

# A model reduction approach for inverse problems with operator valued data

**Matthias Schlottbom**

joint work with Jürgen Dölz (U Bonn), Herbert Egger (TU Darmstadt/Linz)

**CASA Colloquium**

TU Eindhoven

June 30th, 2021

Preprint available at [arxiv.org/abs/2004.11827](https://arxiv.org/abs/2004.11827)

**UNIVERSITY OF TWENTE.**

# Outline

## Fluorescence diffuse optical tomography

- Model

- Inverse problem

- Outline of model reduction approach

## Abstract Analysis: Model reduction for $\mathcal{T}c = \mathcal{V}'\mathcal{D}(c)\mathcal{U}$

- Properties of the forward operator

- Step 1: Tensor product approximation

- Step 2: Quasi-optimal compression

## Model reduction in action: Application to FDOT

- Truth approximation and implementation

- Complexity estimates

- Runtimes and ranks

## Conclusion

## Fluorescence diffuse optical tomography

Model

Inverse problem

Outline of model reduction approach

Abstract Analysis: Model reduction for  $\mathcal{T}c = \mathcal{V}'\mathcal{D}(c)\mathcal{U}$

Properties of the forward operator

Step 1: Tensor product approximation

Step 2: Quasi-optimal compression

Model reduction in action: Application to FDOT

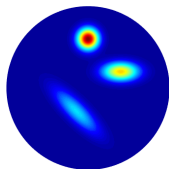
Truth approximation and implementation

Complexity estimates

Runtimes and ranks

Conclusion

# Fluorescence optical tomography: forward problem: $c \mapsto M$



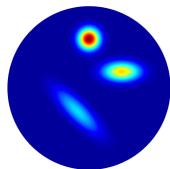
concentration

---

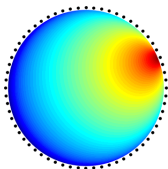
[Arridge, Schotland: Optical tomography: forward and inverse problems, Inverse Problems, 25 (2009)]

[Egger et al: On forward and inverse models in fluorescence diffuse optical tomography, IPI, 4 (2010)]

# Fluorescence optical tomography: forward problem: $c \mapsto M$



concentration



excitation

## Excitation field generated by source $q_j$

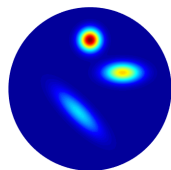
$$\begin{aligned} -\nabla \cdot (\kappa_x \nabla u_{x,j}) + \mu_x u_{x,j} &= 0 & \text{in } \Omega \\ \kappa_x \partial_n u_{x,j} + \rho_x u_{x,j} &= q_j & \text{on } \partial\Omega \end{aligned}$$

---

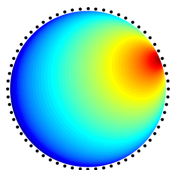
[Arridge, Schotland: Optical tomography: forward and inverse problems, Inverse Problems, 25 (2009)]

[Egger et al: On forward and inverse models in fluorescence diffuse optical tomography, IPI, 4 (2010)]

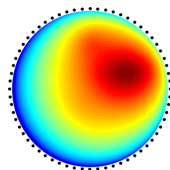
# Fluorescence optical tomography: forward problem: $c \mapsto M$



concentration



excitation



emission

## Excitation field generated by source $q_j$

$$\begin{aligned} -\nabla \cdot (\kappa_x \nabla u_{x,j}) + \mu_x u_{x,j} &= 0 & \text{in } \Omega \\ \kappa_x \partial_n u_{x,j} + \rho_x u_{x,j} &= q_j & \text{on } \partial\Omega \end{aligned}$$

## Emission field for fluorophore concentration $c$ and excitation field $u_{x,j}$

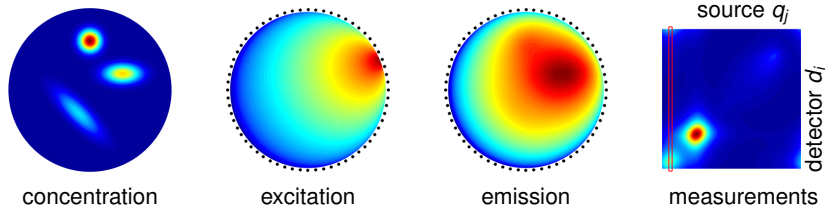
$$\begin{aligned} -\nabla \cdot (\kappa_m \nabla u_{m,j}) + \mu_m u_{m,j} &= c u_{x,j} & \text{in } \Omega \\ \kappa_m \partial_n u_{m,j} + \rho_m u_{m,j} &= 0 & \text{on } \partial\Omega \end{aligned}$$

---

[Arridge, Schotland: Optical tomography: forward and inverse problems, Inverse Problems, 25 (2009)]

[Egger et al: On forward and inverse models in fluorescence diffuse optical tomography, IPI, 4 (2010)]

# Fluorescence optical tomography: forward problem: $c \mapsto M$



## Excitation field generated by source $q_j$

$$\begin{aligned} -\nabla \cdot (\kappa_x \nabla u_{x,j}) + \mu_x u_{x,j} &= 0 & \text{in } \Omega \\ \kappa_x \partial_n u_{x,j} + \rho_x u_{x,j} &= q_j & \text{on } \partial\Omega \end{aligned}$$

