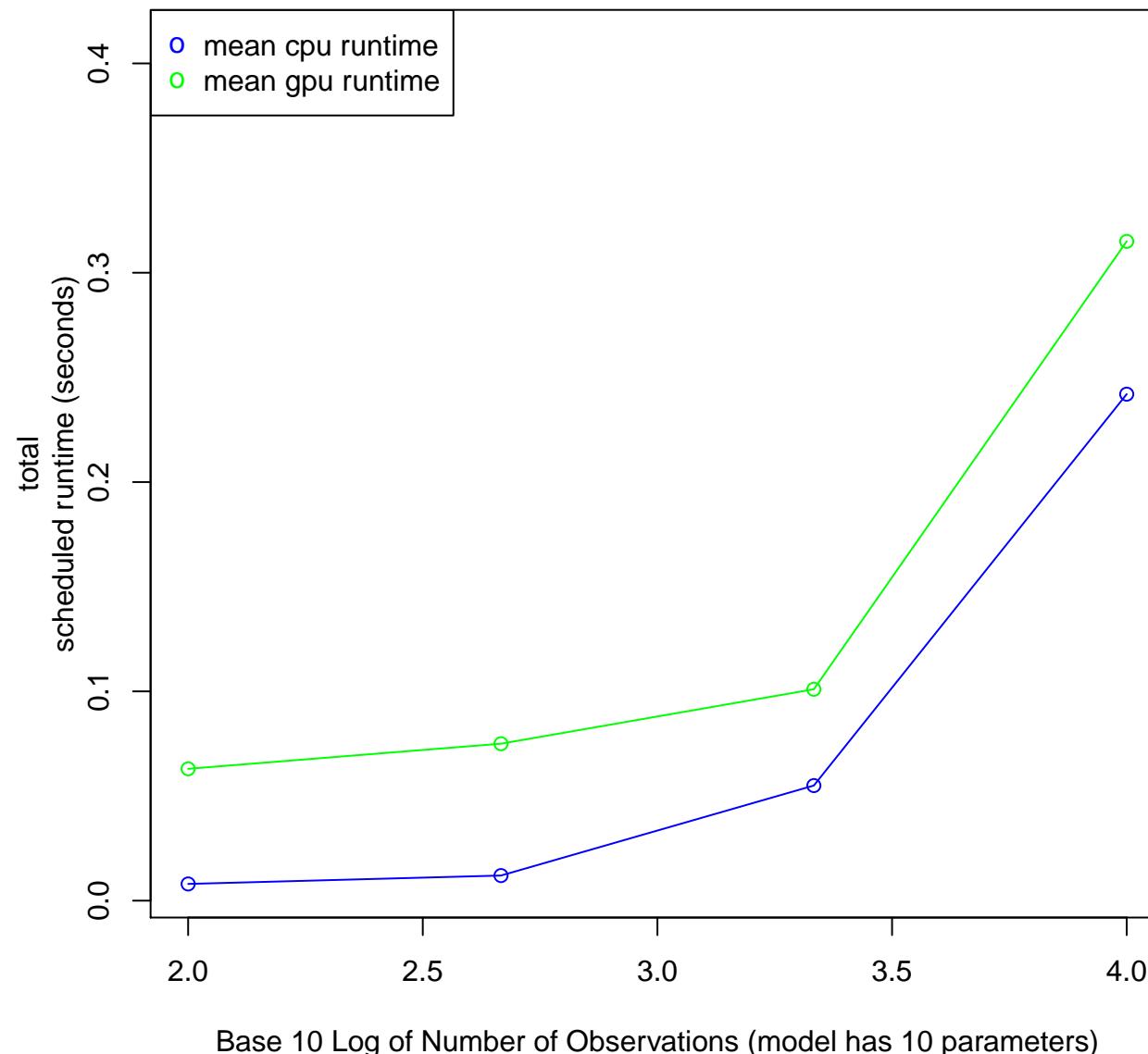
The R script, `gpuLm.r`, compares the performance of `gpuLm(y ~ X)` and `lm(y ~ X)`, where:

- `y` is a random vector of observations.
- `X` is a random design matrix with `length(y)` rows and 100 columns.

