

Scope

Parameter identification related to nonlinear parabolic equations

$$(1) \quad g' - \operatorname{div}(D \operatorname{grad} g) + \lambda g = R\Phi(Wg),$$

on bounded Lipschitz domains $U \subset \mathbb{R}^d$ with nonlinear signal response function Φ

Goals

- Reconstruction of reaction parameters $p = (D, \lambda, R, W)$ from noisy data g^δ
- Application to embryogenesis of *Drosophila* [10]

Ansatz

Ill-posed problem \triangleright regularization needed \triangleright minimization problem

- Tikhonov regularization with Besov penalty term

$$(2) \quad p_\alpha^\delta = \operatorname{argmin}_{p=(D,\lambda,R,W)} \left\| \mathcal{S}(p) - g^\delta \right\|^2 + \alpha |p|_s,$$

with $p \mapsto \mathcal{S}(p) :=$ solution to (1) with parameters p

- Besov penalty term promotes sparse solutions

Tasks

- Efficient solver for the forward problem with optimal convergence rates for prescribed tolerance
- Efficient minimization strategy for (2)

Numerical treatment of the forward problem

I. Parabolic problem

- Solution space for PDE (1)

$$\mathcal{W} = \{u \in L_q(0, T, V_1) : u' \in L_q(0, T, V_2)\},$$

where $V_1 = W_q^1(U, \mathbb{R}^d)$, $V_2 = (W_q^1(U, \mathbb{R}^d))'$

- Implicit discretization by Rothe's method: \triangleright first in time, then in space \triangleright system of elliptic equations per time step:

$$(3) \quad g(t_{n+1}) \approx g^{(n+1)} = g^{(n)} + m_1 g_1$$

$$\left(\frac{1}{h} I - J \right) g_1 = \operatorname{div}(D \operatorname{grad} g^{(n)}) - \lambda g^{(n)} + R\Phi(Wg^{(n)})$$

- Strategy: employ **adaptive methods** (in time/space) to increase efficiency

II. Elliptic problems

Ansatz: adaptive algorithms based on tensor wavelets \triangleright dimension-independent convergence rates

- Construction of generalized anisotropic tensor wavelets

Theorem. Let U be decomposable into cubes \square_i . Let Ψ_i be an anisotropic tensor wavelet basis for $L_2(\square_i)$, scaled: $W_2^s(\square_i)$. Let E be a combination of univariate extension operators, bounded on $\prod_{i=1}^m L_2(\square_i)$ and $\prod_{i=1}^m W_2^s(\square_i)$.

Then

$$\Psi_U := E\{\Psi_i\}_{i=1}^m, \tilde{\Psi}_U := E^{-*}\{\tilde{\Psi}_i\}_{i=1}^m$$

defines a (biorthogonal) wavelet basis for $L_2(U)$, scaled: $W_2^s(U)$.

\triangleright advantages: constructions retains

- tensor structure
- global/local smoothness
- vanishing moments
- piecewise polynomiality

\triangleright dimension-independent approximation rates

Theorem. Given $u \in W_2^m(U)$ there exists an N -term approximation $u_N = \sum_{\lambda=1}^N c_\lambda \psi_\lambda$ from Ψ_U , such that

$$\|u - u_N\|_{W_2^m(U)} \lesssim N^{-(\tau-m)} \left(\prod_{\square_i \subset U} \|u\|_{\mathcal{H}_{m,\theta}^\tau(\square_i)}^2 \right)^{\frac{1}{2}}$$

whenever u is contained in the weighted Sobolev spaces $\mathcal{H}_{m,\theta}^\tau(\square_i)$.