## Emission field for fluorophore concentration $c$ and excitation field $u_{x,j}$

$$\begin{aligned} -\nabla \cdot (\kappa_m \nabla u_{m,j}) + \mu_m u_{m,j} &= c u_{x,j} & \text{in } \Omega \\ \kappa_m \partial_n u_{m,j} + \rho_m u_{m,j} &= 0 & \text{on } \partial\Omega \end{aligned}$$

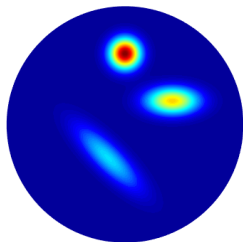
## Measurements at detector (pixel) $d_i$ : $M_{ij} = \int_{\partial\Omega} d_i(x) u_{m,j}(x) d\sigma(x)$

[Arridge, Schotland: Optical tomography: forward and inverse problems, Inverse Problems, 25 (2009)]

[Egger et al: On forward and inverse models in fluorescence diffuse optical tomography, IPI, 4 (2010)]

# Inverse Problem

- ▶  $\mathbb{M} \approx \mathcal{M} = \mathcal{M}(c) : q \rightarrow u_m|_{\partial\Omega}$  (infinite dim.) measurement operator
- ▶ Use of  $\mathcal{M}$  yields algorithms that are independent of the discretization

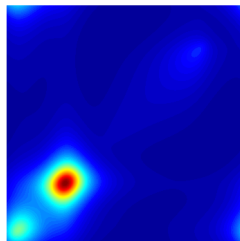


concentration  $c$

$$\xrightarrow{\mathcal{T} : c \mapsto \mathcal{M}}$$

$$\xleftarrow{\quad}$$

$$\text{solve } \mathcal{T}c = \mathcal{M}^\delta$$

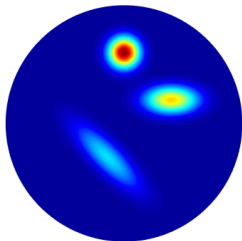


measurements:  $\mathcal{M}$



# Inverse Problem

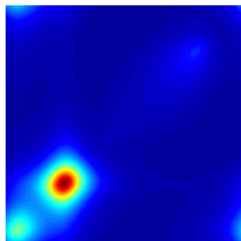
- ▶  $\mathbb{M} \approx \mathcal{M} = \mathcal{M}(c) : q \rightarrow u_m|_{\partial\Omega}$  (infinite dim.) measurement operator
- ▶ Use of  $\mathcal{M}$  yields algorithms that are independent of the discretization



concentration  $c$

$$\xrightarrow{\mathcal{T} : c \mapsto \mathcal{M}}$$

$$\xleftarrow{\text{solve } \mathcal{T}c = \mathcal{M}^\delta}$$



measurements:  $\mathcal{M}$

**Tikhonov regularization**

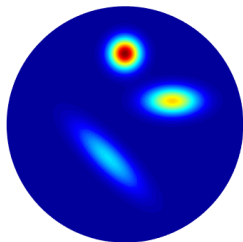
$$\|\mathcal{T}c - \mathcal{M}^\delta\|^2 + \alpha\|c\|^2 \rightarrow \min$$

**Regularized normal equations**

$$(\mathcal{T}^*\mathcal{T} + \alpha\mathcal{I})c_\alpha^\delta = \mathcal{T}^*\mathcal{M}^\delta$$

# Inverse Problem

- ▶  $\mathbb{M} \approx \mathcal{M} = \mathcal{M}(c) : q \rightarrow u_m|_{\partial\Omega}$  (infinite dim.) measurement operator
- ▶ Use of  $\mathcal{M}$  yields algorithms that are independent of the discretization

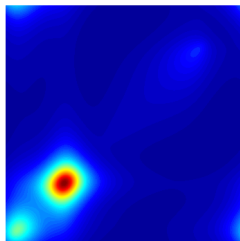


concentration  $c$

$$\xrightarrow{\mathcal{T} : c \mapsto \mathcal{M}}$$

$$\xleftarrow{\quad}$$

$$\text{solve } \mathcal{T}c = \mathcal{M}^\delta$$



measurements:  $\mathcal{M}$

**Tikhonov regularization**

$$\|\mathcal{T}c - \mathcal{M}^\delta\|^2 + \alpha\|c\|^2 \rightarrow \min$$

**Regularized normal equations**

$$(\mathcal{T}^*\mathcal{T} + \alpha\mathcal{I})c_\alpha^\delta = \mathcal{T}^*\mathcal{M}^\delta$$

- ▶ solve with conjugate gradients (apply  $\mathcal{T}c$  and  $\mathcal{T}^*M$  (its truth approximation))
- ▶ expensive for large parameter space and many measurements

---

[Freiberger et al: High-performance image reconstruction in fluorescence tomography on desktop computers and graphics hardware, Biomed. Opt. Express, 2 (2011)]

# Pathway to model reduction via projections

## Projection

$$\mathcal{T}_N = \mathcal{Q}_N \mathcal{T}$$

## Error bound

$$\|\mathcal{Q}_N \mathcal{T} - \mathcal{T}\| \leq \delta.$$

## Reconstruction

$$(\mathcal{T}_N^* \mathcal{T}_N + \alpha \mathcal{I}_N) \mathbf{c}_{\alpha, N}^\delta = \mathcal{T}_N^* \mathcal{M}_N^\delta$$

