ESCI, Bioinformatics

Discrete Mathematics and Optimization. Final Exam: 15th of December 2021
Write problems in separate sheets 3h

Problem 1 (Enumeration and graph theory, 3 points)**.** Let W be the set of words of length 4 over the alphabet $\{1, 2, 3, 4\}$ which contain two distinct symbols each repeated twice (for instance $(1, 2, 1, 2)$ and $(3, 4, 4, 3)$ are words in W, but $(2, 2, 3, 1)$ is not).

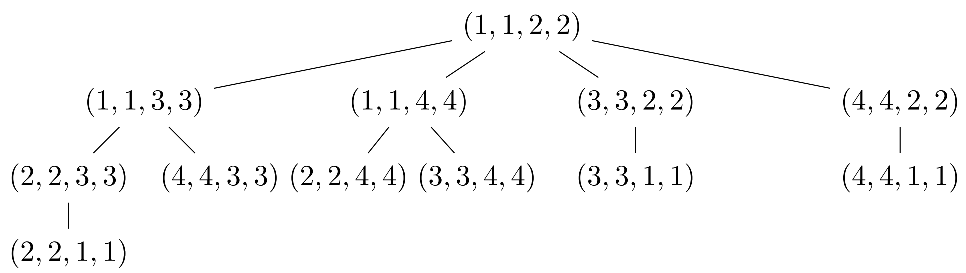
(a) How many words are in W?

(b) Let $G = (V, E)$ be the graph with vertex set $V = W$ and two words are adjacent if they have the same symbol in the same positions (for instance $(1, 2, 1, 2)$ and $(1, 3, 1, 3)$ are adjacent). Run the breath first search algorithm on G starting at the vertex $(1, 1, 2, 2)$ and display the resulting tree. Is the graph G connected?

(c) Label each vertex of the tree found in the above breath first search according to its first appearance in the algorithm (so $(1, 1, 2, 2)$ is labeled 1). Run the Prüfer algorithm on this labeled tree and display its Prüfer code (display the steps for obtaining the code).

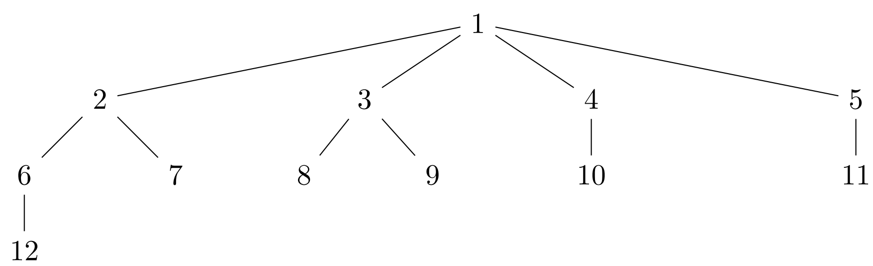
Solution. (a) Choose two of the symbols to place in the word, there are $\binom{4}{2}$ choices. Choose the two positions where to place the smaller of the two, $\binom{4}{2}$ choices, and place the larger in the remaining two positions. This way we count every word in W precisely once, giving $\binom{4}{2}^2 = 36$ words.

(b) Starting with the vertex $(1, 1, 2, 2)$, an execution of the breadth first search produces the following tree:



Since the breadth first search tree finds only 12 of the 36 vertices in G, the graph is not connected.

(c) The labeled tree is



The Prüfer code has length 10. Its first entry is the label of the vertex adjacent to the smallest leave. By running the Prüfer algorithm we get the code

$$\begin{gathered}
(2,*,*,*,*,*,*,*,*,*) \\
(2,3,*,*,*,*,*,*,*,*) \\
(2,3,3,*,*,*,*,*,*,*) \\
(2,3,3,1,*,*,*,*,*,*) \\
(2,3,3,1,4,*,*,*,*,*) \\
(2,3,3,1,4,1,*,*,*,*) \\
(2,3,3,1,4,1,5,*,*,*) \\
(2,3,3,1,4,1,5,1,*,*) \\
(2,3,3,1,4,1,5,1,6,*) \\
(2,3,3,1,4,1,5,1,6,2)
\end{gathered}$$

Problem 2 (Linear Programming, 3 points)**.** A population is divided into three groups A, B, C, where each group has more than 1000 individuals. A lot of 1000 vaccines for a contagious illness is to be distributed to the population. The 10% of vaccinated people in group A is expected to go to the hospital for this illness. The analogous percentages for groups B and C are 20% and 30%, respectively. The number of individuals vaccinated in group B must be at least twice the number in group A, and the number in group C at least twice the number in B plus the number in A. We want to minimize the expected number of individuals going to hospital with the above conditions.

