Master in Mathematics and Applications - Técnico, Lisbon
Numerical Functional Analysis and Optimization - Fall Semester 2020

Computational Assignment - Version 3

1. Consider the unconstrained minimization problem

$$\min_{x\in\mathbb{R}^2} f(x)\,, \quad \text{where} \quad f(x_1,x_2) = \Big(x_2 - \frac{5}{4\pi^2}\,x_1^2 + \frac{5}{\pi}\,x_1 - 6\Big)^2 + 10\Big(1 - \frac{1}{8\pi}\Big)\cos x_1 + 10\,.$$

a) Find all the stationary points of f and classify them according to whether they are saddle points, strict/nonstrict local/global minimum/maximum points.

b) Approximate the local minimizers of f by the BFGS Method and the steepest descent method with exact line search. Consider different starting values $x_0 \in \mathbb{R}^2$ and different stopping criteria and investigate whether the methods converge to all stationary points or only to local minimizers.

c) SR1 (*Symmetric rank–1*) is a quasi-Newton method in which the update formula, generating symmetric approximations of the Hessian matrix of f, is given by

$$H_{k+1} = H_k + \frac{(y_k - H_k s_k)(y_k - H_k s_k)^T}{(y_k - H_k s_k)^T s_k}\,.$$

Approximate the minimizers by the SR1 method. Consider different initial approximations $x_0 \in \mathbb{R}^2$ and $B_0 \in \mathbb{R}^{2\times 2}$, a symmetric matrix, and different stopping criteria, and investigate whether the method converges to all stationary points or only to local minimizers.

d) Analyse experimentally the rate of local convergence of the proposed methods.

e) Modify your methods by converting them into inexact line search strategies. Consider Armijo backtracking for the BFGS method, constant step size for the the steepest descent method (consider different values for α) and a modification of the SR1 method obtained by adding a diagonal matrix γI (consider different values for $\gamma > 0$) to H_k before determining the new search direction. Consider different initial approximations and comment on whether the methods converge globally, or at least in a larger neighbourhood of the stationary points than the exact line search strategies considered previously.

2. Consider the following constrained minimization problem

$$\min_{x\in\mathbb{R}^2} f(x) \qquad \text{subject to} \qquad c_1(x) = 0\,, \tag{1}$$

where $f(x) = (x_1 - 2)^4 + (x_1 - 2\,x_2)^2$ and $c_1(x) = x_1 - x_2^2$.

a) Write out the first and the second order necessary and sufficient conditions of optimality for problem (1) and determine the local and global solutions.

b) Approximate the KKT points of problem (1) by Newton's method and Broyden's method.

c) Approximate the solutions of problem (1) by the quadratic penalty method, i.e. by minimizing the objective function

$$Q(x;\mu) = f(x) + \frac{1}{2\mu}\,c_1^2(x)\,,$$

where $\mu > 0$ is a penalty parameter. Solve the unconstrained minimization problems by the BFGS method and the steepest descent method.

d) Approximate the solutions of (1) by the augmented Lagrangian method, i.e. by minimizing the objective function

$$\mathcal{L}_A(x,\lambda_1;\mu) = f(x) - \lambda_1\,c_1(x) + \frac{1}{2\mu}\,c_1^2(x)\,.$$

Solve the unconstrained minimization problems by the BFGS method and the steepest descent method.

3. A nonlinear least squares problem (NLLS) can be written as the following unconstrained minimization problem

$$\min_{x\in\mathbb{R}^N} f(x)\,, \tag{2}$$

where $f(x) = \frac{1}{2}\sum_{j=1}^{M} f_j^2(x)$, $N < M$, with $f_j : \mathbb{R}^N \to \mathbb{R}$, $j = 1, \ldots, M$, denoting some nonlinear functions. Defining the *residual function* $F : \mathbb{R}^N \to \mathbb{R}^M$ by $F(x) = (f_1(x), f_2(x), \ldots, f_M(x))$, the NLLS problem can be written equivalently as

$$\min_{x\in\mathbb{R}^N} \frac{1}{2}\, F(x)^T F(x)\,. \tag{3}$$

Given that

$$\nabla f(x) = J_F(x)^T F(x)\,, \qquad H_f(x) = J_F(x)^T J_F(x) + S(x)\,, \tag{4}$$

where $J_F(x) \in \mathbb{R}^{M\times N}$ is the Jacobian matrix of F and $S(x) = \sum_{j=1}^{M} f_j(x)\, H_{f_j}(x)$, Pure Newton's method for approximating the solutions of the minimization problem (2) reads as

Pure Newton's Algorithm

Choose $x_0 \in \mathbb{R}^N$. For $k = 0, 1, \ldots$

1. Solve the linear system $\Big(J_F(x_k)^T J_F(x_k) + S(x_k)\Big)\, p_k = -\, J_F(x_k)^T F(x_k)$.
2. Compute $x_{k+1} = x_k + p_k$.

Gauss–Newton method is an iterative method, similar to Newton's method, where the term $S(x)$ is omitted from the Hessian matrix $H_f(x)$. It can be written as

Pure Gauss-Newton Algorithm

Choose $x_0 \in \mathbb{R}^N$. For $k = 0, 1, \ldots$

1. Solve the linear system $J_F(x_k)^T J_F(x_k)\, p_k = -\, J_F(x_k)^T F(x_k)$.
2. Compute $x_{k+1} = x_k + p_k$.

a) Show that Gauss-Newton method solves the linear least squares problem in one iteration. Consider $F(x) = Ax - b$, where $A \in \mathbb{R}^{M\times N}$, with $\operatorname{rank}(A) = N$.

b) Consider the objective function $f : \mathbb{R}^2 \to \mathbb{R}$ defined by

$$f(x) = \frac{1}{2}\sum_{j=1}^{4}\Big(\sin(t_j\, x_1) + \cos(t_j\, x_2) - y_j\Big)^2\,, \tag{5}$$

where $t_1 = 0.2, t_2, = 0.5, t_3 = 1.0, t_4 = 1.5$, and $y_1 = 0.9, y_2 = 0.6, y_3 = -0.6, y_4 = -0.7$. Approximate the global minimizers of f by Pure Newton's method and by the Gauss-Newton method.

c) Based on your numerical results, estimate the rate of local convergence of the proposed methods.

d) Approximate the global minimizers of (5) by considering a line search Gauss-Newton method with inexact search of the step length.