Statistical and Mathematical Software on HPC systems

Jefferson Davis
Research Analytics

Plan of Attack

- Look at three packages on Karst: SAS, R, Matlab.
- Look at running a common task in all three.
- Discuss a bit on how the different packages take advantage of multicore or parallel functionality.

What modules am I using?

```
module load matlab
module load java
module load curl
module load r
module load sas
# Modules for GPU Matlab on BRII
module load ccm
module load cudatoolkit
```

Three roads to parallelism

- Implicit parallelism (my favorite)
- Small modifications to existing code
- Fiddling around with mpi

SAS: background

- First developed in 1966 at North Carolina State for regression and analysis of variance.
- Commercialized in 1976 when the SAS Institute incorporates.
- Solid workhorse statistical package
- Still has not been used as a New York Times crossword clue, but both "Special Air Service" and "Scandinavian Airlines System" have.

SAS: starting it up

~> `module load sas`

SAS data analysis and management system version 9.4 loaded.

~> `sas -nodms`

More common to write the sas program and run it as a script

~> `sas lineExample.sas`

A SAS program has two steps: a data step and a proc step.

SAS: sample Karst script

```
#!/bin/bash
#PBS -l nodes=1:ppn=16,walltime=1:00:00
#PBS -M username@iu.edu
#PBS -m abe
#PBS -N JobName
#PBS -o sas_output
#PBS -e sas_error

cd /N/u/username/Karst/new_directory
sas lineExample.sas
```

SAS: loading data and regressing

Look at the example of fitting a line through some data.

The csv file faithful.csv has 272 values.

We use SAS to find the line of best fit.

	A	B
1	3.6	79
2	1.8	54
3	3.333	74
4	2.283	62
5	4.533	85
6	2.883	55
7	4.7	88
8	3.6	85
9	1.95	51
10	4.35	85
11	1.833	54
12	3.917	84
13	4.2	78
14	1.75	47
15	4.7	83
16	2.167	52
17	1.75	62
18	4.8	84
19	1.6	52
20	4.25	79
21	1.8	51
22	1.75	47

SAS: loading data and regressing

The file lineExample.sas

```
data faithful;
 infile "faithful.csv" delimiter=",";
 input x y;
run;
proc reg;
  model y = x;
run;
```

```
~>sas lineExample.sas
```

The output goes to lineExample.lst

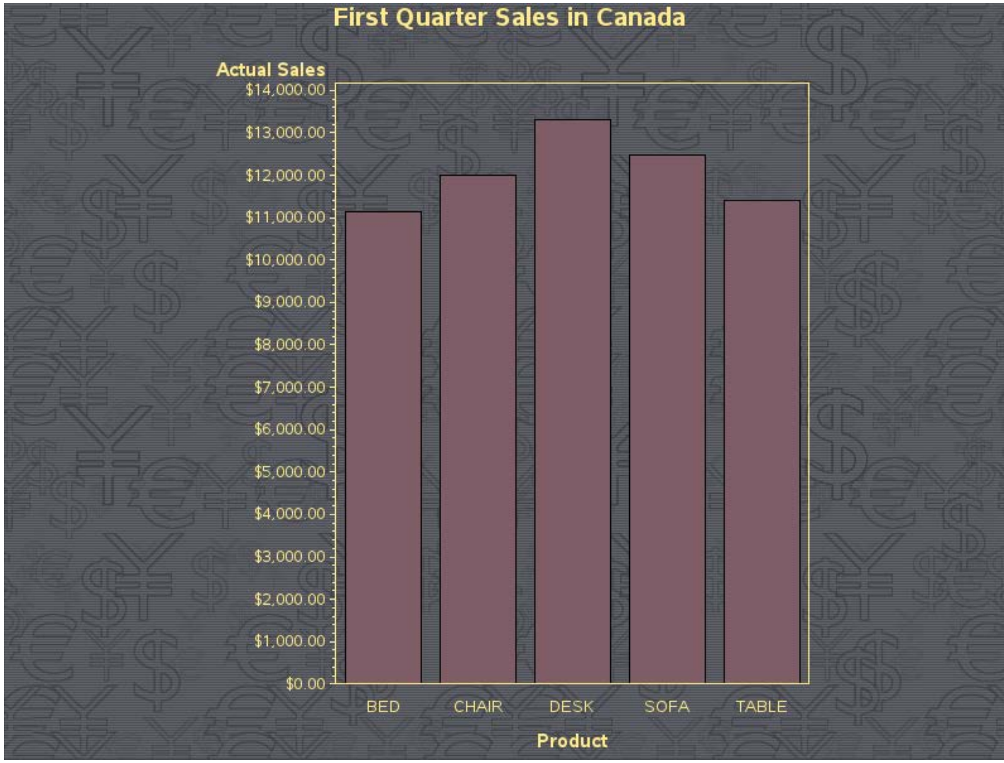
SAS: loading data and regressing

```
~> tail -n 7 lineExample.lst
               Parameter Estimates

               Parameter   Standard
Variable  DF    Estimate      Error     t Value  Pr > |t|

Intercept  1    33.47440    1.15487   28.99     <.0001
x          1    10.72964    0.31475   34.09     <.0001
```

