On the optimal initial conditions for an inverse problem of model parameter estimation

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Introduction

- The aim of this contribution is to establish the link between experimental conditions (experimental protocol) and the accuracy of the resulting model parameter estimate.
- The idea is presented in a simplified case study of FRAP (Fluorescence Recovery After Photobleaching) data processing.
- It serves as a paradigmatic example of the inverse problem of the diffusion parameter estimation from spatio-temporal measurements.
- A natural question is how to design an experiment optimaly, i.e., how the experimental settings influence the accuracy of resulting parameter estimates.

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 is to find the value of the diffusion coefficient δ from spatio-temporal measurements of the concentration $u^M(r, t)$.

The measured data:

$$u^M(r_i, t_j), \qquad \begin{aligned} i &= 0 \dots n, \quad r_0 = 0, \quad r_n = 1, \\ j &= 0 \dots m, \quad t_0 = 0, \quad t_n = 1, \end{aligned}$$

The data points are uniformly distributed in spatio-temporal grid.

When solving the inverse problem to (1)-(2):
Noise in data $\Rightarrow$ an estimated value $\overline{\delta}$.

The expected relative error in δ depends on the data noise and the sensitivity measure S_{GRS} (global sensitivity):

$$\mathbb{E}\left(\left|\frac{\overline{\delta}-\delta}{\delta}\right|^2\right) \sim \frac{\sigma^2}{S_{GRS}}, \tag{3}$$

where σ^2 denotes the variance of the additive Gaussian noise.

The sensitivity measure S_{GRS} is

$$S_{GRS} := \delta^2 \sum_{i=0}^{n} \sum_{j=1}^{m} \left[\frac{\partial}{\partial \delta} u(r_i, t_j)\right]^2, \tag{4}$$

If the noise level is fixed, the estimation of δ can only be improved by an experimental design with a higher sensitivity S_{GRS}.

Initial bleach as the experimental design parameter

We look for an optimal initial bleach shape (pattern), i.e., we aim to select initial conditions in such a way that S_{GRS} is maximized and hence the expected error in δ is minimized.

The class of designs:

$$u_0(r) = \begin{cases} 1, & r \in B, \\ 0, & \text{else}, \end{cases} \tag{5}$$

where B is an open subset of $[0,1]$.

We seek

$$B_{opt} = \arg\max_{B \subset [0,1]} S_{GRS}. \tag{6}$$

We use a finite difference Crank-Nicholson (CN) scheme to compute a numerical solution $u(r_i, t_j),\ i = 0 \dots n-1,\ j = 1 \dots m$, of the initial boundary value problem (1)-(2).

Replacing the derivative with a finite difference, the sensitivity measure S_{GRS} can be approximated with a value S_{app} as follows

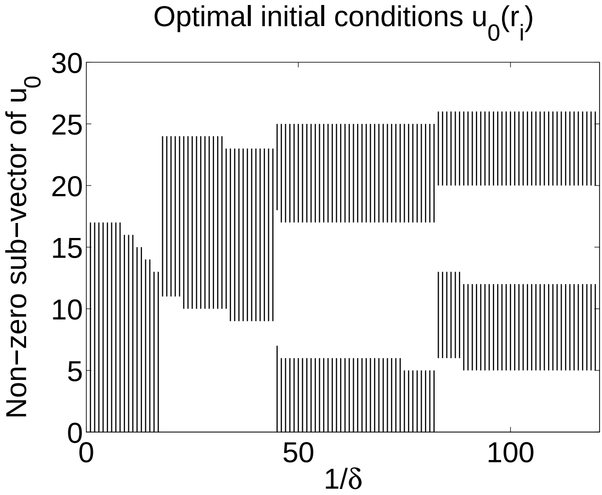
$$S_{GRS} \approx S_{app} = \sum_{j=1}^{m} j^2 \sum_{i=0}^{n} \left[u(r_i, t_j) - u(r_i, t_{j-1})\right]^2 . \qquad (7)$$

The values $u(r_i, t_j)$ are computed from $u(r_i, t_{j-1})$ using the CN scheme, thus no extra work is necessary.