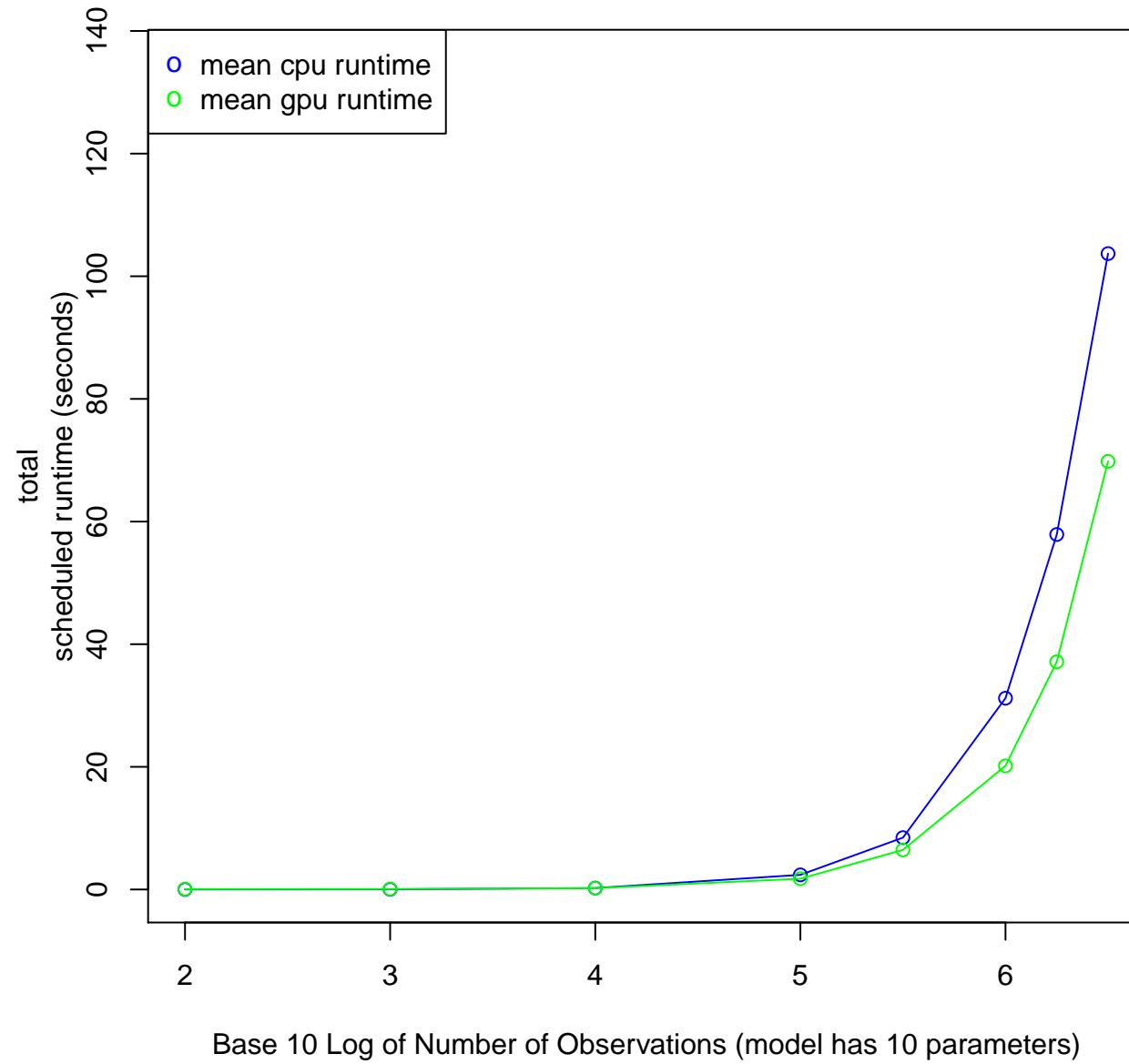
The script times each function with varying `length(y)` and `nrow(X)`.