Sure, y = 10.72964 x + 33.47440 seems okay.

SAS: producing graphics

```
ods listing close;
ods html style=money
file="CanadaGraph.html" ;
proc gchart
   data=sashelp.prdsale;
vbar Product / sumvar=actual;
title1 "First Quarter
   Sales in Canada";
where Quarter=1
   and Country="CANADA";
run;
quit;
ods html close;
ods listing;
```




```
~>sas canada.sas
```

SAS: implicit parallelism exapmple

- SAS will create threads to run faster on multicore environments.
- This happens by default but we can see the improvement if we force SAS to run without threads
- The next example involves taking the mean of a set of 500,000,000 random numbers

SAS: implicit parallelism exapmple

```
%let NObs = 500000000;
data Unif(keep=u);
call streaminit(123);
do i = 1 to &NObs;
   u = rand("Uniform");    /*
U[0,1] */
   output;
end;
run;

proc means data=unif;

var u ;
run;
```

```
NOTE: PROCEDURE MEANS used
(Total process time):
      real time   13.45 seconds
      cpu time    28.80 seconds
```

```
%let NObs = 500000000;
data Unif(keep=u);
call streaminit(123);
do i = 1 to &NObs;
   u = rand("Uniform");    /*
U[0,1] */
   output;
end;
run;

proc means data=unif;
options nothreads;
var u ;
run;
```

```
NOTE: PROCEDURE MEANS used
(Total process time):
      real time    24.91 seconds
      cpu time     23.91 seconds
```

R: background

- First created in the early 1990s by Ross Ihaka and Robert Gentleman as an implementation of S.
- Development soon shifted to a larger core group.
- Distributed under the GNU General Public License.
- Academic statisticians like R much more than developers do.

R: starting it up

```
~> module load java
~> module load curl
~> module load r
~> R
```

One Karst node is running an Rstudio server

https://rstudio.iu.edu/

R: some useful tidbits

- The question mark will display a function's help text. This is a shortcut for the help() function
  `? sin`
- The command `R CMD BATCH --no-save R_input.R` runs in batch
- The up arrow key will go back to previous commands
- The command `system()` is used for shell commands
  `system("rm core")`
- The rm() command clears variables
  `rm(list=ls(all=TRUE))  #Clear all variables`
- The hash tag is used for comments
  `#This is an R comment`

R: sample Karst script

```
#!/bin/bash
#PBS -l nodes=1:ppn=16,walltime=1:00:00
#PBS -M username@iu.edu
#PBS -m abe
#PBS -N JobName
#PBS -o r_output
#PBS -e r_error

cd /N/u/username/Karst/new_directory
R CMD BATCH --no-save R_input.R
```

R: loading data and regressing

Let’s load the file faithful.csv again and rerun the earlier regression.

