MATH661 Homework 6 - Optimization problems

Posted: Nov 15, Due: 11:55PM, Nov 22 (theoretical exercises), Dec 6 (computational application)

1 Problem statement

Optimization problems arise throughout scientific computing. Typically, problem-specific considerations impose constraints on allowable solutions. In this homework, some basic procedures of finding optimal solutions are considered.

2 Theoretical exercises

1. K&C, 10.1.5, p. 688.

   Solution. This is good practice on proving set equalities and understanding set of convex combinations. By definition the convex hull of set S, $\mathrm{co}(S) = \{z \colon \exists x, y \in S, \exists \theta, 0 \leqslant \theta \leqslant 1, z = \theta x + (1-\theta) y\}$, i.e., the set of all convex combinations of points in S. Prove the requested set equalities by double inclusion. In all the following assume $0 \leqslant \theta \leqslant 1$, $x, y \in S$

   a) $\mathrm{co}(\lambda S) \subseteq \lambda \mathrm{co}(S)$: $\forall z \in \mathrm{co}(\lambda S)$, $z = \theta(\lambda x) + (1-\theta)(\lambda y) = \lambda w$, with $w = \theta x + (1-\theta) y$, and $w \in \mathrm{co}(S)$ ✓.

   b) $\lambda \mathrm{co}(S) \subseteq \mathrm{co}(\lambda S)$: $\forall z \in \mathrm{co}(S)$, $z = \theta x + (1-\theta) y$, hence $\lambda z = \theta(\lambda x) + (1-\theta)(\lambda y) \in \mathrm{co}(\lambda S)$ ✓.

   c) $\mathrm{co}(S+T) \subseteq \mathrm{co}(S) + \mathrm{co}(T)$: $\forall z \in \mathrm{co}(S+T)$, $z = \theta u + (1-\theta) v$, with $u, v \in S+T$, hence $u = x+p$, $v = y+q$, $x, y \in S$, $p, q \in T$. Replacing u, v into expression for z gives

   $$z = \theta(x+p) + (1-\theta)(y+q) = \theta x + (1-\theta) y + \theta p + (1-\theta) q = a + b$$

   with $a \in \mathrm{co}(S), b \in \mathrm{co}(T)$ ✓.

   d) $\mathrm{co}(S) + \mathrm{co}(T) \subseteq \mathrm{co}(S+T)$: $\forall a \in \mathrm{co}(S)$, $b \in \mathrm{co}(T)$, $\exists x, y < S$, $\exists p, q \in T$ such that $a = \theta x + (1-\theta) y$, $b \in \theta p + (1-\theta) q$, hence $a + b \in \mathrm{co}(S+T)$ ✓.

2. K&C, 10.1.21, p. 688.

   Solution. This is a very useful exercise to gain understanding of the concepts of convexity, open and closed sets, dimensionality, and critical points. Read through the solution carefully. The important aspect is how the sequence of reasoning steps leads to the example asked for in this problem. At each step something is learned about the required properties of the example asked for. Unsuccesful attempts to come up with an example are marked ✠, the final example is marked ✓.

   i. First, note that if S is convex, then $S = \mathrm{co}(S)$, so the convex hull of a convex set S has all the properties of S. Therefore, the example asked for in the problem cannot be convex.

   ii. Recall that a closed set is a set whose complement is open, and O is an open set if any point in O has a neighborhood contained in O.

iii. Try to form a closed, non-convex set on the real axis, $S = U \cup V$.

a) First try to form a non-convex set by union of subsets of lower dimension $S = \{0\} \cup \{1\}$. The complement of S is $\mathbb{R} \backslash S = (-\infty, 0) \cup (0, 1) \cup (1, \infty)$ and is open, hence S is closed. The convex hull of S is $\mathrm{co}(S) = [0, 1]$ and is closed. In general the convex hull of a union of disjoint points on the real axis will be the closed interval defined by the extremal points, and itself be closed. ✠

b) Next try to form a non-convex closed set by union of subsets of the same dimension, say $S = [-2, -1] \cup [1, 2]$. The convex hull is $\mathrm{co}(S) = [-2, 2]$ and is closed. In general, the convex hull of closed non-convex intervals on the real axis will just yield the enclosing closed interval. ✠

Deduce from the above that the example must be sought in $\mathbb{R}^n$ with $n > 1$. Note that the sequence of attempted steps was: $\dim U = \dim V = 0$, $\dim U = \dim V = 1$. An attempt through $\dim U = 0$, $\dim V = 1$ would have led to the same result.

