Efficient Parametric Model Reduction for Tomographic Reconstruction

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Modern Challenges in Imaging, In the footsteps of Allan MacLeod Cormack,
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Collaborators & Acknowledgements

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- Applications: tomography (DOT/EIT), topology optimization, model reduction, acoustics, quantum Monte Carlo, CFD

Overview

- Applications of Interest: Tomography, Topology Optimization, PDE-Constrained Optimization
- Forward Problem and High Computational cost
- More General Look at the Discrete Problems to Solve
- How to Solve/Optimize/Invert/Sample Faster?
- (Interpolatory) Parametric Model Reduction
- Randomization to efficiently compute ROMs
- Experimental Results
- Cheap updated ROMs with stochastic accuracy estimate
- Summary and Future Work

Why Tomography?

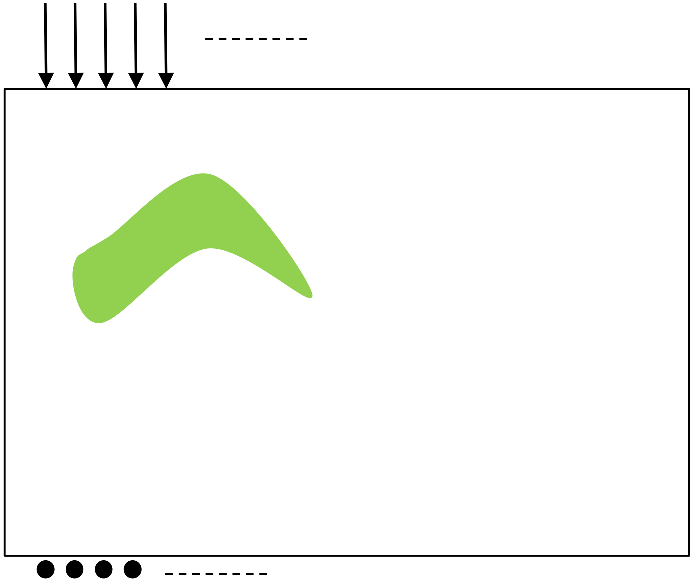
Diffuse Optical Tomography (DOT)

[Arridge IP'99]

- Tissue illuminated by near infra-red, freq. modulated, light
- Light detected in arrays
- Tumors different optical properties than surrounding tissue
- Recover images of optical properties $D(x)$ and $\mu(x)$ in

$$-\nabla \cdot \left(D(x)\nabla\eta\right) + \left(\mu(x) + \frac{i\omega}{\nu}\tilde{I}\right)\eta = b$$

- Problem ill-posed, underdetermined, and noisy



Forward Model & High Computational Costs

DOT forward problem typically solved in frequency domain

$$-\nabla \cdot \left(D\left(x;p\right)\nabla\eta\right) + \left(\mu\left(x;p\right) + \frac{i\omega}{\nu}\tilde{I}\right)\eta = b_j$$

Discretized: $C^T\left(sE - A\left(p\right)\right)^{-1}B$ (C^T from detectors)

Minimize misfit: $\left\|R\left(p\right)\right\|_F^2 = \left\|C^T\left(sE - A\left(p\right)\right)^{-1}B - D\right\|_F^2$

For n_s sources and n_f frequencies, solve $n_s n_f$ large 3D PDEs per step

Jacobian: $-C^T\left(sE - A\left(p\right)\right)^{-1}\frac{\partial A\left(p\right)}{\partial p}\left(sE - A\left(p\right)\right)^{-1}B$

Newton-type methods: extra $n_d n_f$ 3D PDE solves for transpose/adjoint

So, computational costs are very large

More General Look at Discrete Problems

- Many problems lead to minimizations of the form

$$\left\| C^T A\left(p\right)^{-1} B - D \right\|_F^2 \qquad \text{or} \qquad \operatorname{trace}\left(F^T K\left(p\right)^{-1} F \right)$$

- Require approximations of bilinear and quadratic forms involving linear inverse
- Approximations of more general bilinear forms

$$C^T f\left(A(p)\right) B$$

- Can be approximated by combinations of methods discussed and Krylov subspace approximation techniques

- Tomography, topology optimization (structural design), optimization of QOI using error transport/sensitivity equations, …

How to Solve Problems Faster?

- Reduce parameter space: PaLS [Aghasi, Kilmer, Miller SIIMS'11]
- Better optimization steps – faster convergence, especially useful in inverse problems: TREGS [dS, Kilmer SISC'11]
- Make each step faster
  - Exploit slowly changing systems – faster convergence & better initial guess
    - Krylov recycling / Recycling preconditioners [Parks, dS et al '06; Kilmer, dS '06; Feng et al '09&'13; Soodhalter et al '14; …]
  - Model reduction for inversion [Druskin et al SISC'13; Borcea et al'13; dS et al SISC'15], more for optimization/UQ: [Sachs et al; Bui et al'08 (2x), …]
  - Simultaneous random sources [Haber et al SIOPT'12; Roosta et al'14 and '15]
  - Random and optimized src/dets [Aslan,dS,Kilmer SISC'19]
  - Randomization for cheap ROMs [Aslan, dS, Gugercin (prep); Aslan thesis'18]
  - Estimate bilinear forms directly [many people]

