Identification of non-linearities in transport-diffusion models of crowded motion

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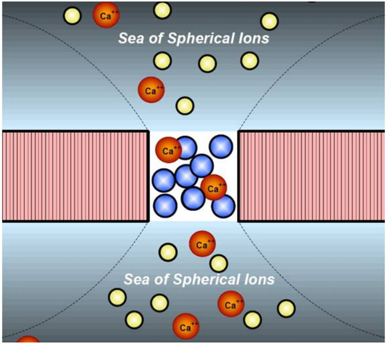
Introduction

Definitions

- Crowded motion: movement in confined geometries where finite size effects matter.

Some Examples



The Inverse Problem

$$\partial_t u = \operatorname{div}(D(u)(\nabla E'(u) - \nabla V)),$$

Non-linear Drift-/Convection-Diffusion Equation

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Aim: Identify (reconstruct)

- the mobility $D = D(u)$
- the entropy $E = E(u)$

given "some measurements".

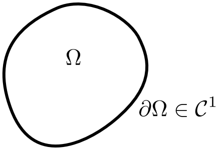
Forward Problem

Stationary case:

$$\operatorname{div}(G(u)\nabla u - D(u)\nabla V) = 0,$$

with

$$G(u) = D(u)E''(u)$$



Boundary conditions:
$$u|_{\partial\Omega} = f \in H^2(\Omega).$$

Assumptions:

(A1) $G(u) \geq \epsilon > 0,\ D(u) > 0$ for $0 < u < 1$, $\epsilon > 0$.

(A2) $E \in \mathcal{C}^2(\mathcal{I}),\ E''(u) \geq 0$, $\mathcal{I} = [0, 1]$

(A3) $D \circ (E')^{-1}$ exists,

(A4) $V \in W^{1,\infty}(\Omega)$.

Direct Problem - Well-Posedness

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Theorem (Existence)

Let $n = 1, 2, 3$ and $F'(u) = (D(H^{-1}(u)))'$, $H' = G$, continuous and bounded for all $0 < a \leq u \leq b < 1$. Then, there exists a solution $u \in L^\infty(\Omega) \cap H^1(\Omega)$

Proof:

- Transformation to entropyvariables:

$$\varphi = \partial_u \mathcal{E}(u), \quad \mathcal{E}(u) := \int_\Omega E(u(x)) - u(x)UV(x)dx.$$

- Linearisation + a-priori bounds (maximum principle) + fixed point arguments
- Uniqueness only for U small

Assumptions/Inverse Problem

Available data:

- Flux measurements (robust, easy to obtain)
- Density estimation from trajectories

Data available from artificial experiments, video recordings

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Inverse Problem:

$(\mathcal{IP})$ Identify the functions $G,\ D$ from flux measurements

$$j_{meas} = \int_{\Gamma \subset \partial\Omega} j \, d\sigma = \int_{\Gamma \subset \partial\Omega} (G(u)\nabla u - D(u)\nabla V) \cdot n \, d\sigma$$

where (U, V, f) are taken from a subset of $\mathbb{R} \times W^{1,\infty}(\Omega) \times H^2(\Omega)$.

Linearisations, Simple Cases

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One spatial dimension, $\Omega = [0,1]$, linear potential $V = Ux$

$$\partial_x(G(u)\partial_x u - D(u)U) = 0$$

Measurements = flux measurements on boundary

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Reconstruction of D:

- $u(0) = u(1) = u_0 \ \Rightarrow$ constant stationary solutions u_0

$$j_{meas} = G(u_0)\underbrace{\partial_x u_0}_{=0} - D(u_0)U$$

$$\Rightarrow D(u_0) = -\frac{j_{meas}}{U}$$

$\Rightarrow$ Can identify D from flux measurements

Linearisations, Simple Cases

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Reconstruction of G:

Linearise around equal Dirichlet boundary conditions, i.e. $u_R = u_L + \epsilon$:

$$\partial_x (G(u_0)\nabla u - D'(u_0)uU) = 0.$$

Linearised flux:

$$j_{meas} = G(u_0)\nabla u - D'(u_0)uU$$

Transformation $u = e^{cx}v$ (Semiconductors) and Integration yields

$$G(u_0) = -D'(u_0)U \Bigg/ \log\left(1 - \frac{\epsilon}{u_R + \frac{j_{meas}}{D'(u_0)U}}\right)$$

Numerical Examples

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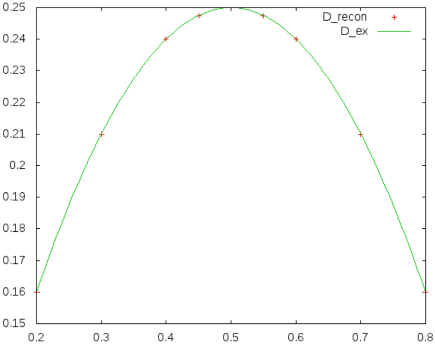
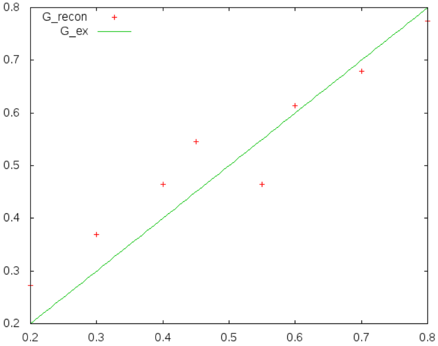
$G(u) = u,\ D(u) = u(1-u)$