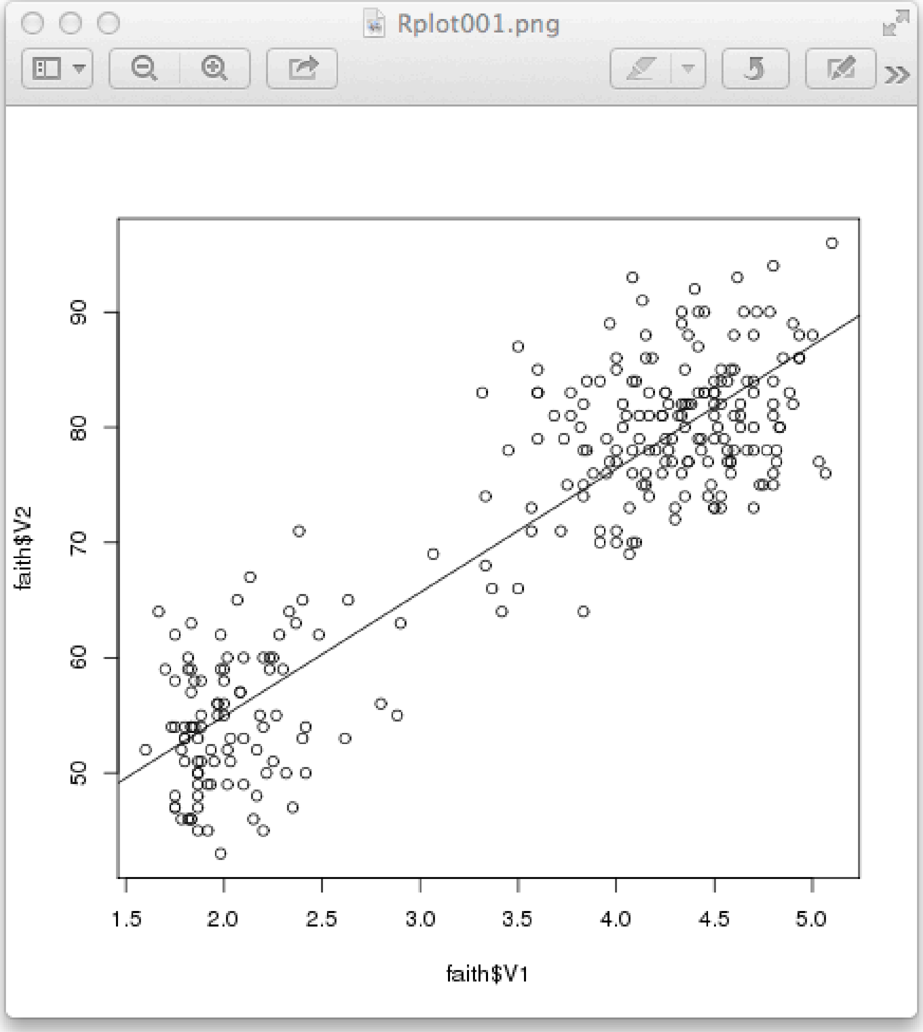
```
 faith <- read.csv("faithful.csv", header=FALSE)
 faith
      V1 V2
1   3.600 79
2   1.800 54
 lm(faith$V2 ~ faith$V1)
Call:
lm(formula = faith$V2 ~ faith$V1)
Coefficients:
(Intercept)     test2$V1
33.47           10.73
```

R: plotting data

```
fit<-lm(faith$V2~faith$V1)
png()
plot(faith$V1,faith$V2)
abline(fit$coefficients)
dev.off()
```

Default name is "Rplot001.png".

Multiple plots are saved in multiple files.