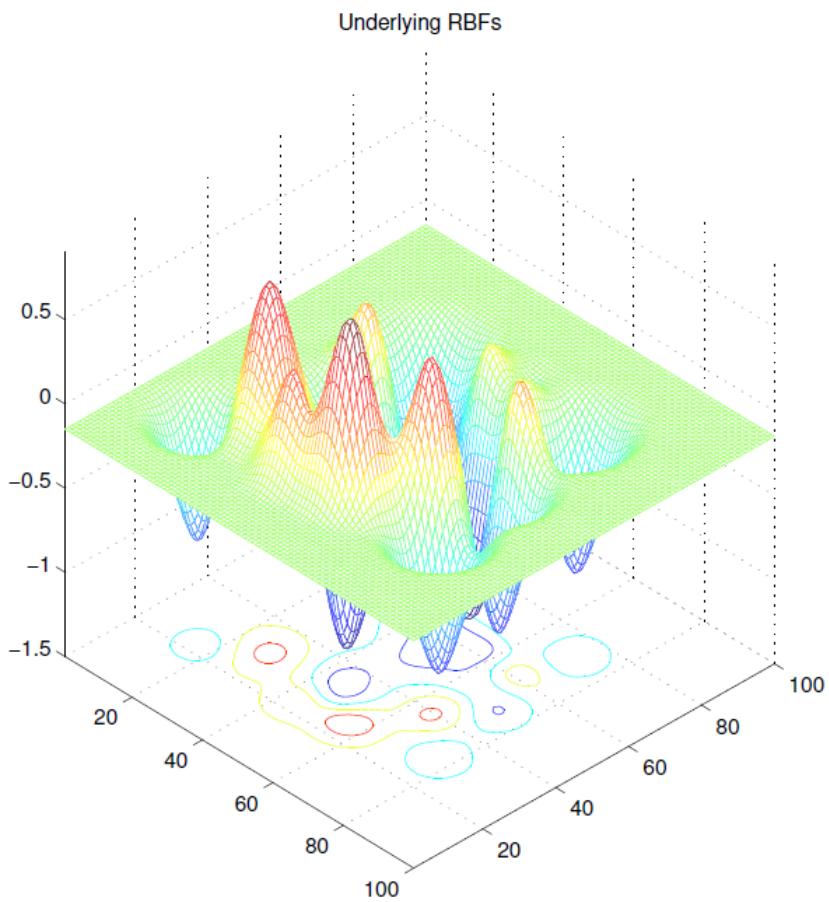
Parameterized Tomography

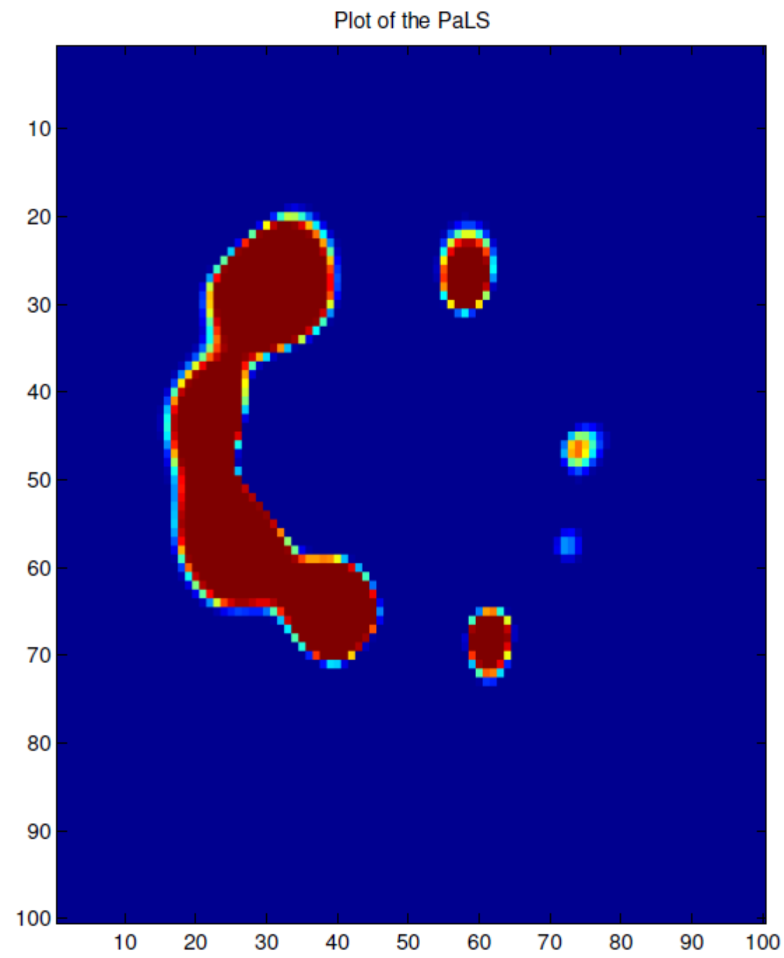
Rather than solve full inverse problem, parameterize the medium and solve for parameters – nonlinear least squares problem

$$\min_{\mathbf{p}} \|M(\mathbf{p}) - \mathbf{d}\|^2 \quad \left(+\lambda^2 \Gamma(\mathbf{p}) \right)$$