## Reconstruction error bound

$$\|\mathbf{c}_{\alpha, N}^\delta - \mathbf{c}_\alpha^\delta\| \leq C(\alpha) \delta$$

---

[Bakushinsky, Kokurin: Iterative Methods for Approximate Solution of Inverse Problems. Springer 2004]

[Neubauer: An a posteriori parameter choice for Tikhonov regularization in the presence of modeling errors. APNUM 4 (1988)]

# Offline-Online decomposition

**Offline.** Setup of the approximations  $\mathcal{Q}_N$ ,  $\mathcal{T}_N^*$ , and  $\mathcal{T}_N\mathcal{T}_N^*$ .

**Online.** Computation of the regularized solution requires

step	computations	complexity	memory
compression	$\mathcal{M}_N^\delta = \mathcal{Q}_N\mathcal{M}^\delta$	$Nk^2$	$Nk^2$
analysis	$z_{\alpha,N}^\delta = g_\alpha(\mathcal{T}_N\mathcal{T}_N^*)\mathcal{M}_N^\delta$	$N^2$	$N^2$
synthesis	$c_{\alpha,N}^\delta = \mathcal{T}_N^*z_{\alpha,N}^\delta$	$Nm$	$Nm$

**Truth approximation**  $\mathcal{T} \in \mathbb{R}^{m \times k^2}$

# Offline-Online decomposition

**Offline.** Setup of the approximations  $\mathcal{Q}_N$ ,  $\mathcal{T}_N^*$ , and  $\mathcal{T}_N\mathcal{T}_N^*$ .

**Online.** Computation of the regularized solution requires

step	computations	complexity	memory
compression	$\mathcal{M}_N^\delta = \mathcal{Q}_N\mathcal{M}^\delta$	$Nk^2$	$Nk^2$
analysis	$z_{\alpha,N}^\delta = g_\alpha(\mathcal{T}_N\mathcal{T}_N^*)\mathcal{M}_N^\delta$	$N^2$	$N^2$
synthesis	$c_{\alpha,N}^\delta = \mathcal{T}_N^*z_{\alpha,N}^\delta$	$Nm$	$Nm$

**Truth approximation**  $\mathcal{T} \in \mathbb{R}^{m \times k^2}$

$\mathcal{T}_N$  being a truncated SVD of  $\mathcal{T}$  is the benchmark, but expensive!

see, e.g., [Hochstenbach 2001, Markel et al 2003, Stoll 2012, Chaillat et al 2012, Musco et al 2015,...]

# A decomposition of the forward operator: $\mathcal{T} = \mathcal{V}'\mathcal{D}(\cdot)\mathcal{U}$

## Adjoint emission problem

$$\begin{aligned} -\nabla \cdot (\kappa_m \nabla v_m) + \mu_m v_m &= 0 & \text{in } \Omega \\ \kappa_m \partial_n v_m + \rho_m v_m &= q_m & \text{on } \partial\Omega \end{aligned}$$

## Solution operators of excitation and adjoint emission problem

$$\mathcal{U} : q_x \mapsto \mathcal{U}q_x := u_x$$

$$\mathcal{V} : q_m \mapsto \mathcal{V}q_m := v_m.$$

## Multiplication operator

$$\mathcal{D}(c)u = cu, \quad \text{i.e. } \langle \mathcal{D}(c)u, v \rangle = \int_{\Omega} c u v \, dx.$$

One can show that  $u_m|_{\partial\Omega} = \mathcal{V}'\mathcal{D}(c)u_x$  in correct functional analytic setting, i.e.,

$$\mathcal{T}c = \mathcal{V}'\mathcal{D}(c)\mathcal{U}.$$

# Procedure for setting up the projection for $\mathcal{T} = \mathcal{V}'\mathcal{D}(\cdot)\mathcal{U}$

## 1. Accurate projections

$$\mathcal{U}_K = \mathcal{U}\mathcal{Q}_{K,\mathcal{U}} \quad \text{and} \quad \mathcal{V}_K = \mathcal{V}\mathcal{Q}_{K,\mathcal{V}}$$

lead to

$$\mathcal{T}_{K,K}\mathbf{c} = \mathcal{Q}_{K,K}\mathcal{T}\mathbf{c} = \mathcal{V}'_K\mathcal{D}(\mathbf{c})\mathcal{U}_K, \quad \mathcal{M}_{K,K}^\delta = (\mathcal{Q}'_{K,\mathcal{V}}\mathcal{M}^\delta)\mathcal{Q}_{K,\mathcal{U}}$$

with error bound  $\|\mathcal{T}_{K,K} - \mathcal{T}\| \leq \delta$

**2. Further compression** of  $\mathcal{T}_{K,K}$  gives rise to desired projection

$$\mathcal{Q}_N = \mathcal{P}_N\mathcal{Q}_{K,K}, \quad \mathcal{M}_N^\delta = \mathcal{P}_N\mathcal{M}_{K,K}^\delta$$

**Remark.** Computation of  $\mathcal{M}_{K,K}^\delta = (\mathcal{Q}'_{K,\mathcal{V}}\mathcal{M}^\delta)\mathcal{Q}_{K,\mathcal{U}}$  requires only  $O(Kk + K^2)$  mem instead of  $O(Nk^2)$  if **tensor structure** is used.

