Numerische Methoden der Physik

WiSe 2023-2024 – Prof. Marc Wagner

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Exercise sheet 12

To be handed in on 17.01.2024 and discussed on 19.01.2024 and 22.01.2024.

Exercise 1 [*Equivalence between the standard error and the jackknife error*] (4 pts.)

For a set of measurements $f^{(1)}, \ldots f^{(S)}$, the mean value f and error σ can be estimated via

$$f = \frac{1}{S}\sum_{s=1}^{S} f^{(s)}, \qquad \sigma = \left(\frac{1}{S(S-1)}\sum_{s=1}^{S}(f^{(s)} - f)^2\right)^{1/2}.$$

In the jackknife method, the $f^{(s)}$ are combined to reduced samples

$$a^{(s)} = \frac{1}{S-1}\sum_{r\neq s} f - f^{(r)},$$

with jackknife mean and jackknife error

$$a = \frac{1}{S}\sum_{s=1}^{S} a^{(s)}, \qquad \sigma^{\text{red.}} = \left(\frac{S-1}{S}\sum_{s=1}^{S}(a^{(s)} - a)^2\right)^{1/2}.$$

Show that, in this particular case, the jackknife method is equivalent to the standard method, i.e.

$$f = a \quad \text{and} \quad \sigma = \sigma^{\text{red.}}.$$

Explain, why in other cases, the equation for f and σ cannot be applied and the jackknife method is mandatory. Discuss in this context briefly the computation of $\ln(f)$ (mean value and error), as well as a χ^2-minimization fit to data points (mean values and errors of the fit parameters).

Exercise 2 [*Minimization of a paraboloid*] (6 + 4 + 6 = 16 pts.)

(i) Implement the golden section search to minimize a 1-dimensional function $f(x)$ for a given starting interval $[a^{(0)}, c^{(0)}]$ with $c^{(0)} > a^{(0)}$. Choose the intermediate point b as given in the script, by fixing $w = (3-\sqrt{5})/2$. Terminate the procedure, if the condition

$$c - a < \tau,$$

with $\tau = 10^{-5}$, is fulfilled, or $N = 100$ iterations have passed. Test your implementation by minimizing the parabola

$$f(x) = x^2 + 1,$$

with $a^{(0)} = -1$ and $c^{(0)} = 1$. Present the evolution of a and c in one common plot and discuss your observations.

(ii) Repeat task (i), but instead of fixing $w = (3 - \sqrt{5})/2$, use $b^{(0)} = -0.1$ to compute $y^{(0)}$ and determine $(a, b, c) \to (a', b', c')$ with the criteria from the lecture. How has the evolution of a and c changed?

(iii) Now, consider the $D = 2$ dimensional paraboloid

$$g(x, y) = \frac{x^2 + y^2 + 2xy}{2h_1^2} + \frac{x^2 + y^2 - 2xy}{2h_2^2},$$

with $h_1 = 100$ and $h_2 = 0.01$.

Minimize g, by repeating 1-dimensional minimizations along straight lines parametrized by

$$\boldsymbol{s}_{2i}(t) = \boldsymbol{r}_{2i} + t\boldsymbol{p}_1 \quad \text{and} \quad \boldsymbol{s}_{2i+1}(t) = \boldsymbol{r}_{2i+1} + t\boldsymbol{p}_2,$$

with $\boldsymbol{p}_1 = (1, 0)$, $\boldsymbol{p}_2 = (0, 1)$ and $i = 0, 1, \ldots$.

Start the first minimization at $\boldsymbol{r}_0 = (0, 1)^t$. For this, find a way to algorithmically select two points $\boldsymbol{a}_0$, $\boldsymbol{c}_0$ on $\boldsymbol{s}_0(t)$, such that the minimum $\boldsymbol{x}_0^{\min}$ of $g(x, y)|_{(x,y)\in \boldsymbol{s}_0}$ is in between.

Repeat the process to find the minima $\boldsymbol{x}_i^{\min}$ of $g(x, y)|_{(x,y)\in \boldsymbol{s}_i}$ with $\boldsymbol{r}_i = \boldsymbol{x}_{i-1}^{\min}$, until you find the minimum of g within machine precision. How many iterations do you need?

Are $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ as given above efficient choices for search directions? What is the ideal search direction $\boldsymbol{p}_2$ for step 2?