Numerical optimization of the non-axisymmetric bleaching pattern for FRAP experiments

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Problem formulation & Results & 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 [2]-[5]. In contrast to our previous papers, we will concentrate on non-axisymmetric domain. For this reason we consider the Fickian diffusion equation in polar coordinates

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

where $r \in (0,1],\ \theta \in [0, 2\pi],\ t \in [0,1]$, with the initial and Neumann boundary conditions

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

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 $u(r,\theta,t)$, see, e.g., [1].
The measured data are discrete uniformly distributed in a finite domain

$$\begin{array}{llll} u(r_i,\theta_k,t_j), & i = 0\dots n, & r_i = i\,\Delta r, & \Delta r = 1/n \\ & k = 0\dots p{-}1, & \theta_k = k\,\Delta\theta, & \Delta\theta = 2\pi/p \\ & j = 0\dots m, & t_j = j\,\Delta t, & \Delta t = 1/m \end{array}$$

(note that $\theta_0 = \theta_p$). The initial condition $u_0(r,\theta)$ is considered as an $(np+1)$-dimensional vector $u_0 \in \mathcal{R}^{np+1}$ containing p rays (angles) each divided into n points and one center point $r = 0$. The diffusion coefficient δ can be computed numerically by solving the inverse problem to (1)-(2) using the CN scheme.

A key issue is to find the narrowest confidence interval of the true diffusion parameter δ_T. This can be done by maximizing the so called sensitivity measure

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

see [4], where

$$u_j = (u_{0,0,j},\ u_{1,0,j}, \dots, u_{n,0,j},\ u_{1,1,j}, \dots, u_{n,1,j},\ \cdots,\ u_{1,p-1,j}, \dots, u_{n,p-1,j})^T \in \mathcal{R}^{np+1},$$

$$u_{i,k,j} := u(r_i,\theta_k,t_j), \quad i = 1\dots n, \quad k = 0\dots p-1, \quad j = 1\dots m.$$

Note that the subvector $u_{1,k,j}, \dots, u_{n,k,j}$ is the k-th ray (angle) of the domain.

The optimal initial condition giving the narrowest confidence interval is a solution of the following optimization problem

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

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 the $(np+1)$-dimensional hypercube. Thus, u_0^{opt} is a $\{1,0\}$-function, see also [2].

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

$$A^{(j)} u_j = A^{(j-1)} u_{j-1}$$

for $u_j \in \mathcal{R}^{np+1},\ j = 1\dots m$.

To find a global solution of problem (3), small values of n, p have to be used due to a combinatory problem of a boundary solution and a large dimension $(np+1)$. Thus, for our preliminary results, we first put $n = 10,\ p = 8$ and $m = 21$ to obtain a global solution. Optimal initial condition obtained is shown in the tables below, where the k-th row corresponds to the k-th ray (the values for $\theta_0, \dots, \theta_{p-1}$). Left table is for $\delta = 1.0\text{D}0$, right table is for $\delta = 1.0\text{D}6$.

	r_0	r_1	r_2	r_3	r_4	r_5	r_6	r_7	r_8	r_9	r_{10}
θ_0	0	0	1	0	1	0	1	0	1	0	1
θ_1		1	0	1	0	1	0	1	1	0	1
θ_2		0	1	0	1	0	1	0	1	1	0
θ_3		1	0	1	0	1	0	1	0	1	0
θ_4		0	1	0	1	0	1	0	1	0	1
θ_5		1	0	1	0	1	0	1	0	1	0
θ_6		0	1	0	1	0	1	0	1	0	1
θ_7		1	0	1	0	0	1	0	1	0	1

	r_0	r_1	r_2	r_3	r_4	r_5	r_6	r_7	r_8	r_9	r_{10}
θ_0	1	1	1	0	0	0	0	1	0	0	1
θ_1		1	1	1	0	1	1	0	0	0	0
θ_2		1	1	1	1	0	1	0	0	0	1
θ_3		0	1	1	1	0	1	0	1	0	0
θ_4		1	0	1	1	1	1	1	0	1	0
θ_5		0	0	1	1	0	0	0	0	0	0
θ_6		0	1	1	1	0	1	0	0	0	1
θ_7		1	0	0	1	0	1	1	0	0	1

Second, we used a finer grid and sought for only a local solution using several randomly chosen starting points for the optimization process. We put $n = 25,\ p = 24$ and $m = 21$. Below there are four rays for $k = 0,1,2,3$ of optimal u_0^{opt} giving the best function value S_{app} for $\delta = 1.0\text{D}0$ and $\delta = 1.0\text{D}6$.

	r_0	r_1	r_2	r_3	r_4	r_5	r_6	r_7	r_8	r_9	r_{10}	r_{11}	r_{12}	r_{13}	r_{14}	r_{15}	r_{16}	r_{17}	r_{18}	r_{19}	r_{20}	r_{21}	r_{22}	r_{23}	r_{24}	r_{25}
θ_0	1	0	1	0	1	1	0	1	0	1	0	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0
θ_1		1	0	1	0	1	1	0	1	0	1	1	0	1	0	1	1	0	1	0	1	1	0	1	1	0
θ_2		1	1	0	1	1	0	0	1	0	1	0	1	0	1	0	1	1	0	1	0	1	0	1	0	1
θ_3		0	1	1	0	1	0	1	0	1	0	1	0	0	1	0	1	1	0	1	0	1	0	1	0	1

	r_0	r_1	r_2	r_3	r_4	r_5	r_6	r_7	r_8	r_9	r_{10}	r_{11}	r_{12}	r_{13}	r_{14}	r_{15}	r_{16}	r_{17}	r_{18}	r_{19}	r_{20}	r_{21}	r_{22}	r_{23}	r_{24}	r_{25}
θ_0	1	0	1	0	1	1	1	0	1	1	0	1	1	1	1	0	0	1	1	0	1	0	0	0	0	0
θ_1		0	0	0	0	1	0	0	1	0	0	1	0	0	1	0	1	0	0	1	1	1	0	0	1	0
θ_2		1	1	1	1	1	0	0	0	0	0	1	1	1	1	1	0	1	0	0	1	1	0	0	0	1
θ_3		1	1	1	1	0	0	1	1	1	0	1	0	1	0	0	1	0	0	1	1	0	0	0	1	1

To compare the results also with some symmetric structures, we computed the values S_{app} also for optimal disc, optimal rays (only subvectors $u_{1,k,0}, \dots, u_{n,k,0}$ have nonzero components for $k \in \{0, \dots, p-1\}$), and optimal cross (combination of disc and rays) with $\delta = 1.0\text{D}0$. The table below shows the results.

u_0	optimal of all	optimal disc	optimal rays	optimal cross
S_{app}	64.51	3.75	19.75	4.56

From the preliminary results above we deduce that optimal patterns need not be symmetric at all. For small values of δ we see more jumps between ones and zeros in optimal initial condition than for larger values of δ. It corresponds to our previous results obtained in [4].

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