---

Related to step 1.: [Herrmann et al 2009, Krebs et al 2009, Roosta-Khorasani et al 2014, Markel et al 2019]

## Fluorescence diffuse optical tomography

Model

Inverse problem

Outline of model reduction approach

### Abstract Analysis: Model reduction for $\mathcal{T}c = \mathcal{V}'\mathcal{D}(c)\mathcal{U}$

Properties of the forward operator

Step 1: Tensor product approximation

Step 2: Quasi-optimal compression

### Model reduction in action: Application to FDOT

Truth approximation and implementation

Complexity estimates

Runtimes and ranks

## Conclusion



## Abstract setting

**Assumptions.**  $\mathcal{U}, \mathcal{V}, \mathcal{X}, \mathcal{Y}, \mathcal{Z}$  separable Hilbert spaces

$$\mathcal{U} \in \text{HS}(\mathcal{Y}, \mathcal{U}), \quad \mathcal{V} \in \text{HS}(\mathcal{Z}, \mathcal{V}), \quad \mathcal{D} \in \mathcal{L}(\mathcal{X}, \mathcal{L}(\mathcal{U}, \mathcal{V}'))$$

---

**recall:** Any  $\mathcal{S} \in \mathcal{L}(\mathbb{A}, \mathbb{B})$  compact has singular value decomposition (SVD)

$$\mathcal{S}a = \sum_{k=1}^{\infty} (a, a_k)_{\mathbb{A}} \sigma_{k, \mathcal{S}} b_k$$

with ONBs  $\{a_k\} \subset \mathbb{A}$  and  $\{b_k\} \subset \mathbb{B}$ . Truncated SVD

$$\mathcal{S}_K a = \sum_{k=1}^K (a, a_k)_{\mathbb{A}} \sigma_{k, \mathcal{S}} b_k.$$

Error  $\|\mathcal{S} - \mathcal{S}_K\|_{\mathcal{L}(\mathbb{A}, \mathbb{B})} = \sigma_{K+1, \mathcal{S}}$ ,

$\mathcal{S} \in \text{HS}(\mathbb{A}, \mathbb{B})$  iff  $\{\sigma_{k, \mathcal{S}}\}_k \in \ell_2$ , and  $\|\mathcal{S}\|_{\text{HS}(\mathbb{A}, \mathbb{B})}^2 = \sum_{k=1}^{\infty} \sigma_{k, \mathcal{S}}^2$

---

see, e.g., [Hackbusch: Tensor spaces and numerical tensor calculus. Springer. 2014]

## Properties of the forward operator

$U, V, X, Y, Z$  separable Hilbert spaces

$$U \in \text{HS}(Y, U), \quad V \in \text{HS}(Z, V), \quad \mathcal{D} \in \mathcal{L}(X, \mathcal{L}(U, V'))$$

**Lemma.**  $\mathcal{T}(c) = \mathcal{V}' \mathcal{D}(c) \mathcal{U}$  defines a bounded linear compact operator  $\mathcal{T} : X \rightarrow \text{HS}(Y, Z')$ .

# Properties of the forward operator

$U, V, X, Y, Z$  separable Hilbert spaces

$$U \in \text{HS}(Y, U), \quad V \in \text{HS}(Z, V), \quad D \in \mathcal{L}(X, \mathcal{L}(U, V'))$$

**Lemma.**  $\mathcal{T}(c) = V' D(c) U$  defines a bounded linear compact operator  $\mathcal{T} : X \rightarrow \text{HS}(Y, Z')$ .

**Proof (sketch).**

- ▶ Consider TSVDs:  $U_K = U Q_{K,U}$  and  $V_K = V Q_{K,V}$  with rank  $K$  such that

$$\|U - U_K\|_{\mathcal{L}(Y,U)} \lesssim K^{-1/2} \quad \text{and} \quad \|V - V_K\|_{\mathcal{L}(Z,V)} \lesssim K^{-1/2}$$

- ▶ Define  $\mathcal{T}_{K,K} : X \rightarrow \text{HS}(Y, Z')$  by  $\mathcal{T}_{K,K} c = V'_K D(c) U_K$
- ▶  $\text{rank } \mathcal{T}_{K,K} \leq K^2$ .
- ▶ Show  $\|\mathcal{T} - \mathcal{T}_{K,K}\|_{\mathcal{L}(X, \text{HS}(Y, Z'))} \lesssim K^{-1/2}$  via triangle inequality.

## Step 1: Tensor product approximation of $\mathcal{T}$

**Corollary.** For any  $\delta > 0$  there exists  $K \in \mathbb{N}$  with  $K \lesssim \delta^{-2}$  such that

$$\|\mathcal{U} - \mathcal{U}_K\|_{\mathcal{L}(\mathbb{Y}, \mathbb{U})} \leq \delta \quad \text{and} \quad \|\mathcal{V} - \mathcal{V}_K\|_{\mathcal{L}(\mathbb{Z}, \mathbb{V})} \leq \delta,$$

and  $\mathcal{T}_{K,K}c = \mathcal{V}'_K \mathcal{D}(c) \mathcal{U}_K$  satisfies

$$\|\mathcal{T} - \mathcal{T}_{K,K}\|_{\mathcal{L}(\mathbb{X}, \text{HS}(\mathbb{Y}, \mathbb{Z}'))} \lesssim \delta.$$

If  $\sigma_{k,\mathcal{U}}, \sigma_{k,\mathcal{V}} \lesssim k^{-\alpha}$  for  $\alpha > 1/2$ , then  $K \simeq \delta^{-1/\alpha}$  and  $\text{rank}(\mathcal{T}_{K,K}) \lesssim \delta^{-2/\alpha}$ .

