POLITECNICO
MILANO 1863

Parameter estimation in PDE-regularized spatial regression via parameter cascading

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Data:

- $\mathbf{p}_1, ..., \mathbf{p}_n$ n locations in $\Omega \subset \mathbb{R}^2$
- $t_1, .., t_m$ time steps in $T \subset \mathbb{R}$
- z_{ij} variable of interest observed at $(\mathbf{p}_i, t_j)$

Space-Time model:

- $f : \Omega \times T \to \mathbb{R}$ deterministic spatio-temporal field
- $z_{ij} = f(\mathbf{p}_i, t_j) + \epsilon_{ij}, \qquad i = 1, ..., n, \quad j = 1, ..., m$
- ϵ_{ij} i.i.d. residuals with zero mean and finite variance σ^2

Goal: estimate f minimizing

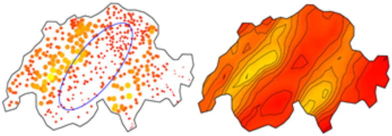
$$J_{\rho,\gamma}(f) = \frac{1-\rho}{nm} \sum_{i=1}^{n} \sum_{j=1}^{m} (z_{ij} - f(\mathbf{p}_i, t_j))^2 + \frac{\rho}{|\Omega|} \int_T \int_\Omega (\gamma \frac{\partial f}{\partial t} + Lf - u)^2$$

- $\rho \in (0,1)$ smoothing parameter
- $Lf = -\nabla \cdot (K \nabla f), \qquad K \in \mathbb{R}^{2x2}$ diffusion matrix
- $u = 0$
- γ unknown PDE parameter to estimate via profiling estimation (parameter cascading)

Reference Papers

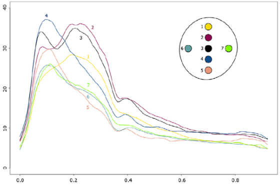
Bernardi et al., 2018, JMVA

- Space only
- Estimation of the anisotropy matrix K via parameter cascading
- Switzerland rainfall data



Arnone et al., 2019, JMVA

- Space-time
- Blood-flow velocity field in a carotid artery affected by atherosclerosis

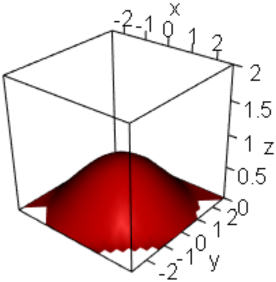


$$J_\rho(f, K) = \frac{1-\rho}{n} \sum_{i=1}^{n} (z_i - f(\mathbf{p}_i))^2 + \frac{\rho}{|\Omega|} \int_\Omega (\nabla \cdot (K \nabla f))^2$$

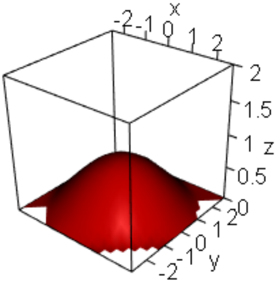
$$J_\lambda(f) = \sum_{i=1}^{n} \sum_{j=1}^{m} (z_{ij} - f(\mathbf{p}_i, t_j))^2 + \lambda \int_T \int_\Omega \left(\frac{\partial f}{\partial t} + Lf - u\right)^2$$

Aim of the Project

Analyze and implement a **statistical technique** to estimate f and γ by means of **parameter cascading**



True field



Estimated field

Parameter Cascading

For fixed increasing values of ρ, perform:

Step 1: Estimate $\hat{f}$ keeping γ fixed, minimizing J:

$$J_{\rho,\gamma}(f) = (1-\rho)\frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{m}(z_{ij} - f(\mathbf{p}_i, t_j))^2 + \rho\frac{1}{|\Omega|}\int_T\int_\Omega(\gamma\frac{\partial f}{\partial t} - K\Delta f)^2$$

Step 2: Estimate $\hat{\gamma}$ keeping $\hat{f}$ fixed, minimizing H:

$$H(\gamma) = \sum_{i=1}^{n}\sum_{j=1}^{m}(z_{ij} - \hat{f}_{\rho,\gamma}(\mathbf{p}_i, t_j))^2$$

In our case, we chose:
$\rho = (0.01, 0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 0.95, 0.99)$

Pseudo-code

Algorithm 1 Estimation of γ through parameter cascading

```
Create a vector with n different values of ρ
for ρ_i,  i = 1, ..., n do
    if i = 1 then
        Set γ to an initial value (e.g. 1)
    else
        Set γ to the estimate of the previous step
    end if
    Minimize the functional H and find the optimal γ
end for
```

GitHub Library

For the project, the R/C++ library *fdaPDE* from Github was used:

`github.com/fdaPDE/fdaPDE`

In particular, the function *smooth.FEM.time* was used to perform the final estimation of the paramater ρ (via GCV) and the field f.

