A model reduction approach to numerical inversion for parabolic partial differential equations

Liliana Borcea[1]
Alexander V. Mamonov[2], Vladimir Druskin[3], Mikhail Zaslavsky[3]

[1]University of Michigan, Ann Arbor
[2]University of Houston
[3]Schlumberger Doll Research, Boston

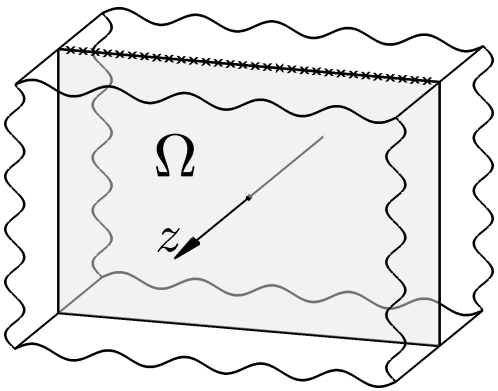
Controlled Source Electromagnetics

Inverse problem: determine underground resistivity $r(\mathbf{x})$ from measurements of the magnetic field $\mathbf{H}(t, \mathbf{x})$ at the surface.

Model: diffusion Maxwell system (negligible displacement current)

$$-\nabla \times \Big[r(\mathbf{x}) \nabla \times \mathbf{H}(\mathbf{x}, t) \Big] = \partial_t \mathbf{H}(\mathbf{x}, t)$$

Setup: $\mathbf{x} = (x, z)$, $\quad r := r(x)$ for $x \in \Omega \subset \mathbb{R}^n$, simply connected with boundary $\mathcal{B} = \mathcal{B}_A \cup \mathcal{B}_I$.



- Measurements are on accessible $\mathcal{B}_A$.
- Polarization $\mathbf{H}(\mathbf{x}, t) = u(x, t)\mathbf{e}_z$ and the boundary conditions $\mathbf{n} \cdot \nabla u(\cdot, t)\Big|_{\mathcal{B}_A} = 0$ and $u(\cdot, t)\Big|_{\mathcal{B}_I} = 0$.
- Excitation is in initial conditions and measurements are $u(\cdot, t)\Big|_{\mathcal{B}_A}$

Generic parabolic problem

$$\partial_t u(x,t) = \nabla \cdot (r(x)\nabla u(x,t)), \quad x \in \Omega, \quad t > 0$$

- Boundary conditions $u(\cdot,t)|_{\mathcal{B}_I} = 0, \quad \mathbf{n} \cdot \nabla u(\cdot,t)\Big|_{\mathcal{B}_A} = 0.$
- Initial conditions $u(x,0) = u_o(x)$ supported on $\mathcal{B}_A$.
- The sources/receivers are on $\mathcal{B}_A$ and give knowledge of the measurement operator

$$\mathcal{M}(u_o) = u(x,t)\Big|_{\mathcal{B}_A} \quad \text{for all } u_o \text{ supported in } \mathcal{B}_A \text{ and } t > 0.$$

Inverse problem is to find $r(x)$ given $\mathcal{M}$.

Model reduction

- The measurement operator $\mathcal{M}$ is nonlinear in the unknown $r(x)$, but it depends linearly on the initial conditions u_o.
- Suffices to consider integral kernel of mapping from u_o to $\mathcal{M}(u_o)$.

  In 1-D we have $\Omega = [0, 1]$, with $\mathcal{B}_A = \{0\}$ and $\mathcal{B}_I = \{1\}$ and

  $$u(0, t) = u_o \mathcal{M}(\delta(x)) \text{ with scalar response } y(t) := \mathcal{M}(\delta).$$

  In 2-D $\mathcal{B}_A$ is a line segment and $y_{ij}(t) := \mathcal{M}(\delta(x_j))\Big|_{x_i}, \; x_i, x_j \in \mathcal{B}_A$.
- Laplace transform of $y(t)$ is the transfer function of the system.
- Reduced model $\rightsquigarrow$ rational interpolation of transfer function.

Model reduction motivation

- Benefit for forward problem:
  - Reduced model is small (fast computations) and yet approximates well the transfer function.
  - We may relate the model to a finite difference spatial discretization of the PDE on a special grid, with few points.
- Benefit for inversion:
  - The nonlinear map $\mathcal{R}$ from the function space of the unknown resistivity $r(x)$ to the low-dimensional space of the discrete resistivities may be used to precondition the inversion.
  - We can adapt the size of the reduced model to the noise level (regularization) so we get a natural stability-resolution trade-off.

1-D case. Semi-discrete case (for simplicity).

- Discretize $\Omega = [0, 1]$ on a fine grid with spacing $h = \frac{1}{N+1}$

$$\partial_t \mathbf{u}(t) = A(\mathbf{r})\mathbf{u}(t), \quad \mathbf{u}(0) = \frac{1}{h}\mathbf{e}_1$$

Differential operator $\nabla \cdot (r\nabla)$ is replaced by the matrix

$$A(\mathbf{r}) = -D^T \mathrm{diag}(\mathbf{r}) D, \quad \mathbf{r} \in \mathbb{R}_+^N$$

- Inverse problem: given $y(t; \mathbf{r}) = \mathbf{e}_1^T \mathbf{u}(t)$ find $\mathbf{r} \in \mathbb{R}_+^N$.

Forward model reduction: we know $\mathbf{r}$ and seek a reduced model that approximates y.

Inverse model reduction: obtain a reduced model from y, then find $\mathbf{r}$ which has this reduced model.

Model reduction

- Transfer function of full model $A(\mathbf{r}) \in \mathbb{R}^{N\times N}$, $\mathbf{b} \in \mathbb{R}^N$

$$G(s;\mathbf{r}) = \int_0^\infty dt\, y(t;\mathbf{r})e^{-st} = \mathbf{b}^T(sI - A(\mathbf{r}))^{-1}\mathbf{b}, \quad s > 0, \quad \mathbf{b} = \frac{\mathbf{e}_1}{\sqrt{h}}$$

- Reduced model $(A_m, \mathbf{b}_m)$ with $A_m \in \mathbb{R}^{m\times m}$, $\mathbf{b}_m \in \mathbb{R}^m$ and $m \ll N$

$$G_m(s) = \mathbf{b}_m^T(sI_m - A_m)^{-1}\mathbf{b}_m = \sum_{j=1}^{m} \frac{c_j}{s+\theta_j}$$

with $-\theta_j =$ eigenvalues of A_m, and $c_j = (\mathbf{b}_m^T\mathbf{z}_j)^2$, where $\mathbf{z}_j =$ normalized eigenvectors.

- Rational interpolation $\partial_s^k G_m(\sigma_j) = \partial_s^k G(\sigma_j)$ at nodes $\sigma_j \in [0, +\infty)$, for $j = 1, \ldots, \ell$, $k = 0, \ldots, 2M_j - 1$ and $m = \sum_{j=1}^{\ell} M_j$.