See the results on the next slides.

**total
scheduled runtime (seconds):
lm() vs gpuLm()**



total
scheduled runtime (seconds):
lm() vs gpuLm()



A COMPARISON OF `gpuGlm()` AND `glm()`

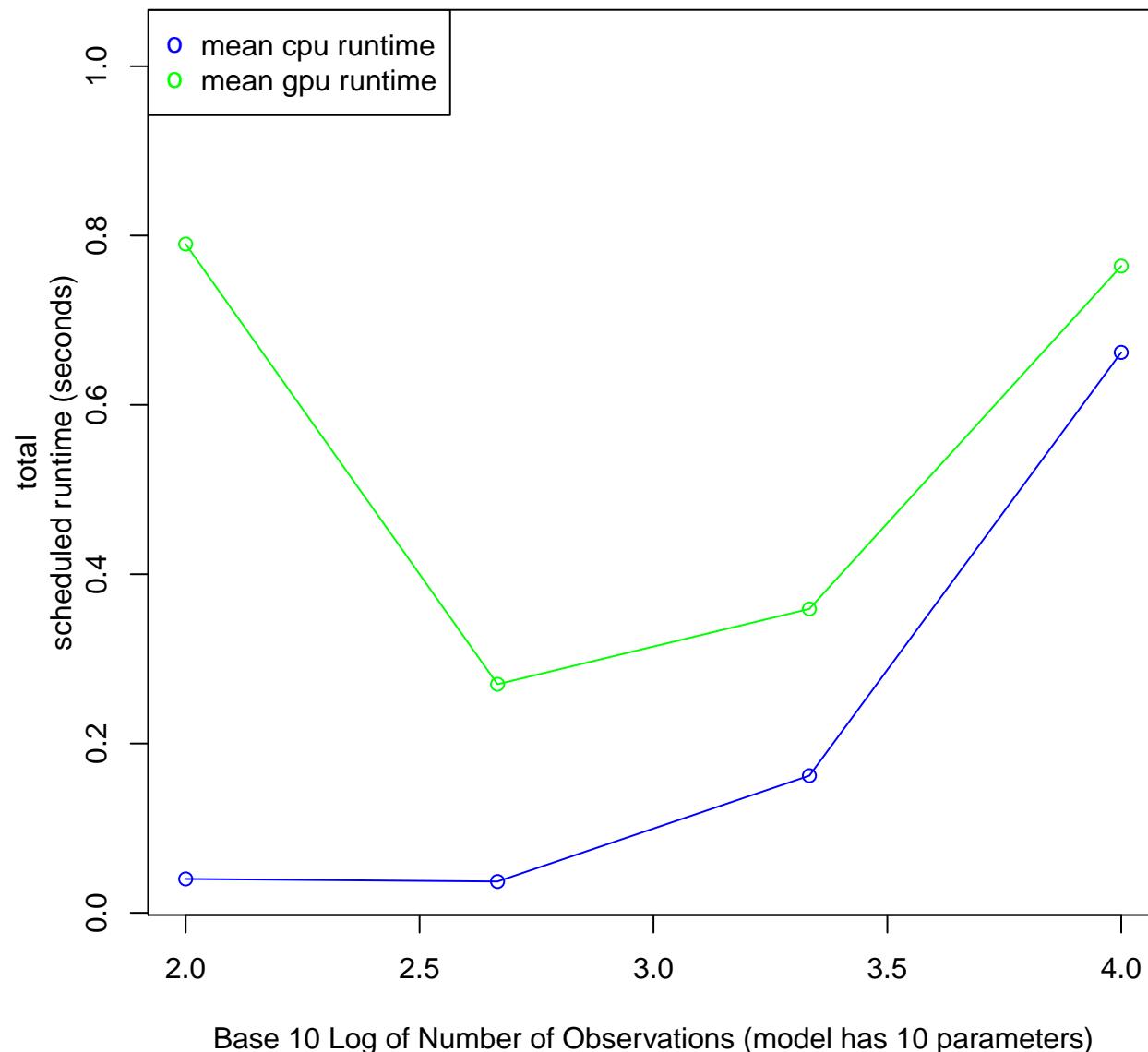
The R script, `gpuGlm.r`, compares the performance of `gpuGlm(y ~ X, family = poisson())` and `glm(y ~ X, family = poisson())`, where:

- `y` is a random vector of observations.
- `X` is a random design matrix with `length(y)` rows and 100 columns.