iv. Choose $n = 2$. Seek a non-convex set S formed by union of closed subsets U, V, $S = U \cup V$. As before, systematically go through $\dim U, \dim V \in \{0, 1, 2\}$

a) $U = \{(0, 0)\}$, $V = \{(a, b)\}$. Convex hull is line segment from (0,0) to (a, b) and is closed. ✠

b) $U = \{(0, 0)\}$, $V = \{(0, y) \colon 0 \leqslant y \leqslant 1\}$. Convex hull is line segment from $(0, 0)$ to $(0, 1)$ and is closed. ✠

c) $U = \{(x, 0) \colon x \geqslant 0\}$,$V = \{(0, y) \colon y \geqslant 0\}$. Convex hull is first quadrant and is closed. ✠

d) $U = \{(x, 0) \colon x \geqslant 0\}$,$V = \{(0, y) \colon 1 \geqslant y \geqslant 0\}$. By definition, the convex hull is $\mathrm{co}(S) = \{w \colon w = \theta u + (1 - \theta) v, u \in U, v \in V, 0 \leqslant \theta \leqslant 1\}$, and can be written as

$$\mathrm{co}(S) = \{(x, y) \colon x \geqslant 0, 0 \leqslant y < 1\} \cup \{0, 1\}. \checkmark$$

Note what occurs in the construction of the convex hull in this case. The only way to obtain point (x, y) with $y = 1$ is to choose $\theta = 0$ in which case $x = 0$. The resulting convex hull is now not closed (e.g., the complement would contain a point $(a, 1)$, with $a > 0$ for which no neighborhood can be defined that would be enclosed in the complement), and the required example has been determined. Indeed, $(0, 1)$ is a critical point of the convex hull.

Examples that solve this exercise can readily be found through a web search. You should ask yourself though whether your objective is expertise in employing a search engine or understanding mathematics. If the later, follow the train of reasoning that leads to the solution. Though apparently abstract with little relevance to practical application, this topic frequently arises in optimization of linear functionals, and in fact appears in the solution to the computational problem proposed in this homework.

3. K&C, 10.2.1, 10.2.2, p. 694

Solution. 10.2.1. From linear algebra, $\boldsymbol{A} \in \mathbb{R}^{m \times n}$, $\mathbb{R}^m = C(\boldsymbol{A}) \oplus N(\boldsymbol{A}^T)$,

$$m = \dim C(\boldsymbol{A}) + \dim N(\boldsymbol{A}^T). \tag{1}$$

$\boldsymbol{A}^T\boldsymbol{y} > 0$ implies $N(\boldsymbol{A}^T) = 0$ and $\dim N(\boldsymbol{A}^T) = 0$, while $\boldsymbol{A}\boldsymbol{x} = 0$ for $\boldsymbol{x} \geqslant \boldsymbol{0}$ implies columns of $\boldsymbol{A}$ are linearly dependent hence $\dim C(\boldsymbol{A}) < m$, contradicting (1). The statement is also a direct application of Theorem 6 (p.693) with $\boldsymbol{b} = \boldsymbol{0}$.

10.2.2. Apply Theorem 7 (p.693) with $\boldsymbol{b} = \boldsymbol{0}$.

4. K&C, 10.2.6, p. 694

   Solution. Accept all results from 10.2.3-10.2.5, and follow the hint.

5. K&C, 10.3.1, p. 700

   Solution. Recall that standard form $(\boldsymbol{A}, \boldsymbol{b}, \boldsymbol{c})$ is

$$\max \boldsymbol{c}^T\boldsymbol{x}, \boldsymbol{A}\boldsymbol{x} \leqslant \boldsymbol{b}, \boldsymbol{x} \geqslant \boldsymbol{0},$$

and the dual is $(-\boldsymbol{A}^T, -\boldsymbol{c}, -\boldsymbol{b})$.

(a) $\min(3x_1 + x_2 - 5x_3 + 2) \Leftrightarrow \min(3x_1 + x_2 - 5x_3) \Leftrightarrow \max(-3x_1 - x_2 + 5x_3)$

Replace: $x_1 = u_1 - u_4, x_2 = -u_2, x_3 = u_3 - u_5$, with $\boldsymbol{u} \geqslant 0$ to obtain

$$\max(-3u_1 + u_2 + 5u_3 + 3u_4 - 5u_5)$$

$x_1 \geqslant x_2 \Rightarrow x_2 - x_1 \leqslant 0 \Rightarrow -u_2 - u_1 + u_4 \leqslant 0 \Rightarrow -u_1 - u_2 + u_4 \leqslant 0$

