Computational Astrophysics I: Introduction and basic concepts

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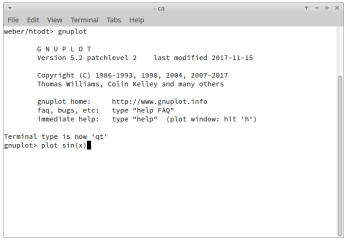
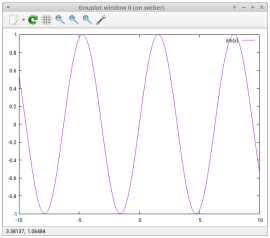
Brief introduction to gnuplot

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 termial via
  `gnuplot`





- quit gnuplot by command
  `exit`

Plotting functions

- 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 only over a specific x-range (also for fitting):
  `plot [-2.5:+3] cos(x)`
- plotting only over a specific y-range:
  `plot [] [-1:+1] sin(x)`
- plotting only over a specific x- and y-range:
  `plot [-2.5:+3] [-1:1] cos(2*x)`

Labels

- 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 type `replot`

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
```

- Columns are separated by blanks. Can be changed before plotting, e.g.,
  `set datafile separator "," # (comma seprated)`
  `set datafile separator "\t" # (separated by tabs)`
- `plot "file.txt"`
  → default: 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)

Creating a histogram I

Histogram

is the **graphical** representation of the frequency distribution of some quantity x.

- → requires the division of the data (quantity) into **bins** of a **width** Δx (can be constant or variable)
- → representation usually by rectangles of width Δx and height corresponding to frequency of occurrence
- → can be used to estimate the **probability density function** $p(x)$ of a continuous random variable x

Creating a histogram II

Example: normal distribution / Gaussian distribution

A data set of 10^3 random variables drawn from a Gaussian distribution with

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

where the mean value was set to $\mu = 0$ and the variance to $\sigma = 1$, hence the distribution is $N(x,0,1) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{1}{2} \cdot x^2) \rightarrow$ so-called standard normal distribution
in some file `"gauss.dat"`

10-DM banknote with a Gaussian distribution

Creating a histogram III

Graphical representation with gnuplot:

1. Define the (constant) width of the bins ("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 to next larger integer

2. The number of data points (for normalization):

```
gnuplot> N=1000
```

   one can also use

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

Creating a histogram IV

3. The histogram is then created via:

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

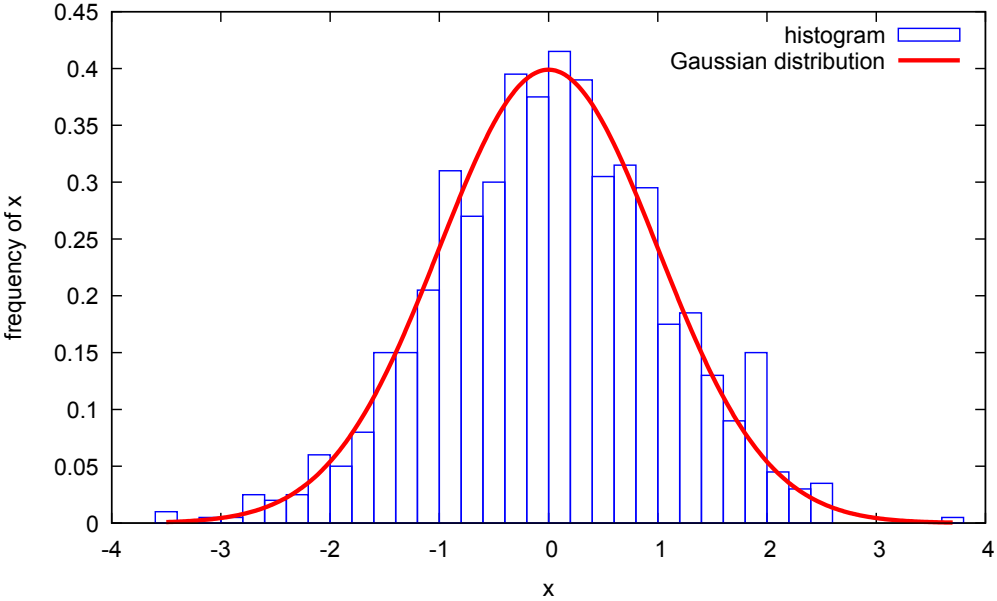
4. Plot together with the underlying probabilty density function

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

in the same diagram:

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

Creating a histogram V



Fitting data

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)
   ```

If the fit should be done only for a specific x-range:

```
fit [100:300] f(x) "data.txt" via a, b
```

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 or incomplete PDF 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}`	$\Theta\pi$

Scripts in gnuplot

In addition to the 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