Projection-based model reduction

- Grimme 1997 showed that interpolation is equivalent to projection-based model reduction:

$$A_m = V^T A V \in \mathbb{R}^{m\times m}, \qquad \mathbf{b}_m = V^T \mathbf{b} \in \mathbb{R}^m,$$

$V \in \mathbb{R}^{N\times m}$ has orthonormal columns spanning rational Krylov space

$$\mathcal{K}_m(\boldsymbol{\sigma}) = \text{span}\left\{(\sigma_j I - A)^{-k}\mathbf{b} \mid j = 1,\ldots,\ell;\ k = 1,\ldots,M_j\right\}$$

- The choice of the points σ_j matter as we shall see!

Connection to finite differences

- The matrix A_m is dense in general, so how do we connect the reduced model to a finite difference scheme?
- We have the (Stieltjes) continued fraction representation

$$G_m(s) = \cfrac{1}{\widehat{\kappa}_1 s + \cfrac{1}{\kappa_1 + \cfrac{1}{\ddots + \cfrac{1}{\widehat{\kappa}_m s + \cfrac{1}{\kappa_m}}}}}$$

- $G_m(s) = W_1(s)$ the response of second-order difference scheme

$$\frac{1}{\widehat{\kappa}_j}\left(\frac{W_{j+1} - W_j}{\kappa_j} - \frac{W_j - W_{j-1}}{\kappa_{j-1}}\right) - sW_j = 0, \qquad j = 1, \ldots, m$$

where $r(x)$ is encoded in $\{\kappa_j, \widehat{\kappa}_j\}$.

Optimization formulation

- Data is $d(t) = y(t; \mathbf{r}^{\text{true}}) + \mathcal{N}(t)$ where $\mathcal{N}(t) =$ noise and discretization error.
- Reconstruction is $\mathbf{r}^\star = \arg\min_{\mathbf{r} \in \mathbb{R}^N_+} \frac{1}{2} \|\mathcal{Q}(d(t)) - \mathcal{Q}(y(t; \mathbf{r}))|_2^2$
- Instead of minimizing misfit between $d(t)$ and $y(t; \mathbf{r}) = [\mathcal{F}(\mathbf{r})](t)$, where $\mathcal{F}$ is the forward map, we work with $\mathcal{R}(\mathbf{r}) = \mathcal{Q} \circ \mathcal{F}(\mathbf{r})$ where $\mathcal{Q}$ is used as a preconditioner.
- We seek $\mathbf{r}$ that gives the reduced model calculated for the measurements $d(t)$.

The map $\mathcal{R}(\mathbf{r}) = \mathcal{Q}(y(\cdot;\mathbf{r})) = \mathcal{Q} \circ \mathcal{F}(\mathbf{r})$.

$$\mathcal{R}: \ \mathbf{r} \overset{(a)}{\to} A(\mathbf{r}) \overset{(b)}{\to} V \overset{(c)}{\to} A_m \overset{(d)}{\to} \{(c_j, \theta_j)\}_{j=1}^m \overset{(e)}{\to} \{(\log \kappa_j, \log \widehat{\kappa}_j)\}_{j=1}^m$$

(a) is definition $A(r) = -D^T \mathrm{diag}(\mathbf{r}) D$.

(b) is calculation of orthonormal basis of rational Krylov subspace $\rightsquigarrow$ projection matrix V.

(c) is definition $A_m = V^T A(\mathbf{r}) V$ and $\mathbf{b}_m = V^T \mathbf{b}$.

(d) here $-\theta_m$ are the eigenvalues of A_m and $c_j = (\mathbf{b}_m^T \mathbf{z}_j)^2$, where $\mathbf{z}_j$ are the eigenvectors.

(e) Conversion of rational interpolant to continued fraction (Lanczos) and then logarithm of the coefficients.

Here all the steps are stable!

The chain of mappings in $\mathcal{Q}(d(t)$

$$\mathcal{Q} \,:\, d(t) \overset{\text{(a)}}{\to} G(s) \overset{\text{(b)}}{\to} G_m(s) \overset{\text{(c)}}{\to} \{(c_j, \theta_j)\}_{j=1}^m \overset{\text{(d)}}{\to} \{(\log \kappa_j, \log \widehat{\kappa}_j)\}_{j=1}^m.$$

(a) is Laplace transform of measured data.

(b) is rational (Padé) interpolation . This is the only ill-conditioned step and we regularize by reducing m until we get positive continued fraction coefficients.

(c) Calculate the poles $-\theta_j$ and residues c_j of the rational $G_m(s)$.

(d) Calculate the continued fraction coefficients (Lanczos iteration).

The map $\mathcal{R}(r) = \mathcal{Q} \circ \mathcal{F}(r)$ and discrete resistivities

- Change coordinates $x \to \xi$ so that $r^{1/2}\partial_x = \partial_\xi$ and $w(\xi, s) =$ Laplace transform of $u(x, t)$ satisfies

$$r^{-1/2}\partial_\xi(r^{1/2}\partial_\xi w) - sw = 0$$

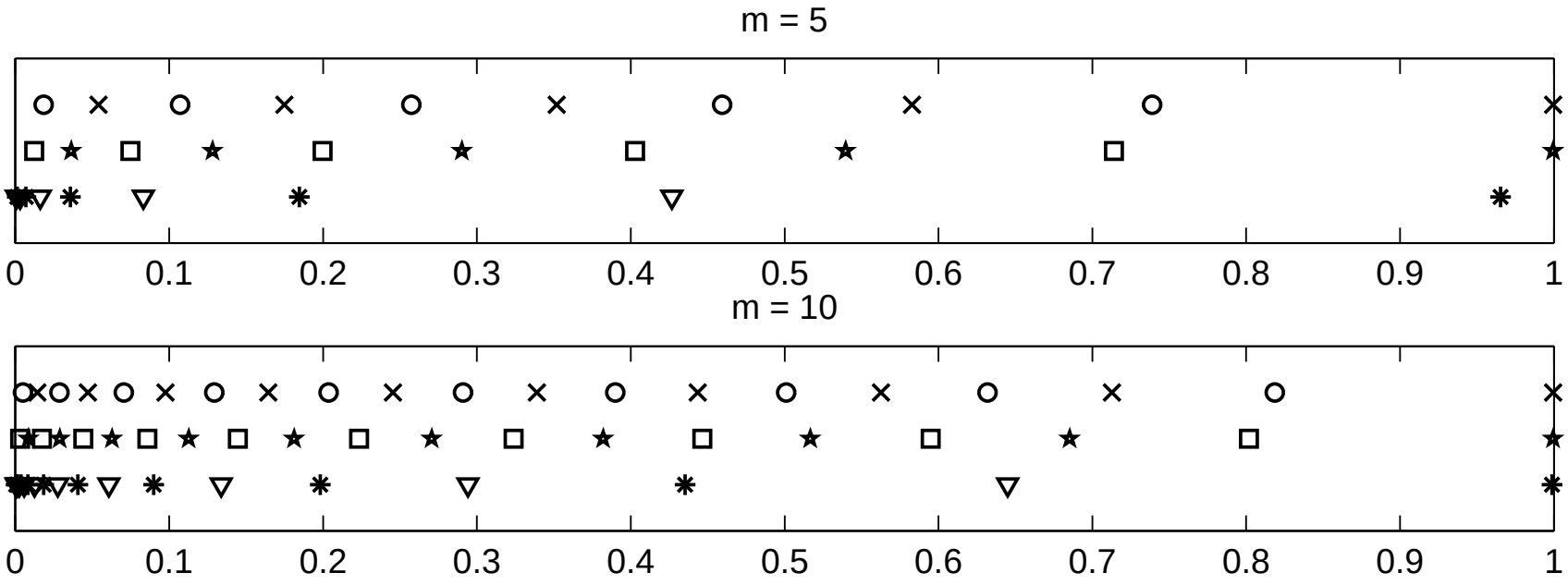
- Reduced model corresponds to

$$\frac{1}{\widehat{\kappa}_j}\left(\frac{W_{j+1} - W_j}{\kappa_j} - \frac{W_j - W_{j-1}}{\kappa_{j-1}}\right) - sW_j = 0 \ldots, m$$

- The discrete resistivity is defined by $\widehat{\kappa}_j^2$ and κ_j^{-2} up to scaling by mesh steps, which we do not need to know. In the optimization we work with the log of $\widehat{\kappa}_j$ and κ_j, so grid factors cancel out.

