Exercise 13

MC Application, Linear Algebra

(handed out: 24.07.2023)

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1. Task *Bootstrapping* (20 extra P)

Implement the bootstrapping method in C++ to check the result of the linear regression applied on the data in `xydaten.txt` (clickable URL).

The values in the first column are $\lambda^2\,1/I\,dI/d\lambda$ in $4.67 \times 10^{-13}\,\mathrm{G}^{-1}$ with wavelength λ and intensity I. The data in the second column are the ratio of Stokes V to Stokes I (fraction of the circularly polarized light), such that the slope of the straight line fit corresponds to a magnetic field strength $\langle B_z \rangle$ in G. The errors $\sigma_{V/I}$ are given in the third column.

a) Implement the *linear regression* for the case of

i. given errors $\sigma_{V/I}$ (weighting of data points)

ii. without taking these errors into account, hence without weighting.

What is the result for the slope B_z and the error σ? Plot the data points and the straight line fit (e.g., via `gnuplot`). Think about a reasonable scaling of the axes. (5 extra P)

b) Your bootstrapping program should now create a random sample j of size n from the imported n data points (so combinations with repetition) and apply a linear regression to this sample, taking the errors $\sigma_{V/I}$ into account. Create m sample, where $m \gg n$. Print out the $B_z(j)$ of every run into a file, where each line just contains the value of $B_z(j)$. (5 extra P)

c) Plot a histogram of the obtained values of B_z (e.g., with `gnuplot`). Choose an appropriate bin size. (2 extra P)

d) What does the distribution look like? What is the expectation value and the variance? (Hint: Can be obtained from `gnuplot` or *recursively* when writing $B_z(j)$ to the file within the program.)

Judge on the significance of the "measured" magnetic field with help of the histogram and the calculated statistical quantities. (3 extra P)

e) Repeat the bootstrapping analysis, but this time without taking the errors $\sigma_{V/I}$ into account. (2 extra P)

2. Task *Nonlinear fit* (10 extra P)

Fit the Breit-Wigner formula

$$f(E) = \frac{f_\mathrm{r}}{(E - E_\mathrm{r})^2 + \Gamma^2/4} \tag{1}$$

via the parameters $f_\mathrm{r}, E_\mathrm{r}, \Gamma$ to the cross section data from the lecture. For this purpose write a program that fits the parameters with help of the Newton-Raphson method, i.e., by iteration and computing the Jacobian matrix. How sensitive the solution is to the

initial guesses for a_1, a_2, a_3?
Plot the resulting function together with the data. Determine with the mentioned method E_r and Γ (width of the resonance).

3. Task *Solving systems of linear equations* (10 extra P)
Let

$$\boldsymbol{A} = \begin{pmatrix} \frac{\pi}{3} & \frac{\pi}{3} & \dots & \dots & \dots & \frac{\pi}{3} \\ 0 & \frac{\pi}{3} & \dots & \dots & \dots & \frac{\pi}{3} \\ 0 & 0 & \frac{\pi}{3} & \dots & \dots & \frac{\pi}{3} \\ 0 & 0 & 0 & \ddots & \dots & \frac{\pi}{3} \\ 0 & 0 & 0 & \dots & \frac{\pi}{3} & \frac{\pi}{3} \\ 0 & 0 & 0 & & \dots & \frac{\pi}{3} \end{pmatrix} \in \mathbb{R}^{n\times n} \qquad \text{and} \qquad \boldsymbol{b} = \begin{pmatrix} n \\ n \\ \vdots \\ \vdots \\ n \\ n \end{pmatrix} \in \mathbb{R}^n \tag{2}$$

for different values of $n \geq 1000$.
Write a program in C/C++ that solves $\boldsymbol{Ax} = \boldsymbol{b}$ for $\boldsymbol{x}$ numercially

a) column-wise

b) row-wise

and measure the runtime of both versions with help of, e.g., `omp_get_wtime()`. Make n sufficiently large to get significant different runtimes. Explain the difference.
Hint: While the row-wise version might be straightforward to program (outer loop over first index i from $n-1$ to 1), the column-wise implementation (outer loop over second index j from $n-1$ to 1) looks in pseudo code like that:

```
for j = n-1 ... 1
  for i = 1 ... j
      b[i] = b[i] - a[i][j+1] * x[j]
  x[j] = b[j] / a[j][j]
```