



Introduction to Numerical Methods for Computer Simulation

Exercises No. 9

E 25: *Convergence radius of Newton's method.*

The nonlinear system

$$F(x, y) \equiv \begin{pmatrix} x^2 - y - 2 \\ xy + 1 \end{pmatrix} = 0$$

exhibits exactly three zeros. The zero $(x^*, y^*) = (1, -1)$ shall be approximated by Newton's method.

- Prove that the Jacobian matrix $DF(x, y)$ is invertible in (x^*, y^*) .
- Determine a radius r such that Newton's method converges to (x^*, y^*) for all starting values $(x^0, y^0) \in \mathcal{K}$, where

$$\mathcal{K} := \{(x, y) \in \mathbb{R}^2 : \max\{|x - x^*|, |y - y^*|\} \leq r\}.$$

E 26: *Modified Newton method.*

To solve the nonlinear system $F(x) = 0$ with $F : D \rightarrow \mathbb{R}^n (D \subset \mathbb{R}^n)$, consider the modified Newton method

$$\begin{aligned} &\text{starting value: } x^0 \\ &k = 0, 1, 2, \dots : \\ &\Delta x^k = -DF(x^k)^{-1} F(x^k) \\ &x^{k+1} = x^k + \lambda^k \Delta x^k. \end{aligned}$$

Assuming $F \in C^1(D)$, the corresponding Jacobian matrix is denoted by DF . Let x^* be the unique zero of F . The arising parameters λ^k have to be chosen appropriately.

Given a matrix $A \in \mathbb{R}^{n \times n}$ with $\det A \neq 0$, the test function

$$T(x, A) := \frac{1}{2} \|AF(x)\|^2$$

is defined applying the Euclidean norm $\|\cdot\|$.

a) *search direction.*

Consider a search direction $p^k \neq 0$ satisfying

$$(p^k)^T \text{grad}T(x^k, A) < 0. \quad (\star)$$

Prove that

$$\exists \mu^k > 0 \quad \forall 0 < \lambda \leq \mu^k : \quad T(x^k + \lambda p^k, A) < T(x^k, A).$$

Which matrices A fulfill (\star) in the case $p^k = \Delta x^k$?

b) *natural scaling.*

Show the equivalences

$$\begin{aligned} T(x, A) = 0 &\Leftrightarrow F(x) = 0 \Leftrightarrow x = x^* \\ T(x, A) \neq 0 &\Leftrightarrow F(x) \neq 0 \Leftrightarrow x \neq x^* \end{aligned}$$

Which choice of A implies that the Newton direction Δx^k represents the steepest descent of $T(x, A)$ in the point x^k ?

c) *invariance w.r.t. basis transformations.*

An iterative method is called invariant with respect to a basis transformation, if the produced sequence of points is independent of the chosen basis.

Consider the basis transformation

$$\tilde{e}_i = Qe_i, \quad i = 1, \dots, n$$

involving a matrix Q , which represents a diagonal matrix, an orthogonal matrix or an arbitrary regular matrix. Examine Newton's method for $F(x) = 0$ using $\lambda^k = 1$ and the method of the steepest descent for $T(x, A)$ with regard to invariance.

d) *λ -strategy.*

A common strategy for choosing the parameters λ^k is given by the demand

$$\|AF(x^{k+1})\|^2 \leq (1 - \tau\lambda^k)\|AF(x^k)\|^2,$$

where $0 < \tau \leq \frac{1}{2}$ is a constant, for example $\tau = \frac{1}{4}$. Now $0 < \lambda^k \leq 1$ is selected as large as possible such that the above property is still satisfied.

What is the meaning of the term $\tau\lambda^k$?

What advantage results, if $A = DF(x^k)^{-1}$ is chosen in each step?

E 27: Least-squares problems.

We consider two radiant sources in a single reservoir. The corresponding constants of collapse are $\lambda_l = -\ln 2/T_l$; $l = 1, 2$, where T_1, T_2 denote the two half-life periods. Consequently, the quantities $c_1(t)$ and $c_2(t)$ of the two species decrease in time. At many time points t_i , the intensity y_i of radiation is measured. We assume

$$y(t) = \alpha_0 + \alpha_1 c_1(t) + \alpha_2 c_2(t) = \alpha_0 + \alpha_1 c_1(0)e^{\lambda_1 t} + \alpha_2 c_2(0)e^{\lambda_2 t},$$

where α_0 represents the natural radiation in the environment and α_1, α_2 depend on the radiation intensity of the corresponding source. Thus the data (t_i, y_i) for $i = 1, \dots, m$ arises.

We observe the following two cases.

- a) Given the constants λ_1, λ_2 and the physical parameters $\alpha_0, \alpha_1, \alpha_2$, an approximation of the concentrations $c_1(0), c_2(0)$ at the beginning shall be determined.
- b) Given the quantities $c_1(0), c_2(0)$ at the beginning, an approximation of all physical parameters $\alpha_0, \alpha_1, \alpha_2, \lambda_1, \lambda_2$ shall be determined.

Formulate the corresponding least-squares problem in each case, i.e. specify the involved vectors, matrices or functions. What is the difference between the arising problems? Which numerical methods are appropriate to solve the respective problem?