

Introduction to Computational Astrophysics

Helge Todt

Astrophysics
Institute of Physics and Astronomy
University of Potsdam

SoSe 2019



Brief introduction to gnuplot

Starting gnuplot

- gnuplot is available for almost every platform (operating system): Linux, MacOS X, Windows, ...
- download, e.g, from <http://gnuplot.info/>
- under Linux: start interactive session in terminal via `gnuplot`
- quit gnuplot by command `exit`

- gnuplot can plot basic functions (independent variable / dummy variable is x) and combinations of them, default plot symbol for functions: solid line
- examples
 - plot $\sin(x)$
 - plot $x^{**3} + 0.5*\sqrt{2}$
- plotting more than one function by using comma separated list:
plot $\sin(x)$, $\cos(1/x)$, $\tanh(x+2)$

Plotting data

gnuplot plots data from files in ascii table format, i.e.

```
# this is a comment  
4.5 91 -0.5  
5.6 70  0.8  
19   200 1.1
```

- plot “file.txt” → plots 2nd column over 1st column
- plot ‘filexyz.txt’ using (\$2):(\$3) → plots 3rd column over 2nd column
- plot ‘data.txt’ u (log10(\$1)): (log10(\$2)) → plots the decadic logarithm of the data in columns 1 and 2 (double-logarithmic plot)

with help of the Levenberg-Marquardt algorithm gnuplot can fit any function with free parameters to data:

① define function: $f(x) = a * x + b$

② fitting examples:

```
fit f(x) 'data.txt' via a, b
```

```
fit f(x) 'data.txt' u (log10($1)):(log10($2)) via a, b
```

③ plotting data and function:

```
plot 'data.txt', f(x)
```

- x- and y-axis labels: `set xlabel 'd in pc',
set ylabel 't in Ga'`
- key (legend): is automatically generated, can be written by option
`title: plot 'data.txt' title 'observation (1998)' \
, f(x) t 'model 17-04'`

→ requires execution of previous plot command (or just `replot`)

Creating PDFs for output

gnuplot supports many different output formats (see → help terminal)

- ① set terminal pdf enhanced color → sets terminal (output format) to colorized pdf with special characters
- ② set output 'myplot.pdf' → name of the file for output (don't forget it!)
- ③ plot 'data.txt', f(x), or replot
- ④ either: set term qt (resetting terminal to previous output format) or quit
→ this assures that the plot is *written* to the file (otherwise: empty file)

Special characters

if output is written to PDF or PS file, via option enhanced:

Input	Output in PDF/PS
T_0	T_0 (subscript)
e^{-x}	e^{-x} (superscript)
{/Symbol Qp}	$\Theta\pi$

besides interactive mode, gnuplot supports also non-interactive script mode

- write all instructions into an ASCII text file (e.g., “myplot.gplt”) comments begin with a # (like in makefile and shell)
line continuation via backslash \

