Point source identification in non-linear advection-diffusion-reaction systems

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Point source identification in non-linear advection-diffusion-reaction systems

1. Problem formulation and identification algorithm
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   - Initial guess
2. Adaptive measurement placement
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   - Sensitivity approach
   - Level set approach
3. Numerical results
   - Source detection with adaptive measurement placement
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4. Conclusions and future work

Motivation

Problem: Identify the locations and intensities of point sources in a chemical system from sparse measurements of concentrations of the species

- Detection of pollutant (hazardous substance) release
- Environmental (atmospheric, marine) and security applications
- Wind and current propagation requires advection modeling
- Dozens of non-linearly reacting chemical species
- Placement of sensors, measurement strategies

Source: http://kaunewsbriefs.blogspot.com, http://crag.org/our-work/water-quality-wetlands/

Forward model

- Parabolic system with n species $\boldsymbol{u}(\boldsymbol{x},t) = (u_1(\boldsymbol{x},t),\ldots,u_n(\boldsymbol{x},t))^T$

$$\boldsymbol{u}_t = \boldsymbol{D}\boldsymbol{\Delta}\boldsymbol{u} - \boldsymbol{w}\cdot\nabla\boldsymbol{u} + \boldsymbol{R}(\boldsymbol{u})\boldsymbol{u} + \boldsymbol{f}, \quad \boldsymbol{x}\in\Omega, \quad t\in[0,T]$$

$$\boldsymbol{u}|_{\Gamma_D} = \boldsymbol{u}_D, \quad \left.\frac{\partial\boldsymbol{u}}{\partial\nu}\right|_{\Gamma_N} = \psi, \quad \partial\Omega = \Gamma_D\cup\Gamma_N, \quad \boldsymbol{u}(\boldsymbol{x},0) = 0$$

- Diffusion and advection terms are linear
- Non-linearity is in the reaction term

$$\boldsymbol{R}(\boldsymbol{u})\boldsymbol{u} = \boldsymbol{L}\boldsymbol{u} + \boldsymbol{Q}(\boldsymbol{u})\boldsymbol{u},$$

- Numerical results are for $\boldsymbol{R}(\boldsymbol{u})$ quadratic in $\boldsymbol{u}$ ($\boldsymbol{Q}(\boldsymbol{u})$ linear in $\boldsymbol{u}$), but stronger non-linearities are possible
- Source term is of the form

$$f_k(\boldsymbol{x},t) = \sum_{j=l_k+1}^{l_{k+1}} a_j h_j(t)\delta(\boldsymbol{x}-\boldsymbol{y}^j), \quad k=1,\ldots,n,$$

point-like in space and either point-like $h_j(t) = \delta(t-\tau_j)$, or step-like $h_j(t) = H(t-\tau_j^{(1)}) - H(t-\tau_j^{(2)})$ in time

Forward problem: existence and uniqueness

- Constructive proofs of existence and uniqueness rely on fixed-point iteration
- Proofs for systems of equations require many technicalities
- Typical result for a scalar elliptic equation

$$Au + R(u) + f(\boldsymbol{x}) = 0, \quad \boldsymbol{x} \in \Omega, \tag{1}$$

  under conditions on the reaction term

$$\frac{\partial R}{\partial u} + \kappa > 0, \quad (\boldsymbol{x}, u) \in \overline{\Omega} \times [m, M], \quad \kappa, m, M > 0.$$

- The iteration

$$(A - \kappa)u^{q+1} = -\left(R(u^q) + f(\boldsymbol{x}) + \kappa u^q\right), \quad q = 0, 1, 2, \dots$$

  has a unique fixed point that is the solution of (1)
- Proof relies on regularity of solutions of elliptic equations, which may be problematic if point sources are present
- Here we assume that $\boldsymbol{u}(\boldsymbol{x}, t) = \lim_{q \to \infty} \boldsymbol{u}^q(\boldsymbol{x}, t)$, where

$$\boldsymbol{u}_t^{q+1} = \left(\boldsymbol{D\Delta} - \boldsymbol{w} \cdot \boldsymbol{\nabla} + \boldsymbol{L} + \boldsymbol{Q}(\boldsymbol{u}^q)\right) \boldsymbol{u}^{q+1} + \boldsymbol{f}, \quad q = 0, 1, \dots$$

Adjoint problem

- The formal adjoint is

$$-\boldsymbol{v}_t = \boldsymbol{D}\Delta\boldsymbol{v} + \boldsymbol{w}\cdot\nabla\boldsymbol{v} + \boldsymbol{L}^T\boldsymbol{v} + \boldsymbol{Q}^T(\boldsymbol{u})\boldsymbol{v} + \boldsymbol{g}.$$

  runs backwards in time from $t = T$ to $t = 0$

- Forward and adjoint solutions satisfy the *adjoint relation*

$$\langle \boldsymbol{f}, \boldsymbol{v}\rangle_{\Omega,T} + c(\boldsymbol{u}, \boldsymbol{v}) = \langle \boldsymbol{g}, \boldsymbol{u}\rangle_{\Omega,T},$$

  where the *correction term* is

$$\begin{aligned} c(\boldsymbol{u}, \boldsymbol{v}) \quad = \quad & -\langle \boldsymbol{u}, \boldsymbol{v}\rangle_{\Omega}\Big|_{t=0}^{t=T} + \langle \boldsymbol{v}, \boldsymbol{D}\nu\cdot\nabla\boldsymbol{u}\rangle_{\partial\Omega,T} - \langle \boldsymbol{u}, \boldsymbol{D}\nu\cdot\nabla\boldsymbol{v}\rangle_{\partial\Omega,T} \\ & - \langle \boldsymbol{u}, (\nabla\cdot\boldsymbol{w})\boldsymbol{v}\rangle_{\Omega,T} + \langle \boldsymbol{u}, (\nu\cdot\boldsymbol{w})\boldsymbol{v}\rangle_{\partial\Omega,T}. \end{aligned}$$