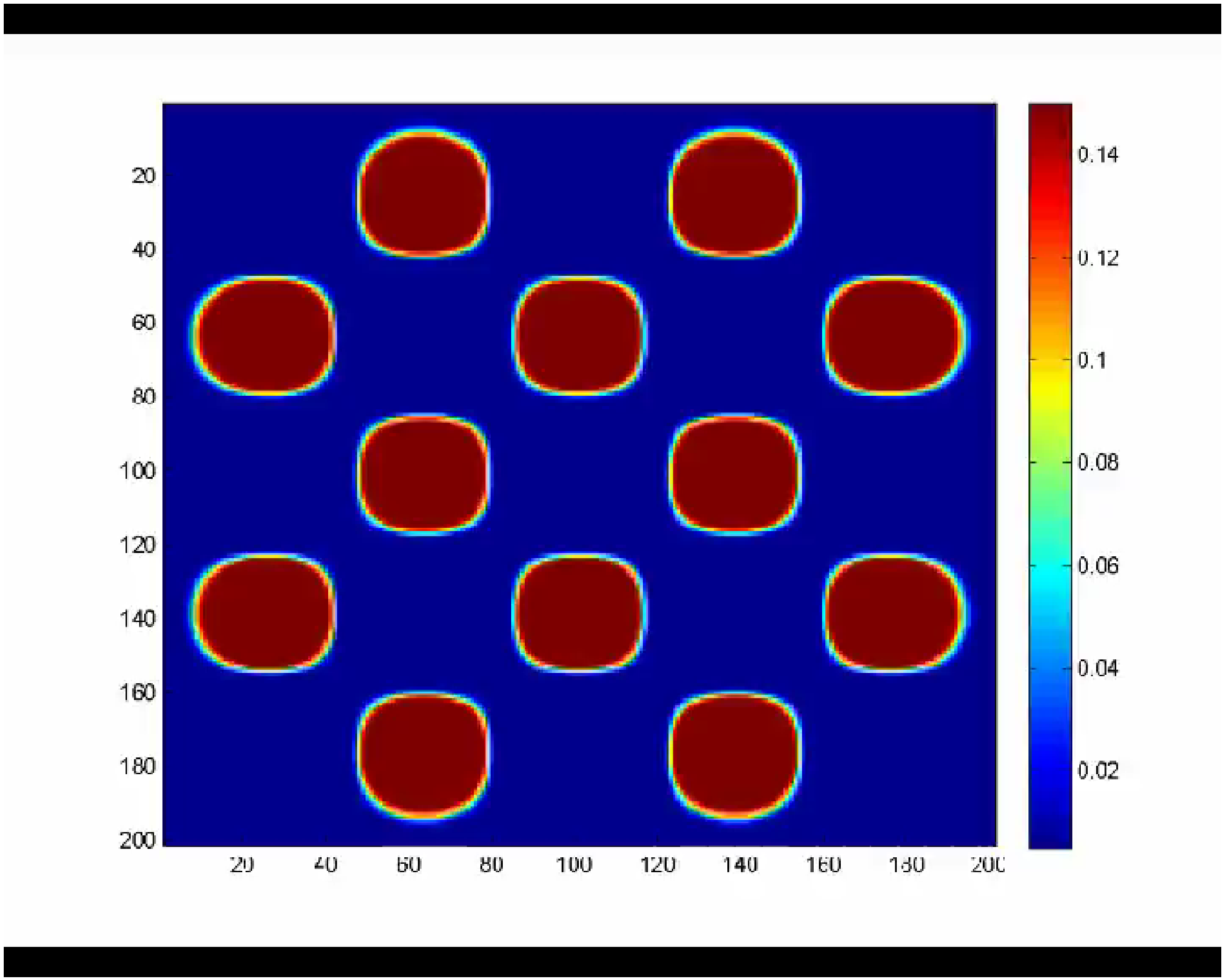
- Parameterize D and μ by expansion in compactly supported radial basis functions (CSRBF) and map to near 0-1 function using approx. Heavyside function and level set [Aghassi, Kilmer, Miller 2011]
- This parameterization yields regularized solution (some caveats)
- Solve using trust region method with regularized Gauss-Newton search directions [EdS/Kilmer 2011]
- Objective function and Jacobian require large number of linear system solves

Radial Basis Functions and Level Sets





What’s in the box?



Interpolatory Parametric Model Reduction

Time domain $E\dot{x}(t) = A(p)x(t) + Bu(t), \quad y(t) = C^T x(t)$

where $E, A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$, and $C \in \mathbb{R}^{n\times p}$

Transfer function: $G(p,s) = C^T \left(A(p) - sE\right)^{-1} B$

Project dynamics onto r dimensional subspace

Choose trial space V_r and take $x(t) \approx V_r x_r(t)$

Choose test space W_r and apply Petrov-Galerkin condition:

$$W_r^T \left(EV_r\dot{x}_r - A(p)V_r x_r - Bu\right) = 0 \quad \text{and set} \quad y_r = C^T V_r x_r$$

With $E_r = W_r^T E V_r$, $A_r(p) = W_r^T A(p) V_r$, $B_r = W_r^T B$, $C_r = V_r^T C$