---

Compare to: [Markel et al: Fast linear inversion for highly overdetermined inverse scattering problems, Inverse Problems, 35 (2019)]

## Step 1: Tensor product approximation of $\mathcal{T}$

**Corollary.** For any  $\delta > 0$  there exists  $K \in \mathbb{N}$  with  $K \lesssim \delta^{-2}$  such that

$$\|\mathcal{U} - \mathcal{U}_K\|_{\mathcal{L}(\mathbb{Y}, \mathbb{U})} \leq \delta \quad \text{and} \quad \|\mathcal{V} - \mathcal{V}_K\|_{\mathcal{L}(\mathbb{Z}, \mathbb{V})} \leq \delta,$$

and  $\mathcal{T}_{K,K}c = \mathcal{V}'_K \mathcal{D}(c) \mathcal{U}_K$  satisfies

$$\|\mathcal{T} - \mathcal{T}_{K,K}\|_{\mathcal{L}(\mathbb{X}, \text{HS}(\mathbb{Y}, \mathbb{Z}'))} \lesssim \delta.$$

If  $\sigma_{k,\mathcal{U}}, \sigma_{k,\mathcal{V}} \lesssim k^{-\alpha}$  for  $\alpha > 1/2$ , then  $K \simeq \delta^{-1/\alpha}$  and  $\text{rank}(\mathcal{T}_{K,K}) \lesssim \delta^{-2/\alpha}$ .

Can we do better?

---

Compare to: [Markel et al: Fast linear inversion for highly overdetermined inverse scattering problems, Inverse Problems, 35 (2019)]

## Step 1': Hyperbolic cross approximation of $\mathcal{T}$

**Lemma.** Let  $\sigma_{k,\mathcal{U}} \lesssim k^{-\beta}$  and  $\sigma_{k,\mathcal{V}} \lesssim k^{-\alpha}$  for  $\beta > 1/2$  and  $\alpha > \beta + 1/2$ . Then for any  $\delta > 0$ , we can construct  $\mathcal{T}_{\hat{K}}$  with  $\text{rank} \lesssim \delta^{-1/\beta}$  :

$$\|\mathcal{T} - \mathcal{T}_{\hat{K}}\|_{\mathcal{L}(\mathbb{X}, \text{HS}(\mathbb{Y}, \mathbb{Z}'))} \lesssim \delta.$$

## Step 1': Hyperbolic cross approximation of $\mathcal{T}$

**Lemma.** Let  $\sigma_{k,U} \lesssim k^{-\beta}$  and  $\sigma_{k,V} \lesssim k^{-\alpha}$  for  $\beta > 1/2$  and  $\alpha > \beta + 1/2$ . Then for any  $\delta > 0$ , we can construct  $\mathcal{T}_{\hat{K}}$  with  $\text{rank} \lesssim \delta^{-1/\beta}$  :

$$\|\mathcal{T} - \mathcal{T}_{\hat{K}}\|_{\mathcal{L}(\mathbb{X}, \text{HS}(\mathbb{Y}, \mathbb{Z}'))} \lesssim \delta.$$

### Remarks.

- (i)  $\text{rank } \mathcal{T}_{K,K} = K^2 \simeq \delta^{-2/\alpha}$ , with  $\mathcal{T}_{K,K}c = \mathcal{V}'_K \mathcal{D}(c) \mathcal{U}_K$
- (ii)  $\text{rank } \mathcal{T}_{\hat{K}} \lesssim \delta^{-1/(\alpha - (1/2 + \epsilon))} \implies$  **rank  $\mathcal{T}_{K,K}$  is not optimal if  $\alpha > 1$**
- (iii)  $\mathcal{T}_{\hat{K}}$  can be realized as a **hyperbolic cross approximation** of  $\mathcal{T}_{K,K}$ .

## Step 1': Hyperbolic cross approximation of $\mathcal{T}$

**Lemma.** Let  $\sigma_{k,\mathcal{U}} \lesssim k^{-\beta}$  and  $\sigma_{k,\mathcal{V}} \lesssim k^{-\alpha}$  for  $\beta > 1/2$  and  $\alpha > \beta + 1/2$ . Then for any  $\delta > 0$ , we can construct  $\mathcal{T}_{\widehat{K}}$  with rank  $\lesssim \delta^{-1/\beta}$ :

$$\|\mathcal{T} - \mathcal{T}_{\widehat{K}}\|_{\mathcal{L}(\mathbb{X}, \text{HS}(\mathbb{Y}, \mathbb{Z}'))} \lesssim \delta.$$

### Remarks.

- (i) rank  $\mathcal{T}_{K,K} = K^2 \simeq \delta^{-2/\alpha}$ , with  $\mathcal{T}_{K,K}c = \mathcal{V}'_K \mathcal{D}(c) \mathcal{U}_K$
- (ii) rank  $\mathcal{T}_{\widehat{K}} \lesssim \delta^{-1/(\alpha - (1/2 + \epsilon))} \implies$  rank  $\mathcal{T}_{K,K}$  is not optimal if  $\alpha > 1$
- (iii)  $\mathcal{T}_{\widehat{K}}$  can be realized as a hyperbolic cross approximation of  $\mathcal{T}_{K,K}$ .