- Choose boundary and initial conditions for $\boldsymbol{v}$ to get $c(\boldsymbol{u}, \boldsymbol{v}) = 0$
- Solve N_m adjoint systems, one for each measurement $\boldsymbol{g}^{(i)}$, $i = 1, \ldots, N_m$

$$\begin{aligned} \text{Instantaneous:} \quad g_j^{(i)}(\boldsymbol{x}, t) &= \delta_{j,m_i}\delta(t-\theta_i)\delta(\boldsymbol{x}-\boldsymbol{z}^i), \quad j = 1, \ldots, n, \\ \text{Time-integrated:} \quad g_j^{(i)}(\boldsymbol{x}, t) &= \delta_{j,m_i}\delta(\boldsymbol{x}-\boldsymbol{z}^i), \quad j = 1, \ldots, n. \end{aligned}$$

Source identification

- The adjoint relation for point sources and sparse measurements is

$$\sum_{k=1}^{n} \sum_{j=l_k+1}^{l_{k+1}} a_j \int_0^T h_j(t) v_k^{(i)}(\boldsymbol{y}^j, t) dt = d_i, \quad i = 1, \ldots, N_m \tag{2}$$

- Unknown intensities a_j and spatial locations $\boldsymbol{y}^j$, also temporal locations τ_j
- Measured **data** is

$$d_i = \left\langle \boldsymbol{g}^{(i)}, \boldsymbol{u} \right\rangle_{\Omega, T}$$

- In matrix-vector form (2) for $\boldsymbol{s}^j = (\boldsymbol{y}^j, \tau_j)$ becomes

$$\boldsymbol{V}(\boldsymbol{s})\boldsymbol{a} = \boldsymbol{d} \tag{3}$$

- **Source identification:** for measured $\boldsymbol{d}$ find $\boldsymbol{s}$, $\boldsymbol{a}$ that solves (3)
- Linear case ($\boldsymbol{Q}(\boldsymbol{u}) \equiv 0$): adjoint solutions $\boldsymbol{v}^{(i)}$ do not depend on (unknown) $\boldsymbol{u}$, so (3) is a system of non-linear algebraic equations
- Non-linear case: $\boldsymbol{V}$ in (3) implicitly depends on $\boldsymbol{u}$

Linear problem

- Optimization formulation
$$\underset{\boldsymbol{a},\boldsymbol{s}}{\text{minimize}} \|\boldsymbol{V}(\boldsymbol{s})\boldsymbol{a} - \boldsymbol{d}\| \tag{4}$$
- Possible approach: discretize $\boldsymbol{s}$ on a grid, allow for sources at every grid point, search for sparse solutions
$$\begin{aligned} \text{minimize} \quad & \|\widetilde{\boldsymbol{a}}\|_0 \\ \text{s.t.} \quad & \widetilde{\boldsymbol{V}}\widetilde{\boldsymbol{a}} = \boldsymbol{d} \end{aligned} \tag{5}$$
- Standard compressed sensing approach: replace 0-norm in (5) with L_1 norm
- L_1 relaxation of (5) only works under some additional assumptions on $\widetilde{\boldsymbol{V}}$ (e.g. restricted isometry property, etc.)
- Heat operator does not satisfy RIP (Li, Osher, Tsai, 2011), application to parabolic problems requires some modifications
- Alternatively, eliminate the intensities
$$\boldsymbol{a} = \left(\boldsymbol{V}^T(\boldsymbol{s})\boldsymbol{V}(\boldsymbol{s})\right)^{-1} \boldsymbol{V}^T(\boldsymbol{s})\boldsymbol{d}$$
- Use the 2-norm in (4), solve the optimization problem
$$\underset{\boldsymbol{s}}{\text{maximize}}\, \boldsymbol{d}^T \boldsymbol{V}(\boldsymbol{s}) \left(\boldsymbol{V}^T(\boldsymbol{s})\boldsymbol{V}(\boldsymbol{s})\right)^{-1} \boldsymbol{V}^T(\boldsymbol{s})\boldsymbol{d}$$

Non-linear problem: forward-adjoint iteration

- How to resolve the implicit dependency of $\boldsymbol{V}$ on $\boldsymbol{u}$?
- Run the forward and the adjoint iterations concurrently

Forward-Adjoint iteration:

1. Obtain an initial guess $\boldsymbol{u}^0$ from

$$\boldsymbol{u}_t^0 = (\boldsymbol{D}\boldsymbol{\Delta} - \boldsymbol{w} \cdot \boldsymbol{\nabla} + \boldsymbol{L})\boldsymbol{u}^0$$

For $q = 1, 2, \ldots$ **do**

2. Solve for the current adjoint solution iterate

$$-\boldsymbol{v}_t^{(i),q} = (\boldsymbol{D}\boldsymbol{\Delta} + \boldsymbol{w} \cdot \boldsymbol{\nabla} + \boldsymbol{L}^T + \boldsymbol{Q}^T(\boldsymbol{u}^{q-1}))\boldsymbol{v}^{(i),q} + \boldsymbol{g}^{(i)}, \quad i = 1, \ldots, N_m$$

3. Solve the optimization problem for the source location iterate

$$\boldsymbol{s}^q = \operatorname{argmax} \boldsymbol{d}^T \boldsymbol{V}(\boldsymbol{s}) \left(\boldsymbol{V}^T(\boldsymbol{s}) \boldsymbol{V}(\boldsymbol{s}) \right)^{-1} \boldsymbol{V}^T(\boldsymbol{s}) \boldsymbol{d}$$

   and compute the source term iterate $\boldsymbol{f}^q$.

4. Update the forward solution iterate by solving

$$\boldsymbol{u}_t^q = (\boldsymbol{D}\boldsymbol{\Delta} - \boldsymbol{w} \cdot \boldsymbol{\nabla} + \boldsymbol{L} + \boldsymbol{Q}(\boldsymbol{u}^{q-1}))\boldsymbol{u}^q + \boldsymbol{f}^q$$

Forward-adjoint iteration

- Mimics the behavior of the fixed point iteration for forward problem
- Convergence analysis complicated by the coupling to a non-linear optimization problem in step 3
- What method to use to solve the optimization problem in step 3?
- The most computationally expensive part is the solution of multiple adjoint problems in step 2
- Optimization in step 3 is cheap in comparison, derivative-free search methods can be employed
- Convergence of optimization in step 3 can provide the stopping criterion for the forward-adjoint iteration
- Premature termination of the forward-adjoint iteration yields an accurate estimate for $\boldsymbol{s}$ (less accurate for $\boldsymbol{a}$) and saves computational effort
- How to choose an initial guess for $\boldsymbol{s}$?

