04-Plotting_data

March 8, 2018

1 04-Graphing and analyzing data

1.1 4.1 physica

physica is a CLI-driven data plotting and analysis program that is using full MINUIT fitting package to combine outstanding data analysis capabilities with publication-quality output generation. It's been used at Brock for more than 20 years, and is embedded into all of our Y1 lab experiments (in a simplified form). It exists in both a tcl-wrapped physicalab and an online variants, the latter with a brief tutorial and an extensive online help facility.

physica has a flexible macro language, Fortran-like in its syntax.

Below is a brief introduction to its basic functionality:

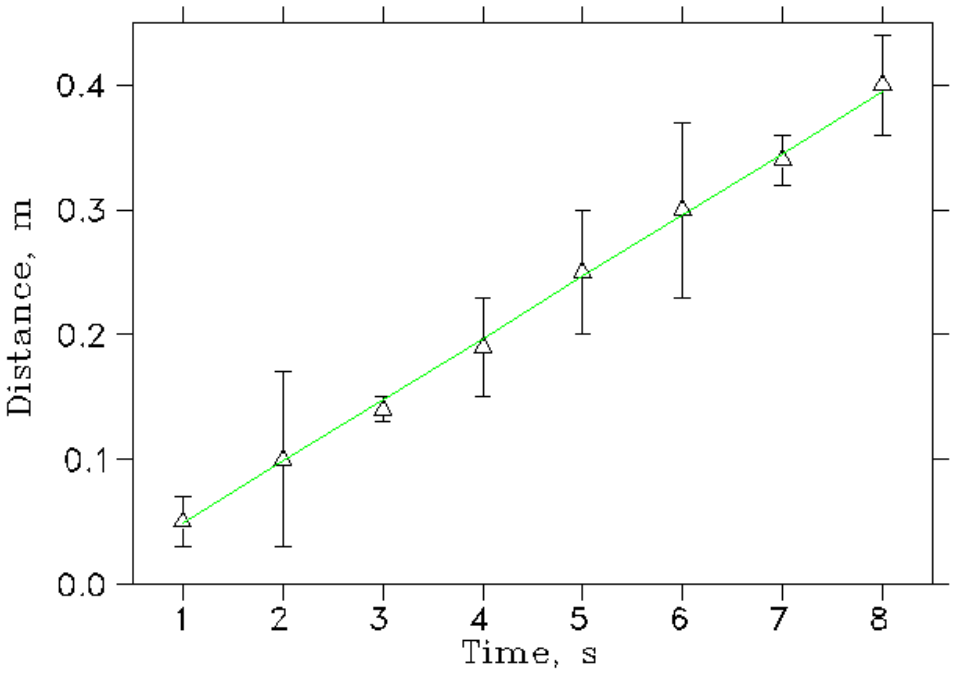
```
In [1]: %%file graph2d.pcm
        x=[1:8]
        y=[0.05;0.10;0.14;0.19;0.25;0.30;0.34;0.40]
        dy=[0.02;0.07;0.01;0.04;0.05;0.07;0.02;0.04]

        label\x `Time, s'
        label\y `Distance, m'
        set pchar -10
        graph x,y,dy

        scalar\vary a
        fit y=a*x
        fit\update f

        set pchar 0
        graph\noaxes x,f

        hardcopy PNG
        quit
```

```
Overwriting graph2d.pcm
```

We can execute a non-interactive version of physica and pass this set of commands to it.

```
In [2]: %%bash
        physica-www < graph2d.pcm > graph2d.png
```

There are multiple ways of displaying the resulting output within the notebook. The first two require the use of a markdown-type cell, which is quick and seamless, but unfortunately, may not update properly since the browser caching cannot be easily turned off, so even if the figure changes - you modify and re-run the script - the copy shown in the notebook may well be the stale cached version.