**Proof (sketch).** Let  $\{\sigma_{k,*}, a_{k,*}, b_{k,*}\}$  denote the singular systems for  $\mathcal{U}$  and  $\mathcal{V}'$ , respectively. The hyperbolic cross approximation

$$\mathcal{T}_{\widehat{K}}(c) = \sum_{k \geq 1} \sum_{\ell=1}^{L_k} \sigma_{\ell,\mathcal{U}} \sigma_{k,\mathcal{V}'} (\cdot, a_{\ell,\mathcal{U}})_{\mathbb{Y}} \langle \mathcal{D}(c) b_{\ell,\mathcal{U}}, a_{k,\mathcal{V}'} \rangle_{\mathbb{V}' \times \mathbb{V}} b_{k,\mathcal{V}'},$$

with the choice  $L_k = \lfloor \widehat{K}/k^{1+\epsilon} \rfloor$ ,  $\widehat{K} \simeq \delta^{-1/\beta}$ , and  $\epsilon = (\alpha - \beta - 1/2)/(2\beta) > 0$  has the required properties.

cf. [Dung et al: Hyperbolic cross approximation, Birkhäuser/Springer, Cham, 2018.]



## Step 2: Quasi-optimal low-rank approximation via TSVD

**Lemma.** Let  $\delta > 0$  and let  $\mathcal{T}^\delta : \mathbb{X} \rightarrow \text{HS}(\mathbb{Y}, \mathbb{Z}')$  be a linear compact operator such that  $\|\mathcal{T}^\delta - \mathcal{T}\|_{\mathcal{L}(\mathbb{X}, \text{HS}(\mathbb{Y}, \mathbb{Z}'))} \leq C\delta$  for some  $C > 0$ . Let  $\mathcal{P}_{N^\delta}^\delta \mathcal{T}^\delta$  denote the truncated singular value decomposition of  $\mathcal{T}^\delta$  with minimal rank  $N^\delta$  such that

$$\|\mathcal{T}^\delta - \mathcal{P}_{N^\delta}^\delta \mathcal{T}^\delta\|_{\mathcal{L}(\mathbb{X}, \text{HS}(\mathbb{Y}, \mathbb{Z}'))} \leq (C + 1)\delta.$$

Then  $N^\delta \leq N^{\text{svd}}$ , the rank of the TSVD of  $\mathcal{T}$  that yields a  $\delta$  error, and

$$\|\mathcal{T} - \mathcal{P}_{N^\delta}^\delta \mathcal{T}^\delta\|_{\mathcal{L}(\mathbb{X}, \text{HS}(\mathbb{Y}, \mathbb{Z}'))} \leq (2C + 1)\delta,$$

i.e.,  $\mathcal{P}_{N^\delta}^\delta \mathcal{T}^\delta$  is a  $\delta$ -approximation for  $\mathcal{T}$  with quasi-optimal rank.

## Proof: Step 1. Perturbation of singular values

**Claim.** (cf [Kato1966]): Let  $\|\mathcal{T}^\delta - \mathcal{T}\| \leq C\delta$ . For each  $k \in \mathbb{N}$  one has

$$\sigma_k - C\delta \leq \sigma_k^\delta \leq \sigma_k + C\delta,$$

where  $\{\sigma_k\}$  and  $\{\sigma_k^\delta\}$  denote the singular values of  $\mathcal{T}$  and  $\mathcal{T}^\delta$ , respectively.

Choose  $\varepsilon > 0$ , and let  $\mathcal{P}_M^{\text{svd}}\mathcal{T}$  denote the TSVD of  $\mathcal{T}$  with optimal rank  $M$  s.t.

$$\|\mathcal{P}_M^{\text{svd}}\mathcal{T} - \mathcal{T}\| \leq \varepsilon.$$

Optimality of  $M$  and the non-expansiveness of the projection implies

$$\begin{aligned}\sigma_{M+1}^\delta &= \|(\mathcal{I} - \mathcal{P}_M^\delta)\mathcal{T}^\delta\| \leq \|(\mathcal{I} - \mathcal{P}_M^{\text{svd}})\mathcal{T}^\delta\| \\ &\leq \|(\mathcal{I} - \mathcal{P}_M^{\text{svd}})\mathcal{T}\| + \|(\mathcal{I} - \mathcal{P}_M^{\text{svd}})(\mathcal{T} - \mathcal{T}^\delta)\| \leq \varepsilon + C\delta.\end{aligned}$$

For  $\varepsilon = \sigma_{k+1}$ , we have  $M = M(\varepsilon) = k$ , and we conclude that

$$\sigma_{k+1}^\delta \leq \sigma_{k+1} + C\delta.$$

The second inequality follows by interchanging the roles of  $\mathcal{T}$  and  $\mathcal{T}^\delta$ .

## Proof: Step 2.

Let  $N^\delta$  be as in the lemma:  $\sigma_{N^\delta+1}^\delta \leq (C+1)\delta < \sigma_{N^\delta}^\delta$ .

Let  $N^{\text{svd}} = M(\delta)$  as defined in Step 1:  $\sigma_{N^{\text{svd}}+1} \leq \delta$ .