(a) Write a Linear Program for the stated minimization problem.

(b) Write the LP in equational form.

(c) Run the simplex algorithm and find a solution for the number of individuals in each group to be vaccinated.

Solution. (a) Let x, y, z be the number of individuals (in hundreds) to be vaccinated in groups A, B, C respectively. The function to be minimized is

$$c = c(x, y, z) = 0.1x + 0.2y + 0.3z$$

The conditions are

$$\begin{aligned}
y &\geq 2x \\
z &\geq 2x + y \\
x + y + z &= 10 \\
x \geq 0, y &\geq 0, z \geq 0
\end{aligned}$$

(b) We only have to solve for x and y as $z = 10 - x - y$. The linear program in equational form is

$$\begin{array}{ll}
\text{Maximize} & 0.2x + 0.1y - 3 \\
\text{Subject to} & 2x - y + t = 0 \\
 & 3x + 2y + u = 10 \\
 & x, y, t, u \geq 0
\end{array}$$

(c) Setting $x = y = 0$ we obtain the basic feasible condition $(0, 0, 0, 10)$. The initial tableau is

$$\begin{array}{rl|l} t & = -2x + y & \\ u & = 10 - 3x - 2y & \\ \hline c & = 0.2x + 0.1y - 3 & -3 \end{array}$$

The variable x is constrained by the first equation to $x \leq 0$, so make it entering will not change the basic feasible condition. We let y enter, which is not constrained by the first equation and gives $y \leq 5$ by the second one. We let u be the leaving variable. The updated tableau is

$$\begin{array}{rl|l} t & = 5 - (7/2)x - u/2 & \\ y & = 5 - (3/2)x - u/2 & \\ \hline c & = (1/20)x - (1/20)u - (5/2) & -5/2 \end{array}$$

with the basic feasible condition $(0, 5, 5, 0)$. We must now enter x to increase the objective function, which is restricted by $x \leq 10/7$ from the first equation and by $x \leq 10/3$ from the second one, so we let t be leaving. The updated tableau is

$$\begin{array}{rl|l} x & = (10/7) - 2t/7 - u/7 & \\ y & = (20/7) - 3t/14 - 4u/14 & \\ \hline c & = -t/70 - 3u/70 - 34/14 & -34/14 \end{array}$$

Threfore the solution is $x = 10/7, y = 20/7$ and $z = 40/7$ with an expected number of $17/7$ hundreds of hospital entries.

Problem 3 (Non–linear optimisation, 4 points)**.**

(a) Determine the critical points of $f(x, y) = 2x^3 - 6xy + 3y^2$ and their nature.

(b) Perform one iteration of the steepest descent method on $f(x, y)$ with initial point $(1, -1)$.

(c) Write $g(x, y) = x^2 - 2xy + 2y^2 - x + 2y + 3$ in quadratic form and show that it admits a unique global minimum in $\mathbb{R}^2$.

(d) Find the global minimum of $g(x, y)$ via the Newton method with initial point $(1, 1)$.

Solution. (a) The gradient of $f(x, y)$ is $\nabla f(x, y) = (6x^2 - 6y, 6y - 6x)$. The critical points of $f(x, y)$ are thus solutions of

$$\begin{cases} 6x^2 - 6y = 0, \\ 6y - 6x = 0. \end{cases} \Leftrightarrow \begin{cases} 6x^2 - 6x = 0, \\ y = x. \end{cases} \Leftrightarrow \begin{cases} 6x(x-1) = 0, \\ y = x. \end{cases} \Rightarrow \begin{array}{lll} x = 0 & \text{and} & y = 0, \\ \text{or} \quad x = 1 & \text{and} & y = 1, \end{array}$$

i.e. the critical points of $f(x, y)$ are $(0, 0)$ and $(1, 1)$. The Hessian matrix of $f(x, y)$ is

$$H_f(x, y) = \begin{pmatrix} 12x & -6 \\ -6 & 6 \end{pmatrix} \implies H_f(0, 0) = \begin{pmatrix} 0 & -6 \\ -6 & 6 \end{pmatrix} \text{ and } H_f(1, 1) = \begin{pmatrix} 12 & -6 \\ -6 & 6 \end{pmatrix}.$$

