Disc vs. annulus: On the bleaching pattern optimization for FRAP experiments

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Problem formulation & Results & Conclusion

WE consider the Fickian diffusion equation

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

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

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

The measured data are discrete uniformly distributed in a finite domain

$$u(r_i, t_j), \quad i = 0 \dots n, \quad j = 0 \dots m,$$

Let $N_{\text{data}} := (m + 1) \times (n + 1)$. We define a forward map

$$F : D \in \mathcal{R} \to u(r_k, t_k)_{k=1}^{N_{\text{data}}} \in \mathcal{R}^{N_{\text{data}}}.$$

Our regression model is now $F(D) = \text{data}$, where the data are modeled as contaminated with additive white noise

$$\text{data} = F(D_T) + e = u(r_k, t_k)_{k=1}^{N_{\text{data}}} + (e_k)_{k=1}^{N_{\text{data}}}. \tag{3}$$

where D_T is a true coefficient. A least-squares solution D_c is found

$$\| \text{ data} - F(D_c) \|^2 = \min_{D>0} \| \text{ data} - F(D) \|^2 . \tag{4}$$

The expected relative error in D_T satisfies

$$\mathbb{E}\left(\left|\frac{D_c - D_T}{D_T}\right|^2\right) \sim \frac{\sigma^2}{S_{GRS}}, \tag{5}$$

where $\mathbb{E}$ is the expected value, σ^2 is the variance of the noise, and

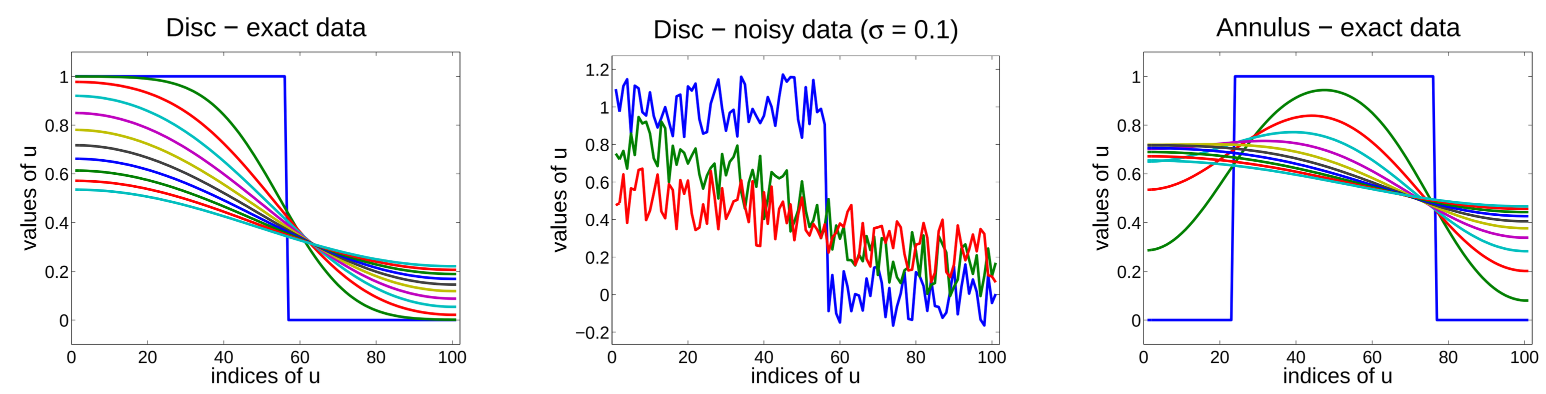
$$S_{GRS} = D_T^2 \sum_{i=0}^{n} \sum_{j=1}^{m} \left[\frac{\partial}{\partial D} u(r_i, t_j)|_{D=D_T}\right]^2 \approx \sum_{j=1}^{m} j^2 \sum_{i=0}^{n} [u_{i,j} - u_{i,j-1}]^2 =: S_{app}, \tag{6}$$