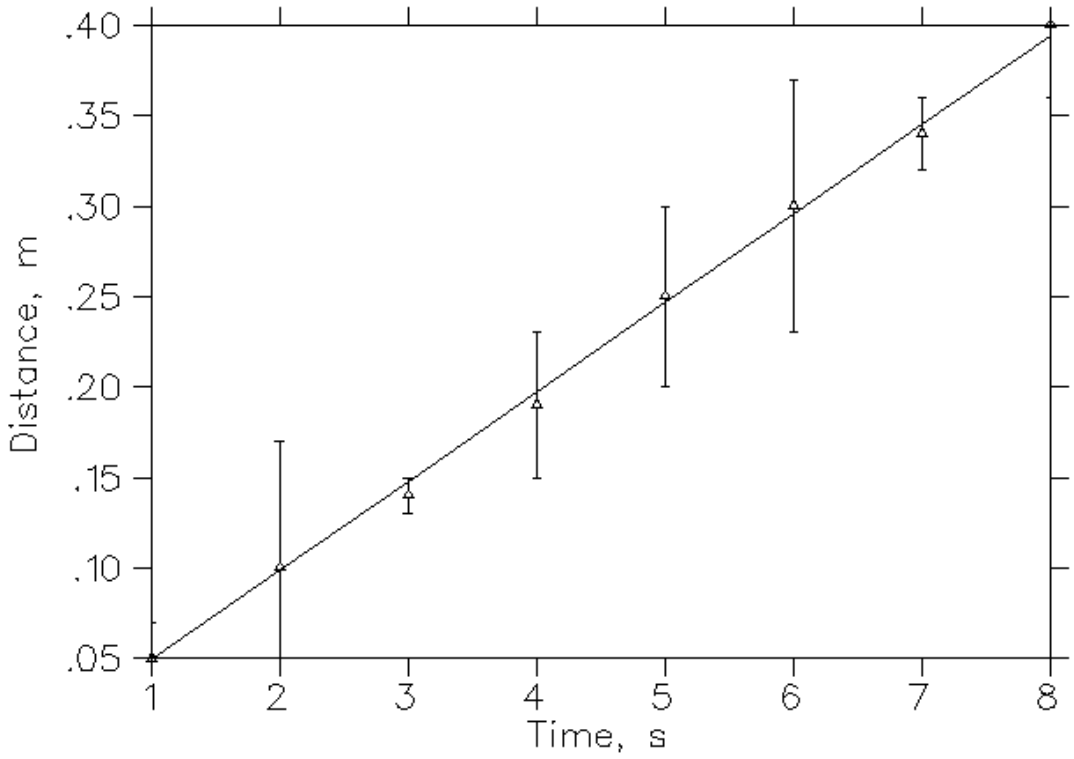
from physica

```
In [3]: %%html
        <img src="graph2d.png">
```

```
<IPython.core.display.HTML object>
```

A more robust way is to execute some native python code which bypasses the caching by the browser.

```
In [4]: from IPython.display import display, Image
        display(Image('graph2d.png'))
```



Here's a slightly more elaborate version of the same macro, with slightly refined annotation and colour use.

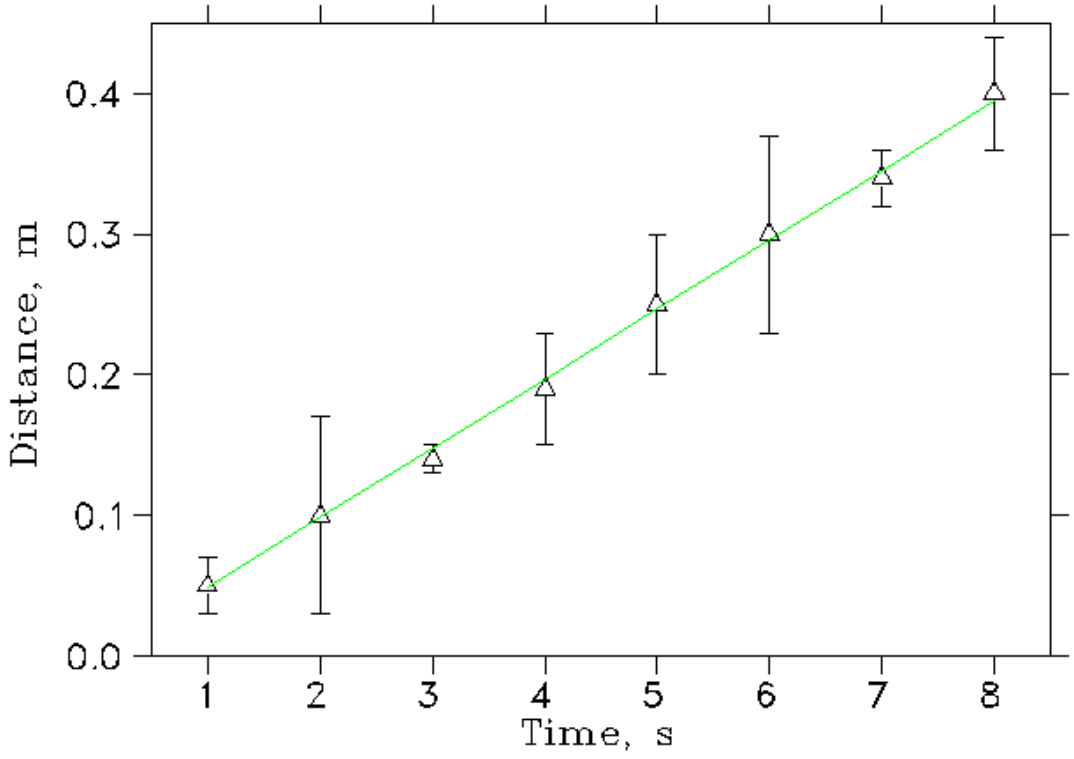
```
In [5]: %%file graph2d.pcm
        ! graph2d.pcm
        !   - a simple data plot, with a fit to a linear dependence
        !
        ! By:        edward.sternin@brocku.ca
        ! Completed: 2018.02
        !

        x=[1:8]
        y=[0.05;0.10;0.14;0.19;0.25;0.30;0.34;0.40]
        dy=[0.02;0.07;0.01;0.04;0.05;0.07;0.02;0.04]

        scales 0.5 8.5 7 0 0.45 4
        set
          xvmin 1
          xvmax 8
          yvmax 0.4
          font triumf.2
          %charsz 2
```

```
  yleadz 1

scalar\vary a
fit y=a*x
fit\update f

label\x `Time, s'
label\y `Distance, m'

set pchar -10
graph x,y,dy

set pchar 0
set colour 3
graph\noaxes x,f

hardcopy PNG
quit
```

```
Overwriting graph2d.pcm
```