$-x_1 + 4x_3 \geqslant 0 \Rightarrow x_1 - 4x_3 \leqslant 0 \Rightarrow u_1 - u_4 - 4u_3 + 4u_5 \leqslant 0 \Rightarrow u_1 - 4u_3 - u_4 + 4u_5 \leqslant 0$

$x_1 + x_2 + x_3 = 0 \Rightarrow x_1 + x_2 + x_3 \leqslant 0 \,\text{and}\, x_1 + x_2 + x_3 \geqslant 0$ leading to

$-u_1 + u_2 - u_3 + u_4 + u_5 \leqslant 0$ and $u_1 - u_2 + u_3 - u_4 - u_5 \leqslant 0$. The standard form is

$$\boldsymbol{A} = \begin{pmatrix} -1 & -1 & 0 & 1 & 0 \\ 1 & 0 & -4 & -1 & 4 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 \end{pmatrix}, \boldsymbol{b} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \boldsymbol{c} = \begin{pmatrix} -3 \\ 1 \\ 5 \\ 3 \\ -5 \end{pmatrix}.$$

The dual form written out in full is

$$\max(-\boldsymbol{b}^T\boldsymbol{y}), \boldsymbol{A}^T\boldsymbol{y} \geqslant \boldsymbol{c}, \boldsymbol{y} \geqslant 0 \Leftrightarrow \boldsymbol{A}^T\boldsymbol{y} \geqslant \boldsymbol{c}, \boldsymbol{y} \geqslant 0 \,\text{since}\, \boldsymbol{b} = \boldsymbol{0}.$$

(b) Replace: $u_1 = -x_1 \geqslant 0$, $x_2 = u_2 - u_4$, $u_2, u_4 \geqslant 0$, $u_3 = x_3 - 2 \geqslant 0$. Rewrite remaining constraints

$$\begin{array}{lll} x_1 - x_2 = 5 \;\Rightarrow\; -u_1 - u_2 + u_4 \leqslant 5 & \text{and} & u_1 + u_2 - u_4 \leqslant 5 \\ x_2 - x_3 = 7 \;\Rightarrow\; u_2 - u_4 - u_3 \leqslant 5 & \text{and} & -u_2 + u_3 + u_4 \leqslant 5 \end{array}$$

Objective function becomes

$$|x_1 + x_2 + x_3| = |-u_1 + u_2 - u_4 + u_3 + 2|.$$

Recall that $|x|$ is shorthand for two function branches, hence

$$\min|-u_1 + u_2 - u_4 + u_3 + 2| = \begin{cases} \max(u_1 - u_2 - u_3 + u_4 - 2) & \text{if} -u_1 + u_2 + u_3 - u_4 + 2 \geqslant 0 \\ \max(-u_1 + u_2 + u_3 - u_4 + 2) & \text{if} -u_1 + u_2 + u_3 - u_4 + 2 \leqslant 0 \end{cases}$$

The two problems are therefore

$$\max \boldsymbol{c}_1^T \boldsymbol{u}_1,\ \boldsymbol{A}_1 \boldsymbol{u}_1 \leqslant \boldsymbol{b}_1,\ \boldsymbol{u}_1 \geqslant \boldsymbol{0},$$

$$\boldsymbol{A}_1 = \begin{pmatrix} -1 & -1 & 0 & 1 \\ 1 & 1 & 0 & -1 \\ 0 & 1 & -1 & -1 \\ 0 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 \end{pmatrix}, \boldsymbol{b}_1 = \begin{pmatrix} 5 \\ 5 \\ 5 \\ 5 \\ 2 \end{pmatrix}, \boldsymbol{c}_1 = \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}.$$

$$\max \boldsymbol{c}_2^T \boldsymbol{u}_2,\ \boldsymbol{A}_2 \boldsymbol{u}_2 \leqslant \boldsymbol{b}_2,\ \boldsymbol{u}_2 \geqslant \boldsymbol{0},$$

$$\boldsymbol{A}_2 = \begin{pmatrix} -1 & -1 & 0 & 1 \\ 1 & 1 & 0 & -1 \\ 0 & 1 & -1 & -1 \\ 0 & -1 & 1 & 1 \\ -1 & 1 & 1 & -1 \end{pmatrix}, \boldsymbol{b}_2 = \begin{pmatrix} 5 \\ 5 \\ 5 \\ 5 \\ -2 \end{pmatrix}, \boldsymbol{c}_2 = \begin{pmatrix} -1 \\ 1 \\ 1 \\ -1 \end{pmatrix}.$$

The overall solution to the problem would be given by $\max(\max \boldsymbol{c}_1^T \boldsymbol{u}_1, \max \boldsymbol{c}_2^T \boldsymbol{u}_2)$.

