On the optimal initial conditions for a model parameter estimation problem: A complementarity principle

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Problem formulation & Numerical issues & Conclusion

We continue to look for an optimal bleaching pattern used in FRAP (Fluorescence Recovery After Photobleaching), being the initial condition of the Fickian diffusion equation maximizing a sensitivity measure [1-5].
Consider the Fickian diffusion equation

$$\frac{\partial u}{\partial t} = \delta \left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} \right), \tag{1}$$

where $r \in (0,1],\ t \in [0,1]$, with the initial and Neumann boundary conditions

$$u(r,0) = u_0(r), \quad \frac{\partial u}{\partial r}(1,t) = 0. \tag{2}$$

The main issue in FRAP and related estimation problems is to find the value of the diffusion coefficient δ from spatio-temporal measurements of the concentration $u(r,t)$, cf. [1, 5].
The measured data are discrete uniformly distributed in a finite domain

$$\begin{array}{lllll} u(r_i,t_j), & i = 0\dots n, & r_0 = 0, & r_n = 1, & \Delta r = 1/n \\ & j = 0\dots m, & t_0 = 0, & t_n = 1, & \Delta t = 1/m \end{array}$$

and the initial condition $u_0(r)$ can be considered as an $(n+1)$-dimensional vector $u_0 \in \mathcal{R}^{n+1}$.
The diffusion coefficient δ can be computed numerically by solving the inverse problem to (1)-(2) using the CN scheme.
Further, we define an optimization problem by looking for the narrowing of confidence interval of the true diffusion parameter δ_T. This can be done by maximizing the so called sensitivity measure

$$S_{app}(u_0) = \sum_{j=1}^{m} j^2 \|u_j - u_{j-1}\|^2,$$

where $u_j = (u_{0,j},\dots,u_{n,j})^T \in \mathcal{R}^{n+1},\ u_{i,j} := u(r_i,t_j),\ i = 0\dots n,\ j = 1\dots m$ [4].

The optimization problem is then formulated as follows

$$\boxed{u_0^{opt} = \arg\max_{u_0 \in \mathcal{R}^{n+1}} S_{app}(u_0) \quad \text{subject to} \quad 0 \le u_0 \le 1} \tag{3}$$

When computing a numerical solution $u_{i,j}$ of the IBV problem (1)-(2), the finite difference CN scheme is used. Starting with an initial $u_0 \in \mathcal{R}^{n+1}$ and after some algebraic manipulation we arrive at a linear system with a three-diagonal symmetric positive definite matrix

$$Au_j = Bu_{j-1} \tag{4}$$

for $u_j = (u_{0,j},\dots,u_{n-1,j})^T \in \mathcal{R}^n,\ j = 1\dots m$. The Neumann boundary condition implies the last component $u_{n,j} = u_{n-1,j}$.
Denote

$$C = A^{-1}B.$$

Then $\varrho(C) \le 1,\ u_j = C^j u_0,\ j = 1,\dots,m,$ and

$$S_{app}(u_0) = \sum_{j=1}^{m} j^2 \|C^{j-1}(C-I)u_0\|^2. \tag{5}$$

The function S_{app} is quadratic and nonnegative. The maximum is achieved at a vertex of the constrained set $0 \le u_0 \le 1$, which is $(n+1)$-dimensional hypercube. Thus, u_0^{opt} is a $\{1,0\}$-function, see also [2].
Moreover, since $(C-I)e = 0,\ e = (1,\dots,1)^T$, we have

$$S_{app}(\alpha e) = 0, \quad \alpha \in [0,1]. \tag{6}$$

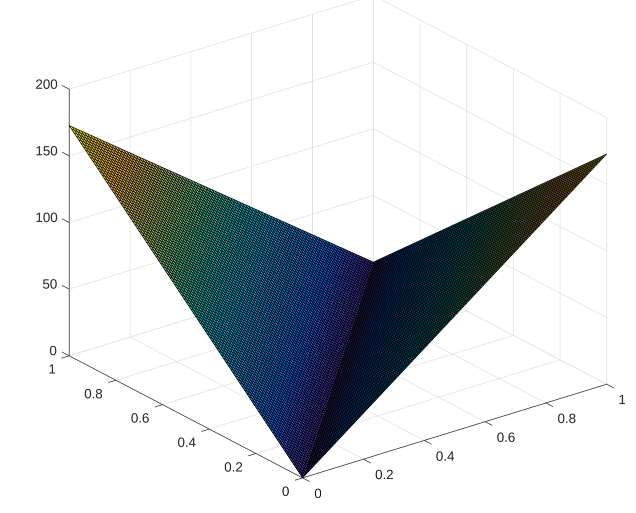
The most important property of the function S_{app} is

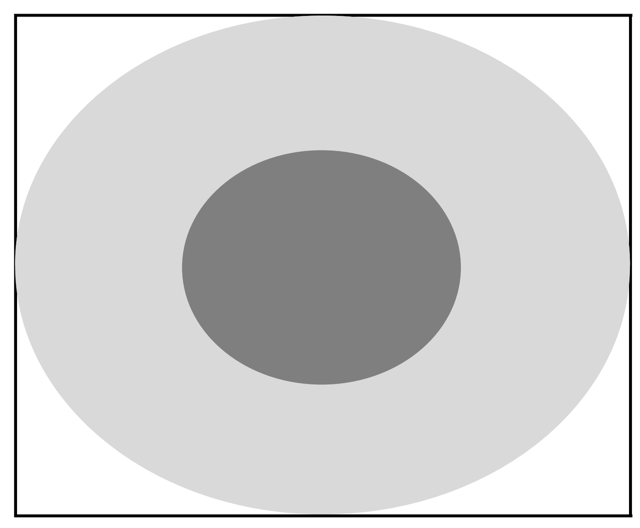
$$S_{app}(u_0) = S_{app}(e - u_0). \tag{7}$$

This implies that if u_0^{opt} is an optimal vertex solution to problem (3), then also $e - u_0^{opt}$ is a solution with the same function value, see the left figure.

In practice it means that if e.g. the disc is an optimal bleaching pattern, then also its complement (the annulus touching the bleached domain) is an optimal bleaching pattern and thus whichever of them can be used in practice, see the right figure.

Complementarity principle *Having prescribed δ and other parameters reflecting the experimental protocol, there exist two corresponding optimal initial conditions (and hence optimal bleach sizes and shapes).*





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