In [6]:
```
%%bash
physica-www < graph2d.pcm > graph2d.png
```

In [7]:
```
from IPython.display import display, Image
display(Image('graph2d.png'))
```



1.2 4.2 gnuplot

gnuplot is one of the most widely used programs, and is available for a wide variety of platforms (even for Android!). It has a quick learning curve for simple graphs, but anything elaborate or requiring some serious computations, even if possible, gets to be quite difficult quickly. The current version of gnuplot is 5.2 and there is an excellent reference book:

gnuplot home page, including
the official user manual

a large collection of sample scripts
an inexpensive and very comprehensive e-book

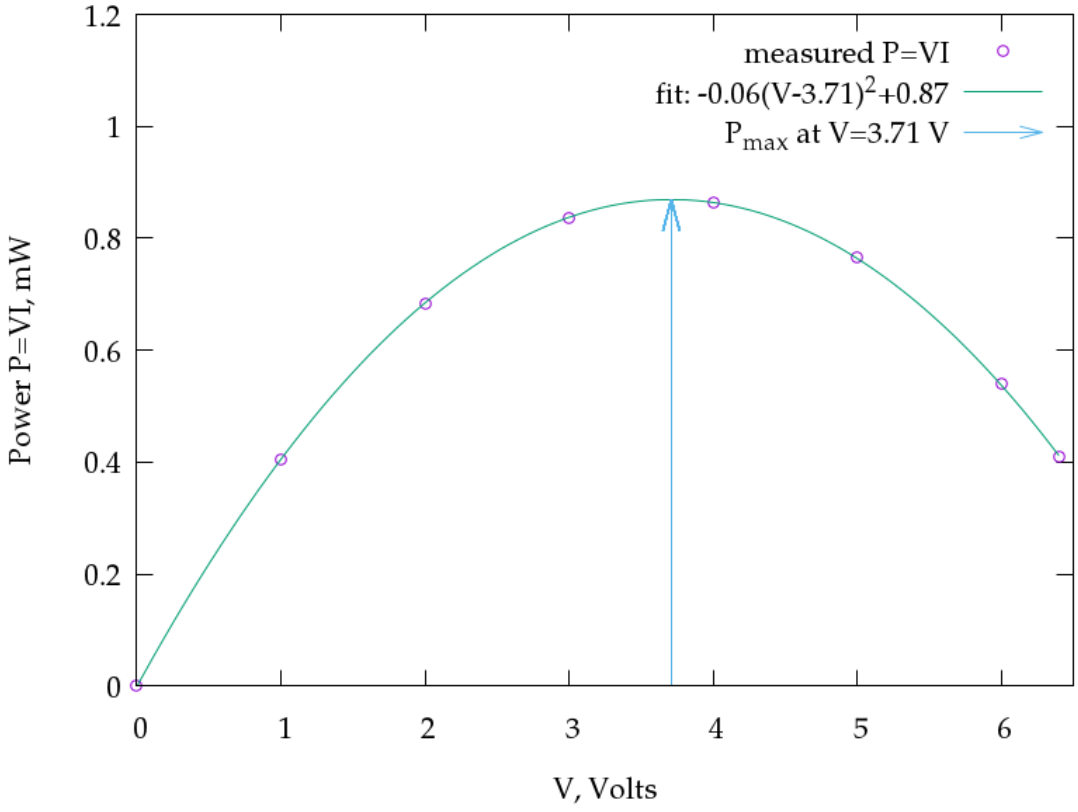
We have already seen some basic use in the previous part of the course. Here's a slightly more elaborate example which involves fitting and some annotation.