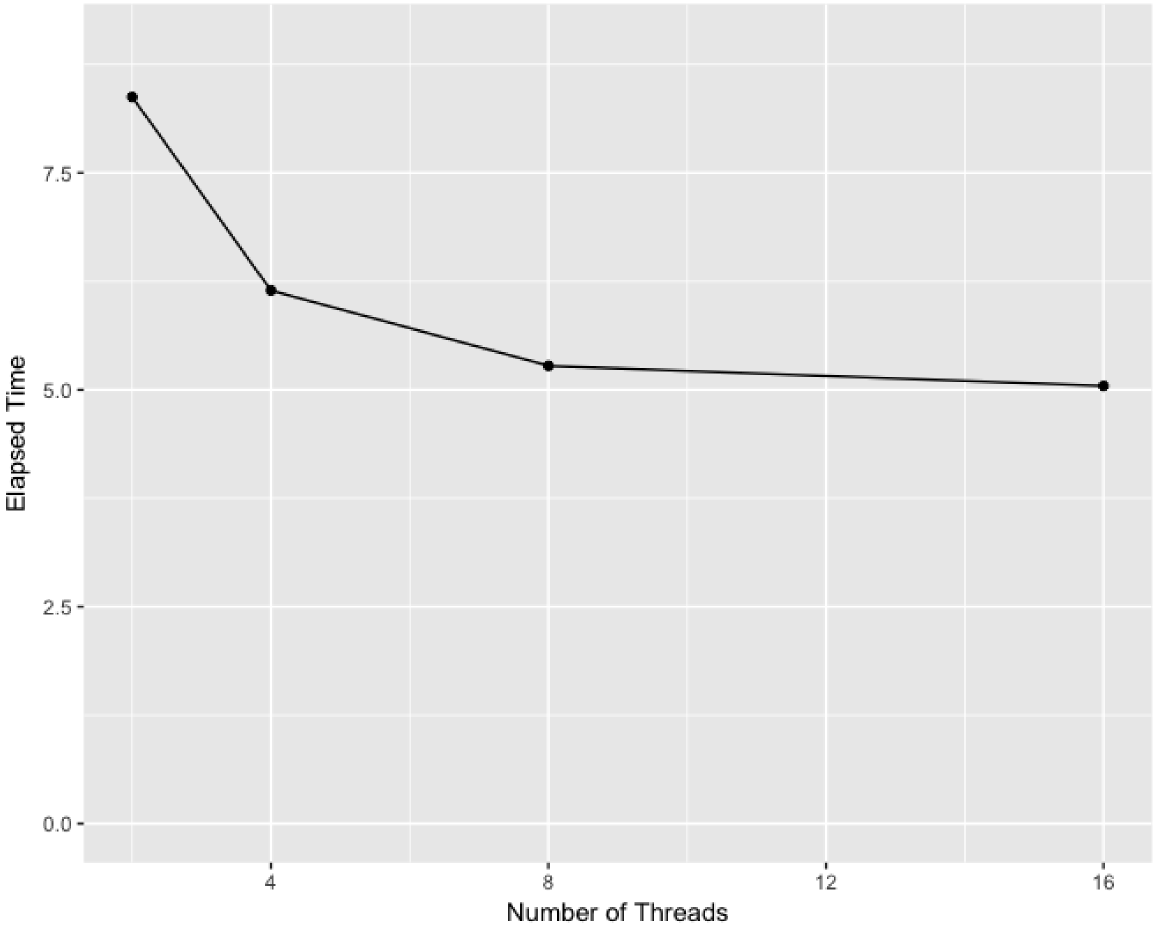
R: Using the MKL Libraries on Karst

The current version of R on Karst is built against the MKL libraries.

~> export MKL_NUM_THREADS=2 ~> R N <- 2000 A <- matrix(rnorm(N * N), N, N) t3 <- sapply(1 : T, function(t) system.time(eigen(A)) ['elapsed']) besttime <- apply(time, 2, min)	~> export MKL_NUM_THREADS=16 ~> R N <- 2000 A <- matrix(rnorm(N * N), N, N) t3 <- sapply(1 : T, function(t) system.time(eigen(A)) ['elapsed']) besttime <- apply(time, 2, min)
elapsed 8.376	elapsed 5.046

R: Using the MKL Libraries on Karst

Increasing the number of threads scales as expected.



R: multicore versions of apply()

R has many mapping functions that apply a function to the elements of a list, vector, what-have-you.

The function lapply() applies a function to the elements of a list. The function mclapply() is a multicore version of lapply.

The function rep(m,n) repeats m for n time. So lapply(rep(100,1000000),rnorm) returns 1000000 lists of 100 random numbers from a normal distribution.

st<-system.time(
  lapply(rep(100,1000000),
  rnorm))
st[3]
	library(parallel)
	stm<-system.time(
	  mclapply(rep(100,1000000),
	  rnorm,mc.cores=15))
	stm[3]

elapsed 18.733	elapsed 2.927

Matlab: background

- Developed by Cleve Moler in the 1970s to give students easier access to numerical libraries for linear algebra (Matrix Laboratory)
- MathWorks company founded in 1984 for commercial development
- About 1900 IU network users 2013-14 academic year
- Decent support for parallelism

Matlab: starting it up

```
~> module load matlab
MATLAB numerical calculation framework version
2015a loaded.
~> matlab
```

To run myInput.m in batch

```
~> matlab -r matlab_input
```

```
~> matlab < matlab_input.m
```