- Design of adaptive method

- main building block of adaptive methods: approximation of biinfinite matrix/vector-multiplication $\text{APPLY}[\mathbf{A}, \mathbf{x}, \delta] \rightarrow v_\delta$ finitely supported with $\|\mathbf{A}\mathbf{x} - v_\delta\| \leq \delta$
- design of **APPLY** possible if \mathbf{A} is compressible

Theorem. Let \mathbf{A} be the stiffness matrix according to (3) with respect to Ψ_U . Then there exist matrices \mathbf{A}^M with $\mathcal{O}(M^{\frac{1-\varepsilon}{2}} d)$ many entries per column, such that

$$\|\mathbf{A} - \mathbf{A}^M\| \lesssim 2^{-M}.$$

\triangleright Adaptive method converges with **optimal order!**

Parameter identification problem

I. Parameter-to-state map

- Parameters $p = (D, \lambda, R, W)$

◦ $D \in L_\infty([0, T], L_\infty(U, \mathbb{R}^d))$ ◦ $\lambda, R \in L_r([0, T], L_r(U, \mathbb{R}^d))$, $W \in L_r([0, T], L_r(U, \mathbb{R}^{d \times d}))$

◦ pointwise global bounds, $r \in (2, \infty)$ chosen respectively for λ, R, W \triangleright admissible sets are non-complete metric spaces

- In practice: noisy data measurements $g_t^\delta \in L(\mathbf{t}, L_2(U, \mathbb{R}^d))$ at discrete time points $\mathbf{t} = \{t_i\}_{i=1}^k \subset [0, T]^k$

◦ need sampling operator $\mathcal{P} : L_2([0, T], L_2(U, \mathbb{R}^d)) \rightarrow L_2(\mathbf{t}, L_2(U, \mathbb{R}^d))$

- Resulting parameter identification problem

$$(4) \quad \mathcal{P}\mathcal{S}(p) = g_t^\delta$$

Theorem. The parameter-to-state map \mathcal{S} is continuously differentiable with Hölder continuous derivative \mathcal{S}' on convex, bounded, admissible sets.

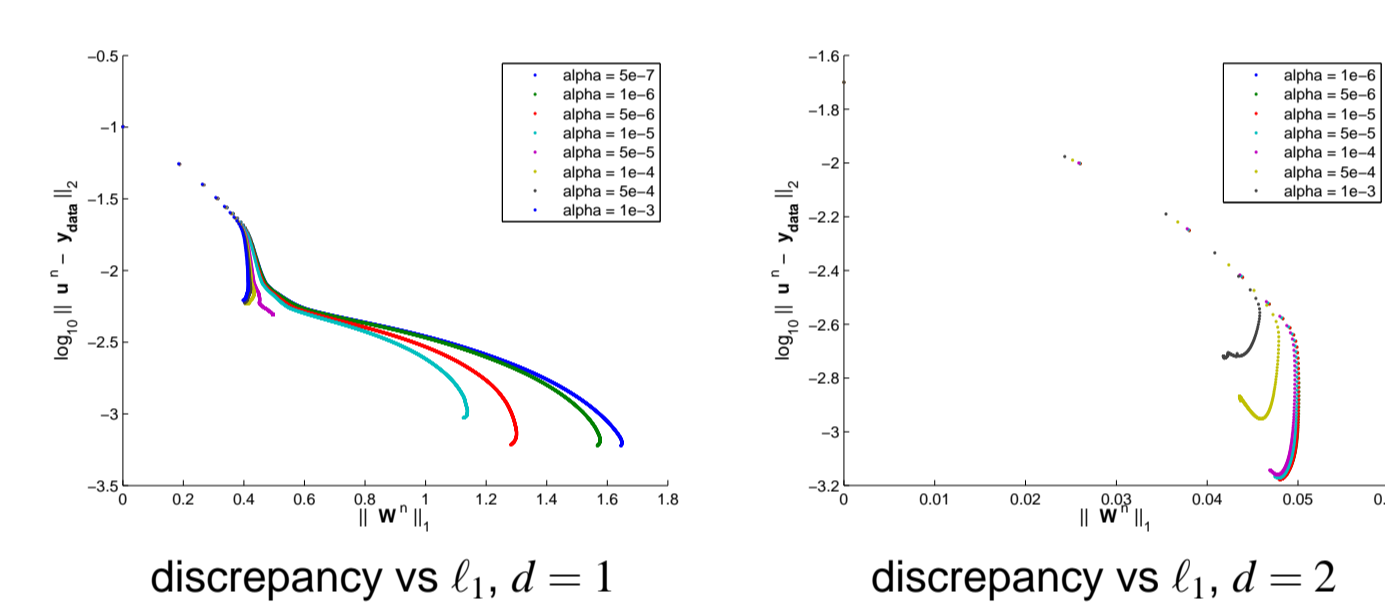
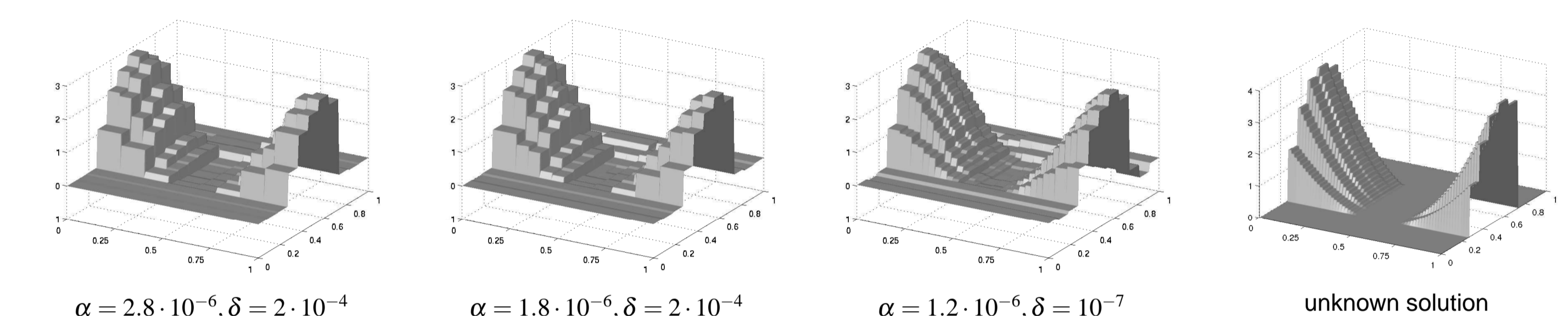
II. Regularization