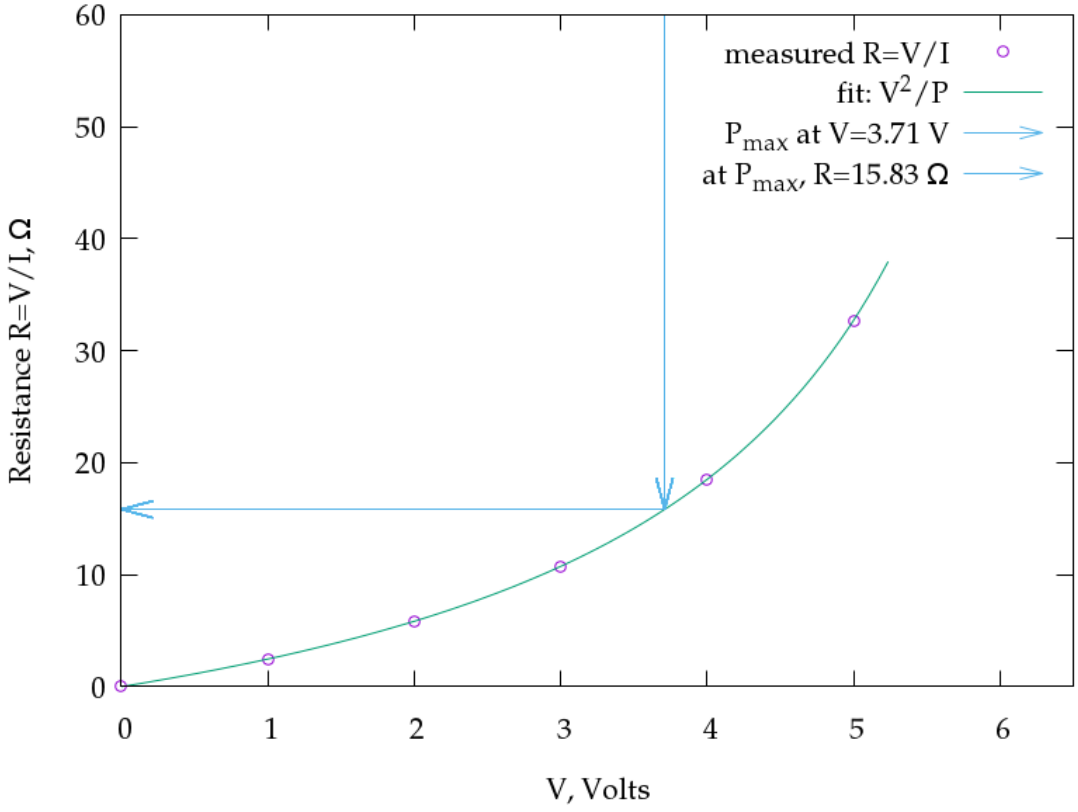
```
In [8]: # This loads the gnuplot kernel extension, for embedded gnuplot use
        %load_ext gnuplot_kernel
        %gnuplot inline pngcairo size 800,1200 font "Palatino,16"

In [9]: %%file VI.dat
        #  V    I,mA
          0   0.468
```

```
 1   0.405
 2   0.342
 3   0.279
 4   0.216
 5   0.153
 6   0.090
 6.4 0.064

Overwriting VI.dat
```

In [10]:
```
%%gnuplot
## a sample script to demonstrate some more advanced features of gnuplot
## By edward.sternin@brocku.ca
## 2018.02

## outside of the jupyter notebook, can use these lines instead of a separate data file
## and then use $DATA instead of every occurrence of 'VI.dat' below.  It's a limitation
## jupyter, and not of gnuplot.

#$DATA << EOD
##  V   I,mA
#  0   0.468
#  1   0.405
#  2   0.342
#  3   0.279
#  4   0.216
#  5   0.153
#  6   0.090
#  6.4 0.064
#EOD

# scan through the data file
stats 'VI.dat'
# a few examples of useful values:
#x_max=STATS_max_x
#y_min=STATS_min_y
#Npts=STATS_records
#  etc.

## fit the data
set dummy v
P(v)=a*(v-Vo)**2+b
Vo=4
a=-15
b=0.85
# fit does NOT like zero starting values for any parameters, so do not skip the previou
fit P(v) 'VI.dat' using ($1):($1)*($2) via Vo,a,b
```

```
# two rows, one column is the layout of outputs for our multiple "plot ..." commands
set multiplot layout  2,1

## upper frame, P vs. V
set xlabel 'V, Volts'
set ylabel 'Power P=VI, mW'
plot[0:6.5] [0.:1.2] 'VI.dat' using ($1):($1)*($2) with points pt 6 ps 1.25 t 'measured
        [STATS_min_x:STATS_max_x] P(v) t sprintf("fit: %.2f(V-%.2f)^2+%.2f",a,Vo,b),\
        '+' using (Vo):(-0.4):(0):(0.4+b) with vectors t sprintf("P_{max} at V=%.2f V",

## lower frame, R vs. V
Ro=Vo**2/b
set xlabel 'V, Volts'
set ylabel 'Resistance R=V/I, {/Symbol W}'
plot [0:6.5] [0:60] 'VI.dat' using ($1):($1)/($2) with points pt 6 ps 1.25 t 'measured
        [STATS_min_x:STATS_max_x] (v<=5.3 ? v**2/P(v) : NaN ) t 'fit: V^2/P',\
        '+' using (Vo):(60):(0):(-60+Ro) with vectors ls 3 t sprintf("P_{max} at V=%.2f
        '+' using (Vo):(Ro):(-Vo):(0) with vectors ls 3 t sprintf("at P_{max}, R=%.2f {

unset multiplot
```


measured P=VI
fit: -0.06(V-3.71)^2+0.87
P_max at V=3.71 V
Power P=VI, mW
V, Volts
0
0.2
0.4
0.6
0.8
1
1.2
0
1
2
3
4
5
6