- $\mathcal{R}$ takes r to the (log of) discrete resistivities. If we interpolated these grid values in Ω, we would expect that $\mathcal{R}(r)$ would be close to the identity for smooth r i.e., $\mathcal{Q}$ is like inverse of $\mathcal{F}$.

Optimal grids calculated from $\widehat{\kappa}_j^o$ and κ_j^o for $r^o \equiv 1$



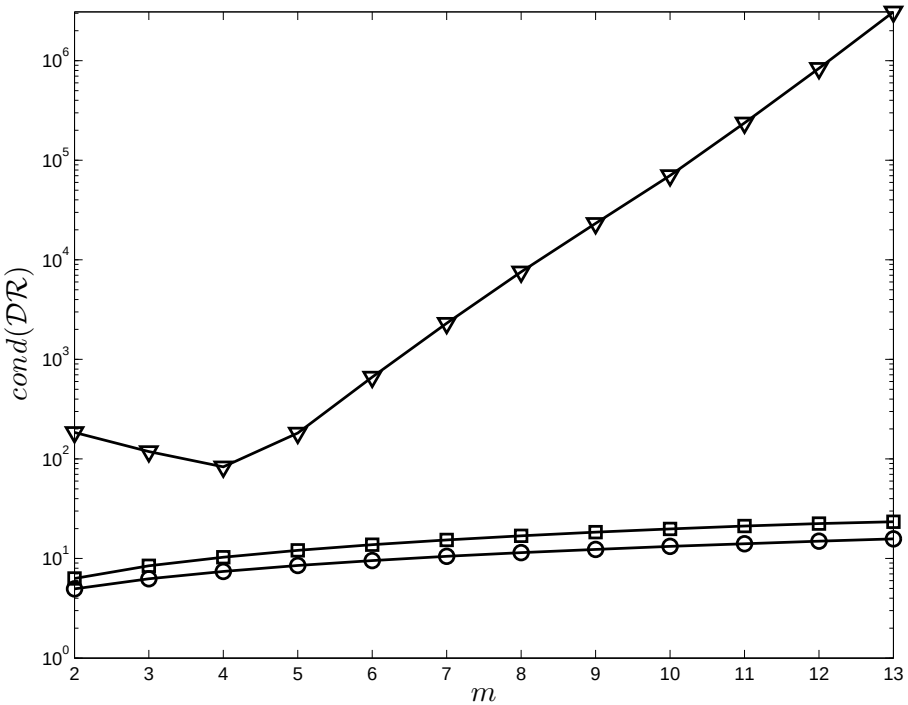
Compare three choices of matching conditions:

$(\circ, \times)$ Moment matching at zero, $\mathcal{K}_m(0) = \text{span}\left\{A^{-1}\mathbf{b}, A^{-2}\mathbf{b}, \ldots, A^{-m}\mathbf{b}\right\}$

$(\square, \star)$ Interpolation $\mathcal{K}_m(\boldsymbol{\sigma}) = \text{span}\left\{(\sigma_j I - A)^{-1}\mathbf{b} \mid j = 1, \ldots, m\right\}$ at geometrically spaced nodes $\sigma_j = \sigma_1 \left(1 + 12/m\right)^{j-1}$

$(*, \bigtriangledown)$ Interpolation at faster growing nodes $\boldsymbol{\sigma}^\star$

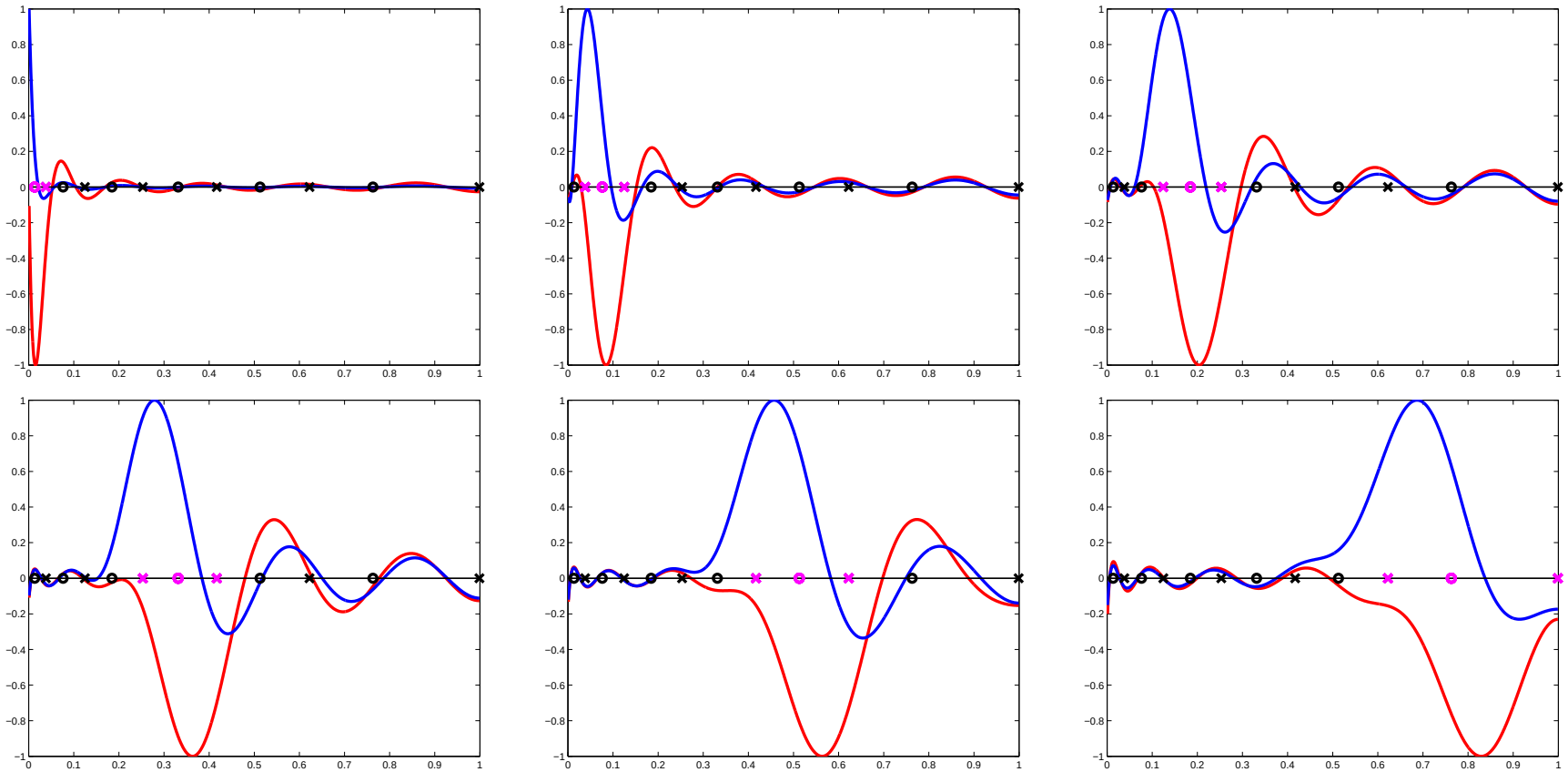
Conditioning of the Jacobian $\mathcal{DR}$