- Tikhonov approach yields regularization scheme: $p_\alpha^\delta \rightarrow p$ for a suitable parameter choice rule for α
- Minimization problem (2) is solved by generalized conditional gradient method (iterative soft-shrinkage)

$$p_{n+1} = \text{Shrink}_\alpha(p_n - (\mathcal{S}'(p_n))^* \mathcal{P}^*(\mathcal{P}\mathcal{S}(p_n) - g_t^\delta)) \rightarrow p_\alpha^\delta$$

with Besov ℓ_s penalty term on coefficients with respect to wavelet basis/frame

Numerical realization



- Linearized model problem, $d = 1, 2$
- Reconstruction of coupling parameter $W(t, x)$
- Adaptive (tensor) wavelet approach
- Based on Marburg software library

Objectives and work schedule

Forward problem: adaptive tensor product wavelet schemes for elliptic/parabolic equations

I. Finetuning of adaptive algorithms

- Vector-valued case
- Parallelization strategies

II. Generalization to nonlinear problems

- Sparse evaluation of nonlinear functionals applied to tensor wavelet expansions
- Generalization to vector-valued case

III. Theoretical justification

- Investigate regularity of solution in generalized weighted Sobolev spaces
- Generalizations to nonlinear problems

Inverse problem: parameter identification with sparsity constraints

I. Convergence aspects

- Convergence theory and rates in case of inexact solution of forward problem
- Exploration of different approaches encompassing positivity constraints

II. Acceleration strategies

- Speed-up for iterated soft shrinkage \triangleright decreasing thresholding
- Investigate alternative minimization procedures

Numerical realization and application

I. Fully adaptive solver in time and space

- Efficient sparse evaluation of nonlinearity Φ • Vector-valued case
- Adaptive discretization in time • Parallelization
- Based on Marburg software library

II. Application to full embryogenesis model

- Combination of new forward solver with iterated soft shrinkage • Complex geometry
- High-dimensional parameter space