The determinant of $H_f(0, 0)$ is $-36 < 0$ thus, by Sylvester's criterion, $(0, 0)$ is a saddle point of $f(x, y)$.

Furthermore, the two leading principal minors of $H_f(1, 1)$ are both positive: its top-left corner is 12 and its determinant is 36, so that, by Sylvester's criterion, $H_f(1, 1)$ is definite positive. This implies that $(1, 1)$ is a strict local minimum of $f(x, y)$.

(b) We have $\nabla f(1,-1) = (12,-12)$, so that the first iteration of the steepest descent method applied to $f(x,y)$ and starting at $(1,-1)$ is given by the point

$$(x_1, y_1) = (1,-1) - t_0 \nabla f(1,-1),$$

such that t_0 minimises the function $\phi_0(t) = f\left((1,-1) - t\nabla f(1,-1)\right)$. In particular, t_0 is determined by $\phi_0'(t) = 0$ and $\phi_0''(t) \geq 0$. Using the chain rule, we first have

$$\begin{aligned}
\phi_0'(t) &= -\nabla f(1,-1) \cdot \nabla f\left((1,-1) - t\nabla f(1,-1)\right) \\
&= -(12,-12) \cdot \nabla f(1-12t, -(1-12t)) \\
&= (-12,12) \cdot (6(1-12t)^2 + 6(1-12t), -12(1-12t)) \\
&= -72(1-12t)(4-12t).
\end{aligned}$$

Thus $\phi_0'(t) = 0 \implies t = 1/12$ or $t = 1/3$. Furthermore,

$$\phi_0''(t) = 12 \cdot 72(1 - 12t + 4 - 12t) = 866(5 - 24t),$$

where $\phi_0''(1/3) < 0$, while $\phi_0''(1/12) > 0$. This means that $t_0 = 1/12$. And finally,

$$(x_1, y_1) = (1,-1) - \frac{1}{12}(12,-12) = (1,-1) - (1,-1) = (0,0).$$

(c) The quadratic form of $g(x,y)$ is given by

$$g(x,y) = \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} 1 & -1 \\ -1 & 2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} -1 \\ 2 \end{pmatrix} + 3.$$

Using this form, we obtain

$$\nabla g(x,y) = \begin{pmatrix} 2 & -2 \\ -2 & 4 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} -1 \\ 2 \end{pmatrix} \quad \text{and} \quad H_g(x,y) = \begin{pmatrix} 2 & -2 \\ -2 & 4 \end{pmatrix}.$$

In particular, for any $(x,y) \in \mathbb{R}^2$ and by Sylvester's criterion, $H_g(x,y)$ is definite positive as its two leading principal minors are postive: the top-left corner is equal to 2 while the determinant equals 4. This implies that $g(x,y)$ is striclty convex in $\mathbb{R}^2$ and thus admits a unique global minimum.

(d) Because $g(x,y)$ is a quadratic function, the first iteration of the Newton method will already give its global minimum. Starting at $(1,1)$, the next iteration is the point

$$\begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} - H_g(1,1)^{-1} \nabla g(1,1),$$

where

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

and

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

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

$$\begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} - \frac{1}{4} \begin{pmatrix} 4 & 2 \\ 2 & 2 \end{pmatrix} \begin{pmatrix} -1 \\ 4 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} - \frac{1}{4} \begin{pmatrix} 4 \\ 6 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} - \begin{pmatrix} 1 \\ 3/2 \end{pmatrix} = \begin{pmatrix} 0 \\ -1/2 \end{pmatrix},$$

with $g(0,-1/2) = 5/2$.