Dynamical system $E_r \dot{x}_r = A_r x_r + B_r u$ and $y_r = C_r^T x_r$

and transfer function: $G_r(p,s) = C_r^T \left(A_r(p) - sE_r\right)^{-1} B_r$

Recipe for Interpolatory Parametric ROM

Theorem (under mild assumptions)

[Bauer, Beattie, Benner, Gugercin SISC'11]

- $K_{s,p} = sE(p) - A(p)$
- Given $\{s_1, s_2, \ldots, s_K\} \in \mathbb{C}$ and $\{p_1, p_2, \ldots, p_J\} \subset \mathbb{R}^P$, setting

$$R(V_r) \supset R\left(\left[K_{s_1,p_1}^{-1} B, \ldots, K_{s_K,p_J}^{-1} B\right]\right)$$
$$R(W_r) \supset R\left(\left[K_{s_1,p_1}^{-T} C, \ldots, K_{s_K,p_J}^{-T} C\right]\right)$$

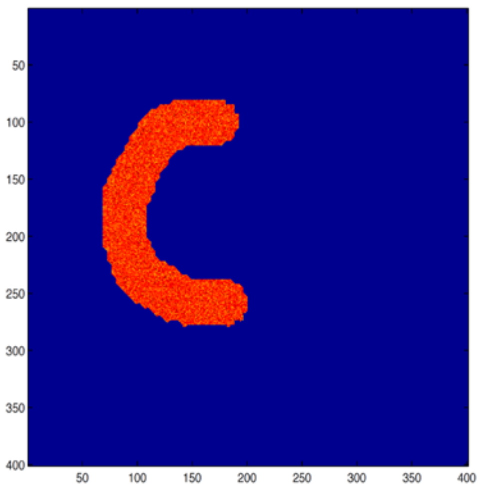
guarantees that

$$\begin{aligned} G_r(s_k, p_j) &= G(s_k, p_j) \\ G_r'(s_k, p_j) &= G'(s_k, p_j) \\ \nabla_p G_r(s_k, p_j) &= \nabla_p G(s_k, p_j) \end{aligned} \qquad \text{for} \quad \begin{cases} k = 1, \ldots, K \\ j = 1, \ldots, J \end{cases}$$

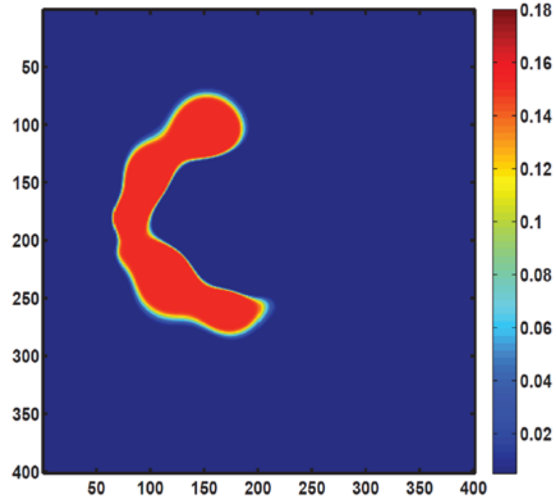
- Shows that space(s) count; not the bases (numerically does)

Reconstruction Example

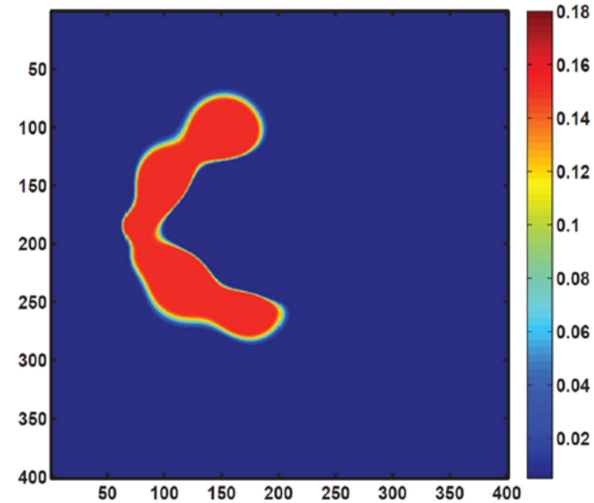
[de Sturler, Gugercin, Kilmer, Chaturantabut, Beattie, O'Connell SISC'15]



True image



Reconstruction using full order model - exact misfit



Reconstruction using ROM - approximate misfit

- 36 src/det, 5 interpolation points, 1 freq: 360 basis vectors
- Full problem: 1120 systems of 160K x 160K
- ROM: 1216 systems of 250 x 250
- Initial cost: 360 systems of 160801 x 160801

Randomization to Reduce Global Basis Cost

- Model reduction very effective, but global basis too expensive
  - Generate many more vectors than needed
  - Rank revealing factorization may reduce set of candidate basis vectors from many 100s or few 1000s to modest nr
- Unnecessary costs:
  - Too many expensive linear solves
  - Expensive rank revealing factorization
- Can we generate the same space at lower cost?
  - Standard candidate basis low rank
  - Approximate basis using randomization/sampling
  - Only needs modestly larger number of vectors than rank
  - [Halko, Martinsson, Tropp SIREV'11]
- Reduces solver cost and rank revealing factorization cost
- Easily be combined with step-wise update [O'Connel et al '17]
- Also opportunity for block-wise parallelization