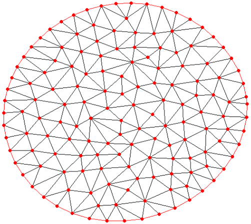
Procedure

- Using FreeFem, we generated the exact solution of:

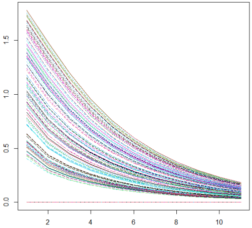
$$\frac{\partial f}{\partial t} - K\Delta f = 0$$

- To test the method, we added error to simulate data

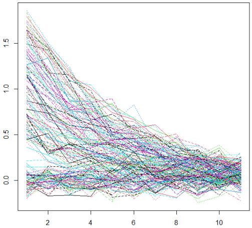
Mesh



Exact observations



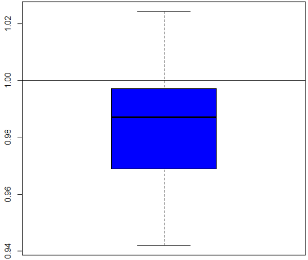
Noisy observations

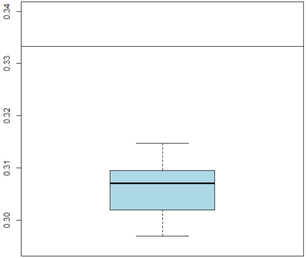


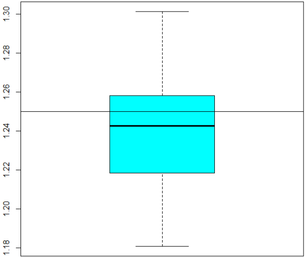
Estimations

We generated data modifying K and we obtained:

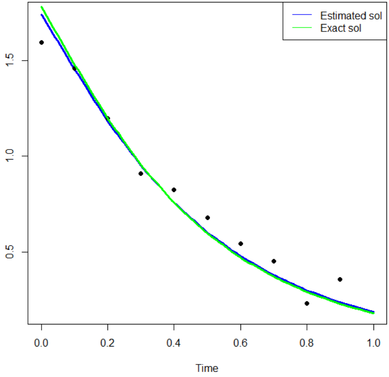
K = 1	**K = 3**	**K = 0.8**
$\hat{\gamma} = 0.9847768$	$\hat{\gamma} = 0.3063712$	$\hat{\gamma} = 1.240424$