measured R=V/I
fit: V^2/P
P_max at V=3.71 V
at P_max, R=15.83 Ω
Resistance R=V/I, Ω
V, Volts
0
10
20
30
40
50
60
0
1
2
3
4
5
6

```
## a sample script to demonstrate some more advanced features of gnuplot
## By edward.sternin@brocku.ca
## 2018.02

## outside of the jupyter notebook, can use these lines instead of a separate data file,
## and then use $DATA instead of every occurrence of 'VI.dat' below.  It's a limitation of
## jupyter, and not of gnuplot.

#$DATA << EOD
##  V   I,mA
#  0   0.468
#  1   0.405
#  2   0.342
#  3   0.279
#  4   0.216
#  5   0.153
#  6   0.090
#  6.4 0.064
#EOD

# scan through the data file
stats 'VI.dat'

* FILE:
  Records:           8
  Out of range:      0
  Invalid:           0
  Column headers:    0
  Blank:             0
  Data Blocks:       1

* COLUMNS:
  Mean:               3.4250          0.2521
  Std Dev:            2.1827          0.1376
  Sample StdDev:      2.3335          0.1472
  Skewness:          -0.1191          0.1168
  Kurtosis:           1.6791          1.6801
  Avg Dev:            1.9250          0.1214
  Sum:               27.4000          2.0170
  Sum Sq.:          131.9600          0.6601

  Mean Err.:          0.7717          0.0487
  Std Dev Err.:       0.5457          0.0344
  Skewness Err.:      0.8660          0.8660
  Kurtosis Err.:      1.7321          1.7321
```

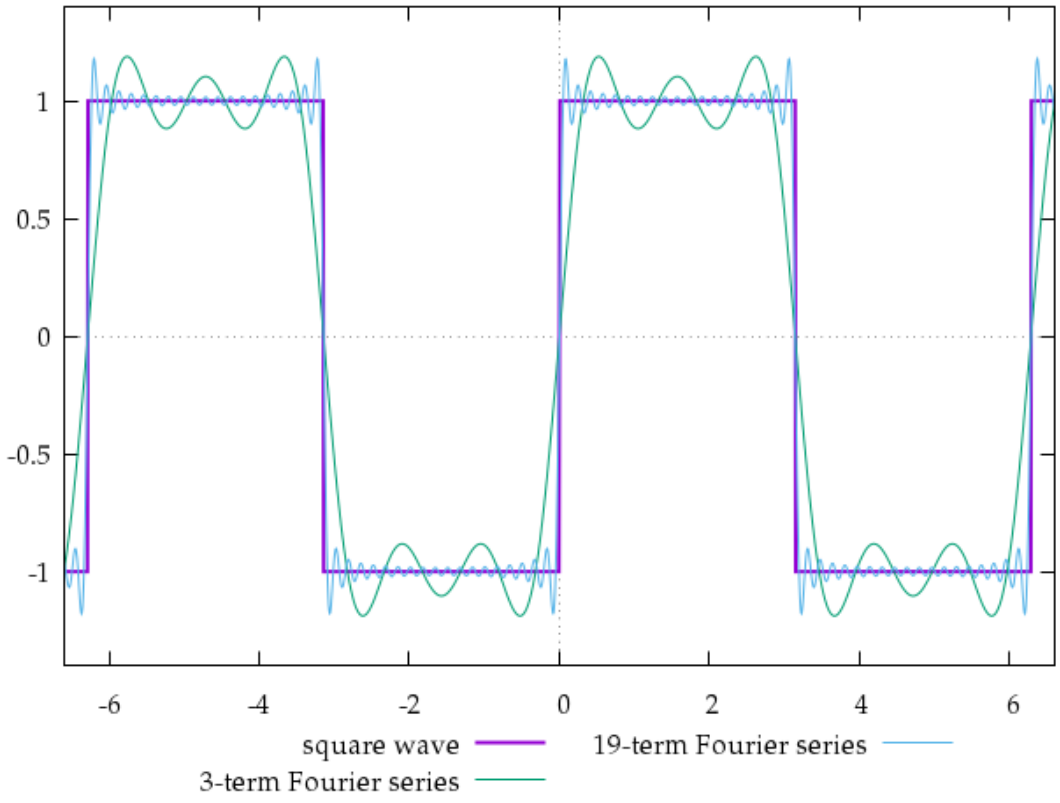
```
  Minimum:              0.0000 [0]        0.0640 [7]
  Maximum:              6.4000 [7]        0.4680 [0]
  Quartile:             1.5000            0.1215
  Median:               3.5000            0.2475
  Quartile:             5.5000            0.3735

  Linear Model:         y = -0.06306 x + 0.4681
  Slope:                -0.06306 +- 4.241e-05
  Intercept:            0.4681 +- 0.0001723
  Correlation:          r = -1
  Sum xy:               4.505

# a few examples of useful values:
#x_max=STATS_max_x
#y_min=STATS_min_y
#Npts=STATS_records
#  etc.

## fit the data
set dummy v
P(v)=a*(v-Vo)**2+b
Vo=4
a=-15
b=0.85
# fit does NOT like zero starting values for any parameters, so do not skip the previous lines
fit P(v) 'VI.dat' using ($1):($1)*($2) via Vo,a,b
iter      chisq       delta/lim  lambda   Vo             a             b
   0 9.0276894603e+04   0.00e+00  1.68e+02    4.000000e+00  -1.500000e+01   8.500000e-01
   1 7.7401581630e+03  -1.07e+06  1.68e+01    3.709145e+00  -4.870474e+00   8.539867e-01
   2 1.4393124873e-01  -5.38e+09  1.68e+00    3.706914e+00  -8.241128e-02   8.560346e-01
   3 1.8474236621e-04  -7.78e+07  1.68e-01    3.711613e+00  -6.232464e-02   8.621812e-01
   4 1.1747302856e-05  -1.47e+06  1.68e-02    3.709792e+00  -6.319534e-02   8.692526e-01
   5 1.1723193296e-05  -2.06e+02  1.68e-03    3.709757e+00  -6.320607e-02   8.693376e-01
   6 1.1723193294e-05  -1.18e-05  1.68e-04    3.709757e+00  -6.320607e-02   8.693376e-01
iter      chisq       delta/lim  lambda   Vo             a             b

After 6 iterations the fit converged.
final sum of squares of residuals : 1.17232e-05
rel. change during last iteration : -1.18416e-10

degrees of freedom    (FIT_NDF)                        : 5
rms of residuals      (FIT_STDFIT) = sqrt(WSSR/ndf)    : 0.00153122
variance of residuals (reduced chisquare) = WSSR/ndf   : 2.34464e-06

Final set of parameters            Asymptotic Standard Error
=======================            ==========================
Vo              = 3.70976          +/- 0.002165     (0.05835%)
```

```
a               = -0.0632061       +/- 0.0001394    (0.2205%)
b               = 0.869338         +/- 0.0008429    (0.09696%)

correlation matrix of the fit parameters:
                Vo     a      b
Vo              1.000
a               0.422  1.000
b              -0.245 -0.762  1.000

# two rows, one column is the layout of outputs for our multiple "plot ..." commands
set output '/tmp/gnuplot-inline-1520556393.8152409.748898697384.png'
set multiplot layout  2,1

## upper frame, P vs. V
set xlabel 'V, Volts'
set ylabel 'Power P=VI, mW'
plot[0:6.5] [0.:1.2] 'VI.dat' using ($1):($1)*($2) with points pt 6 ps 1.25 t 'measured P=VI', [

## lower frame, R vs. V
Ro=Vo**2/b
set xlabel 'V, Volts'
set ylabel 'Resistance R=V/I, {/Symbol W}'
plot [0:6.5] [0:60] 'VI.dat' using ($1):($1)/($2) with points pt 6 ps 1.25 t 'measured R=V/I', [

unset multiplot
unset output
```