Low-Rank Candidate Bases and Princ. Angles

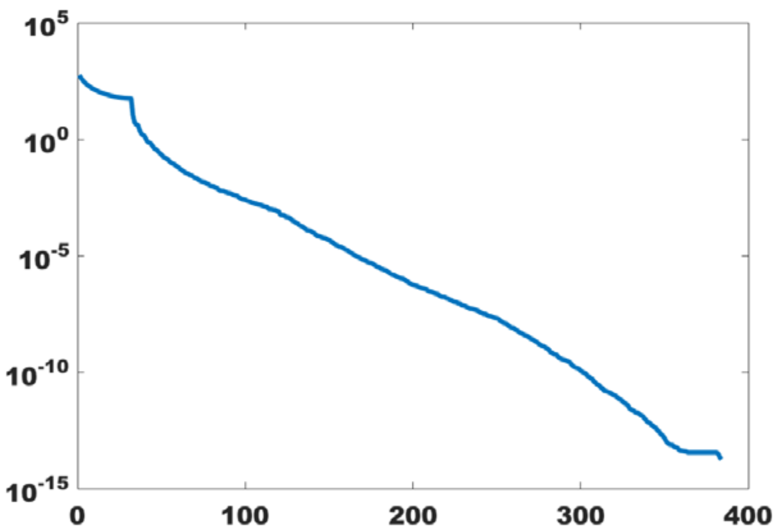


Fig. 4.1: Singular values of the candidate basis $\mathbf{V}$ before computing global basis.

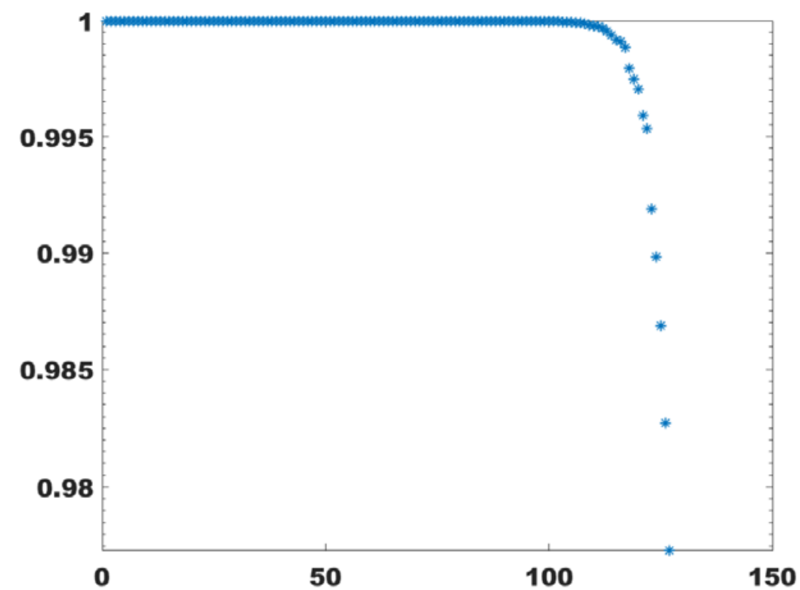


Fig. 4.2: The cosines of the canonical angles between Range($\mathbf{V}_r$) and Range($\widetilde{\mathbf{V}}_r$).

Randomization for Candidate Basis

- Replace standard candidate basis by sampled (randomized) one

$$\left[V_1\ V_2\ \dots\ V_K\right] \rightarrow \left[V_1\ V_2\ \dots\ V_K\right]\Lambda$$

  - where $V_k = \left[\left(\frac{i\omega_1}{\nu}E - A\left(p_k\right)\right)^{-1} B\ \dots\ \left(\frac{i\omega_J}{\nu}E - A\left(p_k\right)\right)^{-1} B\right]$

  - Λ has small fraction of number of columns in candidate basis

- Each element of Λ drawn independently from $\left\{-1,1\right\}$ with equal probability (other distributions possible)

- Solve set of $\left(\frac{i\omega_j}{\nu}E - A\left(p_k\right)\right)^{-1}\left(B\Lambda_k\right)$ (for all j,k)

Theoretical considerations

- Can consider this as using random tangential interpolation
- Alternative would be optimal tangential interpolation
  - Bauer, Beattie, Benner, Gugercin 2009
  - Expensive iteration, but possibly fewer basis vectors

- After few steps, changes in absorption image small
  - ΔA diagonal with modest number nonzeros
  - Small changes in absorption image suggest low rank changes to matrix of candidate basis vectors
  - In general, change is low rank and small
  - Also modest change in reachable and observable states
- Use to analyze required number of samples (a priori number)

Theory – Perturbation Basis Mat.s and Gramians

Assume small anomalies and modest changes per step

Consider change in candidate basis vectors from one parameter vector to next

$$V_1 = \left[\left(s_j E - A\left(p_1\right) \right)^{-1} B \right]_{j=1}^{n_f} \qquad V_2 = \left[\left(s_j E - A\left(p_2\right) \right)^{-1} B \right]_{j=1}^{n_f}$$

$\Delta A = A\left(p_2\right) - A\left(p_1\right)$ is diagonal with modest nr nonzeros