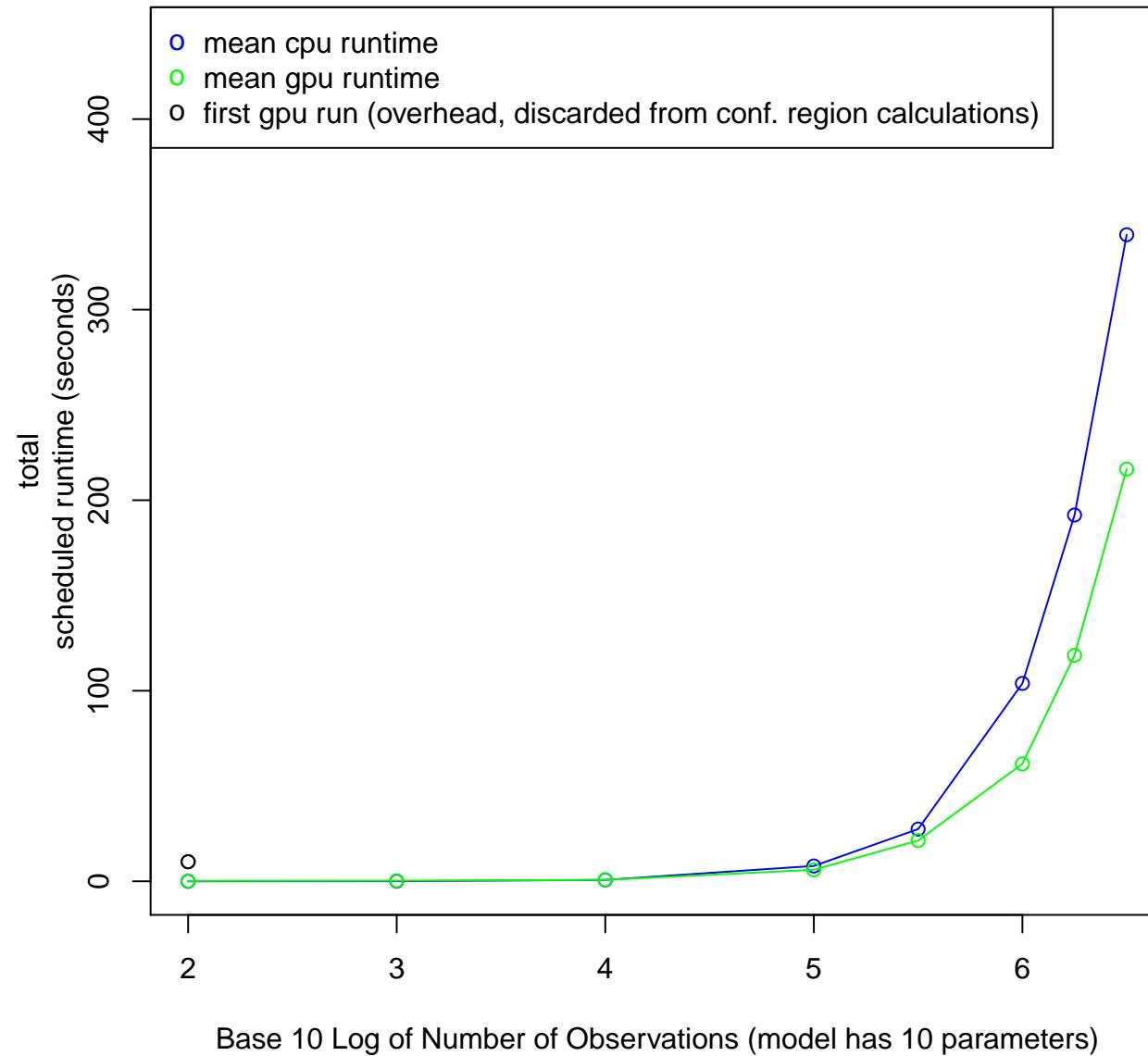
The script times each function with varying `length(y)` and `nrow(X)`.