Rows $\left(\frac{\partial \kappa_1}{\partial r_k}\right)_{k=1}^{N}$ and $\left(\frac{\partial \widehat{\kappa}_1}{\partial r_k}\right)_{k=1}^{N}$ are almost collinear when grid points get too close $\rightsquigarrow$ poor conditioning.

Condition number growth for moment matching at zero ($\circ$), interpolation at $\boldsymbol{\sigma}$ ($\square$), interpolation at $\boldsymbol{\sigma}^\star$ ($\bigtriangledown$)

Sensitivity functions $\frac{\partial \widehat{\kappa}_k}{\partial r}$ (blue) and $\frac{\partial \kappa_k}{\partial r}$ (red)



$k = 1, \ldots m = 6$ from left to right, top to bottom

Reconstruction

- We solve $\min_{\mathbf{r}} \|\mathcal{Q}(d(\,\cdot\,)) - \mathcal{R}(\mathbf{r})\|_2$ with Gauss-Newton iteration.
- Jacobian $\mathcal{DR} \in \mathbb{R}^{2m\times N}$ has a **large null space** $2m \ll N$. At each iteration the Gauss-Newton update is in the $2m$ dimensional range of the pseudoinverse $\mathcal{DR}^\dagger$.
- We can improve results with prior info, by adding correction $\delta\mathbf{r}$ that minimizes regularization term $\mathcal{P}(\mathbf{r}+\delta\mathbf{r})$ over $\delta\mathbf{r} \in \text{null}(\mathcal{DR})$.

  E.g. weighted discrete H^1 seminorm $\mathcal{P}(\mathbf{r}) = \frac{1}{2}\|\mathcal{W}^{1/2}D\mathbf{r}\|_2^2$.

Numerical experiments: 1D setup

- Synthetic noisy data

$$d_j = y(t_j; \mathbf{r}^{\text{true}}) + \mathcal{N}(t_j), \quad j = 1, \ldots, N_T$$

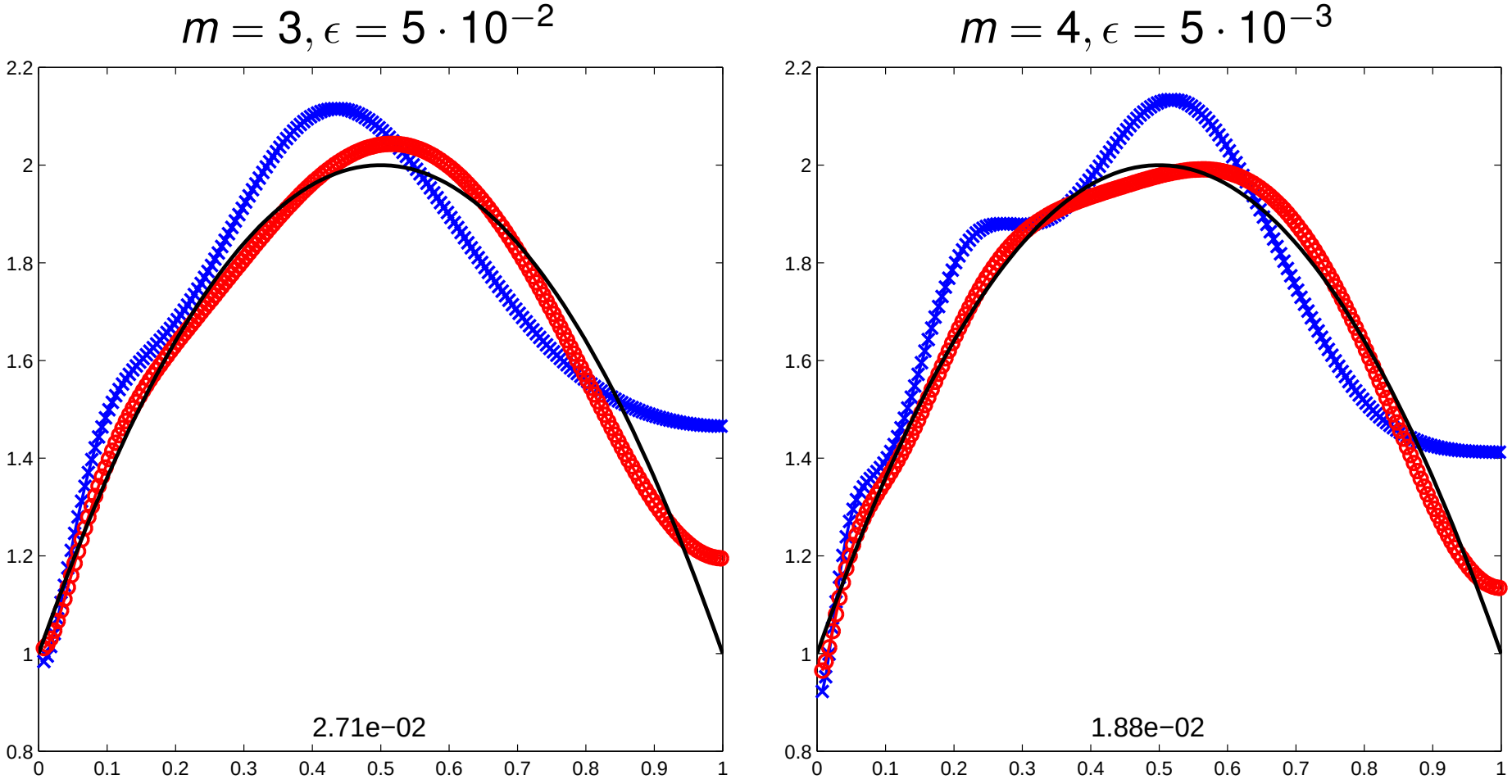
- Noise model $\mathcal{N} = \epsilon\, \text{diag}(\chi_1, \ldots, \chi_{N_T})\mathbf{y}$, with independent χ_k Gaussian mean zero, variance 1.

- Reduced model size m chosen based on noise level ϵ

m	3	4
ϵ	$5 \cdot 10^{-2}$	$5 \cdot 10^{-3}$

- Initial guess $\mathbf{r}^1 \equiv \mathbf{1}$, five Gauss-Newton iterations $n_{GN} = 5$.