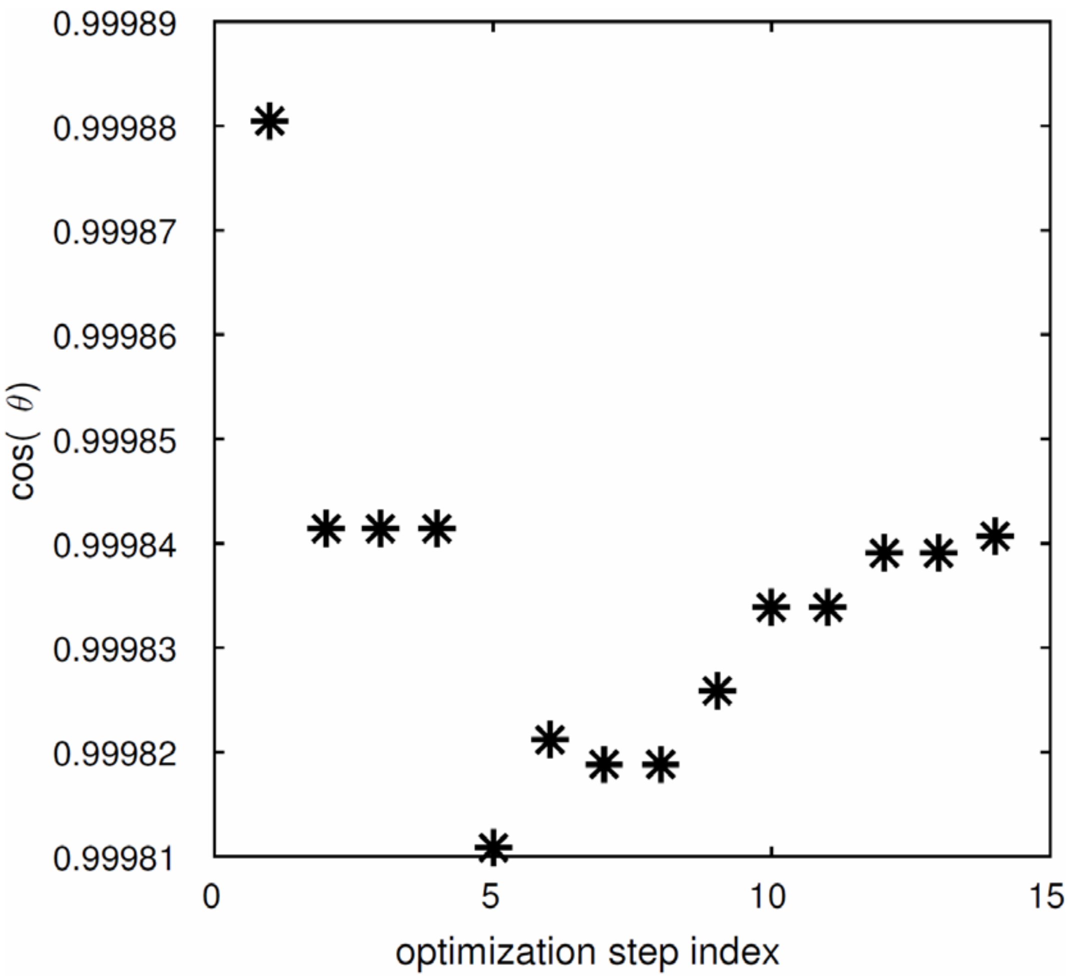
Then $\Delta V = V_2 - V_1$ is low rank and $\dfrac{\left\|\Delta V\right\|}{\left\|V_0\right\|} \leq 2Ch$

Where V_0 is solution for A_0, which corresponds to no anomaly.

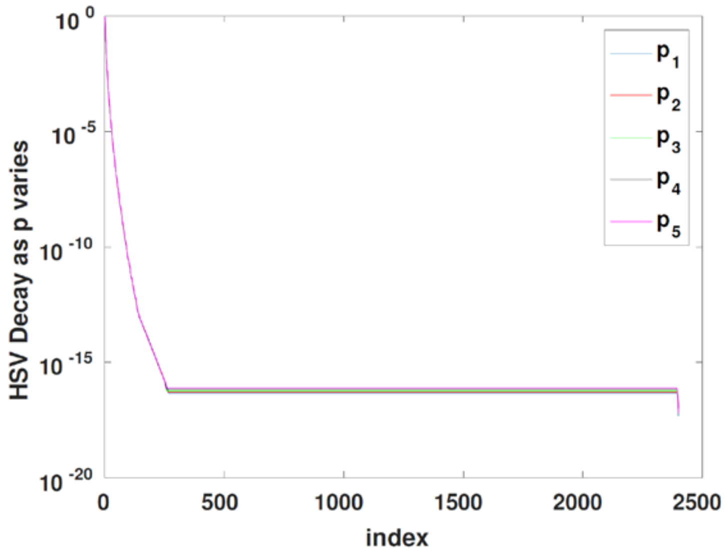
Proof by exploiting structure ΔA and expansion into eigenvector basis for A_0