(c) As above, but now the presence of two absolute values leads to four branches

$$\min(|x_1| - |x_2|) \Leftrightarrow \begin{array}{ll} \max(x_1 - x_2) & \text{if } x_1 \leqslant 0, x_2 \leqslant 0 \\ \max(-x_1 - x_2) & \text{if } x_1 > 0, x_2 \leqslant 0 \\ \max(x_1 + x_2) & \text{if } x_1 \leqslant 0, x_2 > 0 \\ \max(-x_1 + x_2) & \text{if } x_1 > 0, x_2 > 0 \end{array}$$

Replace: $x_1 = u_1 - u_4$, $u_1, u_4 \geqslant 0$, $x_2 = u_2 - u_5$, $u_2, u_5 \geqslant 0$, $u_3 = x_3 - 4 \geqslant 0$. The remaining steps are shown for the first branch only. Objective function

$$\max(x_1 - x_2) \Leftrightarrow \max(u_1 - u_2 - u_4 + u_5)$$

Constraints: $\boldsymbol{u} \geqslant 0$ and

$$\begin{array}{l} u_1 - u_4 \leqslant 0 \\ u_2 - u_5 \leqslant 0 \\ u_1 + u_2 - u_4 - u_5 \leqslant 5 \\ -u_1 - u_2 + u_4 + u_5 \leqslant 5 \\ 2u_1 + 3u_2 - u_3 - 2u_4 - 3u_5 \leqslant 4 \end{array}$$

$$\boldsymbol{A}_1 = \begin{pmatrix} 1 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 & -1 \\ -1 & -1 & 0 & 1 & 1 \\ 2 & 3 & -1 & -2 & -3 \end{pmatrix}, \boldsymbol{b}_1 = \begin{pmatrix} 0 \\ 0 \\ 5 \\ 5 \\ 4 \end{pmatrix}, \boldsymbol{c}_1 = \begin{pmatrix} 1 \\ -1 \\ 0 \\ -1 \\ 1 \end{pmatrix}.$$

6. K&C, 10.4.3, p. 710

Solution. Rewrite inequalities as $\boldsymbol{A}\boldsymbol{x} \leqslant b$, introduce slack variables, and rewrite problem

$$\begin{array}{l} \text{Maximize } F(\boldsymbol{x}) = 2x_1 - 3x_2 + 0x_3 + 0x_4 \\ -2x_1 - 5x_2 + x_3 = -10 \\ x_1 + 8x_2 + x_4 = 24 \\ x_1 \geqslant 0, x_2 \geqslant 0, x_3 \geqslant 0, x_4 \geqslant 0 \end{array}$$

with tableau

$$\begin{array}{cccc|c} 2 & -3 & 0 & 0 & 0 \\ \hline -2 & -5 & 1 & 0 & 10 \\ 1 & 8 & 0 & 1 & 24 \\ \hline 0 & 0 & 10 & 24 & \end{array}$$

First step. Increase x_1 as much as possible, hold $x_2 = 0$ fixed. Constraints:

$$\begin{array}{l} x_3 = -10 + 2x_1 \geqslant 0 \Rightarrow x_1 \geqslant 5 \\ x_4 = 24 - x_1 \geqslant 0 \Rightarrow x_1 \leqslant 24 \end{array},$$

hence choose $x_1 = 24$. New $\boldsymbol{x}$ vector is $\boldsymbol{x} = \left(\begin{array}{cccc} 24 & 0 & 0 & 19 \end{array} \right)^T$, new basic variables are x_1, x_4. Express F in terms of nonbasic variables

$$F(\boldsymbol{x}) = 10 - x_3 - 3x_2.$$

No further increase in F is possible for $x_2, x_3 \geqslant 0$ hence solution is $x_1 = 24$, $x_2 = 0$. Check in Mathematica.

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In[3]:= LinearProgramming[{-2, 3}, {{2, 5}, {-1, -8}}, {10, -24}]
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$\{24, 0\}$

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In[4]:=
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3 Realistic optimization problm

Revisit the diffusion problem from Homework 5 that defines $u(t,x)$, $u: [0,T] \times [0,\pi] \rightarrow \mathbb{R}$, as solution of

$$\begin{array}{l} \dfrac{\partial u}{\partial t} = \dfrac{\partial^2 u}{\partial x^2} + \displaystyle\sum_{i=1}^{n} A_i \exp\left[-\frac{(x-x_i)^2}{(\pi/20)^2}\right] H(t), \\ u(t, x=0) = 0, u(t, x=\pi) = 0, \\ u(t=0, x) = \sin(x). \end{array} \tag{2}$$

This models the evolution of concetration u from initial condition $u(t=0,x)$ due to diffusion and sources placed at positions x_i and intensity A_i turned on after $t > 0$ ($H(t)$ is the Heaviside function). The problem is inspired from cell biology with $[0,\pi]$ the extent of the cell and u the concentration of Ca. Where should additional calcium sources be placed within the cell, and at what intensity should they release calcium such that the resultis a calcium concentration wave $u_0(t,x) = H(x - vt)$, with $v = 6$ over time interval $[0,1]$.

