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.
2. K&C, 10.1.21, p. 688.
3. K&C, 10.2.1, 10.2.2, p. 694
4. K&C, 10.2.6, p. 694
5. K&C, 10.3.1, p. 700
6. K&C, 10.4.3, p. 710

3 Realistic optimization problem

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

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

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), $i=1,...,n$, hence a functional $f:\mathbb{R}^m\to\mathbb{R}$, $m=2n$ 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) $f(\boldsymbol{z})=\sum_{j=1}^{p} b_j \sum_{i=1}^{n} c_i\,[u(t^j,x_i;\boldsymbol{z})-H(x_i-vt^j)]$. 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.