Similar results for reachability and observability Gramians

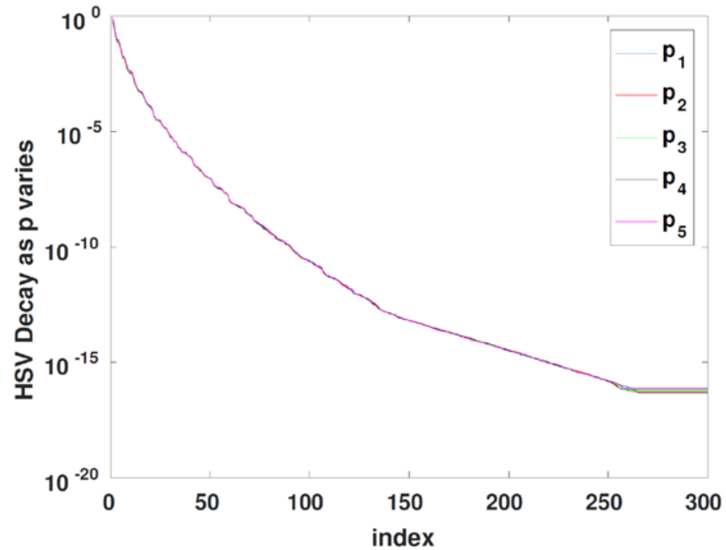
Angles Spans of Candidate Bases Matrices



Hankel Singular Values

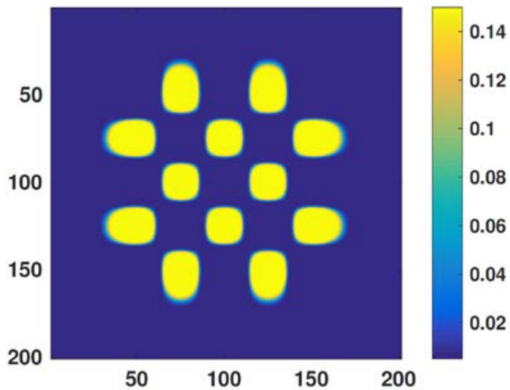


(a)

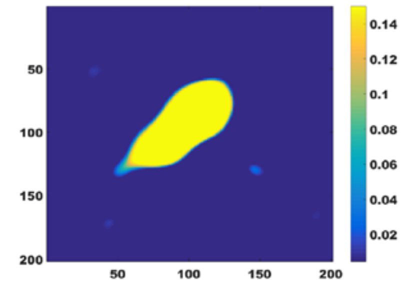


(b)

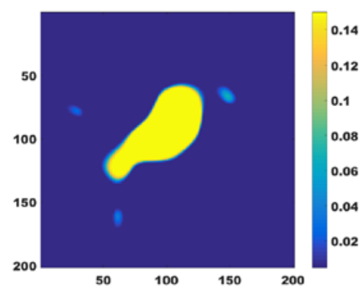
2D Reconstruction – Experiment 1



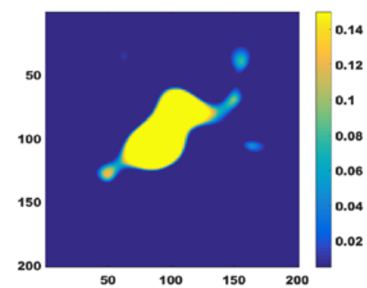
(a) True shape of the anomaly.



(b) Reconstruction using the FOM.



(c) Reconstruction using the standard ROM with all sources and detectors.



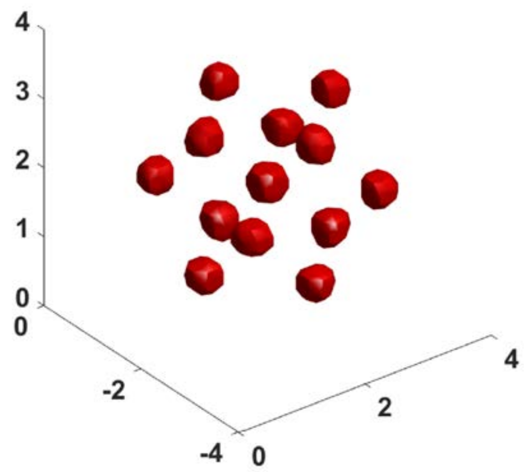
(d) Reconstruction using the ROM with stochastic sources and detectors, $\ell_s = \ell_d = 12$.