gnuplot also has some programming ability. Here's an example of a recursively-defined function. It plots a truncated FT decomposition of a square wave, to an arbitrary order of truncation:

```
In [11]: %gnuplot inline pngcairo size 640,480 font "Palatino,12"

In [12]: %%gnuplot
         # for a clean start, as gnuplot may remember things from previous scripts
         reset

         # set parameters controlling the appearance of the graphs
         set xrange [-2.1*pi:2.1*pi]
         set yrange [-1.4:1.4]
         set samples 2001
         set key below
         set zeroaxis

         # define the Fourier series' expansion iteratively: sin(x)+sin(3x)/3+sin(5x)/5+...
         f(x,n) = (n==1) ? (4/pi)*sin(x) : f(x,n-1) + (4/pi)*sin((2*n-1)*x)/(2*n-1)

         # plot the original square wave, and a couple of interesting approximations
```

```
plot sgn(sin(x)) t 'square wave' lw 2,\
     f(x,3)  t '3-term Fourier series',\
     f(x,19) t '19-term Fourier series'
```




```
# for a clean start, as gnuplot may remember things from previous scripts
reset

# set parameters controlling the appearance of the graphs
set xrange [-2.1*pi:2.1*pi]
set yrange [-1.4:1.4]
set samples 2001
set key below
set zeroaxis

# define the Fourier series' expansion iteratively: sin(x)+sin(3x)/3+sin(5x)/5+...
f(x,n) = (n==1) ? (4/pi)*sin(x) : f(x,n-1) + (4/pi)*sin((2*n-1)*x)/(2*n-1)

# plot the original square wave, and a couple of interesting approximations
set output '/tmp/gnuplot-inline-1520556393.9686322.136613407649.png'
plot sgn(sin(x)) t 'square wave' lw 2,      f(x,3)  t '3-term Fourier series',      f(x,19) t '1
unset output
```

Of course, there are also excellent plotting capabilities within both python, matlab/octave and maple environments, all with much more sophisticated computational capabilities. We will learn these as we go along. However, the flexibility and the ability to generate both screen-friendly bitmap (e.g. PNG) plots and publication-quality scalable vector (SVG, Encapsulated PostScript, LaTeX, etc.) plots makes physica and/or gnuplot useful additions to the scientific toolbox.