Derivative-free search

Derivative-free search: Proceeds by exploring the slices of the objective along the location parameters or one particular source at a time. No differentiation of $\boldsymbol{V}$ is needed. Somewhat more global than derivative-based approaches.

1. Choose an initial guess for $\boldsymbol{s}$.

For $p = 1, 2, \ldots$ **do**

For $j = 1, \ldots, N_s$ **do**

2. Freeze all the components $\boldsymbol{s}^k$ of $\boldsymbol{s}$ for $k \neq j$ and compute the objective

$$J(\boldsymbol{s}) = \boldsymbol{d}^T \boldsymbol{V}(\boldsymbol{s}) \left(\boldsymbol{V}^T(\boldsymbol{s}) \boldsymbol{V}(\boldsymbol{s}) \right)^{-1} \boldsymbol{V}^T(\boldsymbol{s}) \boldsymbol{d}$$

for all possible values of $\boldsymbol{s}^j \in \Omega \times [0, T]$.

3. Update the location of the j^{th} source

$$\boldsymbol{s}^j = \underset{\boldsymbol{r} \in \Omega \times [0,T]}{\operatorname{argmax}} J(\boldsymbol{s}^1, \ldots, \boldsymbol{s}^{j-1}, \boldsymbol{r}, \boldsymbol{s}^{j+1}, \ldots, \boldsymbol{s}^{N_s}).$$

4. If for all $j = 1, \ldots, N_s$ the changes in step 3 are small compared to iteration $p - 1$ then stop.

Initial guess for source locations

Initial guess for $\boldsymbol{s}$: provides a systematic way of obtaining an initial guess. Works good in practice. Prior information may be used instead if available.

1. Given the initial guess $\boldsymbol{u}^0$ from step 1 of the forward-adjoint iteration solve

$$-\boldsymbol{v}_t^{(i)} = (\boldsymbol{D}\boldsymbol{\Delta} + \boldsymbol{w} \cdot \nabla + \boldsymbol{L}^T + \boldsymbol{Q}^T(\boldsymbol{u}^0))\boldsymbol{v}^{(i)} + \boldsymbol{g}^{(i)}, \quad i = 1, \dots, N_m$$

   and assemble $\boldsymbol{V}$ assuming that there is only one source present. Thus $\boldsymbol{V}$ has only one column and depends on $\boldsymbol{s}^1$ only and so does the objective J.

2. Compute the estimate of the first source location as

$$\boldsymbol{s}^1 = \underset{\boldsymbol{r} \in \Omega \times [0,T]}{\text{argmax}} \; J(\boldsymbol{r})$$

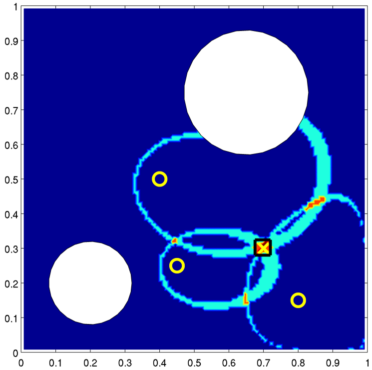
For $k = 2, \dots, N_s$ **do**

3. Assemble $\boldsymbol{V}$ assuming that there are k sources present. Freeze the locations of previously determined sources $\boldsymbol{s}^j$, $j = 1, \dots, k-1$ so that J only depends on $\boldsymbol{s}^k$.

4. Compute the estimate of the k^{th} source location as

$$\boldsymbol{s}^k = \underset{\boldsymbol{r} \in \Omega \times [0,T]}{\text{argmax}} \; J(\boldsymbol{s}^1, \dots, \boldsymbol{s}^{k-1}, \boldsymbol{r})$$

Measurement placement

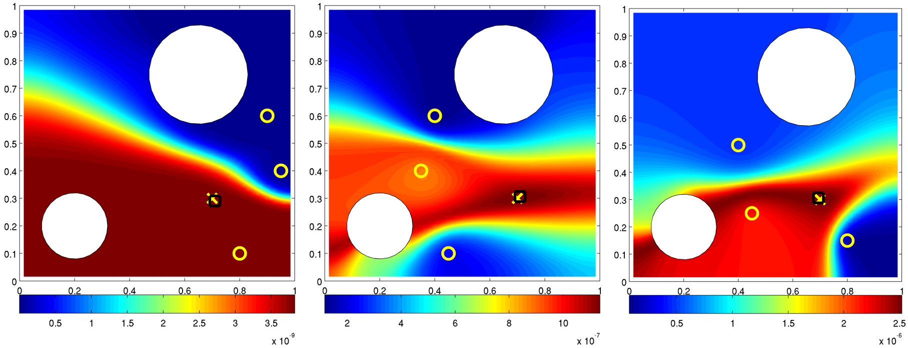


Example: source identification with known intensity $\boldsymbol{V}(\boldsymbol{y}) = \boldsymbol{d}/\boldsymbol{a}$. Source position is an intersection of (d_i/a)-level sets of $v^{(i)}$.

- Measurement placement aspects:
  1. Initial, before measuring anything
  2. Adding more measurements adaptively based on existing data
- Case of one source: in the presence of diffusion three measurements anywhere are enough, but more stable if measured nearby
- Initial placement should aim for **coverage** - uniform sampling of the whole domain
- Adding measurements adaptively based on current estimates of source locations should aim for
  1. **Refinement**: adding measurements near discovered sources
  2. **Separation**: adding measurements between discovered sources

Measurements and advection

When refining, advection should be taken into account:



Upwind Downwind Mixed

Imaging functional $J(\boldsymbol{y}^1)$ for one time-independent source (yellow $\times$) and three measurements (yellow $\bigcirc$). The "wind" blows from right to left. Estimated source location (from noiseless data) is black $\square$.

Geometrical adaptive measurement placement

Spatial adaptive measurement placement in case of time-independent sources:

1. Start with an existing estimate of source locations $\boldsymbol{y}$.
2. Choose a trust radius ρ_T (e.g. based on noise level) and a reference simplex $\boldsymbol{T}$ with vertices $\boldsymbol{T}^k$, $k = 1, \ldots, d+1$. The orientation of the reference simplex is such that one vertex lies upwind and d vertices lie downwind from its center.

