Bioinformatics

Discrete Mathematics and Optimization. Final Exam: 13.12.2022

Write problems in separate sheets

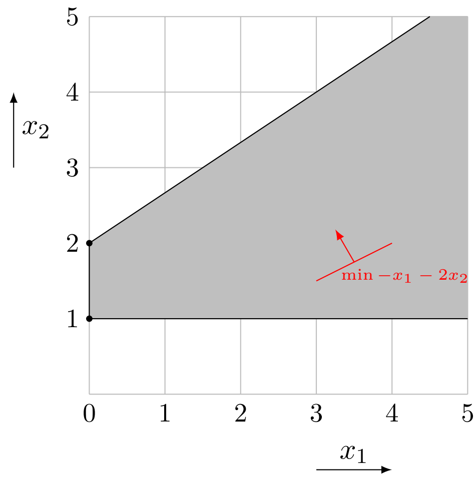
Problem 1 (Linear Programming, 2 points)**.**

Draw the feasible region for the following linear program and discuss its solution.

$$\begin{aligned} \text{minimise} \quad & -x_1 - 2x_2 \\ \text{subject to} \quad & -2x_1 + 3x_2 \leq 6 \\ & x_2 \geq 1 \\ & x_1, x_2 \geq 0. \end{aligned}$$

Solution.

The feasible region is drawn in gray and the objective function corresponds to the red line. If we move the red line in the direction of the arrow we decrease the objective function. Note that we can decrease this indefinitely with the objective function intersecting the feasible region, as the gradient of the objective function is less than that of the boundary line. Therefore the Linear program and its solution are unbounded.



Problem 2 (Nonlinear optimisation and convexity, 3 points)**.**

a) (1.5 pt) Consider the function $f(x, y) = xy(x + y - 1)$. Find all the critical points of f and describe their local nature.

b) (1.5 pt) Determine whether the following functions are convex, concave or neither:

$$\begin{aligned} g_1(x, y) &= x^2 - 5y^3 \\ g_2(x, y) &= -e^{-x} - xy \\ g_3(x, y) &= e^{2x^2 - y - z} \end{aligned}$$

Solution.

a) We have that $f(x,y) = x^2y+y^2x-xy$, the gradient is $\nabla_f(x,y) = (2xy+y^2-y, 2xy+x^2-x)$ and the Hessian is

$$H_f(x,y) = \begin{pmatrix} 2y & 2x+2y-1 \\ 2x+2y-1 & 2x \end{pmatrix}.$$

The gradient is 0 when $2xy+y^2-y = y(2x+y-1) = 0$ and $2xy+x^2-x = x(2y+x-1) = 0$. This is the case when $(x,y) \in \{(0,0),(0,1),(1,0),(1/3,1/3)\}$ and so these are the critical points.

We now use the Hessian to test the nature of the critical points. We have that

$$M_1 = H_f(0,0) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \qquad M_2 = H_f(0,1) = \begin{pmatrix} 2 & 1 \\ 1 & 0 \end{pmatrix}$$
$$M_3 = H_f(1,0) = \begin{pmatrix} 0 & 1 \\ 1 & 2 \end{pmatrix} \qquad M_4 = H_f(1/3,1/3) = \begin{pmatrix} 2/3 & 1/3 \\ 1/3 & 2/3 \end{pmatrix}.$$

We have that each matrix has non-zero determinant and so all the critical points are non-degenerate. M_1 , M_2 and M_3 all have negative determinant and so the matrices are not definite and so $(0,0)$, $(0,1)$ and $(1,0)$ are saddle points. Finally M_4 has first principal minor positive, namely $2/3$, and second principal minor (determinant) positive, namely $1/3$ and so M_4 is positive definite and $(1/3,1/3)$ is a local minimum.

b) g_1 is neither convex or concave as, restricting to $x=0$, we get $-5y^3$ which is convex with y negative but concave with y positive. g_2 has Hessian

$$H_{g_2}(x,y) = \begin{pmatrix} -e^{-x} & -1 \\ -1 & 0 \end{pmatrix},$$

which has first principal minor $-e^{-x}$ (always negative) and determinant 1 (positive) and hence the Hessian is negative definite everywhere and g_2 is concave. Finally, we have that $-y$, $-z$ are negatives of concave functions and so they are convex. Likewise x^2 is convex and so x^2-y-z is a positive linear combination of convex functions and so is convex itself. Therefore as e^x is strictly increasing, g_3 is convex.

Problem 3 (Iterative Methods, 5 points)**.**

a) (1 pt) Write $f(x,y) = x^2-2xy+3y^2+y+8$ as a quadratic form

$$f(x,y) = \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} q_1 & q_2 \\ q_3 & q_4 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} b_1 & b_2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + c$$

with Q symmetric.

b) (2 pt) Apply the Newton method to find the global minimum of $f(x,y) = x^2-2xy+3y^2+y+8$ with initial point $(4,2)$.

c) (2 pt) Perform one iteration of the steepest descent method on $g(x,y) = \frac{1}{3}x^3 + \frac{1}{2}y^2 - xy$ with initial point $(1,4)$.