1.3 Homework

Lord Cavendish was the designer of the original experiment that used a pair of lead spheres and a very sensitive torsional balance to measure the universal gravitational constant, G. A manual for a modern version of such a torsional balance is here. As described there, in Fig.18 on p.13, the following set of data was obtained.

Produce a physica or a gnuplot macro that would plot and analyze the data, and calculate G from it. It appears that a good fit would result from fitting $S(t) = S_0 + Ae^{-(t-t_0)/\tau}\cos[\omega(t-t_0)]$ to each segment of the experiment with S_0, A, t_0, τ and ω the parameters of the fit. Without knowing the exact geometry of the experiment, ΔS between the two equilibrium positions cannot be used, but perhaps the oscillation period can be extracted and used in the analysis. Use the average of the two values obtained for both sections of the data.

A more careful examination reveals that there might be a small drift in the data. Model it by a small linear-in-time correction term, $\alpha(t-t_0)$, and see if the precision of the fit improves.

The data file is in /work/5P10/Cavendish.dat, and you can execute the next cell to save it to your local file space.

```
In [16]: %%file Cavendish.dat
         # Cavendish experiment 2012-02-24
         ## minutes, position_of_dot, cm

         # set spheres to one side at 11:45:00, 45 mins since the start
         45        57.5
         45.5        58
         46        58.5
         46.5        60.5
         47        63
         47.5        66
         48        69
         48.5        72
         49        74.5
         49.5        76.7
         50        78
         50.5        78.7
         51        78.7
         51.5        78
         52        76.7
         52.5        75.
         53        73
         53.5        70.8
```

```
54        69.2
54.5        67.7
55        66.8
55.5        66.4
56        66.5
56.5        67.1
57        68.1
57.5        69.2
58        70.7
58.75        73.2
59        73.8
59.5        74.8
60        75.6
60.5        76.1
61        76.1
61.5        75.8
62        75.1
62.5        74.2
63        73.2
63.5        72.2
64        71.5
64.5        70.7
65        70.1
65.5        69.9
66        69.9
66.5        70.1
67        70.6
67.5        71.2
68        72
68.5        72.7
69        73.4
69.5        74
70        74.2
70.5        74.6
71        74.7
72        74.1
72.5        73.8
73        73.2
73.5        72.8
74        72.2
74.75        71.8
75        71.6
75.5        71.5
76        71.4
76.5        71.6
77        72
77.75        72.6
78        72.8
```

```
78.5        73.1
79        73.5
79.25        73.7
79.5        73.9
79.75        74
80        74.1
80.25        74.1
80.5        74.1
80.75        74.1
81        74.1
81.25        74
81.5        74
81.75        74
82        73.8
82.5        73.7
83        73.4
83.5        73.1
84        72.9
84.5        72.7
85.25        72.7
85.5        72.7
86        72.6
86.5        72.6
87        72.7
87.5        72.8
88        73.1
88.5        73.3
89        73.6
89.5        73.7
90        73.8
90.5        74
91        74
93        73.8
93.5        73.6
94        73.5
98        73.3


# reverse the spheres at 13:25:00, 145 mins since the start
145        75.5
145.5        73.8
146        69.8
146.5        61.5
147        55
147.5        46.5
148        36.5
148.5        31
149        25.8
```

```
149.5       22.6
150       21.6
150.5       23
151       26
151.5       30.8
152       36.6
152.5       42.5
153       48.1
153.5       53.2
154       57.3
154.5       59.5
155       60.2
155.5       59.7
155.75       58.8
156       57.7
156.25       56.2
156.5       54.5
156.75       52.8
157       50.8
157.25       48.7
157.5       46.5
157.75       44.5
158       42.5
158.25       40.6
158.5       38.8
158.75       37.2
159       35.9
159.25       34.8
159.5       34
159.75       33.6
160       33.2
160.25       33.2
160.5       33.6
160.75       34.1
161       35
161.25       35.9
161.5       37
161.75       38.2
162       39.5
162.5       42.5
163       45.3
163.5       48
164       50.1
164.5       51.5
165       52.2
165.5       52.1
166       51.2
166.5       49.8
```

```
167        48
167.5        45.9
168        43.8
168.5        42
169        40.5
169.5        39.2
170        38.9
170.75        39.2
171        39.7
171.5        40.6
172        41.9
172.5        43.6
173        44.9
173.75        46.9
174        47.5
174.5        48.2
175        48.7
175.5        48.7
176        48.4
176.5        47.7
177        47
177.5        46
178        45
178.5        44
179        43.1
179.5        42.7
180        42.3
180.5        42.1
181        42.5
181.5        42.9
182        43.4
182.5        44.1
183        44.7
183.5        45.5
184        46
184.5        46.4
185        46.7
185.5        46.7
186        46.7
186.5        46.4
187        46.1
187.5        45.6
188        45.2
188.5        44.7
189        44.3
189.5        44.1
190        43.9
191        44
```