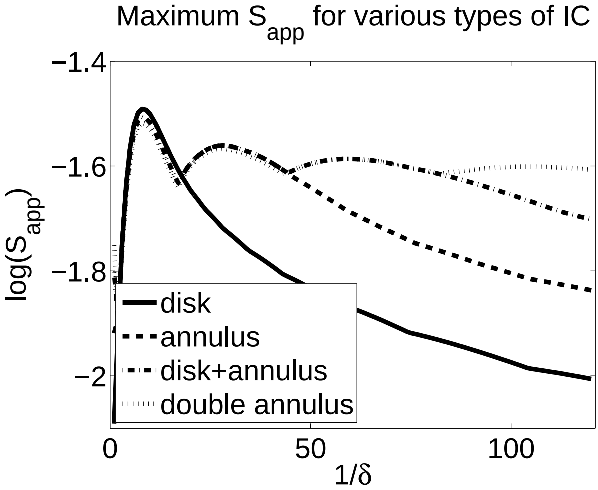
To demonstrate the optimal configurations of the initial condition let us choose $n = 30$, $m = 200$ and find such an initial condition $(u_0(r_0), \ldots, u_0(r_n))^T \in \mathcal{R}^{n+1}$ in form of a $\{1, 0\}$-function, cf. (5), that maximizes the value S_{app} (7) for $1/\delta = 1, 2, \ldots, 120$.

For the sake of simplicity we consider four types of shapes (or patterns) of the initial condition (the sets B in (5)):

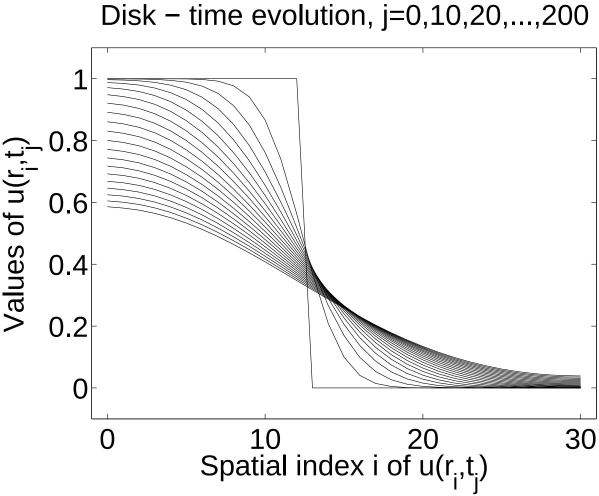
$$\begin{aligned} \text{disc:} \quad & u_0(x) = (\mathbf{1}, 0) \\ \text{annulus:} \quad & u_0(x) = (\mathbf{0}, \mathbf{1}, 0) \\ \text{disc+annulus:} \quad & u_0(x) = (\mathbf{1}, \mathbf{0}, \mathbf{1}, 0) \\ \text{double annulus:} \quad & u_0(x) = (\mathbf{0}, \mathbf{1}, \mathbf{0}, \mathbf{1}, 0) \end{aligned}$$



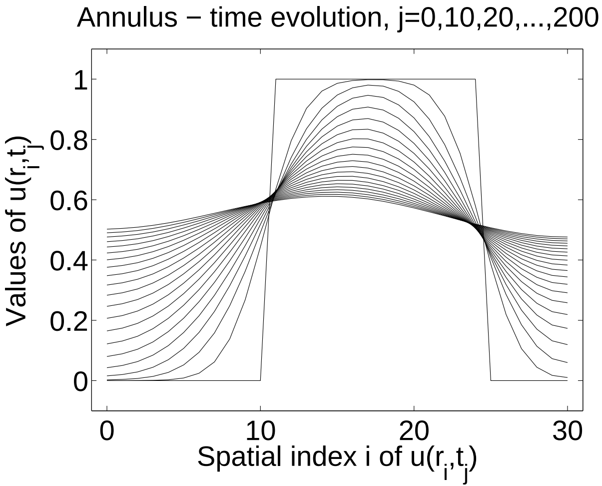
The result of optimization problem (6): each vertical line indicates the non-zero sub-vector of u_0 for which S_{app} is maximal.



Each curve indicates the maximum value of S_{app} determined by initial conditions from the four groups listed above.



Disc – optimal u_0 for $\delta = 0.05$ $(1/\delta = 20)$ and time evolution $u(r, t_j)$ computed using the CN scheme.



Annulus – optimal u_0 for $\delta = 0.05$ $(1/\delta = 20)$ and time evolution $u(r, t_j)$ computed using the CN scheme.

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