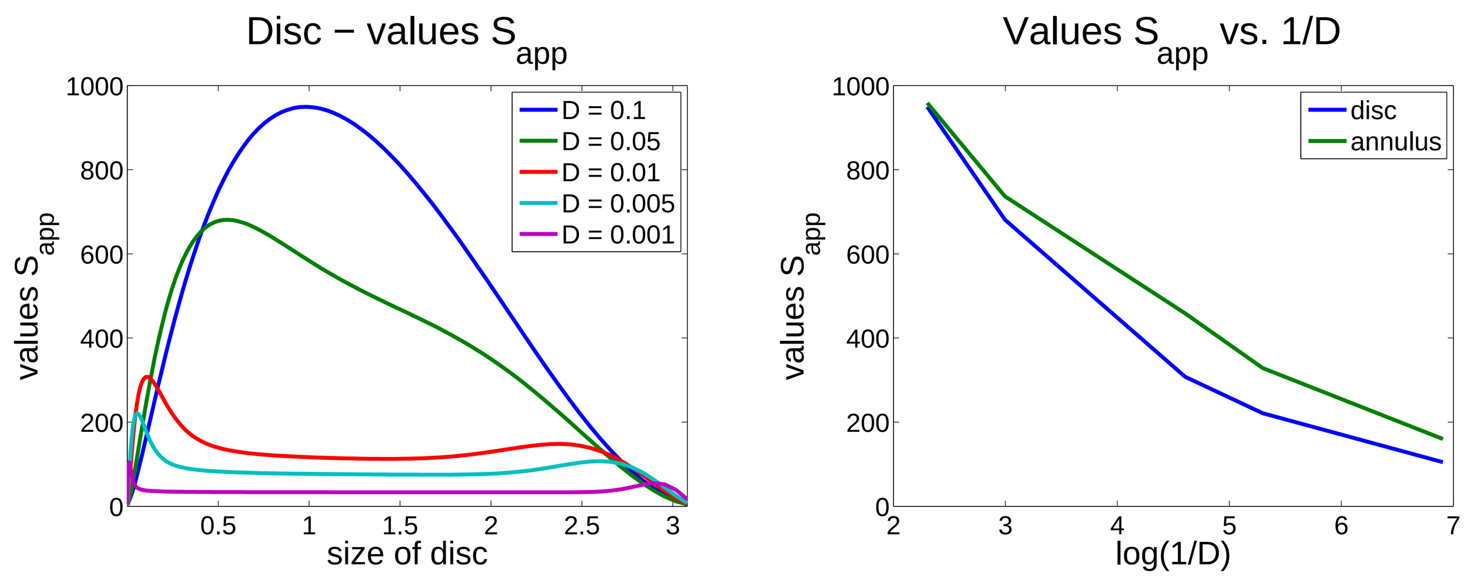
where $u_{i,j}$ is a numerical solution.
The optimization problem is