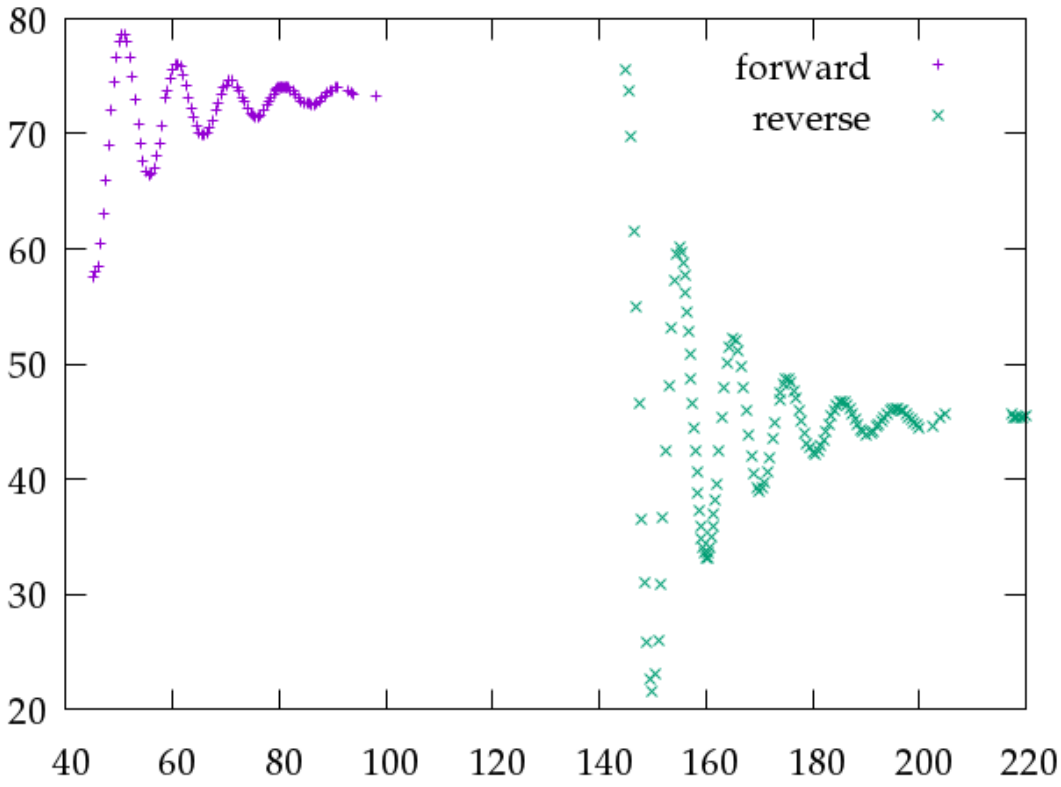
```
191.5        44.2
192         44.6
192.5        44.7
193         45
193.5        45.4
194         45.7
194.5        45.9
195         46.1
195.5        46.1
196         46.1
196.5        46
197         45.9
197.5        45.6
198         45.4
198.5        45.2
199         44.9
199.5        44.7
200         44.5
202.5        44.6
204         45.4
205         45.7
217.5        45.6
217.75        45.4
218         45.4
218.5        45.3
219         45.3
219.5        45.4
220         45.5
```

```
Overwriting Cavendish.dat
```

These two examples (for gnuplot and physica) are a good start:

```
In [14]: %gnuplot inline pngcairo size 640,480 font "Palatino,16"
```

```
In [15]: %%gnuplot
         # for a clean start, as gnuplot may remember things from previous scripts
         reset

         #plot "Cavendish.dat"

         #plot "Cavendish.dat" using ($1 < 140 ? $1: NaN ):($2/100) title "forward",\
         #     "Cavendish.dat" using ($1 > 140 ? $1: NaN ):($2/100) title "reversed"

         ### requires that TWO blank lines separate data into "blocks" in the data file
         plot "Cavendish.dat" index 0 title "forward", "" index 1 title "reverse"
```




```
# for a clean start, as gnuplot may remember things from previous scripts
reset

#plot "Cavendish.dat"

#plot "Cavendish.dat" using ($1 < 140 ? $1: NaN ):($2/100) title "forward", #     "Cavendish.dat

### requires that TWO blank lines separate data into "blocks" in the data file
set output '/tmp/gnuplot-inline-1520556394.1015484.651333514107.png'
plot "Cavendish.dat" index 0 title "forward", "" index 1 title "reverse"
unset output
```

The data is in and is separated into two parts. Complete this homework by adding the fit command, which might look like this, if the dependence were a purely linear function:

Do not skip the step of setting reasonable initial values for each fit parameters, and do not use the initial values of zero, as the fit command chokes on those. By a happy coincidence, an old gnuplot tutorial demonstrates how to do just what we need to do: https://www.cs.hmc.edu/~vrable/gnuplot/using-gnuplot.html

The same, of course, can be done in physica (which is perfectly happy to start with a zero estimate for parameters, and defaults them to 1.0 if not specified):