# Applied Numerical Analysis – Homework  $\#$  6

Optimization: Newton, Golden section, Steepest descent, Conjugate gradient

## Newton's method

Question 1 Consider the function  $f(x) = x^3 \exp(-x) - \sin(x)$ . If Newton is applied to optimise  $f(x)$  with starting point  $x_0 = 5.5$ , what is the value of  $x_1$ ?

A: 6.861 B: 4.879 C: 6.235 D: 3.891

Question 2 The Newton method for higher dimensions involves the Hessian matrix of function  $f(\bar{x}_n)$  evaluated at the current position  $(\bar{x}_n)$  for iteration n. What is the definition of the Hessian evaluated at  $\bar{x}_n$  for  $f(u, v)$ ?

$$
\mathbf{A} \mathbf{:}
$$

B:

A:

B:

 $Hf(\bar{x}_n) = \left[ \begin{array}{c} \frac{\partial f(\bar{x}_n)}{\partial u} \ \frac{\partial f(\bar{x}_n)}{\partial v} \end{array} \right]$  $Hf(\bar{x}_n) = \begin{bmatrix} \frac{\partial^2 f(\bar{x}_n)}{\partial u \partial v} \\ \frac{\partial^2 f(\bar{x}_n)}{\partial v \partial v} \end{bmatrix}$  $\begin{bmatrix} \frac{\partial^2 f(\bar{x}_n)}{\partial u \partial v} & \frac{\partial^2 f(\bar{x}_n)}{\partial u^2} \\ \frac{\partial^2 f(\bar{x}_n)}{\partial v^2} & \frac{\partial^2 f(\bar{x}_n)}{\partial v \partial u} \end{bmatrix}$ C:  $Hf(\bar{x}_n) = \left[ \begin{array}{cc} \frac{\partial^2 f(\bar{x}_n)}{\partial u^2} & \frac{\partial^2 f(\bar{x}_n)}{\partial u \partial v} \ \frac{\partial^2 f(\bar{x}_n)}{\partial v \partial u} & \frac{\partial^2 f(\bar{x}_n)}{\partial v^2} \end{array} \right]$  $\frac{\partial^2 \tilde{f}(\bar{x}_n)}{\partial v^2}$ 1 D:  $Hf(\bar{x}_n) = \begin{bmatrix} \frac{\partial^2 f(\bar{x}_n)}{\partial u^2} & \frac{\partial f(\bar{x}_n)}{\partial u} \\ \frac{\partial f(\bar{x}_n)}{\partial v} & \frac{\partial^2 f(\bar{x}_n)}{\partial v^2} \end{bmatrix}$  $\frac{\partial^2 \breve{f}(\bar{x}_n)}{\partial v^2}$ 1

**Question 3** Consider the function  $f(u, v, w) = \sqrt{u^2 + v \sin(w) + uvw}$ . The Newton method for higher dimensions involves the gradient of function  $f(u, v, w)$  evaluated at the current position. If  $\bar{x}_n(u, v, w) = [14, 5, 3]^T$  is the current position, what is the current gradient?

$$
\nabla f(\bar{x}_n) = \begin{bmatrix} 1.0661 \\ 1.0448 \\ 1.6128 \end{bmatrix}
$$
\nC:  
\n
$$
\nabla f(\bar{x}_n) = \begin{bmatrix} 1.3287 \\ 1.0448 \\ 2.4025 \end{bmatrix}
$$
\nD:  
\n
$$
\nabla f(\bar{x}_n) = \begin{bmatrix} 1.0661 \\ 1.4408 \\ 2.4025 \end{bmatrix}
$$
\nD:  
\n
$$
\nabla f(\bar{x}_n) = \begin{bmatrix} 1.0661 \\ 2.4025 \\ 1.0448 \end{bmatrix}
$$

## Golden section search

Question 4 Apply the golden ratio search to minimise function  $f(x) = \exp(x) - \cos(x)$ . Start at  $a_0 = -2, b_0 = 1, x_{L_0} = -0.8541, x_{R_0} = -0.1459$ . With  $f(x_{L_0}) = -0.2312$  and  $f(x_{R_0}) = -0.1251$ , determine  $[a_1, x_{L_1}, x_{R_1}, b_1].$ 



Question 5 Three iterations of the Golden-Section Search algorithm are applied to the function  $f(x) = x^2 + x - 1$  using the starting interval [-10, 10]. What is the size of the interval after three  $f(x) = x^2 + x - 1$  using the starting interval  $[-10, 10]$ .<br>iterations? [Hint: The golden ratio is  $\phi = \frac{1}{2}(1 + \sqrt{5})$ .]



**Question 6** A Golden-Section search algorithm is applied to a function  $f$ , on an initial interval [22, 113], and at every iteration the left-most interval is selected as containing the minimum. What is the location of the upper-limit of the interval after 10 iterations?