Solution.

a) Multiplying out the second equation, we have that $f(x, y) = q_1x^2 + (q_2 + q_3)xy + q_4y^2 + b_1x + b_2y + c$. Comparing coefficients and imposing that $q_2 = q_3$, we get that

$$Q = \begin{pmatrix} q_1 & q_2 \\ q_3 & q_4 \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ -1 & 3 \end{pmatrix}, \quad b = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad c = 8$$

b) We have that

$$\nabla_f(x, y) = 2Q \begin{pmatrix} x \\ y \end{pmatrix} + b = \begin{pmatrix} 2x - 2y \\ -2x + 6y + 1 \end{pmatrix}$$

and the Hessian is

$$H_f(x, y) = 2Q = \begin{pmatrix} 2 & -2 \\ -2 & 6 \end{pmatrix}.$$

By Sylvester's criterion as both the determinant and first principal minor are positive, we have that the Hessian is positive definite everywhere and so f is convex and has a global minimum.

As we have a quadratic form, we know that the Newton method converges to find the global minimum after one iteration. We get that

$$\begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \begin{pmatrix} 4 \\ 2 \end{pmatrix} - H_f(4, 2)^{-1}\nabla f(4, 2),$$

where

$$\nabla f(4, 2) = \begin{pmatrix} 2 & -2 \\ -2 & 6 \end{pmatrix} \begin{pmatrix} 4 \\ 2 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 4 \\ 5 \end{pmatrix}$$

and

$$H_f(4, 2)^{-1} = \frac{\operatorname{adj}(H_f(4, 2))}{\det(H_f(4, 2))} = \frac{1}{8} \begin{pmatrix} 6 & 2 \\ 2 & 2 \end{pmatrix}.$$

So that the global minimum of $f(x, y)$ is reached at

$$\begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \begin{pmatrix} 4 \\ 2 \end{pmatrix} - \frac{1}{8} \begin{pmatrix} 6 & 2 \\ 2 & 2 \end{pmatrix} \begin{pmatrix} 4 \\ 5 \end{pmatrix} = \begin{pmatrix} 4 \\ 2 \end{pmatrix} - \frac{1}{8} \begin{pmatrix} 34 \\ 18 \end{pmatrix} = \begin{pmatrix} 4 \\ 2 \end{pmatrix} - \begin{pmatrix} 17/4 \\ 9/4 \end{pmatrix} = \begin{pmatrix} -1/4 \\ -1/4 \end{pmatrix},$$

with $f(-1/4, -1/4) = 8$

c) The gradient of $g(x, y)$ is $\nabla g(x, y) = \begin{pmatrix} x^2 - y \\ y - x \end{pmatrix}$. Let $\begin{pmatrix} x_0 \\ y_0 \end{pmatrix} = \begin{pmatrix} 1 \\ 4 \end{pmatrix}$ be the initial point of the steepest descent method. In particular, we have $\nabla g(1, 4) = (-3, 3)$, and the next point is given by

$$\begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} - t_0\nabla g(x_0, y_0),$$

where $t_0 \in \mathbb{R}$ is such that it minimises the function

$$\phi_0(t) = g\left(\begin{pmatrix} x_1 \\ y_1 \end{pmatrix}\right) = g\left(\begin{pmatrix} x_0 \\ y_0 \end{pmatrix} - t\nabla g(x_0, y_0)\right).$$

Remark that t_0 is determined by the equation $\phi_0'(t) = 0$, where using the chain rule

$$\begin{aligned}
\phi_0'(t) = -\nabla g\left(\begin{pmatrix} x_0 \\ y_0 \end{pmatrix}\right) \cdot \nabla g\left(\begin{pmatrix} x_0 \\ y_0 \end{pmatrix} - t\nabla g(x_0, y_0)\right) &= -\begin{pmatrix} -3 \\ 3 \end{pmatrix} \cdot \nabla g\begin{pmatrix} 1+3t \\ 4-3t \end{pmatrix} \\
&= \begin{pmatrix} 3 \\ -3 \end{pmatrix} \cdot \begin{pmatrix} 9t^2 + 9t - 3 \\ 3 - 6t \end{pmatrix} \\
&= 9(3t^2 + 5t - 2).
\end{aligned}$$

So that we have

$$\phi_0'(t) = 0 \implies t = \frac{1}{6}\left(-5 \pm 7\right), \text{ that are the two critcal points of } \phi_0,$$

namely $t = 1/3$ and $t = -2$. To know which one is actually a local minimum of ϕ_0, we compute $\phi_0''(t) = 9(6t + 5)$. And we verify $\phi_0''(-2) = -63 < 0$, while $\phi_0''(1/3) = 63 > 0$. So that the minimum of ϕ_0 is given by $t_0 = 1/3$. And we finally get

$$\begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \begin{pmatrix} 1 \\ 4 \end{pmatrix} - \frac{1}{3}\begin{pmatrix} -3 \\ 3 \end{pmatrix} = \begin{pmatrix} 2 \\ 3 \end{pmatrix}.$$