Frequency Domain Estimation of Spatially Varying Parameters in Heat and Mass Transport

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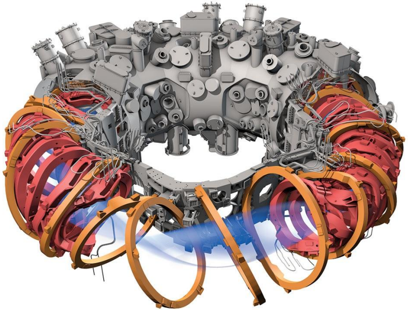
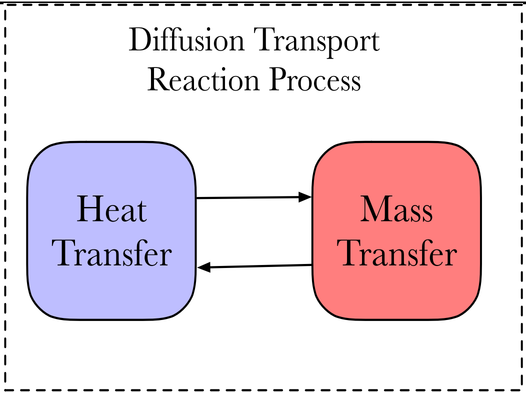
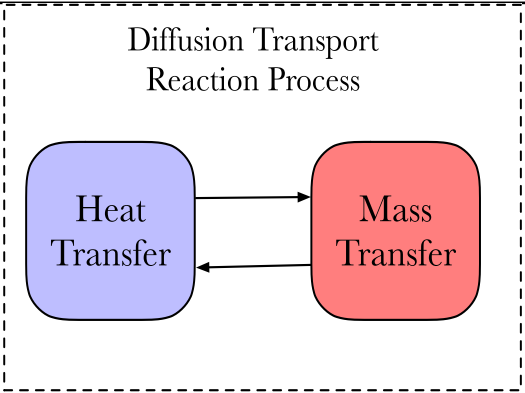



Diffusion Transport
Reaction Process
Heat
Transfer
Mass
Transfer

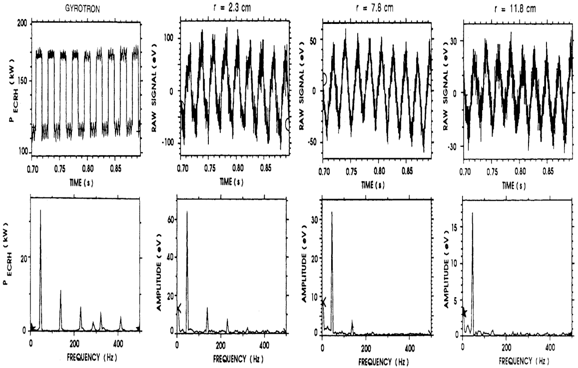


Model Class: Diffusion-Transport-Reaction Equation

$$E(x)\frac{\partial z(x,t)}{\partial t} = D(x)\frac{\partial^2 z(x,t)}{\partial x^2} + U(x)\frac{\partial z(x,t)}{\partial x} + K(x)z(x,t) + P(x)u(t),$$

with suitable boundary conditions

Example: Nuclear Fusion



Giannone, Nuclear Fusion 32 (11), 1992

Few number of harmonics in frequency domain!

Estimating $E(x), D(x), U(x), K(x), P(x)$

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Input $u(t)$

Point-wise outputs $y^m(t) := z(x^1, t), \cdots, z(x^M, t)$

Unknown/free boundary conditions

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Unknown/free boundary conditions

Estimation in time domain is at large solved

Practical Advantages of Frequency Domain

Input signal and output data has same frequency (**important for experiment design**)

Characterization and suppression of noise (**noise model can be incorporated in identification**)

$$\frac{\partial T_e(x,t)}{\partial t} = \chi \frac{\partial^2 T_e(x,t)}{\partial x^2} + P_{ech}(x,t)$$

Alternative Approach: Estimation in Frequency Domain

Practical Advantages of Frequency Domain

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- Characterization and suppression of noise (noise model can be incorporated in identification)

Output Covariance, for frequency points ω_ℓ ($\ell = 1, \ldots, L$)

$$\sigma_y^2(\omega_\ell, \theta) = \sigma_w^2 |H_m(\omega_\ell)|^2 + \sigma_v^2 |G(\omega_\ell, \theta)|^2 |H_e(\omega_\ell)|^2 + \sigma_q^2 |G(\omega_\ell, \theta)|^2$$

$$\theta := \mathrm{col}(E, D, U, K, P)$$

The Basic Idea

Estimation in frequency domain

Estimation in frequency domain

Steps:

1. Find the transfer function from the applied inputs to the sensed outputs
2. Establish an output-error criterion (measured output-modeled output)
3. Minimize the error in least square sense to determine the unknown parameters