Matlab: sample Karst script

```
#!/bin/bash
#PBS -l nodes=1:ppn=16,walltime=1:00:00
#PBS -M username@iu.edu
#PBS -m abe
#PBS -N JobName
#PBS -o matlab_output
#PBS -e matlab_error

cd /N/u/username/Karst/new_directory
matlab < matlab_input.m
```

Matlab: some useful tidbits

- The help command will display a function's help text. The doc command brings up more information
  help sin
  doc sin
- The semi-colon (;) will suppress output
- The up arrow key will go back to previous commands
- Typing and then using the up arrow key goes back to previous commands that start with that text
- The exclamation point is used for shell commands
  ! rm matlab_crash_dump.*
- The percent sign is used for comments
  %This is a Matlab comment

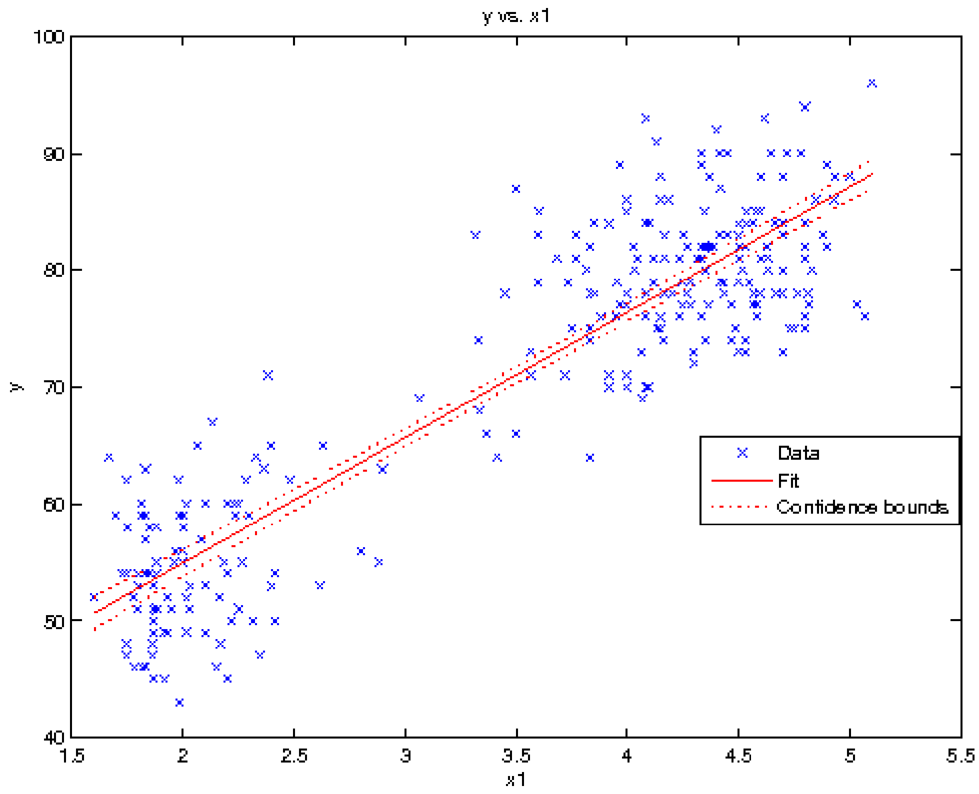
Matlab: loading data and regressing

```
faith=csvread('faithful.csv');
x=faith(:,1);
y=faith(:,2);
fit=fitlm(x,y,'linear')
fit =
Linear regression model:
    y ~ 1 + x1

Estimated Coefficients:
                   Estimate      SE        tStat       pValue
                   ________    _______    ______    __________
(Intercept)        33.474       1.1549    28.985     7.136e-85
x1                  10.73      0.31475    34.089     8.13e-100
```

Matlab: plotting data

```
fit.plot
print( gcf,'-dpng',...
  'MatlabPlot' )
```

This saves the plot as MatlabPlot.png.



Matlab: implicit parallelism in svd

Many functions will recognize the multicore environment and create an appropriate number of threads. A good example is singular value decomposition (SVD), rewriting a matrix as the product of “nice” matrices.

> matlab tic svd(rand(5000)) toc	> matlab -singleCompThread tic svd(rand(5000)) toc
Elapsed time is 15.343513 seconds.	Elapsed time is 157.930566 seconds.