Numerical results: smooth resistivity

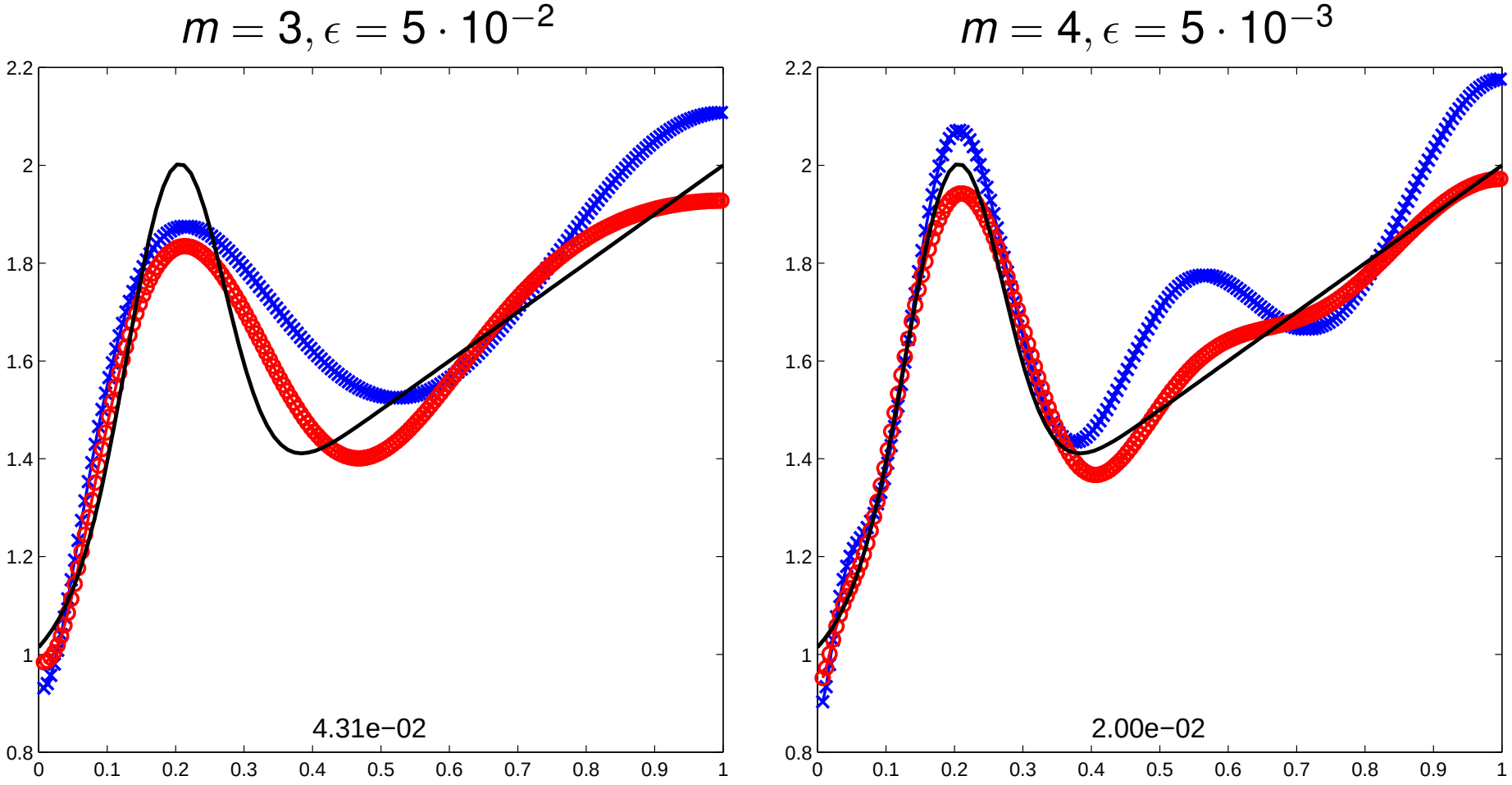


– True resistivity $\mathbf{r}^{\text{true}}$ (quadratic)