Looks ok, but: $U = 0.01$

$$(G(u_0)u_x - D'(u_0)uU)_x = 0$$

Differentiability

Define *parameter-to-solution map*

$$\mathcal{T} : \mathcal{D}(\mathcal{T}) \times \mathbb{R} \times W^{1,\infty}(\Omega) \times H^2(\Omega) \to H^1(\Omega)$$
$$(G, D, V, f) \mapsto u, \ u \text{ solving } \mathcal{DP}(G, D; U, V, g)$$

then:

Theorem

Let $D, G \in \mathcal{C}^1(\mathcal{I})$ (i.e. $E \in \mathcal{C}^3(\mathcal{I})$). Then for given $(V, f) \in W^{1,\infty}(\Omega) \times H^2(\partial\Omega)$ the operator $\mathcal{T}$ is Frechét differentiable with respect to D, G.

Proof (sketch):

$$e(G, D, u) = \operatorname{div}(G(u)\nabla u - D(u)U\nabla V) = 0$$

Generalised inverse function theorem. Main difficulty:

$$\frac{\partial e}{\partial u}(G, D; u)v = \operatorname{div}(G(u)\nabla v + (G'(u)\nabla u - D'(u)U\nabla V)v).$$

Identifiability (I)

Consider two solutions $(u_1; G_1, D)$, $(u_2; G_2, D)$ with fluxes

$$j_i = G_i(u_i)\partial_x u_i - D(u_i)U,\ \ i = 1, 2.$$

Theorem

If $j_1 = j_2$, then the following relation holds:

$$0 = \int_0^1 [(G_1(u_1) - G_2(u_1))\partial_x u_1] \cdot \partial_x \lambda \, dx,$$

where λ is a solution of

$$p(x)\lambda_{xx} + q(x)UV_x\lambda_x = 0, \qquad x \in \Omega = [0, 1],$$

supplemented with

$$\lambda(0) = 0, \quad \lambda(1) = 1,$$

with p, $q \in L^\infty(\Omega)$, $p > 0 \,\mathrm{in}\, \Omega$.

Identifiability (II)

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Definition (Distinguishability, cf. Duchateau (1995))

Two continuous functions $f, g : [a, b] \to \mathbb{R}$ are called distinguishable if $f \neq g$ and $f - g$ changes sign only finitely many times on $[a, b]$.

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Theorem

Let $(u_1; G_1, D)$ and $(u_2; G_2, D)$ denote two solutions. Furthermore assume G_i, $i = 1, 2$ bounded in $L^1(\Omega)$. We define the interval

$$\mathcal{I} = \left[\inf_{x\in\Omega} u, \ \sup_{x\in\Omega} u\right]$$

Then the exists a sets of finitely many Dirichlet B.C.s (u_L^i, u_R^i) (with corresponding fluxes j_1^i, j_2^i) such that the functions (G_1, G_2) are not distinguishable on $\mathcal{I}$ if j_1^i and j_2^i are identical.

Identifiability (Proof)

- Maxiumum principle in $[0, 1]$:

$$sign(u_x) = sign(u_L - u_R),$$
$$\lambda_x > 0$$

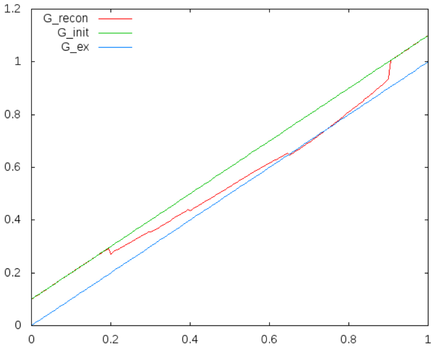
- In each interval $\mathcal{I}_G^k$, we can choose boundary values u_L and u_R such that the values of u_1 lie in this interval (due to the maximum principle). Then we have

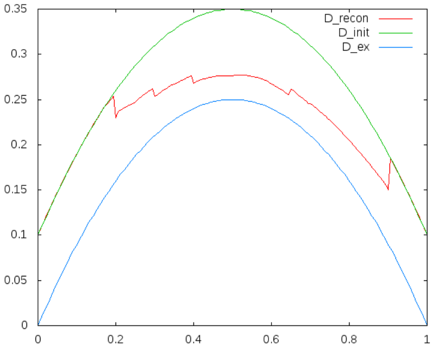
$$0 = \int_\Omega (G_1(u_1) - G_2(u_1))(u_1)_x \lambda_x \, dx.$$

$\Rightarrow$ contradiction and $G_1 = G_2$ on $\mathcal{I}_G^k$.

Numerical Examples

$G(u) = u,\ D(u) = u(1-u),\ U = 0.25$





Conclusion & Outlook

- Well-Posedness of the Direct Problem
- Identifiability (1D)
- Frechét differentiability (strong regularity assumptions)
- Landweber-Kaczmarz scheme

Future Work:

- Time-dependent case
- multiple space dimensions (numerics, identifiability, etc.)

M. Burger, J.-F. P., M.-T. Wolfram
Identification of non-linearities in transport-diffusion models of crowded motion.
Preprint: UCLA-CAM report No. 11-80, 2011

http://www.jfpietschmann.eu