Frequency Domain Estimation- Attempt 1

PDE: $E(x)\frac{\partial z(x,t)}{\partial t} = D(x)\frac{\partial^2 z(x,t)}{\partial x^2} + U(x)\frac{\partial z(x,t)}{\partial x} + K(x)z(x,t) + P(x)u(t)$

Applied Input: $u(\omega_\ell),\ \ell \in \{1, \dots, L\}$ can be either sinusoids/block waves

Measured Output: $y^m(\omega_\ell) = z(x^1;\omega_\ell), \dots, z(x^M;\omega_\ell),\ \ell \in \{1, \dots, L\}$

Estimation Problem: $\min_{\theta := col(E;D;U;K;P)} \sum_{\ell=1}^{L} \int_{X^M} | y^m(\omega_\ell) - H(\omega_\ell; x; \theta)\, q(\omega_\ell) |^2 \, dx$

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Computing $H(\omega_\ell; x; \theta)$ for arbitrary boundary conditions and parameter profile is hard!

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Use finite difference

$$\frac{\partial z}{\partial x} \approx \frac{-z(x_{i-1}) + z(x_{i+1})}{2\Delta x} \qquad + \qquad \frac{\partial^2 z}{\partial x^2} \approx \frac{z(x_{i-1}) - 2z(x_i) + z(x_{i+1})}{(\Delta x)^2}$$

State-space model in terms of unknown sparse matrices E, D, U, K, P. Size depends on mesh-grid

$$E\frac{dz}{dt} = \left(DL_D + UL_U + KL_K\right) z + Pu(t)$$

$$L_D = \begin{bmatrix} \ddots & \ddots & & \\ \ddots & \ddots & \ddots & \\ & \ddots & \ddots & \ddots \\ & & \ddots & \ddots \end{bmatrix}, \quad L_U = \begin{bmatrix} \ddots & & \\ \ddots & \ddots & \\ & \ddots & \ddots \\ & & \ddots \end{bmatrix}, \quad L_K = \begin{bmatrix} \ddots & & \\ & \ddots & \\ & & \ddots \\ & & \ddots \end{bmatrix}, E; \; P = \begin{bmatrix} \ddots & & \\ & \ddots & \\ & & \ddots \\ & & \ddots \end{bmatrix}$$

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For large discretization points difficult to estimate $E; D; U; K; P$

B) Parametrizing spatially varying pro le

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We use orthonormal basis functions

$$(x) \quad \sum_{r=1}^{R} B_r(x)\ _r$$

$$E(\ )\underline{z} = A(\ )z + P(\ )u$$

Example: monomials, B-splines etc.

Sparse, A ne parametrization

$$E(\ ) = \sum_{r=1}^{R} {}^{E}_{r} L^{E}_{r}$$

$$A(\ ) = \sum_{r=1}^{R} \left[{}^{D}_{r} L^{D}_{r} + {}^{U}_{r} L^{U}_{r} + {}^{K}_{r} L^{K}_{r} \right]$$

$$P(\ ) = \sum_{r=1}^{R} {}^{P}_{r} P_r$$

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$$P(\;) = \sum_{r=1}^{R} {}^{P}_{r} P_r$$

Number of parameters to be estimated depends on R

C) Boundary conditions are replaced by measurements

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Input vector $q(t)$ consists of $q(t) = \mathrm{col}(u(t); b_{c;1}(t); b_{c;2}(t))$

$b_{c;1}(t); b_{c;2}(t)$ are the real-time measurement about information at (close to) boundary

Inputs: $q(\omega_\ell) = \mathrm{col}\left(u(\omega_\ell), b_{c,1}(\omega_\ell), b_{c,2}(\omega_\ell)\right), \quad \ell \in \{1, \ldots, L\}$

Finite Difference Discretization of PDEs:

$$\begin{aligned} E(\theta)\dot{z} &= A(\theta)z + B(\theta)q \\ y_m &= C^m z \end{aligned}$$

Estimation Problem:

$$\min_{\theta} \sum_{\ell=1}^{L} \sum_{m=2}^{M-1} \frac{1}{w^m w_\ell} \left| y^m(\omega_\ell) - \underbrace{C^m \left(j\omega_\ell E(\theta) - A(\theta)\right)^{-1} B(\theta)}_{G^m(\omega_\ell;\theta)} q(\omega_\ell) \right|^2$$

The sparse and affine structures of $E(\theta), A(\theta)$ play important role

Least Square Estimation Using Levenberg-Marquardt Algorithm

Optimization Problem: $\min V(\ )$

$$V(\ ) := \sum_{`=1}^{L} \sum_{m=2}^{M\ 1} \frac{1}{w^m w_`} \, j\, y^m(!\,`) \quad G^m(!\,`;\ )\, q(!\,`)\, j^2$$

Descent direction: Combination of Gauss-Newton and Gradient-Descent Method

$$(J_k J_k + \ _i I)h_{lm;i} = J_k V(\ _k)$$

Analytic computation of the Jacobian (J_k)