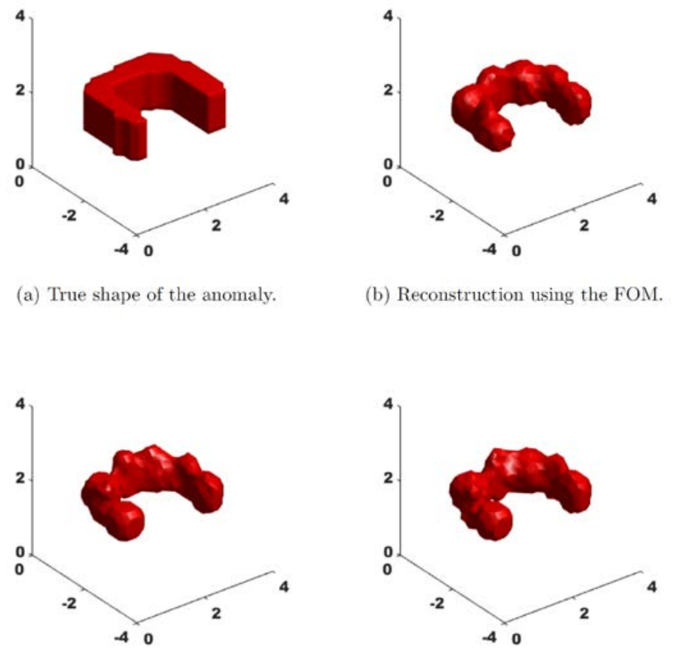
Experiment 1 – 2D Reconstruction

#sources = #detectors = 32, 2 freq.s, 25 CSRBFs, 4 sample points

32 x 32 x 32 mesh, 12 random sample vectors

3D Reconstruction – Experiment 2





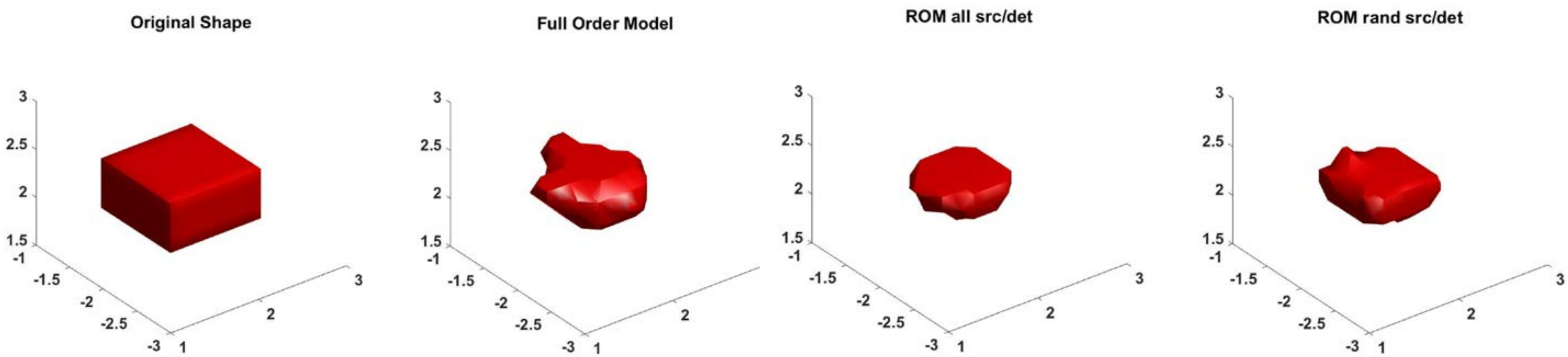
(a) True shape of the anomaly. (b) Reconstruction using the FOM. (c) Reconstruction using the standard ROM with all sources and detectors. (d) Reconstruction using the ROM with stochastic sources and detectors, $\ell_s = 50$.

Experiment 2 – 3D Reconstruction

#sources = #detectors = 225, 3 freq.s, 27 CSRBFs, 4 sample points

32 x 32 x 32 mesh, 50 random sample vectors

3D Reconstruction – Experiment 3



Experiment 3 – 3D Reconstruction

#sources = #detectors = 225, 4 freq.s, 27 CSRBFs, 3 sample points

32 x 32 x 32 mesh, 50 random sample vectors

Results: Reduction of Large Linear Solves

	FOM	ROM (all srcs/det)		ROM (stoch. srcs/dets)	
	large	large	small	large	small
Exp. 1 (n=40401)	1856	512	1792 (r=242)	192	212 (r=212)
Exp. 2 (n=32768)	18900	5400	16875 (r=1368)	1200	17550 (r=1294)
Exp. 3 (n=32768)	47700	5400	21600 (r=1228)	1200	2700 (r=1184)

Conclusions and Future Work

- Significant efficiency improvements using model reduction
- Reduce cost of global basis computation
  - Randomization very effective (tangential interpolation links)
  - Make online ROM building/updating more efficient
  - Subspace angle-based methods to further reduce cost

- Randomization
  - Important how to select right information
  - Make SA methods more robust (at least for Top. Opt.)

- Many problems have similar structure, block bilinear/quadratic form, hence are suitable for these methods
- Interesting opportunities for Krylov methods to efficiently estimate these bilinear/quadratic forms

Some Good Reading

- *Randomization for the efficient computation of reduced order models* – Aslan, de Sturler, Gugercin – arXiv very soon
- *Randomized approach to nonlinear inversion combining random and optimized simultaneous sources and detectors*, Aslan, de Sturler, Kilmer, SISC 2019
- *Stochastic sampling for deterministic structural topology optimization with many load cases: density-based and ground structure approaches*, Zhang, de Sturler, Paulino, Computer Methods in Applied Mechanical Eng., 2017
- *Nonlinear parametric inversion using interpolatory model reduction*, de Sturler, Gugercin, Kilmer, Chaturantabut, Beattie, O'Connell, SISC 2015
- *Computing reduced order models via inner-outer Krylov recycling in Diffuse Optical Tomography*, O'Connell, Kilmer, de Sturler, Gugercin, SISC 2017

- *An effective method for parameter estimation with PDE constraints with multiple rhs*, Haber, Chung, Herrmann, SIOPT 2012
- *Stochastic algorithms for inverse problems involving PDEs and many measurements*, Roosta-Khorasani, van den Doel, Ascher, SISC 2014
- *Assessing stochastic algorithms for large-scale nonlinear least-squares problems*, Roosta-Khorasani, Szekely, Ascher, …, SIAMUQ 2015