For $j = 1, \ldots, N_s$ **do**

3. Place the center of the reference simplex at $\boldsymbol{y}^j$.

   For $k = 1, \ldots, d+1$ **do**

4. Place a new measurement in the direction of the vertex $\boldsymbol{T}^k$ at a distance

$$\rho = \min\left(\rho_T, \kappa_\Omega \operatorname{dist}\left(\boldsymbol{y}^j, \partial\Omega\right), \kappa_{\boldsymbol{y}} \operatorname{dist}\left(\boldsymbol{y}^j, \left\{\boldsymbol{y}^i \mid i \neq j\right\}\right)\right)$$

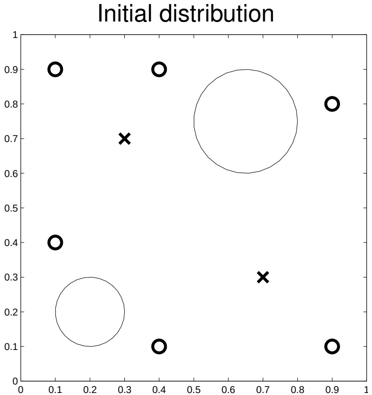
   away from $\boldsymbol{y}^j$, where $\kappa_\Omega, \kappa_{\boldsymbol{y}} \in (0,1)$ determine proximity to $\partial\Omega$ and other sources.

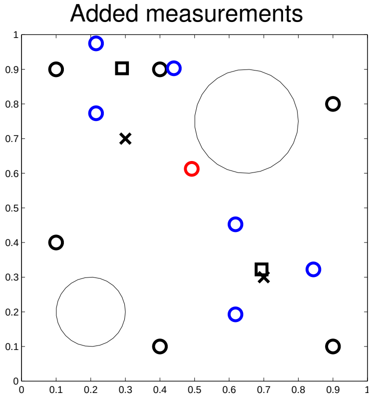
   For $i = 1, \ldots, j-1$ **do**

5. Place a new measurement between $\boldsymbol{y}^j$ and $\boldsymbol{y}^i$.

Geometrical measurement placement: example

Example with $N_s = 2$ sources and $N_m = 6$ initial measurements.





True sources $\times$, initial measurements $\bigcirc$. Estimated sources from 6 measurements $\square$.

Refinement measurements: adjusted copies of reference simplex $\boldsymbol{T}$ are blue $\bigcirc$.

Separation measurement: in between the source estimates is red $\bigcirc$.

Analytical approach: sensitivity analysis

- Geometrical adaptive measurement placement assumes additional measurements are cheap (thus redundancy)
- Sensitivity argument can be used to search for an optimal position of one extra measurement
- Compute the sensitivity using the algorithm:
  1. For a trial measurement $\boldsymbol{z} \in \Omega$ solve
  $$-\boldsymbol{v}_t^{\boldsymbol{z}} = (\boldsymbol{D\Delta} + \boldsymbol{w} \cdot \nabla + \boldsymbol{L}^T + \boldsymbol{Q}^T(\boldsymbol{u}^q))\boldsymbol{v}^{\boldsymbol{z}} + \boldsymbol{g}^{\boldsymbol{z}},$$
  linearized around the last estimate $\boldsymbol{u}^q$ of the forward-adjoint iteration.
  2. "Measure" $d^{\boldsymbol{z}} = \langle \boldsymbol{g}^{\boldsymbol{z}}, \boldsymbol{u}^q \rangle$ and perturb it to obtain
  $$\widetilde{\boldsymbol{V}} = \begin{bmatrix} \boldsymbol{V} \\ \boldsymbol{v}^{\boldsymbol{z}} \end{bmatrix}, \quad \widetilde{d} = \begin{bmatrix} \boldsymbol{d} \\ d^{\boldsymbol{z}} + \epsilon^{\boldsymbol{z}} \end{bmatrix}, \quad \widetilde{J}(\boldsymbol{s}) = \widetilde{\boldsymbol{d}}^T \widetilde{\boldsymbol{V}}(\boldsymbol{s}) \left(\widetilde{\boldsymbol{V}}^T(\boldsymbol{s}) \widetilde{\boldsymbol{V}}(\boldsymbol{s}) \right)^{-1} \widetilde{\boldsymbol{V}}^T(\boldsymbol{s}) \widetilde{\boldsymbol{d}}$$
  3. Solve for the perturbed source estimate $\widetilde{\boldsymbol{s}} = \text{argmax}\ \widetilde{\boldsymbol{J}}(\boldsymbol{s})$
  4. Compute the sensitivity $\sigma(\boldsymbol{z}) = \|\boldsymbol{s}^q - \widetilde{\boldsymbol{s}}\|$
- Place a new measurement where $\sigma(\boldsymbol{z})$ has maximum
- Computationally expensive

Alternative analytical approach: level sets

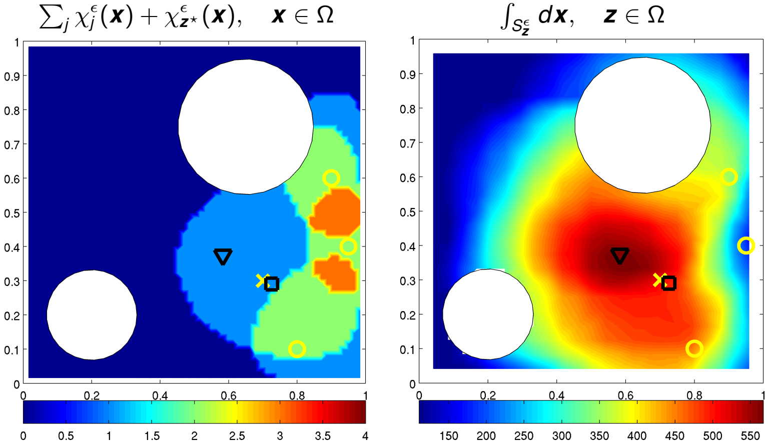
- Combines the geometrical reasoning of the first approach with the analytical structure of the sensitivity approach
- No repeated inversion required

Level set adaptive measurement placement algorithm:

1. For a trial measurement $\boldsymbol{z} \in \Omega$ solve
$$-\boldsymbol{v}_t^{\boldsymbol{z}} = (\boldsymbol{D}\boldsymbol{\Delta} + \boldsymbol{w} \cdot \nabla + \boldsymbol{L}^T + \boldsymbol{Q}^T(\boldsymbol{u}^q))\boldsymbol{v}^{\boldsymbol{z}} + \boldsymbol{g}^{\boldsymbol{z}},$$
linearized around the last estimate $\boldsymbol{u}^q$ of the forward-adjoint iteration.
2. Select the confidence signal level ϵ that can be measured stably
3. Define the indicator functions of ϵ-level sets
$$\chi_{\boldsymbol{z}}^{\epsilon}(\boldsymbol{x}) = \begin{cases} 1, & \boldsymbol{v}^{\boldsymbol{z}}(\boldsymbol{x}) \geq \epsilon \\ 0, & \boldsymbol{v}^{\boldsymbol{z}}(\boldsymbol{x}) < \epsilon \end{cases}, \quad \boldsymbol{x} \in \Omega$$
4. Compute the set
$$S_{\boldsymbol{z}}^{\epsilon} = \{\boldsymbol{x} \in \Omega \mid \textstyle\sum_j \chi_j^{\epsilon}(\boldsymbol{x}) + \chi_{\boldsymbol{z}}^{\epsilon}(\boldsymbol{x}) \geq 2\}$$
5. The new measurement $\boldsymbol{z}^\star$ is a solution of a constrained optimization problem
$$\boldsymbol{z}^\star = \underset{\text{s.t. } \chi_{\boldsymbol{z}}^{\epsilon}(\boldsymbol{y}^{(q)})=1}{\text{argmax}} \int_{S_{\boldsymbol{z}}^{\epsilon}} d\boldsymbol{x}$$

Level sets: example

Single source $\times$ with three upwind measurements $\bigcirc$. Left: sum of level set functions. Right: level set optimization objective for adaptive measurement placement. Source estimate $\boldsymbol{y}^{(q)}$ is $\square$, new measurement location $\boldsymbol{z}^\star$ is $\bigtriangledown$.



Three component chemical system

- We consider a simple, but somewhat realistic chemical system
- Three species (NO, NO_2, O_3) based on Chapman's cycle

$$\begin{aligned} NO + O_3 &\xrightarrow{k_1} NO_2 \\ NO_2 &\xrightarrow{k_2} NO + O_3 \end{aligned}$$

- Reaction rates are $k_1 = 1000$, $k_2 = 2000$, diffusion coefficients of order one, highly non-linear stiff system
- Source emits NO_2, concentrations of NO are measured
- Advection $\boldsymbol{w}$ is modeled via advection potential ϕ

$$\boldsymbol{w} = \nabla\phi, \quad \Delta\phi = 0, \quad \text{in } \Omega$$

- A **preferred** advection direction $\boldsymbol{w}_0$ is enforced via Neumann condition on the outer boundary

$$\frac{\partial\phi}{\partial\nu} = \boldsymbol{w}_0 \cdot \nu$$

- Non-penetrating boundary conditions are enforced on obstacle boundaries

$$\frac{\partial\phi}{\partial\nu} = 0$$

Numerical examples: setup

- Examples in 2D, but the method works in 3D without any modifications
- Finite difference solver in space
- Exponential integrator in time

$$\xi_t = \boldsymbol{E}(t)\xi + \zeta(t)$$

$$\xi^{(k+1)} = \exp\left(\boldsymbol{E}^{(k)} h_k\right)\left(\left(\boldsymbol{E}^{(k)}\right)^{-1}\zeta^{(k)} + \xi^{(k)}\right) - \left(\boldsymbol{E}^{(k)}\right)^{-1}\zeta^{(k)}$$

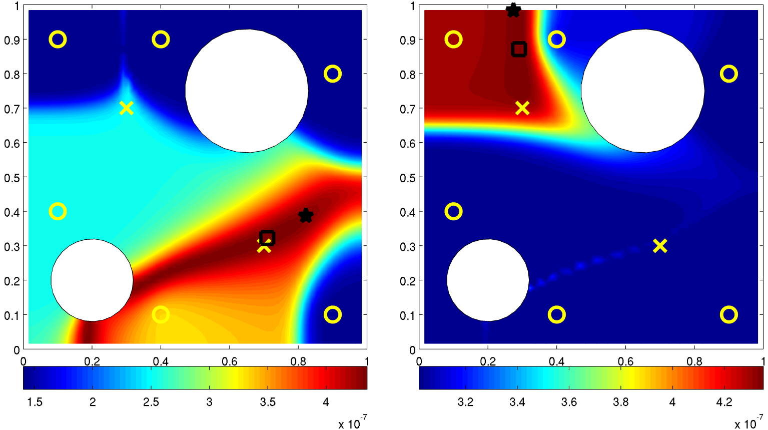
- Action of matrix exponential computed with an efficient algorithm (Al-Mohy, Higham, SISC'2011)
- Adaptive time-stepping for time-dependent source case
- Noise model

$$\boldsymbol{d}^* = (\boldsymbol{I} + \sigma \boldsymbol{N})\boldsymbol{d}, \quad \boldsymbol{N} = \operatorname{diag}\left(X_1, \ldots, X_{N_m}\right),$$

  with zero-mean Gaussian X_j, noise level σ
- Different grids for data simulation and inversion to avoid inverse crime
- Systematic errors even in the absence of noise ($\sigma = 0$)

Two sources: initial recovery

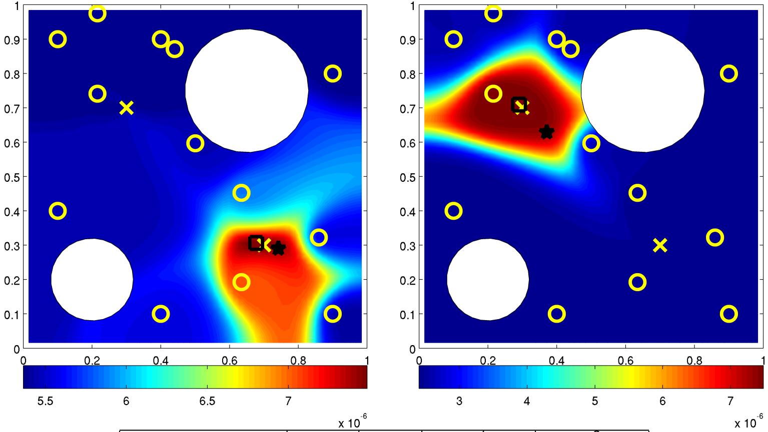
Identifying $N_s = 2$ sources with $N_m = 6$ measurements, 5% noise. Slices of the optimization functional J around the solution $(\boldsymbol{y}^1, \boldsymbol{y}^2)$. True sources $\times$, measurements $\bigcirc$, estimated sources $\square$, initial guess $\bigstar$. Left: $J(\boldsymbol{r}, \boldsymbol{y}^2)$; right: $J(\boldsymbol{y}^1, \boldsymbol{r})$, $\boldsymbol{r} \in \Omega$.