Exploiting sparsity of the matrices, we can speed-up the optimization

Using the Jacobian, we can calculate the uncertainty in the estimation

Uncertainty measure: $Cov(\ _k) \quad Re(2J_k J_k)^{\ 1}$

Results: Using Real Data from Nuclear Fusion Experiments

Input: Block waves with 4 harmonics

Actual Pro le:

$$D^{real}(x) = 5x^3 \quad 0{:}005x + 5$$

Actual Pro le:

$$U^{real}(x) = 15x^2 \quad 0{:}005$$

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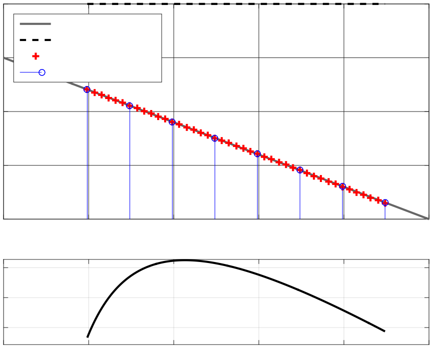

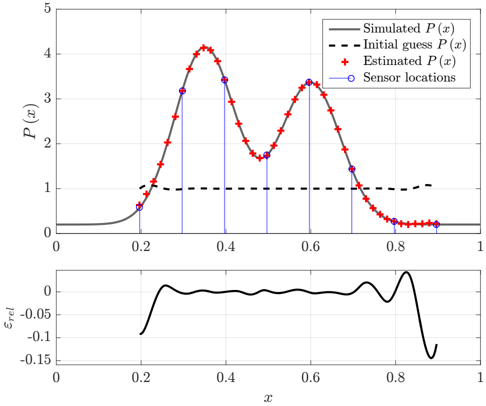

Actual Profile:

$$K^{\text{real}}(x) = -3x$$

Actual Profile:

$$P^{\text{real}}(x) = 0.2 + \frac{7}{\sqrt{\pi}} e^{\frac{-(x-0.35)^2}{(0.1)^2}} + \frac{5.6}{\sqrt{\pi}} e^{\frac{-(x-0.6)^2}{(0.1)^2}}$$

Excitation Signal: Design of Perturbative Experiments

We are using periodic signals

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$$\frac{\partial T_e(x,t)}{\partial t} = \chi \frac{\partial^2 T_e(x,t)}{\partial x^2} + P_{ech}(x,t),$$

$$P_{ech}(x,t) = p(t)\frac{1}{\sigma_w \sqrt{\pi}} \exp\left(-\frac{(x-x_{dep})^2}{\sigma_w^2}\right).$$

Transfer Function:

$$G(\omega,\kappa) = \frac{\Theta(\omega,x_2)}{\Theta(\omega,x_1)} = \exp\left(-\sqrt{\frac{i\omega}{\chi}}\Delta x\right)$$

Use Fisher Information Matrix $F(\theta_0) = \mathrm{E}\left[\left(\frac{\partial \ln(f_z)}{\partial \theta}\right)\left(\frac{\partial \ln(f_z)}{\partial \theta}\right)\right]\Big|_{\theta=\theta_0}$

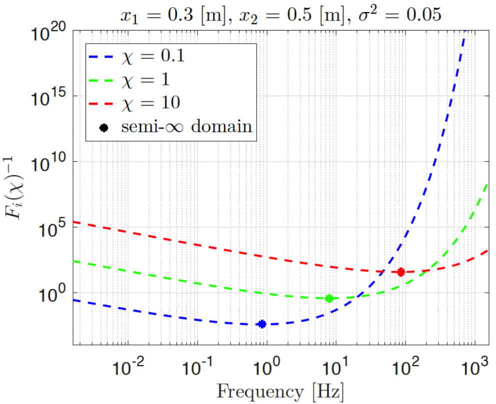
Use Fisher Information Matrix $F(\theta_0) = E\left[\left(\frac{\partial \ln(f_z)}{\partial \theta}\right)\left(\frac{\partial \ln(f_z)}{\partial \theta}\right)^T\right]\Big|_{\theta=\theta_0}$

For one frequency:

$$F(\kappa) = \frac{\Delta x^2}{2\sigma^2\chi^3} \exp\left(-\sqrt{\frac{2\omega}{\chi}}\Delta x\right) |\Theta(\omega, x_1)|^2$$

Upper bound on Modulation Frequency:

$$\omega_{\mathbf{opt}} = \frac{2\chi}{(\Delta x)^2}$$



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* M. van Berkel et.al (2018): "A systematic approach to optimize excitations for perturbative transport experiment"

Exploiting System Identification Tools for Data-Driven Parameter Estimation in PDEs

Conclusion

Basis functions are used to parametrize unknown profile on a discretized domain.

The non-linear least square method uses analytically computed Jacobian.

The unknown boundary conditions are handled by data.

Future work

Handling noisy data for the estimation (Maximum Likelihood Estimation with correlated noise)

Use data find a suitable a basis function (Gaussian regression).

Optimal sensor location (minimizing estimation sensitivity with respect to sensor location).

Thank You!