× Reconstruction $\mathbf{r}^{(2)}$ after one Gauss-Newton iteration

○ Reconstruction $\mathbf{r}^{(6)}$ after five Gauss-Newton iterations

Numerical results: smooth resistivity

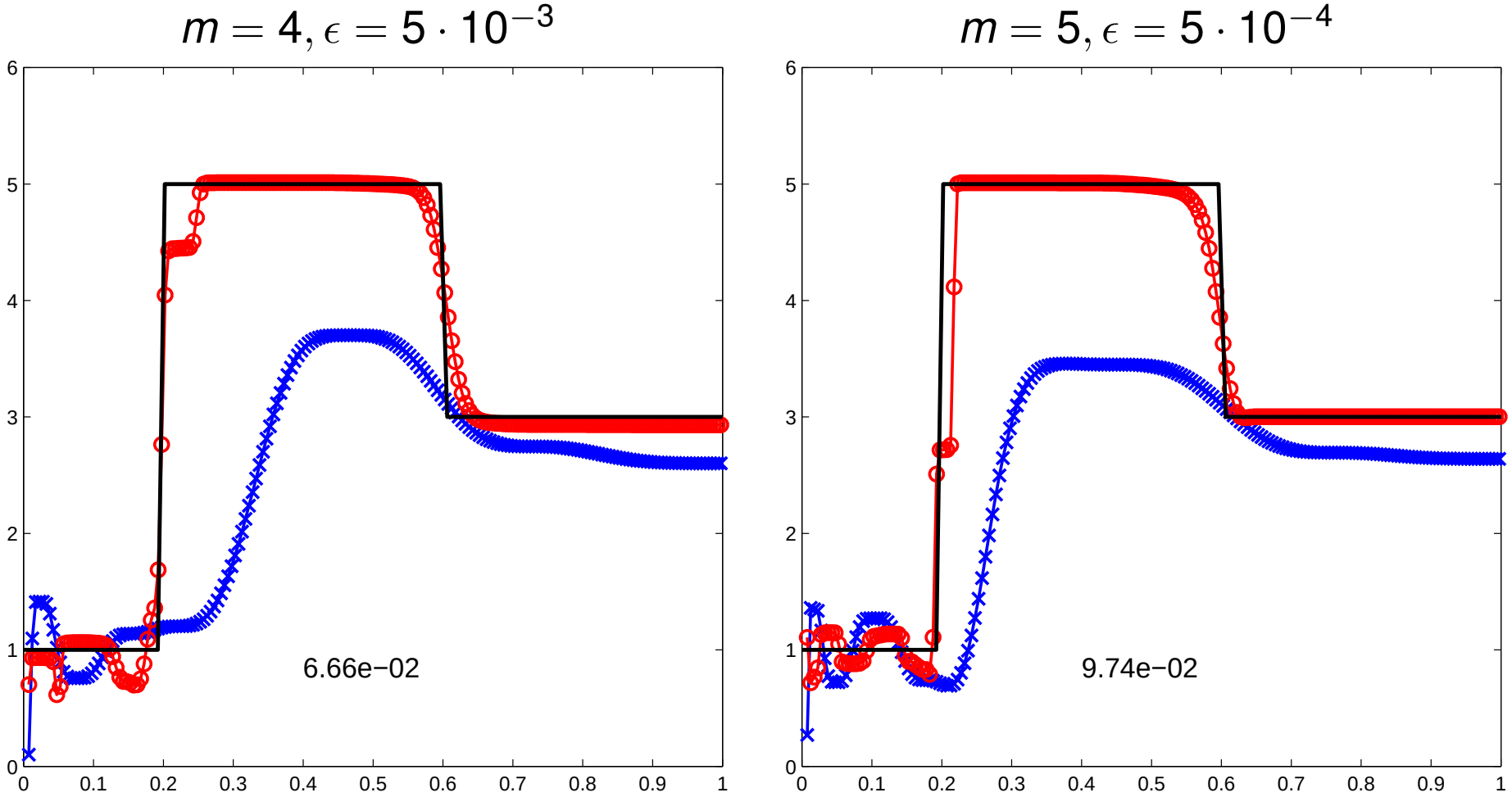


– True resistivity $\mathbf{r}^{\text{true}}$ (linear + Gaussian)

× Reconstruction $\mathbf{r}^{(2)}$ after one Gauss-Newton iteration

○ Reconstruction $\mathbf{r}^{(6)}$ after five Gauss-Newton iterations

Numerical results: piecewise constant resistivity



– True resistivity $\mathbf{r}^{\text{true}}$ (jump of contrast 2)

× Reconstruction $\mathbf{r}^{(2)}$ after one Gauss-Newton iteration

○ Reconstruction $\mathbf{r}^{(6)}$ after five Gauss-Newton iterations

Philosophy

- 1-D problem is formally determined: 1D unknown $r(x)$ and 1D data $y(t)$.
- 2-D problem is **overdetermined**: 2D unknown $r(x)$ but 3D data $y_{ij}(t)$, where (i, j) are source-detector pairs.
- We proceed as in 1-D and construct separately reduced models (i.e., maps $\mathcal{R}_{ij}$) for data subsets indexed by $i, j = 1, \ldots, N_d$.
- The maps $\mathcal{R}_{ij}$ are coupled by their dependence on the same $r(x)$ and are all used in inversion.

Semi-discretization on fine grid with N points

- For the $j-$ source in $\mathcal{B}_A$ (a line on the surface) we have

$$\partial_t \mathbf{u}^{(j)}(t) = A(\mathbf{r})\mathbf{u}^{(j)}(t), \qquad \mathbf{u}^{(j)}(0) = \mathbf{b}^{(j)}.$$

- The response matrix $y_{ij}(t)$ is the restriction of the solution $\mathbf{u}^{(j)}(t) = e^{A(\mathbf{r})t}\mathbf{b}^{(j)}$ to the support of the $i-$th receiver

$$y_{ij}(t) = \mathbf{b}^{(i)^T} e^{A(\mathbf{r})t}\mathbf{b}^{(j)}.$$

  Its Laplace transform is the transfer function $G^{(ij)}(s)$.

- The reduced model is $(A_m^{(ij)}, \mathbf{b}_m^{(ij)})$ and its transfer function is

$$G_m^{(ij)}(s) = \mathbf{b}_m^{(i)^T} \left(sI_m - A_m^{(ij)}\right)^{-1} \mathbf{b}_m^{(j)} = \sum_{q=1}^{m} \frac{c_q^{(ij)}}{s + \theta_q^{(ij)}}$$

Model reduction

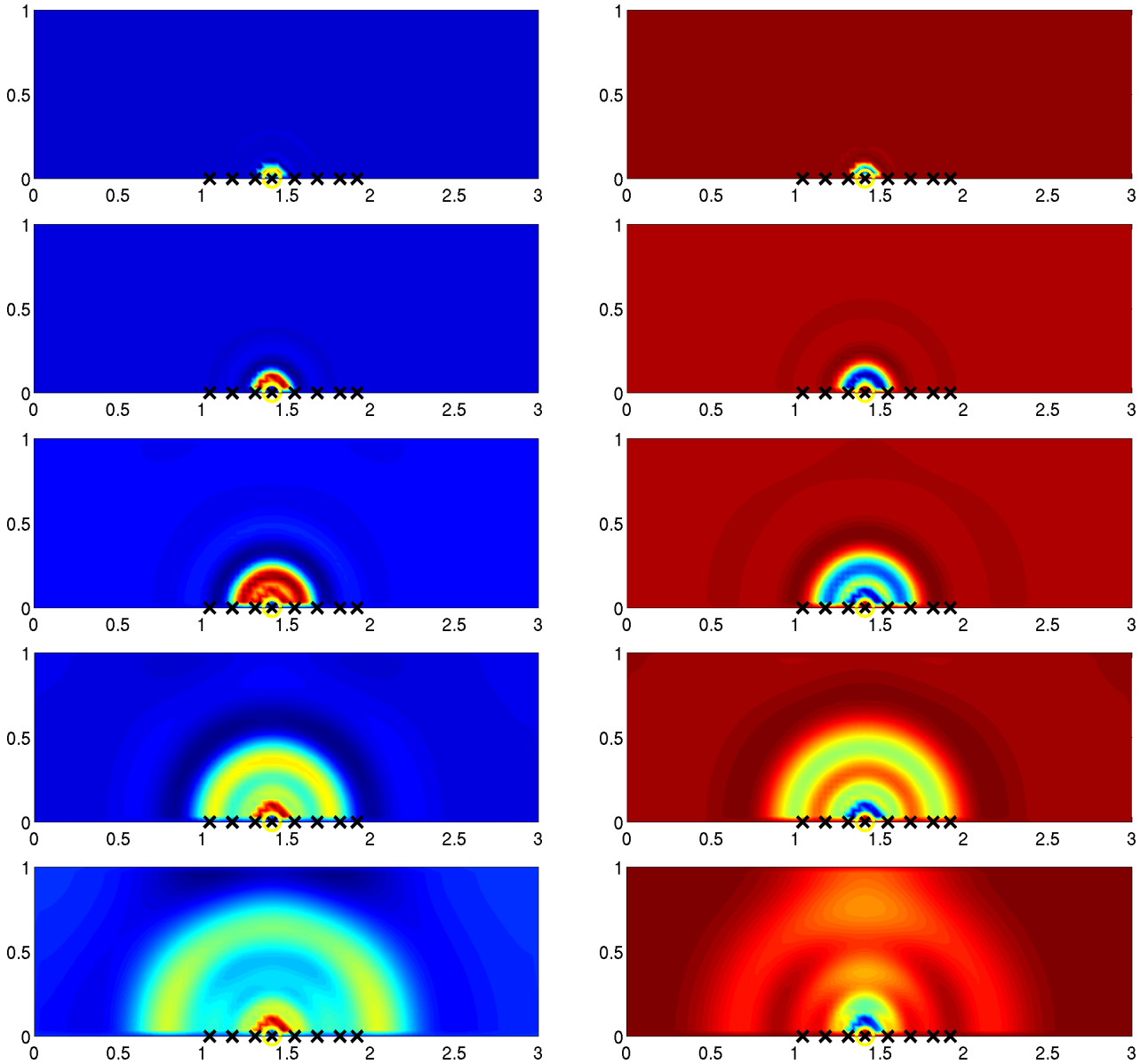
- We can do this for any (i, j), but we are interested in using the continued fraction representation of $G_m^{(ij)}(s)$.
- Coefficients $\left\{\left(\widehat{\kappa}_l^{(ij)}, \kappa_l^{(ij)}\right)\right\}_{l=1}^m$ are guaranteed to be positive if

$$c_q^{(ij)} = \left(\mathbf{b}_m^{(i)^T}\mathbf{z}_q^{(ij)}\right)\left(\mathbf{b}_m^{(j)^T}\mathbf{z}_q^{(ij)}\right) > 0$$