See the results on the next slides.

**total
scheduled runtime (seconds):
glm() vs gpuGlm()**



total
scheduled runtime (seconds):
glm() vs gpuGlm()



CLAIMS FROM THE AUTHORS OF gputools

(All of the following is from
<http://brainarray.mbnl.med.umich.edu/Brainarray/Rgpgpu/.>)

“Tested on a subset of GSE6306, non-GPU enabled fastICA took over four hours while gpuFastICA took just 80 seconds!”

Fig. 1: Speedup (R GPU vs. CPU)

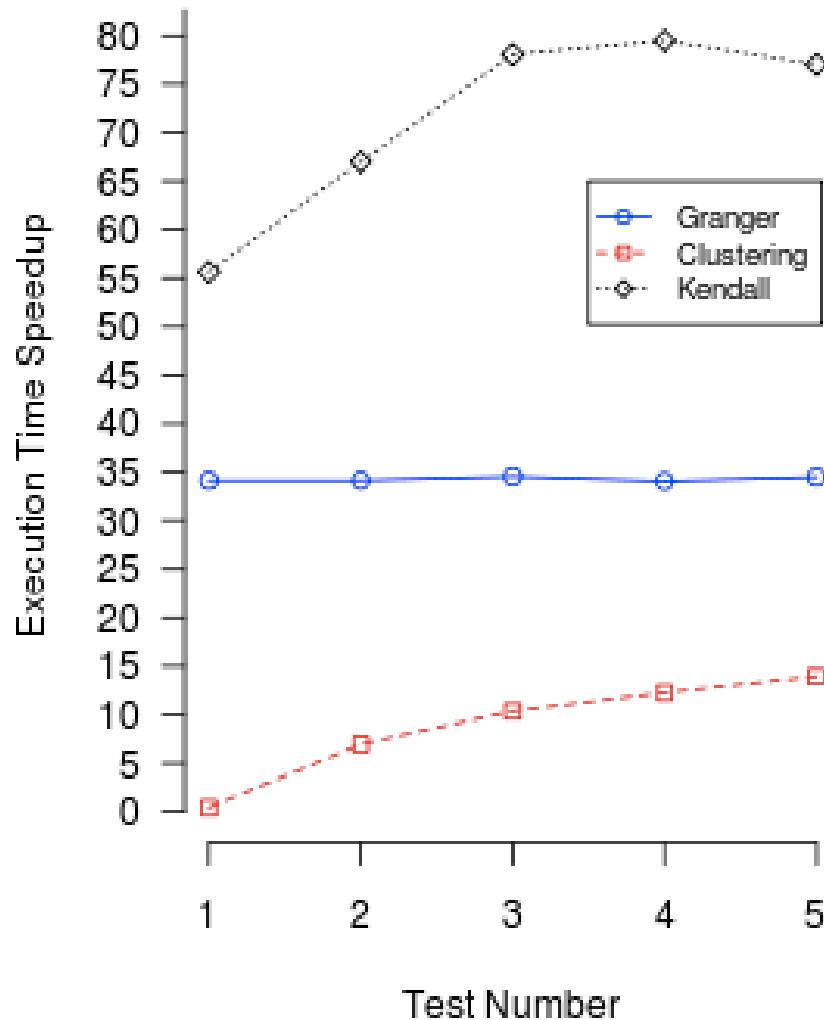


Fig. 2: Granger Times

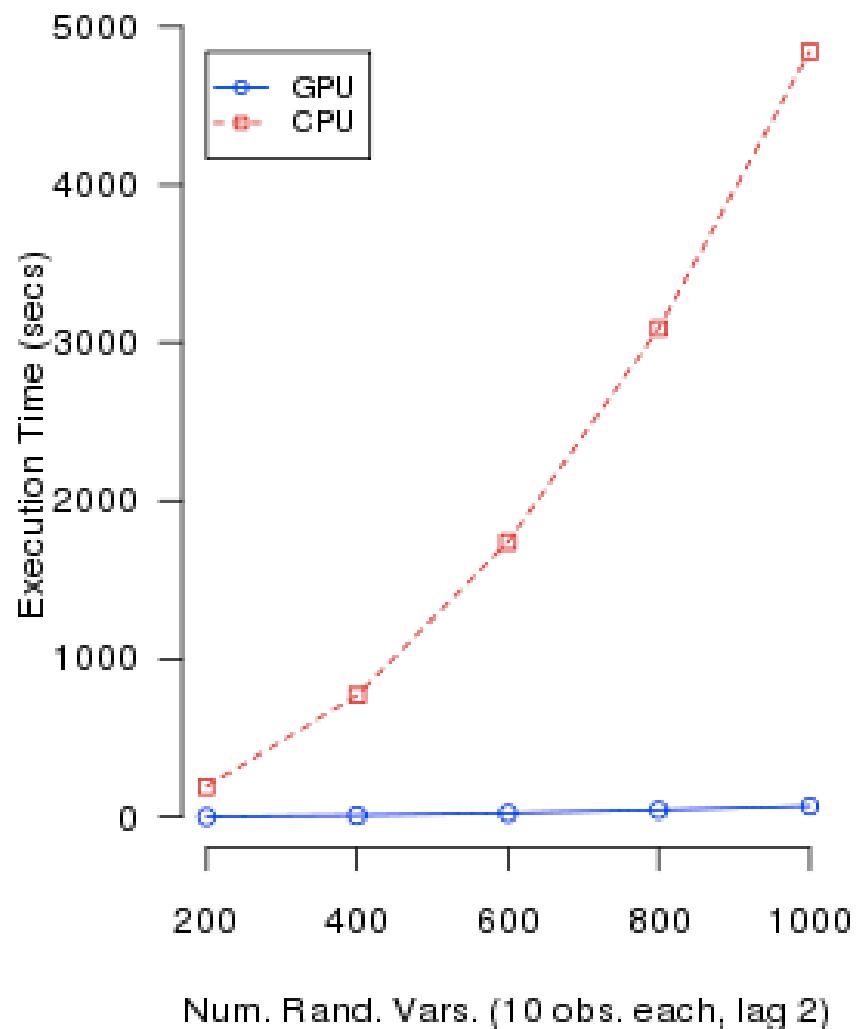


Fig. 3: Cluster Times

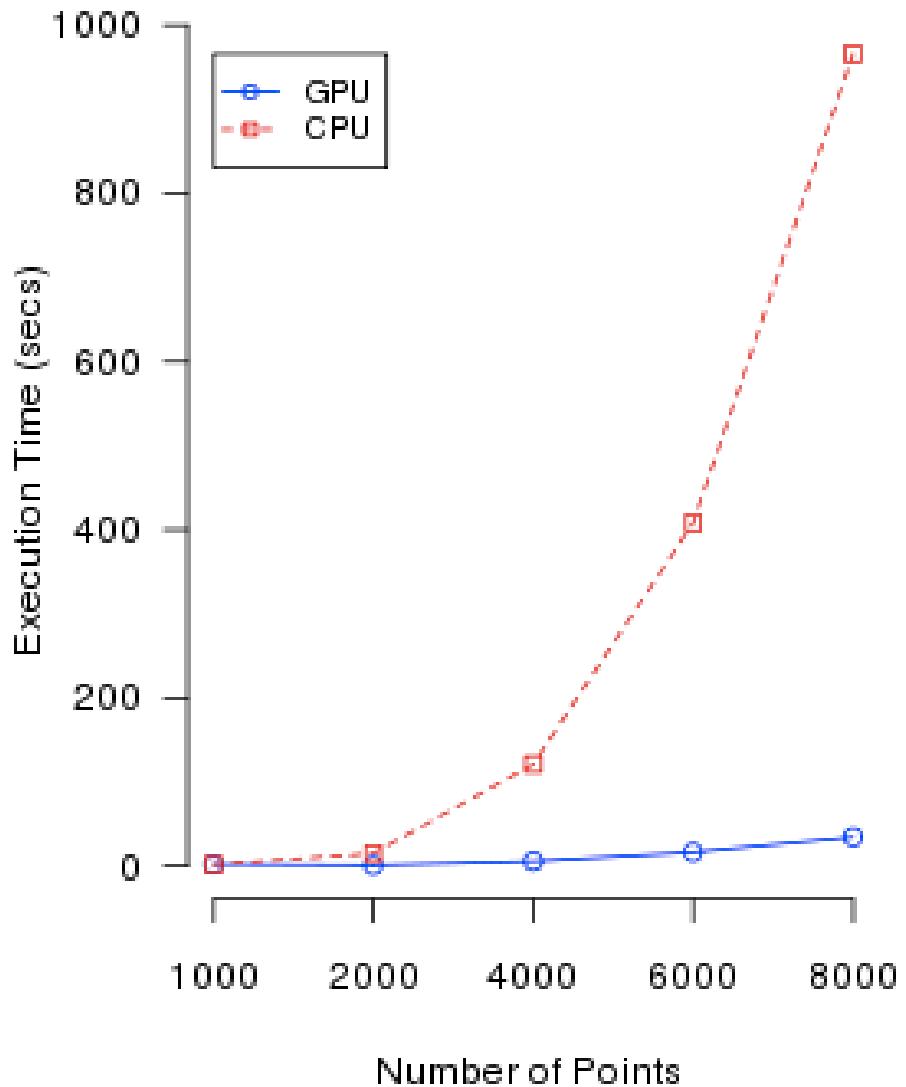
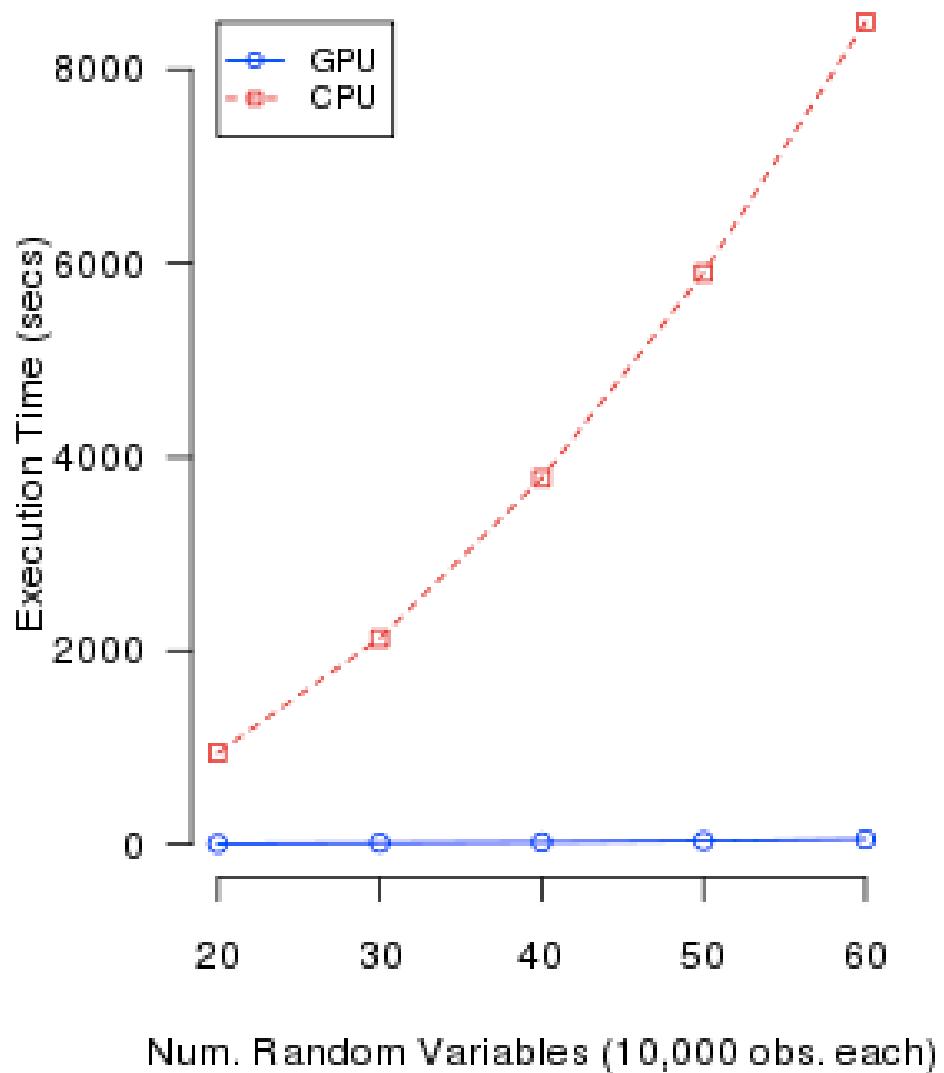