Question 7 Assume the the Golden-Section Search algorithm converges for a particular function  $f(x)$  and initial interval [a, b]. The minimum is approximated on each iteration by the midpoint of the interval. For example the approximation of the minimum given the initial interval is  $x_0 = a + \frac{b-a}{2}$ . What statement one can make about the error  $\epsilon_n = |x_n - x_{\text{exact}}|$  in the approximation of the minimum after n iterations of the method? [Hint:  $\phi$  is the golden ratio from Question 1.]



## Steepest descent

Question 8 Consider the minimization problem

$$
\min_{\mathbf{x}} f(\mathbf{x}).
$$

What is the steepest descent direction  $\mathbf{d}_n$  at  $\mathbf{x}_n$ ?

A: 
$$
\mathbf{d}_n = \nabla f(\mathbf{x}_n)
$$
  
\nB:  $\mathbf{d}_n = -\nabla f(\mathbf{x}_n)$   
\nC:  $\mathbf{d}_n = [\nabla^2 f(\mathbf{x}_n)]^{-1}$   
\nD:  $\mathbf{d}_n = -[\nabla^2 f(\mathbf{x}_n)]^{-1}$ 

Question 9 Apply 1 iteration of the steepest descent method to the quadratic form

$$
Q(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \cdot A \cdot \mathbf{x} - \mathbf{b}^T \cdot \mathbf{x} + c,
$$

where

$$
A = \begin{pmatrix} 1 & 0 \\ 0 & 10 \end{pmatrix}, \quad b = \begin{pmatrix} -4 \\ 4 \end{pmatrix}, \quad c = 1.
$$

with the initial condition  $x_0 = (0, 0)$ . What is the value of  $x_1$ ?



Question 10 The steepest descent method is applied to the quadratic form

$$
Q(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \cdot A \cdot \mathbf{x} - \mathbf{b}^T \cdot \mathbf{x} + c,
$$

where  $A$ ,  $b$  and  $c$ , are matrix, vector and scalar constants. Under what condition on the matrix  $A$ does the steepest descent method converge to the exact minimum in 1 iteration, from *any* initial condition  $x_0$ ? [Hint: If the initial search line  $x_0 + \alpha d_0$  includes the exact minimum of  $Q(x)$ , then the method will converge in 1 iteration.]

- A: A is a multiple of the identity matrix
- B: A is diagonal
- C: A is symmetric
- D: A is positive definite
- E: A has only positive eigenvalues
- F: A is equal to  $bb<sup>T</sup>$
- G: It never converges in 1 iteration
- H: It always converges in 1 iteration

## Nelder-Mead simplex

Question 11 Consider a simplified version of the Nelder-Mead Simplex algorithm for minimizing  $f(x)$  in 2d - as follows: Start with an initial triangle with three nodes:

1. Order the nodes according to the values of  $f$  at the vertices:

$$
f(x_1) \le f(x_2) \le f(x_3)
$$

- 2. Compute  $x_0$ , the average of all points except the worst  $x_3$ .
- 3. REFLECT: Compute  $x_R = x_0 + (x_0 x_3)$ ,
	- If  $f(x_R) < f(x_1)$  then EXPAND.
	- If  $f(x_R) > f(x_2)$  then CONTRACT.
	- Otherwise replace  $x_3$  with  $x_R$  and goto 1.
- 4. EXPAND: Compute  $x_E = x_0 + 2(x_0 x_3)$ ,
	- If  $f(x_E) < f(x_R)$  then replace  $x_3$  with  $x_E$  and goto 1.
	- Otherwise replace  $x_3$  with  $x_R$  and goto 1.
- 5. CONTRACT: Compute  $x_C = x_0 + \frac{1}{2}(x_0 x_3)$ ,
	- Replace  $x_3$  with  $x_C$  and goto 1.

Apply 1 iteration of this algorithm to the function

$$
f(x,y) = 3x^2 + y^2 - 4x + 1
$$

starting from the initial simplex  $(0, 0)$ ,  $(0.5, 0.5)$ ,  $(0.5, 0)$ . What values of f do you find on the nodes of your simplex after 1 iteration?



Question 12 Consider the simplified Simplex algorithm of the previous question. By coincidence, one of the vertices  $(x_1)$ , of the initial simplex is exactly the true global minimum of  $f(\cdot)$ . How does the algorithm behave in this situation?

- A: The algorithm regonizes that the global minimum has been found and stops immediately.
- B: The simplex gets smaller with increasing number of iterations.
- C: The simplex says the same size, but the vertex  $x_1$  is kept at every iteration.
- D: The simplex gets bigger, but the vertex  $x_1$  is kept at every iteration.
- E: The center of the simplex becomes centered on the global minimum.
- F: The simplex stretches in the same direction on every iteration.
- G: The simplex shrinks in the same direction on every iteration.
- H: The algorithm doesn't change the simplex.

## The big picture

Question 13 A minimization problem in  $f(x)$  can be restated as a zero-finding problem by setting  $f'(x) = 0$ . In a similar way a 1d zero-finding problem  $g(x) = 0$  can be rephrased as an minimization problem: Find  $x$  such that

$$
\min_x \frac{1}{2} [g(x)]^2.
$$

This will have a global minimum at every x which satisfies  $g(x) = 0$ , but may also have other local minima  $\tilde{x}_1, \ldots, \tilde{x}_n$ . What equation will these local minima satify?