The claim implies

$$\sigma_{N^{\text{svd}}+1}^\delta \leq \sigma_{N^{\text{svd}}+1} + C\delta \leq (C+1)\delta$$

Monotonicity of the singular values:  $N^\delta \leq N^{\text{svd}}$ .

Finally,

$$\|\mathcal{P}_{N^\delta}^\delta \mathcal{T}^\delta - \mathcal{T}\| \leq \|\mathcal{P}_{N^\delta}^\delta \mathcal{T}^\delta - \mathcal{T}^\delta\| + \|\mathcal{T}^\delta - \mathcal{T}\| \leq (2C+1)\delta,$$

i.e.,  $\mathcal{P}_{N^\delta}^\delta \mathcal{T}^\delta$  is a  $\delta$ -approximation for  $\mathcal{T}$  with quasi-optimal rank  $N^\delta \leq N^{\text{svd}}$ .

## Fluorescence diffuse optical tomography

Model

Inverse problem

Outline of model reduction approach

## Abstract Analysis: Model reduction for $\mathcal{T}c = \mathcal{V}'\mathcal{D}(c)\mathcal{U}$

Properties of the forward operator

Step 1: Tensor product approximation

Step 2: Quasi-optimal compression

## Model reduction in action: Application to FDOT

Truth approximation and implementation

Complexity estimates

Runtimes and ranks

## Conclusion

## Function space setting

**recall:** Assumptions of abstract theory:  $\mathbb{U}, \mathbb{V}, \mathbb{X}, \mathbb{Y}, \mathbb{Z}$  separable Hilbert spaces,

$$\mathcal{U} \in \text{HS}(\mathbb{Y}, \mathbb{U}), \quad \mathcal{V} \in \text{HS}(\mathbb{Z}, \mathbb{V}), \quad \mathcal{D} \in \mathcal{L}(\mathbb{X}, \mathcal{L}(\mathbb{U}, \mathbb{V}'))$$

---

Solution operators

$$\begin{aligned} \mathcal{U} : H^1(\partial\Omega) &\rightarrow H^1(\Omega), & q_x &\mapsto \mathcal{U}q_x := u_x \\ \mathcal{V} : H^1(\partial\Omega) &\rightarrow H^1(\Omega), & q_m &\mapsto \mathcal{V}q_m := v_m. \end{aligned}$$

Multiplication operator

$$\mathcal{D} : L^2(\Omega) \rightarrow \mathcal{L}(H^1(\Omega), H^1(\Omega)'), \quad \mathcal{D}(c)u = cu.$$

Function spaces

$$\mathbb{U} = \mathbb{V} = H^1(\Omega), \quad \mathbb{Y} = \mathbb{Z} = H^1(\partial\Omega), \quad \mathbb{X} = L^2(\Omega).$$

**Lemma.** The operators  $\mathcal{U}$  and  $\mathcal{V}$  are Hilbert-Schmidt and their singular values decay like  $\sigma_{k,\mathcal{U}} \lesssim k^{-3/(2d-2)}$  and  $\sigma_{k,\mathcal{V}} \lesssim k^{-3/(2d-2)}$ .

# Truth approximation via standard FEM

- ▶  $T_h$  a quasi-uniform conforming triangulation of the domain  $\Omega$
- ▶  $\mathbb{P}_1$ -Lagrange finite elements:  $\mathbb{U}_h, \mathbb{V}_h \subset H^1(\Omega)$ ,  $\mathbb{X}_h \subset \mathbb{X}$ ;  $\dim = m \approx h^{-d}$
- ▶ induced boundary finite elements:  $\mathbb{Y}_h, \mathbb{Z}_h \subset H^1(\partial\Omega)$ ;  $\dim = k \approx h^{-d+1}$

$\mathbb{U} \in \mathbb{R}^{m \times k}$  discrete counterpart of the operator  $\mathcal{U}$ :

$$(\mathbb{K}_x + \mathbb{M}_x + \mathbb{R}_x) \mathbb{U} = \mathbb{E}_x \mathbb{Q}_x.$$

$\mathbb{V} \in \mathbb{R}^{m \times k}$  discrete counterpart of the operator  $\mathcal{V}$ :

$$(\mathbb{K}_m + \mathbb{M}_m + \mathbb{R}_m) \mathbb{V} = \mathbb{E}_m \mathbb{Q}_m.$$

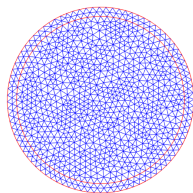
Algebraic form of the truth approximation

$$\mathbb{T}(c) = \mathbb{V}^\top \mathbb{D}(c) \mathbb{U},$$

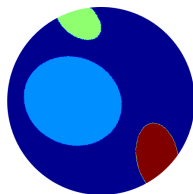
Discrete measurement

$$\mathbb{M}_{ij} = (\mathbb{V}^\top \mathbb{D}(c) \mathbb{U})_{ij} = \mathbb{V}(:, i)^\top \mathbb{D}(c) \mathbb{U}(:, j).$$