Matlab: svd using the gpu

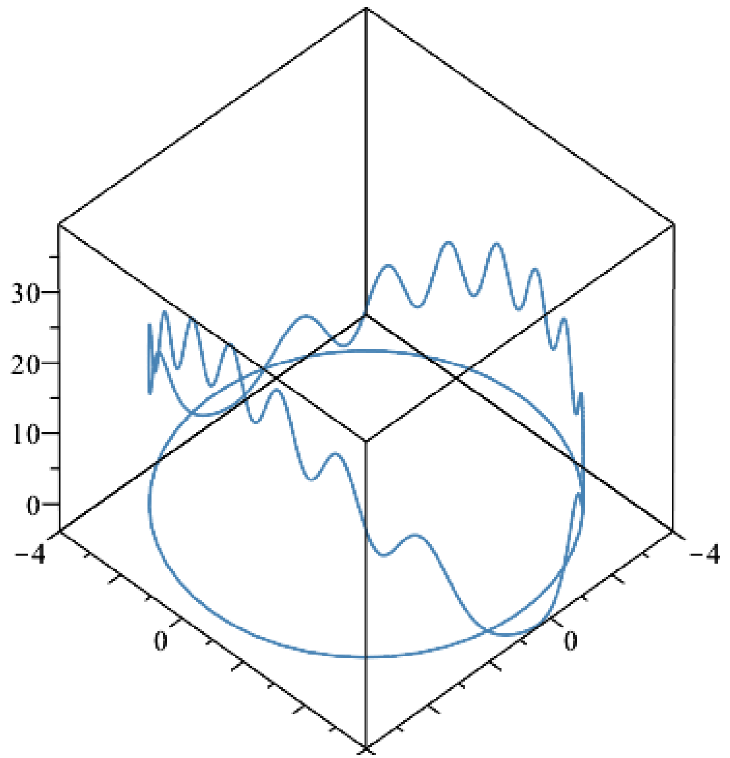
`> qsub -I -q debug_gpu -l gres=ccm`
`> ccmlogin`
`> matlab`
 	
`tic`
`svd(rand(5000))`
`toc`
	`> qsub -I -q debug_gpu -lgres=ccm`
	`> ccmlogin`
	`> matlab`
	
	`tic`
	`svd(rand(5000,'gpuArray'));`
	`toc`

`Elapsed time is 62.310409 seconds.`	`Elapsed time is 16.616624 seconds.`

Matlab: parallel-enabled functions

Many Matlab functions can use a pool of worker processes if you explicitly create them and tell the function to use them.

Sample problem: maximize the function $x_1^2 + 4*\sin(5*x_2)$ subject to the constraint $(x_1-1)^2 + (x_2-1)^2 = 25$



We first write a function to define the constraint mycon.m.

```
function [c,ceq] = mycon(x)
   c = (x(1)-1)^2 + (x(2)-1)^2 - 25
   ceq = [];
```

Matlab: parallel-enabled functions

Then we set up the problem

```
opts = optimset('Algorithm','sqp');
problem = createOptimProblem('fmincon','objective', ...
  @(x) x(1)^2 + 4*sin(5*x(2)),'x0',[3 3],'lb',[-5-5], ...
  'ub',[5 5],'nonlcon',@mycon,'options',opts);
ms = MultiStart;
```

The Matlab Multistart solver runs an optimizer from multiple start points. It's natural to want to run it in parallel.

`ms.UseParallel = false;`
`tic`
`[x,f] =`
`run(ms,problem,2000);`
`toc`
	`ms.UseParallel = true;`
	`tic`
	`[x,f] =`
	`run(ms,problem,2000);`
	`toc`