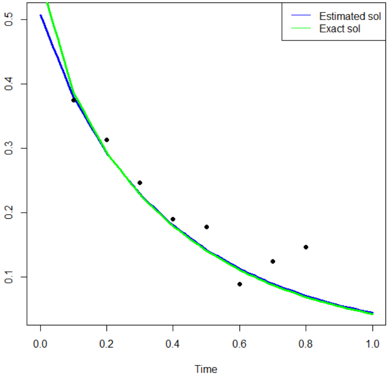




Plots



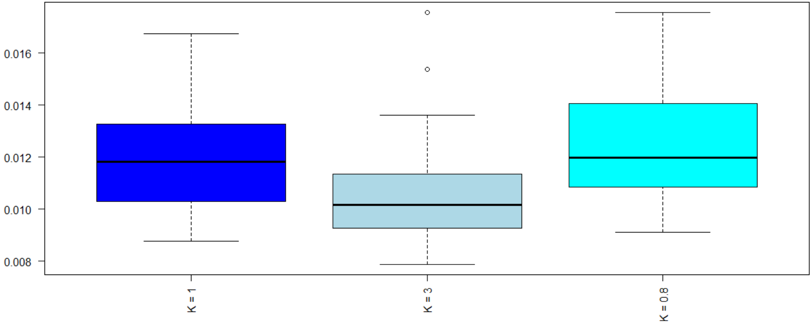
Time evolution near $(0, 0)$



Time evolution near the boundary

Root Mean Squared Errors

K = 1	**K = 3**	**K = 0.8**
$RMSE = 0.01192373$	$RMSE = 0.01172951$	$RMSE = 0.01245426$

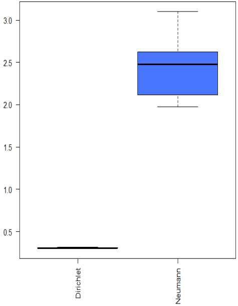


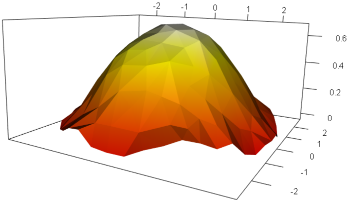
Neumann Boundary Conditions

As expected, the Neumann Boundary Conditions do **not** fulfill the no-slip constraint

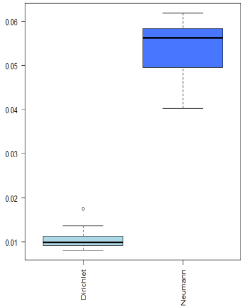
$\hat{\gamma} = 2.433283$

$RMSE = 0.05389998$





Estimated solution



Introducing Anisotropy

Data generation: heat equation with $K = \begin{bmatrix} k-\delta & 0 \\ 0 & k+\delta \end{bmatrix}$

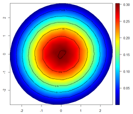
Estimation:

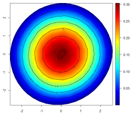
$$J_{\rho,\gamma}(f) = (1-\rho)\frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{m}(z_{ij} - f(\mathbf{p}_i, t_j))^2 + \rho\frac{1}{|\Omega|}\int_T\int_\Omega(\gamma\frac{\partial f}{\partial t} - \Delta f)^2$$

According to δ, ρ properly balances either the adherence to the observations or the PDE penalization.

$\delta = 0$

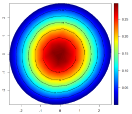
$\hat{\rho} = 0.5685$
$\hat{\gamma} = 0.3064$
$sd(\hat{\gamma}) = 0.0046$
$RMSE = 0.0106$

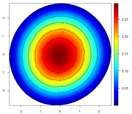




$\delta = 0.01$

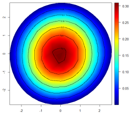
$\hat{\rho} = 0.5685$
$\hat{\gamma} = 0.3064$
$sd(\hat{\gamma}) = 0.0046$
$RMSE = 0.0106$

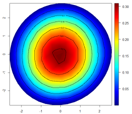




$\delta = 1$

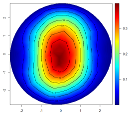
$\hat{\rho} = 0.3299$
$\hat{\gamma} = 0.3149$
$sd(\hat{\gamma}) = 0.0050$
$RMSE = 0.0120$

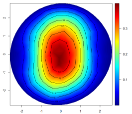




$\delta = 2.95$

$\hat{\rho} = 0.0099$
$\hat{\gamma} = 0.3407$
$sd(\hat{\gamma}) = 0.0047$
$RMSE = 0.0202$





References

[1] E. Arnone, L. Azzimonti, F. Nobile, L. M. Sangalli, Modeling spatially dependent functional data via regression with differential regularization, *Journal of Multivariate Analysis* 170 (2019) 275–295.

[2] L. Azzimonti, F. Nobile, L. M. Sangalli, P. Secchi, Mixed Finite Elements for spatial regression with PDE penalization, *SIAM - ASA Journal on Uncertainty Quantification* (2014), 2 (1), 305-335.

[3] M. S. Bernardi, M. Carey, J. O. Ramsay, L. M. Sangalli, Modeling spatial anisotropy via regression with partial differential regularization, *Journal of Multivariate Analysis* 167 (2018) 15–30.

[4] L. M. Sangalli, Spatial Regression With Partial Differential Equation Regularisation, *International Statistical Review* (2021), 89, 3, 505–531