- execute gnuplot script from shell:

```
gnuplot myplot.gplt
```

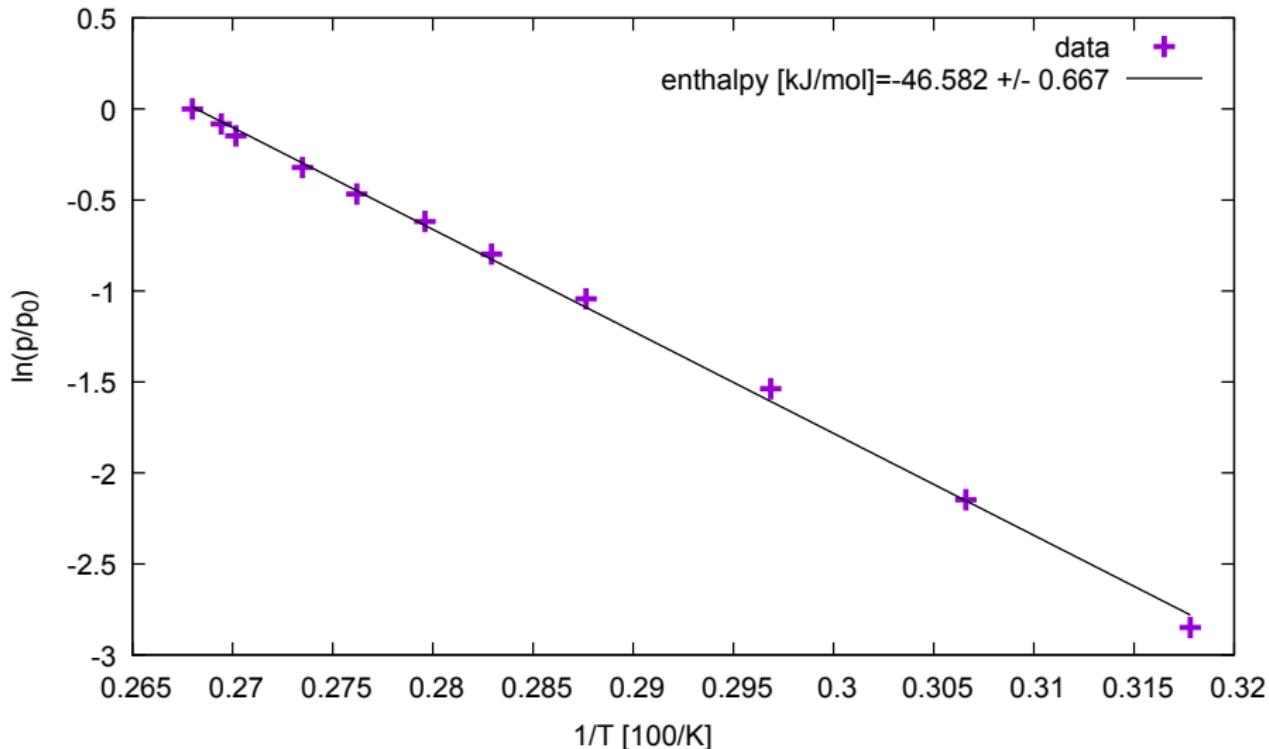
→ useful for automated PDF creation

→ easy re-use of formatting and plot instructions (labels, sizes, . . .)

Example for fitting and pdf output I

```
set terminal pdf enhanced color
set xlabel "1/T [100/K]"
set ylabel "ln(p/p_0)"
ln_p(x) = b + a*x
set fit errorvariables
R=8.314
p_0=1.019
fit [*:*] ln_p(x) 'enthalpie.dat' \
using (1./((\$2)+273.15)):(log((1.019+(\$1))/1.019)) via a,b
set output "enthalpy.pdf"
plot 'enthalpie.dat' \
using (1e2/((\$2)+273.15)):(log((p_0+(\$1))/p_0)) \
with points ps 1 linewidth 3 title "data" \
, ln_p(1e-2*x) with lines linecolor "black" \
t sprintf("enthalpy [kJ/mol]=%5.3f +/- %5.3f",a*R*1e-3,R*a_err*1e-3)
```

Example for fitting and pdf output II



Histogram

is the **graphical** representation of a frequency distribution of a quantity x

- requires the division of the data (erfordert die Einteilung der Daten (measured variable x) into classes, so-called **bins**, whose **width** (Δx) is constant or variable
- for that matter neighboring rectangles are drawn over every bin, such that their heights represent the frequency of the corresponding values

Histograms are also an estimator of the **probability density function** $p(x)$ of a continuous random variable x .

gnuplot allows to compute and plot appropriate representations of a histogram for a given data set

Example

Let the file "gauss.dat" contain 10^3 random numbers from a Gaussian normal distribution with mean value $\mu = 0$ and scatter $\sigma = 1$, hence of the distribution

$$N(x; \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Histograms III

We want to plot the frequency distribution of these values:

- ① define the bin width, Δx :

```
gnuplot> bw=0.2  
gnuplot> set boxwidth bw
```

... and a so-called “binning” function:

```
gnuplot> bin(x,s)=s*ceil(x/s)
```

The function **ceil(x)** rounds *up* the value of x

- ② the number of data points (for normalization)

```
gnuplot> N=1000
```

this can be obtained for **gnuplot > 4.6** also from

```
gnuplot> stats "gauss.dat" ; N = STATS_records
```

- ③ The histogram is computed and plotted:

```
gnuplot> plot "gauss.dat" u (bin($1,bw)-0.5*bw):(1./(N*bw)) \
           smooth frequency with boxes lc rgb "blue"
```