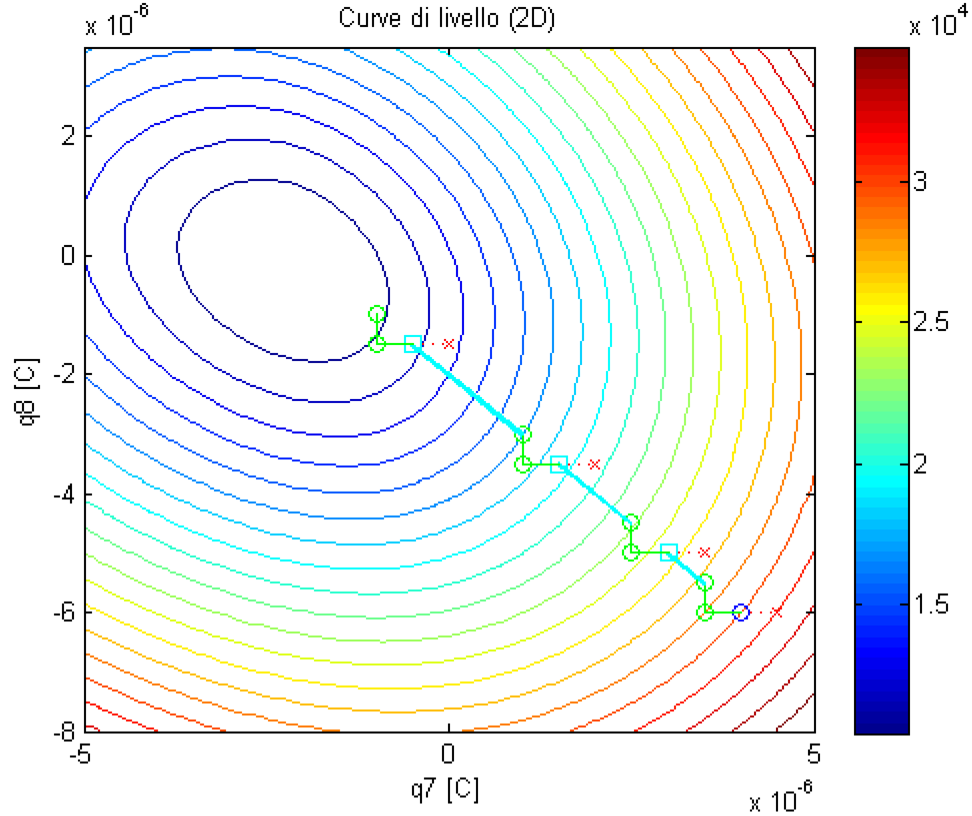
Elapsed time is 52.175676 seconds.	Elapsed time is 5.533175 seconds.

Matlab: parallel-enabled functions

Matlab will more more than happy to let you run things in parallel even is it's a really bad idea.

The optimizer patternsearch is an example. At each step patternsearch checks the values of the objective function at near the current point. The first point with a lower value becomes the current point for the next step.

You can, however, use a pool of workers and check them in parallel. This means checking all the nearby points.



Matlab: parallel-enabled functions

On the right Matlab tries to check all 2^{100} nearby points at each step. Yikes.

<table>
<tr><td>

```
x0=ones(100,1);
tic
patternsearch(@(x)myFun(x),…
x0,[],[],[],[],0*x0,1+0*x0,[
]);
toc
```

</td><td>

```
parpool(15)
options =
psoptimset('UseParallel',
true,…
'CompletePoll', 'on',
'Vectorized', 'off');
x0=ones(100,1);
tic
patternsearch(@(x)myFun(x),…
x0,[],[],[],[],0*x0,1+0*x0,[
],options);
toc

delete(gcp)
```

</td></tr>
<tr><td>Elapsed time is 29.419132 seconds.</td><td>Elapsed time is 160.692717 seconds.</td></tr>
</table>

Matlab: parallel for loops

If you have a pool of parallel workers you can use them to run a for-loop with `parfor`.

`tic`
`for i=1:5000000`
`   a(i)=max(rand(100,1));`
`end`
`toc`
	`parpool(15)`
	`tic`
	`parfor i=1:5000000`
	`   a(i)=max(rand(100,1));`
	`end`
	`toc`
	`delete(gcp)`

Elapsed time is 21.712727 seconds.	Elapsed time is 2.548504 seconds.

Matlab: parallel for loops

The are some restrictions on the loop, but the main one is that the order of evaluation can't matter. So the code below fails

```
%Fibonacci failure
a(1)=1;a(2)=1;
parpool(2)
parfor i=3:100
   a(i)=a(i-1)+a(i-2);
end
delete(gcp)

%Should have used Binet's forumula
```

Contact info

majdavis@iu.edu

researchanalytics@iu.edu

researchtech@iu.edu