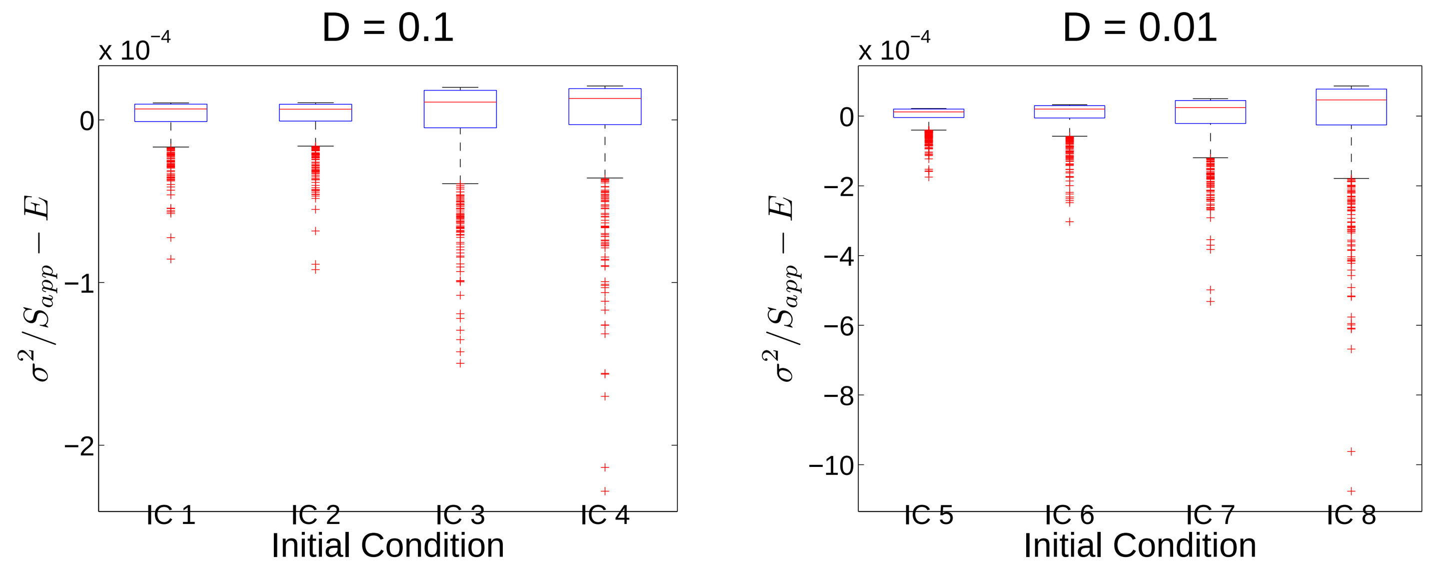
$$\boxed{u_0^{opt} = \arg\max_{u_0 \in \mathcal{R}^{n+1}} S_{GRS}(u_0) \quad \text{subject to} \quad \underline{u_0} \le u_0 \le \overline{u_0}} \tag{7}$$

It can be shown that u_0^{opt} in a discrete form attains only the values $\underline{u_0}$ and $\overline{u_0}$. For our numerical example we chose eight initial conditions IC 1 - IC 8 and parameters $R = 1,\ T = 1,\ n = 100,\ m = 300,\ \underline{u_0} = 0,\ \overline{u_0} = 1,\ \sigma = 0.1$.

D	IC	pattern	1's in u_0	S_{app}	σ^2/S_{app}
0.1	IC 1	optimal annulus	$1,\dots,55$	958.6	1.04e-5
	IC 2	optimal disc	$0,\dots,55$	949.5	1.05e-5
	IC 3	another annulus	$23,\dots,75$	499.9	2.00e-5
	IC 4	another disc	$0,\dots,29$	478.9	2.09e-5
0.01	IC 5	optimal annulus	$19,\dots,51$	458.5	2.18e-5
	IC 6	optimal disc	$0,\dots,18$	307.7	3.25e-5
	IC 7	another annulus	$63,\dots,76$	200.4	4.99e-5
	IC 8	another disc	$0,\dots,57$	115.7	8.64e-5







In this study, the problem of the optimal initial condition for further identification of a diffusion coefficient in FRAP experiments was formulated. Having a bleach size and pattern, which maximizes a sensitivity S_{app} (the optimality criterion considering the sensitivity of measured data w.r.t. parameters to be identified), we expected the minimal error (confidence interval) of the estimated parameter, see (5). Our numerical results confirm this expectation. We used the finite difference scheme to discretize both the scaled initial boundary value problem (1)-(2) and the sensitivity measure S_{app} (6) and we solved the optimization problem (7). We argue that there exists specific optimal initial condition u_0^{opt} that maximizes the sensitivity measure S_{app} and therefore minimizes the error in the model parameter estimate (diffusion coefficient D), see (5). Moreover, we found that in discrete points $r_0, \dots, r_n$, the components of the vector u_0^{opt} attain only two values ($\underline{u_0}$ and $\overline{u_0}$). The jumps between these values represent the discontinuities leading to more complex bleaching patterns (one jump - disc, two jumps - annulus, etc.). We found that the pattern complexity depends on the diffusion coefficient D. The smaller value of D is (i.e., the slower the particle mobility due to the diffusion process is), the larger number of jumps occurs.

Reference

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