Fig. 4: Kendall Times



OTHER R PACKAGES FOR THE GPU

- WideLM - used to quickly fit a large number of linear models to a fixed design matrix and response vector.
- magma - a small linear algebra with implementations of backsolving and the LU factorization.
- cudaBayesreg - implements a Bayesian model for fitting fMRI data.
- gcbd - a Debian package for “benchmarking” linear algebra algorithms such as the QR, SVD and LU factorizations.

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- Usage
- Performance
- Other R packages for the GPU

GPU SERIES MATERIALS

These slides, a tentative syllabus for the whole series, and code are available at:

<https://github.com/wlandau/gpu>.

After logging into you home directory on impact1, type:

```
git clone https://github.com/wlandau/gpu
```

into the command line to download all the materials.

REFERENCES

- Josh Buckner, Mark Seligman, Justin Wilson. “R+GPU”.
<http://brainarray.mbnl.med.umich.edu/Brainarray/Rgpgpu/#introduction>.
- Carten O. Daub, Ralf Steuer, Joachim Selbig, and Sebastian Kloska. 2004. Estimating mutual information using B-spline functions - an improved similarity measure for analysing gene expression data. BMC Bioinformatics. 5:118. Available from
<http://www.biomedcentral.com/1471-2105/5/118>
- Carpenter, Austin. cuSVM: a cuda implementation of support vector classification and regression. <http://patternsonascreen.net/cuSVM.html>
- Dirk Eddelbuettel. “Package gcbd”.
<http://cran.r-project.org/web/packages/gcbd/gcbd.pdf>.
- Hacker R.S. and Hatemi-J A. (2006) ”Tests for causality between integrated variables using asymptotic and bootstrap distributions: theory and application”, Applied Economics, Vol. 38(13), pp. 1489-1500.
- Hand, David J. and Till, Robert J. (2001). A simple generalisation of the area under the ROC curve for multiple class classification problems. Machine Learning. 45, 171-186.

A. Hyvarinen and E. Oja (2000) Independent Component Analysis: Algorithms and Applications, Neural Networks, 13(4-5):411-430. <http://www.cis.hut.fi/aapo/>

A. Hyvarinen. Independent Component Analysis: Recent Advances. Philosophical Transactions of the Royal Society A, in press.
<http://www.cs.helsinki.fi/u/ahyvarin/papers/PTRSA12.pdf>.

Mark Seligman, Chris Fraley. “Package WideLM”.
<http://cran.r-project.org/web/packages/WideLM/WideLM.pdf>.

Brian J Smith. “Package cudaBayesreg”.
<http://cran.r-project.org/web/packages/cudaBayesreg/cudaBayesreg.pdf>.