- Thus, we work only with the diagonal $G_m^{(jj)}(s)$.
- We have as before $\mathcal{R}_j(\mathbf{r}) = \mathcal{Q}\left(y_{jj}(\cdot;\mathbf{r})\right) = \left(\log \widehat{\kappa}_l^{(jj)}, \log \kappa_l^{(jj)}\right)_{l=1}^m$
- We solve optimization

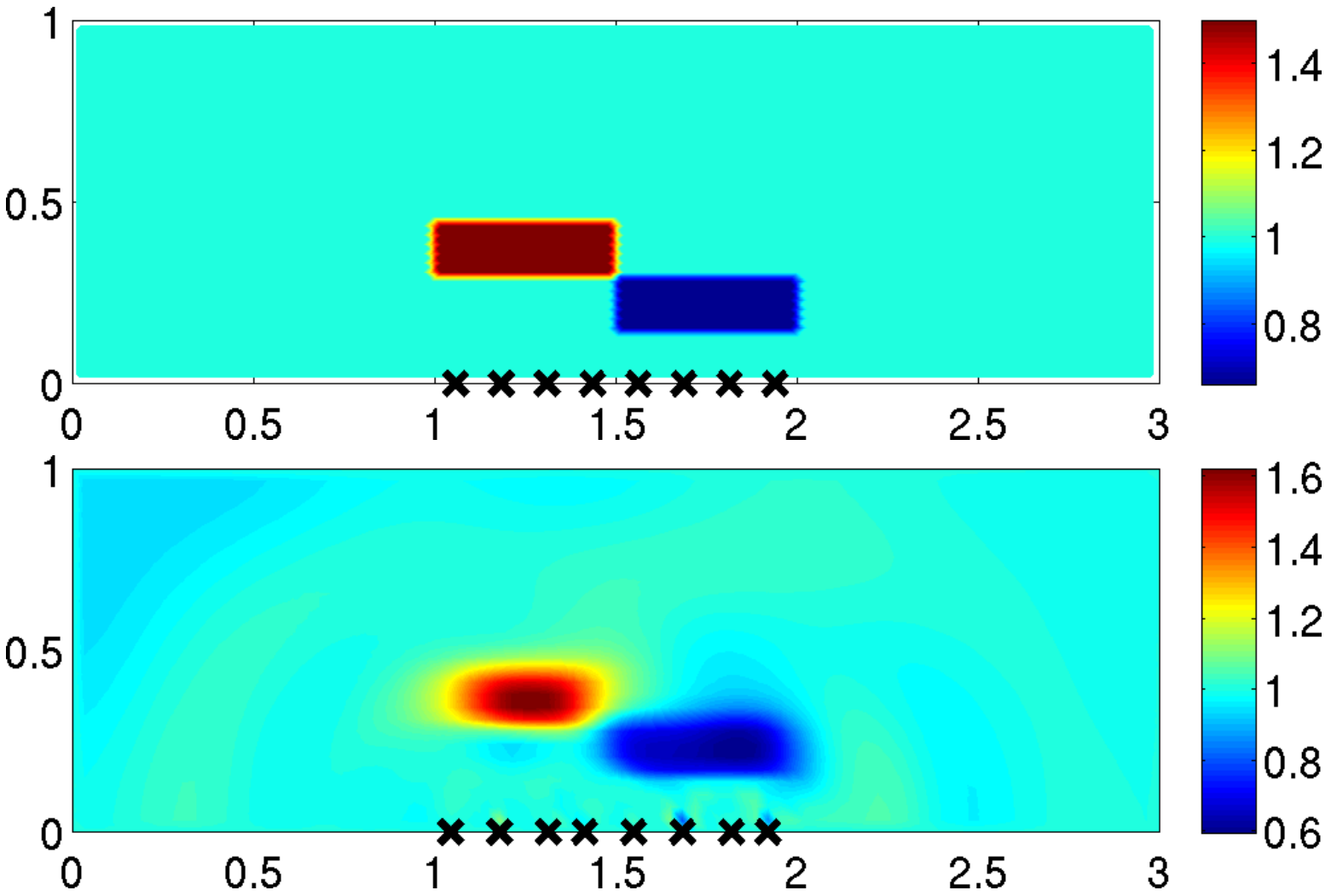
$$\mathbf{r}^\star = \arg\min_{\mathbf{r}\in\mathbb{R}_+^N} \frac{1}{2}\sum_{j=1}^{N_d} \left\|\mathcal{Q}(d_j(t)) - \mathcal{R}_j(\mathbf{r})\right\|_2^2 .$$

Sensitivity functions $\frac{\partial \widehat{\kappa}_k^{jj}}{\partial r}$ (left) and $\frac{\partial \kappa_k^{jj}}{\partial r}$ (right)