Source parameters	a_1	a_2	$\boldsymbol{y}^1$	$\boldsymbol{y}^2$
True	10.00	7.00	(0.70, 0.30)	(0.30, 0.70)
Recovered	13.37	2.27	(0.70, 0.32)	(0.29, 0.87)

Two sources: adaptively added measurements

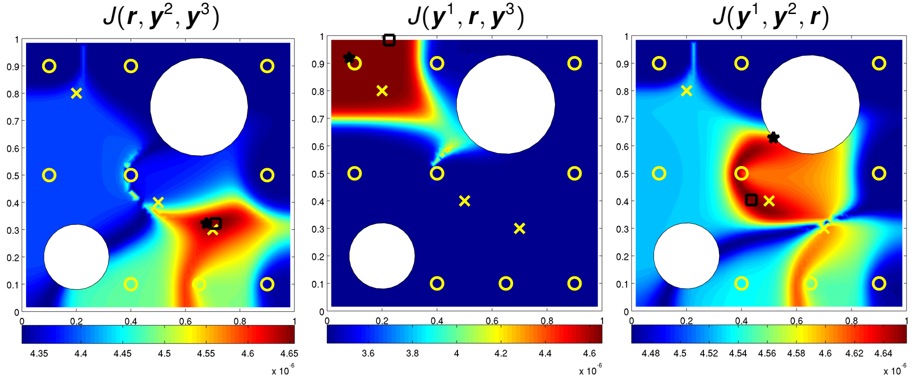
Identifying $N_s = 2$ sources with $N_m = 13$ measurements, 5% noise. Slices of the optimization functional J around the solution $(\boldsymbol{y}^1, \boldsymbol{y}^2)$. True sources $\times$, measurements $\bigcirc$, estimated sources $\square$, initial guess $\bigstar$. Left: $J(\boldsymbol{r}, \boldsymbol{y}^2)$; right: $J(\boldsymbol{y}^1, \boldsymbol{r})$, $\boldsymbol{r} \in \Omega$.



Source parameters	a_1	a_2	$\boldsymbol{y}^1$	$\boldsymbol{y}^2$
True	10.00	7.00	(0.70, 0.30)	(0.30, 0.70)
Recovered	9.62	6.44	(0.67, 0.30)	(0.29, 0.70)

Three sources: initial recovery

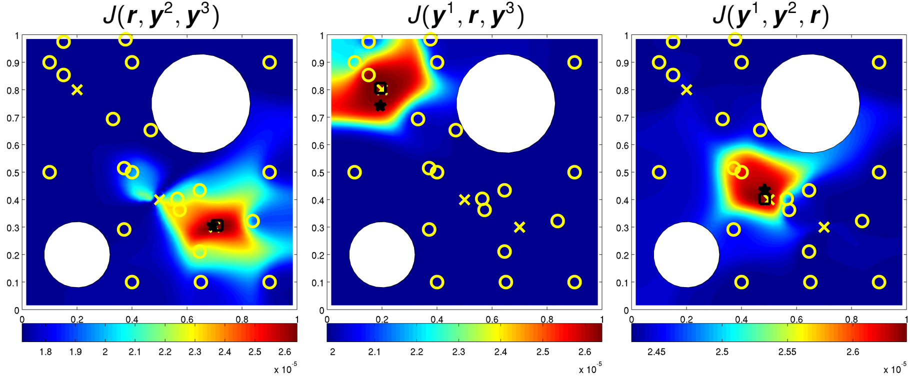
Identifying $N_s = 3$ sources with $N_m = 9$ measurements, 5% noise. Slices of the optimization functional J around the solution $(\boldsymbol{y}^1, \boldsymbol{y}^2, \boldsymbol{y}^3)$. True sources $\times$, measurements $\bigcirc$, estimated sources $\square$, initial guess $\bigstar$.



Parameters	a_1	a_2	a_3	$\boldsymbol{y}^1$	$\boldsymbol{y}^2$	$\boldsymbol{y}^3$
True	10.00	7.00	5.00	(0.70, 0.30)	(0.20, 0.80)	(0.50, 0.40)
Recovered	13.06	21.42	4.22	(0.70, 0.32)	(0.22, 0.98)	(0.43, 0.40)

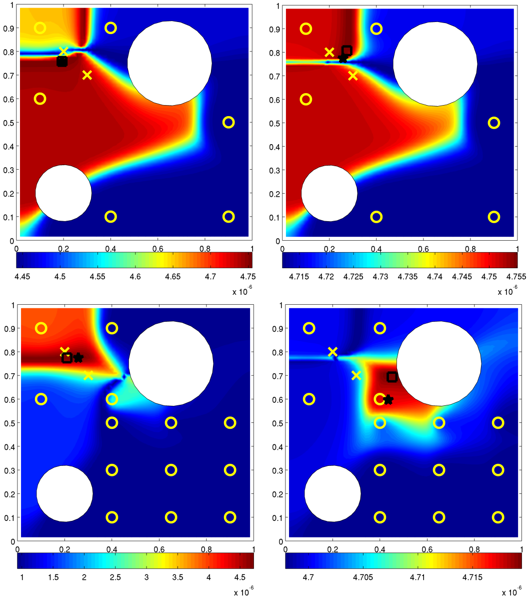
Three sources: adaptively added measurements

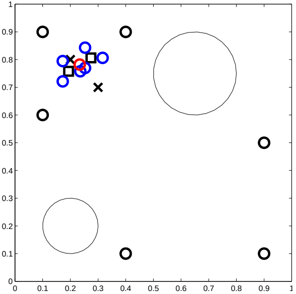
Identifying $N_s = 3$ sources with $N_m = 21$ measurements, 5% noise. Slices of the optimization functional J around the solution $(\boldsymbol{y}^1, \boldsymbol{y}^2, \boldsymbol{y}^3)$. True sources $\times$, measurements $\bigcirc$, estimated sources $\square$, initial guess $\bigstar$.



