**The Inverse Problem of Thermometry**

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Consider a square object of unknown material. Implement and test a program that would estimate thermal conductivity of the object from measurements on the boundary.

Assume the object occupies the domain $\Omega = (0;1)^2$ and $\Gamma$ is its boundary. Heat transfer in governed by the equation,

$$\frac{\partial u}{\partial t} - \frac{\partial}{\partial x}\left(\sigma \frac{\partial u}{\partial x}\right) - \frac{\partial}{\partial y}\left(\sigma \frac{\partial u}{\partial y}\right) = f(x,y,t) \qquad (x,y) \in \Omega, \qquad 0 < t < T$$

$$\frac{\partial u}{\partial n} = 0 \ \text{ on } \Gamma \ \ 0 < t < T \tag{1}$$

$$u(x,y) = 0 \ \text{ at } \ t = 0$$

where $u(x,y,t)$ is the temperature, $\sigma(x,y)$ is the thermal conductivity, $f(x,y,t)$ is the external heating source.

Measurement data $d = d(x,y,t)$ is formed of temperature values at points $(x,y)$ along the domain boundary, $\Gamma$, and within the modelling time, $0 < t < T$, Fig. 1, possibly with an additive noise.

Conductivity is estimated by minimizing the functional,

$$L(\sigma) = \int_0^T \int_\Gamma \big(u(x,y,t) - d(x,y,t)\big)^2 \, dl dt + \alpha \int_\Omega (\sigma(x,y) - \sigma_0)^2 \, dx dy \tag{2}$$

with $\sigma(x,y) > 0$ and $u(x,y,t)$ and $\sigma(x,y)$ related via the heat equation (1), $\sigma_0$ is the initial guess for $\sigma(x,y)$, and $\alpha$ is a weight.

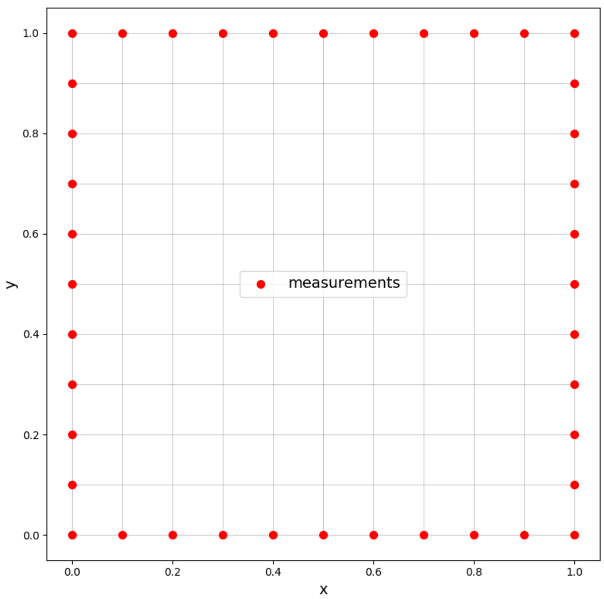


Fig 1. Modelling domain $\Omega$ and measurement points.

**Part 1 – Differentiable forward solver**

Let $M$ be the number of grid cells one direction, then $h = 1/M$ is the grid resolution. Put $x_i = ih,\ y_j = jh$. Similarly, $\tau = T/n$ and $t_k = k\,\tau$.

Denote as $u_{ij}^k$ approximate value of $u(x_i, y_j, t_k)$ and put $\sigma_{ij} = \sigma(x_i, y_j)$, $f_{ij}^k = f(x_i, y_j, t_k)$.

Discretize (1) with explicit the Euler scheme time-stepping scheme combined with the finite-volume method,

$$\frac{u_{ij}^{k+1} - u_{ij}^k}{\tau} + \frac{\sigma_{i+\frac{1}{2}j}\left(u_{ij}^k - u_{i+1\,j}^k\right) + \sigma_{i-\frac{1}{2}\,j}\left(u_{ij}^k - u_{i-1\,j}^k\right)}{h^2} + \frac{\sigma_{i\,j+\frac{1}{2}}\left(u_{ij}^k - u_{i\,j+1}^k\right) + \sigma_{i\,j-\frac{1}{2}}\left(u_{ij}^k - u_{i\,j-1}^k\right)}{h^2} = f_{ij}^k \tag{3}$$

with $\sigma_{i+\frac{1}{2}j}$ denoting the harmonic average of $\sigma_{ij}$ and $\sigma_{i+1j}$ and so on.

Implement (3) in PyTorch or another differentiable framework. **Demonstrate** accuracy of your solver on a test case with known analytical solution for (1), e.g. $u(x, y, t) = (1 - \exp(-t))\cos(\pi x)\cos(\pi y)$ and $\sigma(x, y) = 1$, $h = 0.1$, $T = 1$.

Hint: With this time-stepping, the time step should satisfy for stability limit,

$$\tau \le \frac{h^2}{4\,\sigma_{\max}}.$$

**Part 2 – Optimization**

A discrete dataset $d = (d_{sk})$ should be formed of $m$ values of temperature at several points $(x_s, y_s)$ along the domain boundary and at a sequence of $n$ time points, $t_k$.

Simulate data following (3) with e.g. $\sigma(x, y) = 1 + x + y$, $T = 1$, $h = 0.1$, and for example $f(x, y, t) = \sin(\omega t)$ or other and include 5% noise,

$$d_{sk} = (1 + 0.05\rho\,)u(x_s, y_s, t_k),$$

where $\rho$ is of uniform random distribution ranging from -1 to 1.

The discrete form of (2) is the following,

$$L(\sigma) = h\tau \sum_{k=1}^{n}\sum_{s=1}^{m}\left(u(x_s, y_s, t_k) - d_{ik}\right)^2 + \alpha\, h^2 \sum_{j=1}^{M}\sum_{i=1}^{M}\left(\sigma_{ij} - \sigma_0\right)^2. \tag{4}$$

Starting with $\sigma(x, y) = \sigma_0$ minimize (4) using Adam or another optimizer.

Assuming $\sigma_0 = 2$, **assess** estimated conductivity versus the true one, fitted data versus simulated, functional minimization history.

Consider the impact of the following factors on the quality of the results,

- Source waveform, $\omega$ and other kinds of $f(x, y, t)$.
- Weight $\alpha$.
- transformations of $\sigma$, e.g., $\sigma = \mathrm{a} + \mathrm{b}\tanh(\xi)$.
- Noise level, e.g. 1%, 5%, 10%.