Feel free to collaborate in small groups on how to solve this problem. Here are some questions to consider:

1. How to define a cost functional. The unknowns of the problem are (x_i, A_i), $i = 1, \ldots, n$, hence a functional $f: \mathbb{R}^m \rightarrow \mathbb{R}$, $m = 2n$ must be defined. Some possibilities:

   a) $f(\boldsymbol{z}) = \|u(t,x;\boldsymbol{z}) - H(x - vt)\|_k$, Find $\min_{\boldsymbol{z} \in \mathbb{R}^m} f(\boldsymbol{z})$ for various choices of norm, e.g., $k = 1$, $k = 2$, $k = \infty$

   b) $f(\boldsymbol{z}) = \sum_{j=1}^{p} b_j \sum_{i=1}^{n} c_i \left[u(t^j, x_i; \boldsymbol{z}) - H(x_i - vt^j)\right]$. Here a weighted combination of the difference between the desired distribution $H(x_i - vt^j)$, and that obtained for some choice of $\boldsymbol{z}$ is minimized w.r.t. $\boldsymbol{z}$

2. What algorithm is suitable for minimizing the cost functional? Choices include:
   a) simplex
   b) gradient descent
   c) Nelder-Mead
   d) Genetic algorithms
   e) Simulated annealing

Full credit is awarded for work on one choice of cost functional and one choice of minimization algorithm. The best way to work on this application is for different people in each group to make alternative choices as to cost functional and algorithm and compare results.

This application reflects how scientific computing applications arise in the real world: nobody will state that you have to solve K&C 10.4.5 on page 710. Rather, there exists an interest in a real phenomenon that is transposed into a mathematical model, and then a solution is sought. Furthermore, codes previously developed are reused; in this case the numerical ODE solver from Homework 5 is to be reused to evaluate the cost functional.

In the final Homework, we will solve the same problem using stochastic methods.

Solution.

Define a Runge-Kutta function to advance in time the ODE system resulting from method of lines discretization

```
octave> function [xj,U1]=RK4(m,dt,nt,param)
          h=pi/m; x=(0:m)*h; T=nt*dt; xj=(1:m-1)*h; dt2=0.5*dt;
          U0=f(xj); U0b=[0 U0 0]; sig=dt/h^2; t=0;
          for k=1:nt
            U0b=[0 U0 0]; U0l(1:m-1)=U0b(3:m+1); U0r(1:m-1)=U0b(1:m-1);
            K1=sig*(U0l-2*U0+U0r)+dt*sigma(t,xj,param);
            U1=U0+0.5*K1;
            U1b=[0 U1 0]; U1l(1:m-1)=U1b(3:m+1); U1r(1:m-1)=U1b(1:m-1);
            K2=sig*(U1l-2*U1+U1r)+dt*sigma(t+dt2,xj,param);
            U1=U0+0.5*K2;
            U1b=[0 U1 0]; U1l(1:m-1)=U1b(3:m+1); U1r(1:m-1)=U1b(1:m-1);
            K3=sig*(U1l-2*U1+U1r)+dt*sigma(t+dt2,xj,param);
            U1=U0+K3;
            U1b=[0 U1 0]; U1l(1:m-1)=U1b(3:m+1); U1r(1:m-1)=U1b(1:m-1);
            K4=sig*(U1l-2*U1+U1r)+dt*sigma(t+dt,xj,param);
            U1=U0+(K1+2*K2+2*K3+K4)/6.;
            U0=U1; t=t+dt;
          end;
        end;
octave> function y=f(x)
          y=sin(x).*exp(-(x-pi/2).^2);
        end;
octave> function s=sigma(t,xj,param)
          n=length(param)/3;
          A(1:n)=param(1:n); xi=param(n+1:2*n); ti=param(2*n+1:3*n);
          s=zeros(1,length(xj)); sig=(pi/20.)^2;
          for i=1:n
            if (t>ti(i))
              s = s + A(i)*exp(-(xj-xi(i)).^2/sig);
            end;
          end;
        end;
```