## Quiz 2013 – 60 mins

Question 14 What is the global minimum of

A: Unanswered  
\nB: 0\n  
\n
$$
\begin{array}{ccc}\n & \min_{x \in \mathbb{R}} \left[ 1 - \frac{1}{1 + x^2} \right] ? \\
\text{D: } \frac{1}{4} & \text{E: } \frac{1}{2} \\
\text{E: } \frac{1}{2} & \text{F: } 1\n\end{array}
$$
\nG: 2  
\nB: 0\n  
\nG: 2

Question 15 Apply 1 iteration of Newton's method (for optimization) to approximate the minimum of

$$
f(x) = \frac{1}{4}x^4 + \frac{1}{3}x^3 - x^2,
$$

with an initial guess of  $x_0 = 2$ . What is  $x_1$ ?

A: Unanswered C: 
$$
\frac{10}{7}
$$
 E:  $\frac{13}{7}$  G:  $\frac{15}{7}$   
B: 0 D:  $\frac{12}{7}$  F: 2 H:  $\frac{17}{7}$ 

Question 16 Consider the function  $f(x, y) = 5xy^3 - 15xy + 20$ . Apply 2 iterations of Newton's **Question 16** Consider the function  $f(x, y) = 5xy^3 - 15xy + 20$ . Apply 2 iterations of Newton's method (for optimization) with the initial guess of  $x_0 = [\sqrt{5}, 1]$ . What is the value of the updated guess,  $x_2$ ? [Hint: the Hessian matrix is

$$
f''(x,y) = \begin{pmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{pmatrix}
$$

].



**Question 17** We find the minimum of  $f(x)$  using Golden-section search on the starting interval  $[a_0, b_0] = [0, 10]$ . Assume Golden-section converges. At iteration i, the midpoint of the interval  $[a_i, b_i]$  is taken as the approximation of the minimum of f. On which iteration is the error first less than 0.05? [Note: the Golden-ratio is  $\varphi = \frac{1+\sqrt{5}}{2}$ .]



**Question 18** We want to approximate  $\pi$ . We know that

$$
\pi = \underset{1 \le x \le 5}{\arg \min} \cos(x)
$$

Apply 1 iteration of golden-section search. What is the midpoint of the interval after this single iteration?



**Question 19** The figures below show the contour lines of a function of two variables  $f(x, y)$ . The minimum of this function is computed by three different solution methods:

- 1 Newtons method
- 2 Steepest descent method
- 3 Nelder-Mead simplex method



In all figures the initial guess is  $x_0 = 4$  and  $y_0 = 1$ . The dots in the figures represent the iterative values  $(x_n, y_n)$ . Which figure belongs to which solution method? [Note: for the Nelder-Mead simplex method the midpoint of the triangle is plotted in the figure].



Question 20 Consider the following minimization problem:

$$
\min_{0 \le x \le 3} (x - 1)(x - 2)
$$

Four methods are used to find the minimum:

- Golden-section search.
- Newton's method, with starting point  $x_0 = 0.5$ .
- The true function is sampled at three distinct points, an interpolating polynomial is constructed and the minimum on this interpolant is found analytically.
- A second order Taylor series expansion is constructed around  $x = 2.5$ , after which the minimum on the resulting interpolant is found analytically.

All derivatives are evaluated using second order accurate differencing schemes and the stepsize h. For each method, how many iterations are needed to arrive at the *exact* minimum? [Notes: 1] Assume exact arithmetic, 2) remember results from previous modules, 3) after *n* iterations  $x_n$  is reached.]

A: Unanswered	C: $\infty$ , 2, 2, 2	E: $\infty$ , $\infty$ , 2, 2	G: 14, 2, 2, 2
B: $\infty$ , 1, 1, 1	D: $\infty$ , $\infty$ , 1, 1	F: 14, 1, 1, 1	H: 14, 1, 2, 1

Question 21 Consider the following minimization problem in 2d:

$$
\min_{(x,y)\in\mathbb{R}}\ -\sqrt{\left|1-(x^2+y^2)\,\right|}
$$

Three methods are used to find the minimum:

- Nelder-Mead Simplex, with the following initial triangle:  $(x_1, y_1) = (-1, 0), (x_2, y_2) =$  $\left(-\frac{3}{4},\frac{1}{2}\right), (x_3, y_3) = \left(-\frac{3}{4}, -\frac{1}{2}\right)$
- Steepest descent method, started at  $(x_0, y_0) = (-2, 0)$
- Newton's method, started at  $(x_0, y_0) = (-2, 0)$

All derivatives are evaluated exactly. Which of these methods approaches the local minimum at  $(x, y) = (0, 0)$ ? [Hint: Plot the function, no computations are required!]

- A: Unanswered
- B: Nelder-Mead
- C: Steepest descent
- D: Newton's method
- E: Steepest descent & Newton's method
- F: All
- G: None