Parameters	a_1	a_2	a_3	$\boldsymbol{y}^1$	$\boldsymbol{y}^2$	$\boldsymbol{y}^3$
True	10.00	7.00	5.00	(0.70, 0.30)	(0.20, 0.80)	(0.50, 0.40)
Recovered	9.35	7.26	5.31	(0.70, 0.30)	(0.19, 0.80)	(0.48, 0.40)

Adaptive vs. prior placement of measurements

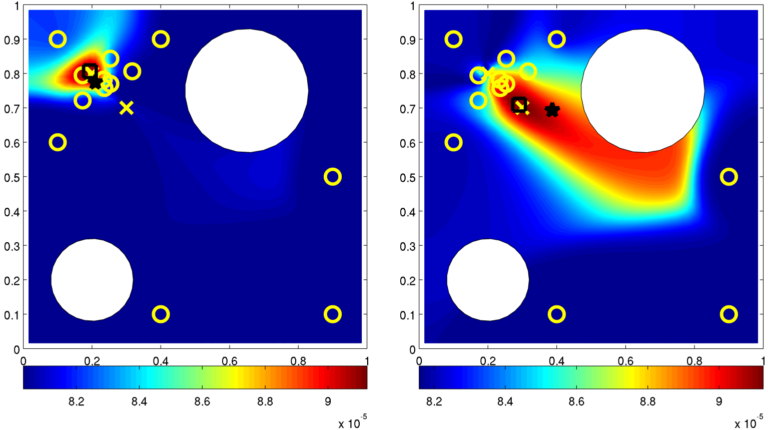




Comparing identification of $N_s = 2$ sources (5% noise).
Top row: $N_m = 6$ and adaptively added measurements for a total of $N_m = 13$.
Bottom row: uniform distribution of $N_m = 13$ measurements for maximum prior coverage.

Adaptive vs. prior placement of measurements

Identification of $N_s = 2$ sources with $N_m = 6 + 7$ adaptively placed measurements, 5% noise. Slices of the optimization functional J around the solution $(\boldsymbol{y}^1, \boldsymbol{y}^2)$. True sources $\times$, measurements $\bigcirc$, estimated sources $\square$, initial guess $\bigstar$.



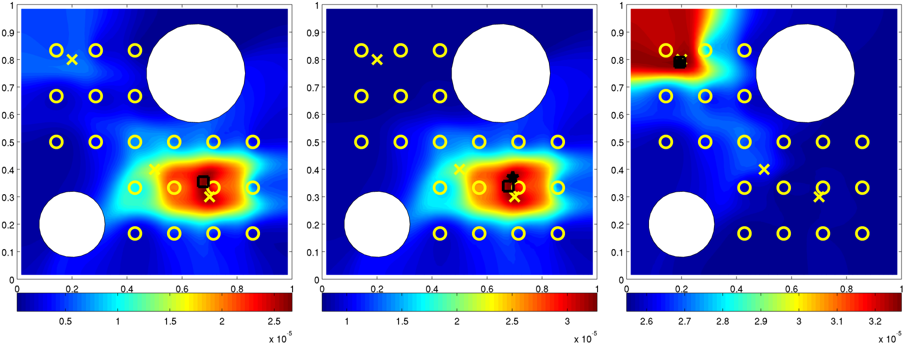
Source parameters	a_1	a_2	$\boldsymbol{y}^1$	$\boldsymbol{y}^2$
True	10.00	7.00	(0.20, 0.80)	(0.30, 0.70)
Recovered	9.46	7.76	(0.19, 0.80)	(0.29, 0.70)

Unknown number of sources

Determining an unknown number of sources:

For $N_s^* = 1, 2, \dots$

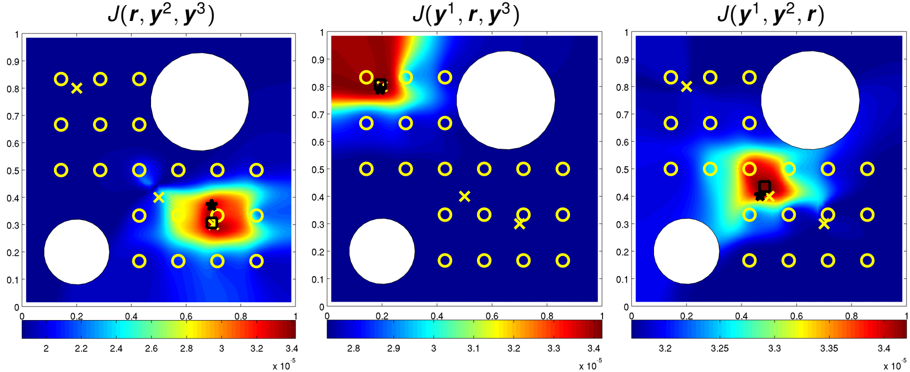
1. Recover N_s^* sources
2. If any $a_j < 0$ then let $N_s = N_s^* - 1$ and quit



Identifying $N_s^* = 1$ (left) and $N_s^* = 2$ (middle and right) sources from $N_m = 20$ fixed measurements, 5% noise. Slices of the optimization functional J around the solution $(\mathbf{y}^1, \dots, \mathbf{y}^{N_s^*})$. True sources $\times$, measurements $\bigcirc$, estimated sources $\Box$, initial guess $\bigstar$.

Unknown number of sources

Identifying $N_s^* = N_s = 3$ sources from $N_m = 20$ fixed measurements, 5% noise. Slices of the optimization functional J around the solution $(\boldsymbol{y}^1, \boldsymbol{y}^2, \boldsymbol{y}^3)$. True sources $\times$, measurements $\bigcirc$, estimated sources $\square$, initial guess $\bigstar$.