The data will be divided into bins ("binned") and by the directive **smooth frequency** each hit of a bin is summed up; the result will be plotted as a function of the bins with "boxes"

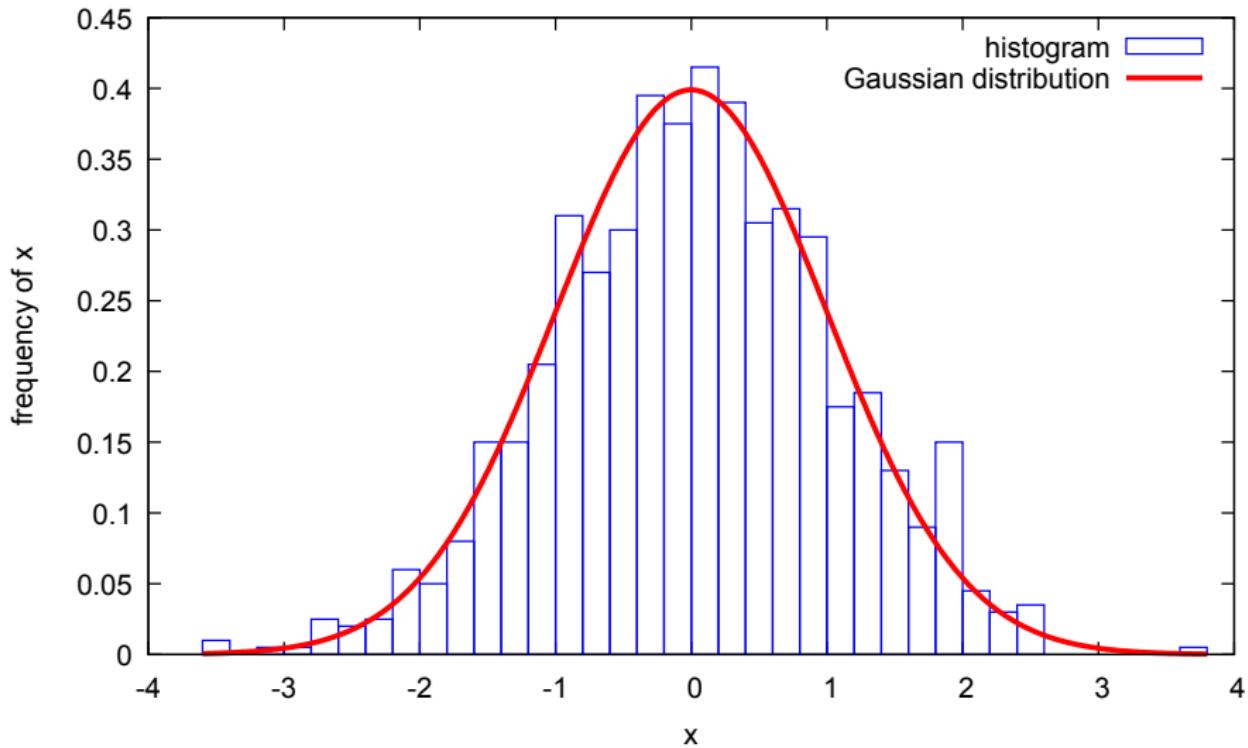
- ④ one can also give the underlying distribution explicitly:

```
gnuplot> gauss(x) = 1./sqrt(2*pi) * exp(-0.5*x**2)
```

and plot it together with the histogram:

```
gnuplot> replot gauss(x) with lines linewidth 3 \
           linecolor rgb "red"
```

Histograms V



Histograms VI

```
set term pdf enhanced color font "Helvetica 20"
set output "histogram_gauss_en.pdf"

set xlabel "x"
set ylabel "frequency of x"

# Box width
bw = 0.2
set boxwidth bw

# number of data points
N = 1000

# Binning function (left aligned)
bin(x,s) = s*(ceil(x/s))

# Gaussverteilung (<x>=0, sigma(x)=1)
gauss(x) = 1./sqrt(2*pi) * exp(-0.5*x**2)

# Plot histogram
plot 'gauss.dat' u (bin($1,bw)-0.5*bw):(1./(N*bw)) smooth frequency \
w boxes lc rgb "blue" t "histogram", gauss(x) w l lt 1 lw 3 \
lc rgb "red" t "Gaussian distribution"
```