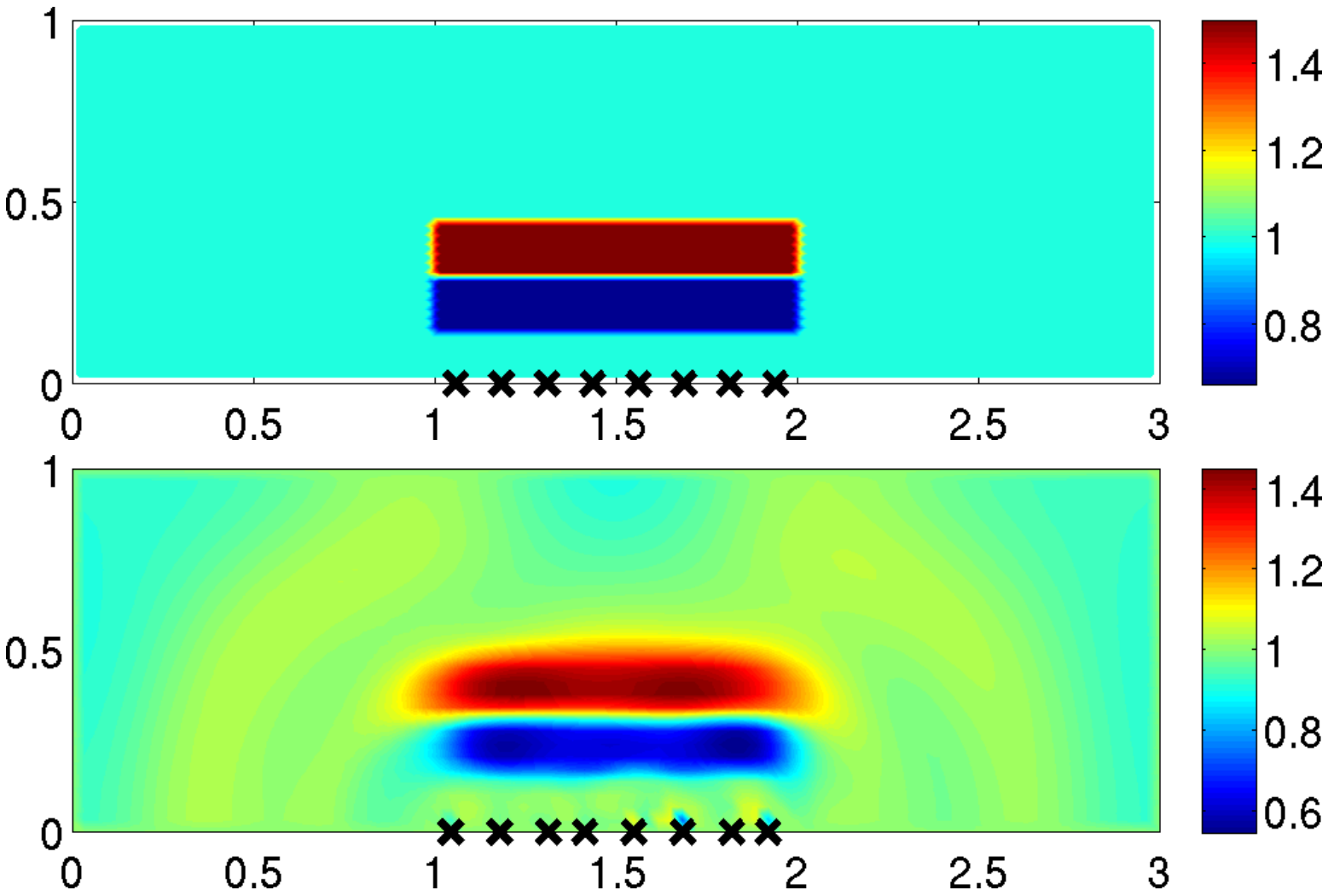
$k = 1, \ldots m = 5$ (top to bottom) for a single source/receiver.

Reconstructions: two checkerboard inclusions



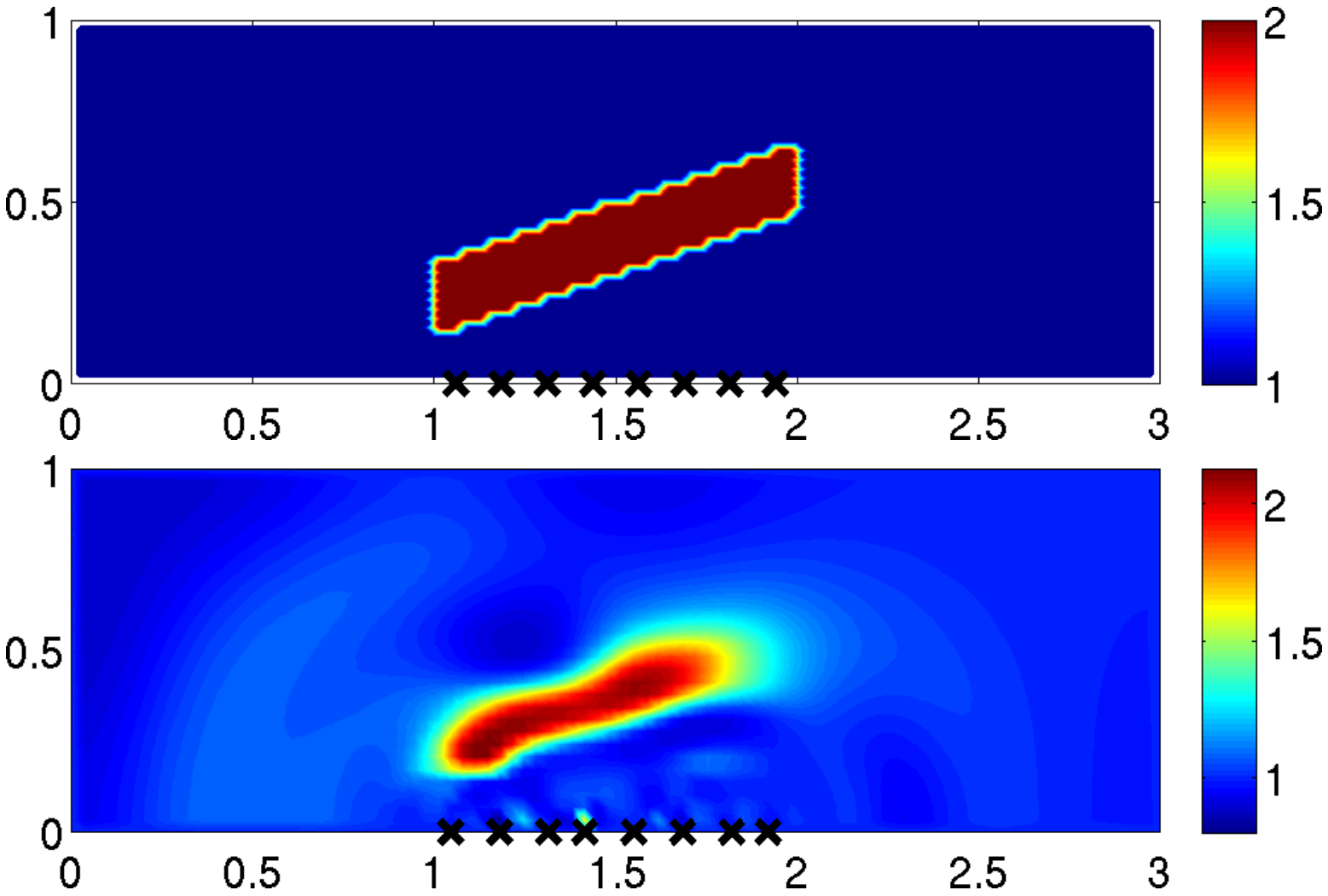
Top: true $r(x, y)$. Bottom: reconstruction after a single Gauss-Newton iteration. Constant initial guess $r_0(x, y) \equiv 1$. Sensors: $\times$.

Reconstructions: two layered inclusions



Top: true $r(x, y)$. Bottom: reconstruction after a single Gauss-Newton iteration. Constant initial guess $r_0(x, y) \equiv 1$. Sensors: $\times$.

Reconstructions: single skewed inclusion



Top: true $r(x, y)$. Bottom: reconstruction after a single Gauss-Newton iteration. Constant initial guess $r_0(x, y) \equiv 1$. Sensors: $\times$.

End notes

- All the details are in: *A model reduction approach to numerical inversion for a parabolic partial differential equation*. L. Borcea, V. Druskin, A.V. Mamonov and M. Zaslavsky, Inverse Problems 30 (2014), 125011 (33pp).
- Still plenty left to be done. The higher dimensional problem treatment is not optimal. Dealing with one source and multiple receivers means doing matrix rational approximation...
- 3-D problems ?