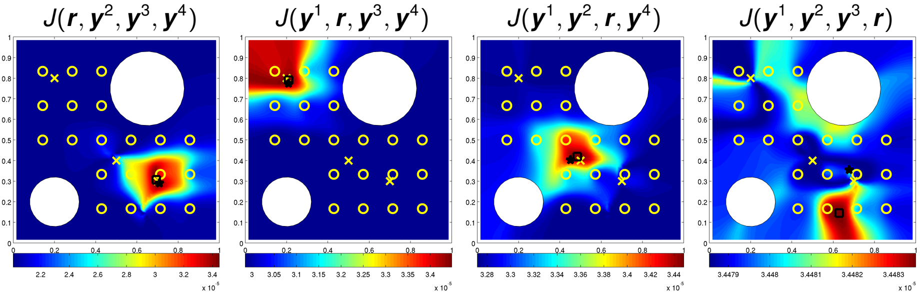


Possible appearances of spurious sources when $N_s^* > N_s$:

1. Small negative intensity (best case possible, easy to detect)
2. Large negative intensity next to a true source (cancellation of intensities)
3. Small positive intensity (may be hard depending on the intensities of true sources)

Unknown number of sources

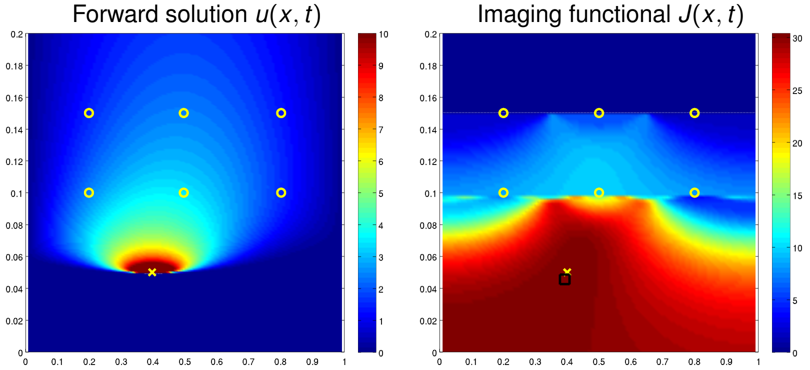
Identifying $N_s^* = 4$ sources from $N_m = 20$ fixed measurements, 5% noise. Slices of the optimization functional J around the solution $(\boldsymbol{y}^1, \boldsymbol{y}^2, \boldsymbol{y}^3, \boldsymbol{y}^4)$. True sources $\times$, measurements $\bigcirc$, estimated sources $\square$, initial guess $\bigstar$.



Case	a_1	a_2	a_3	a_4	$\boldsymbol{y}^1$	$\boldsymbol{y}^2$	$\boldsymbol{y}^3$	$\boldsymbol{y}^4$
True $N_s = 3$	10.00	7.00	5.00	–	(0.70, 0.30)	(0.20, 0.80)	(0.50, 0.40)	–
$N_s^* = 1$	12.29	–	–	–	(0.67, 0.35)	–	–	–
$N_s^* = 2$	12.12	8.13	–	–	(0.67, 0.33)	(0.19, 0.79)	–	–
$N_s^* = 3$	10.44	6.83	4.44	–	(0.69, 0.30)	(0.19, 0.80)	(0.48, 0.43)	–
$N_s^* = 4$	11.30	6.42	4.12	-0.17	(0.69, 0.30)	(0.20, 0.79)	(0.48, 0.41)	(0.62, 0.14)

Time-dependent source: 1D

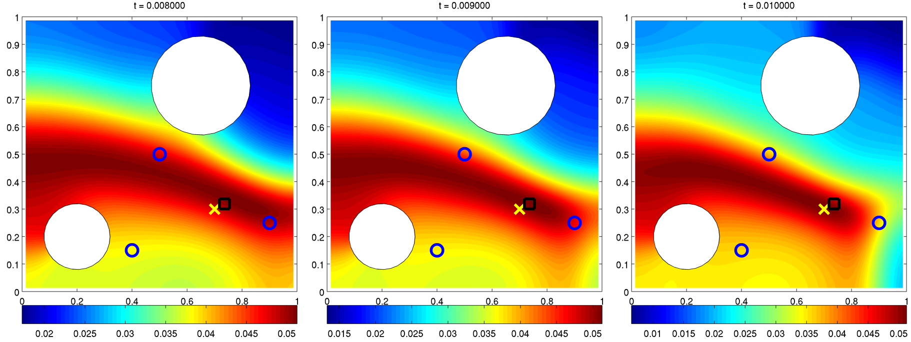
Identifying a source $f(x,t) = a\delta(t-\tau)\delta(x-y)$ in 1D scalar non-linear equation from $N_m = 6$ measurements, three measurements at two time instants $\theta = 0.1,\ 0.15$, $T = 0.2$, 1% noise. Reduced stability compared to time-independent sources and time-integrated measurements. True source $\times$, measurements $\bigcirc$, estimated source $\square$.



Source Parameters	a	y	τ
True	3.000	0.400	0.050
Recovered	3.178	0.392	0.045

Time-dependent source: 2D

Both source and measurements are point in space and time. Identification of a single source from $N_m = 6$ measurements, two groups of three at times $\theta = 0.015,\ 0.020$, $T = 0.03$. Adaptive time stepping to resolve the source/measurement singularity, reduced non-linearity for stability. Spatial locations: true source $\times$, measurements $\bigcirc$, estimated source $\square$. Slices of $J(\boldsymbol{y}, t)$, $\boldsymbol{y} \in \Omega$ at three time instants.



Source Parameters	a	$\boldsymbol{y}$	τ
True	10.00	(0.70, 0.30)	0.010
Recovered	11.18	(0.73, 0.31)	0.009

Conclusions and future work

Conclusions:

- Method for identification of point sources in non-linear parabolic systems from sparse measurements
- Strategy for adaptive measurement placement
- Identifying unknown numbers of sources
- Numerical evidence of good performance

Future work:

- Convergence analysis
- Partial knowledge of the domain and obstacles
- Sensitivity with respect to system parameters (diffusion coefficients, reaction rates, advection term)

Preprint: *Point source identification in non-linear advection-diffusion-reaction systems*. A.V. Mamonov and Y.-H. R. Tsai, arXiv:1202.2373 [math-ph]