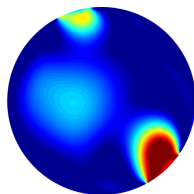
# Numerical example: setup



Computational domain  
and coarse mesh



Minimum norm solution  $c^\dagger$



Reconstruction  $c_{\alpha}^{\delta}$  for  
 $\delta = 10^{-5}$

**Dimensions:**  $m = \dim(\mathbb{X}_h) = \dim(\mathbb{U}_h) = \dim(\mathbb{V}_h)$  and  $k = \dim(\mathbb{Y}_h) = \dim(\mathbb{Z}_h)$   
**discretization error:**  $de_h = \|\mathcal{T}_h - \mathcal{T}\|_{\mathcal{L}(\mathbb{X}, \text{HS}(\mathbb{Y}, \mathbb{Z}'))}$

ref	0	1	2	3	4	5
$m$	993	3881	15345	61025	243393	927161
$k$	88	176	352	704	1408	2816
$de_h$	$6.31 \cdot 10^{-4}$	$1.69 \cdot 10^{-4}$	$4.34 \cdot 10^{-5}$	$1.10 \cdot 10^{-5}$	$2.75 \cdot 10^{-6}$	—

**Remark.** For  $ref = 5$ ,  $\mathbb{T} : \mathbb{R}^{927161} \rightarrow \mathbb{R}^{2816 \times 2816}$ ; storage 56TB of memory; one single evaluation of  $\mathbb{T}(c)$  require approximately 7Tflops.

# Memory and operation cost

## Offline

- ▶ Compression of  $U, V \in \mathbb{R}^{m \times k}$ : mem  $O(km)$ , ops  $O(k^2m + k^3)$   
These steps are at most as expensive as one application of T.
  - ▶ Compression: mem  $O(Km)$ 
    - ▶ tensor product TKK: ops  $O(K^2m)$
    - ▶ hyperbolic cross TK: ops  $O(mK \ln K)$
  - ▶ Recompression to obtain TN with quasi-optimal rank N
    - ▶ of tensor product: ops  $O(mK^4 + K^6)$
    - ▶ of hyperbolic cross: ops  $O(m(K \ln K)^2 + (K \ln K)^4)$
- Use hyperbolic cross approximation TK to compute TN.

## Online (inverse problem)

- ▶ Data compression: mem  $O(Kk)$ , ops  $O(K^2k + Kk^2)$
- ▶ Analysis: depends on N only (cheap!)
- ▶ Synthesis: mem  $O(mN)$ , ops  $O(mN)$



# Truncation ranks $N$ and timings for SVD

of  $T$  (full operator),  $TKK$  (tensor product approx.) and  $TK$  (hyperbolic cross approx.)

refinements	0	1	2	3	4	5
svd( $T$ ) in sec	6.46	28.23	284.33	—	—	—
$N(T)$	231	303	473	—	—	—
svd( $TKK$ ) in sec	6.45	15.05	48.40	248.42	994.66	—
$N(TKK)$	231	276	296	310	314	—
setup of $TK$ , $TKTKt$ in sec	0.01	0.013	1.38	6.31	30.48	140.32
$\text{rank}(TK)$	403	933	1725	1867	1905	1917
svd( $TK$ ) in sec	0.08	0.87	2.57	3.51	3.87	4.03
$N(TK)$	166	266	391	396	401	403

# Timings and error $\|c_\alpha^\delta - c^\dagger\|$ for solving the inverse problem

## Full operator (T) and tensor product approximation (TKK)

refinements	0	1	2	3	4	5
time(T) in sec	1.24	13.91	320.73	—	—	—
time(TKK) in sec	1.22	10.07	65.02	382.76	—	—

## Reduced order model

ref	0	1	2	3	4	5
data compression	0.001	0.005	0.028	0.114	0.457	1.831
regularized normal equations	0.002	0.001	0.002	0.003	0.003	0.003
synthesis	0.001	0.001	0.004	0.015	0.061	0.107
reconstruction error	0.112	0.108	0.107	0.107	0.107	0.107

## Fluorescence diffuse optical tomography

Model

Inverse problem

Outline of model reduction approach

## Abstract Analysis: Model reduction for $\mathcal{T}c = \mathcal{V}'\mathcal{D}(c)\mathcal{U}$

Properties of the forward operator

Step 1: Tensor product approximation

Step 2: Quasi-optimal compression

## Model reduction in action: Application to FDOT

Truth approximation and implementation

Complexity estimates

Runtimes and ranks

## Conclusion

# Conclusion and final remarks

- ▶ Derived a systematic way to obtain a certified reduced order model of quasi-optimal rank for linear operators of the form  $\mathcal{T}c = \mathcal{V}'\mathcal{D}(c)\mathcal{U}$
- ▶ Advantages:
  - ▶ Fast setup time (cost = one single evaluation of forward operator)
  - ▶ Partial compression during recording (access to full data is never required)
- ▶ Problems with a similar structure  $\mathcal{T} = \mathcal{V}'\mathcal{D}(\cdot)\mathcal{U}$ :
  - ▶ Inverse scattering [Colton & Kress, Grinberg & Kirsch, Somersalo et al 1992]
  - ▶ Aeroacoustic source problems [Hohage et al 2020]
- ▶ Compression of  $\mathcal{U}$  and  $\mathcal{V}$  is related to
  - ▶ optimal sources and detectors [Herrmann et al 2009, Krebs et al 2009, van den Doel 2012, Roosta-Khorasani et al 2014]
  - ▶ optimal experimental design [Pukelsheim 2006]

---

[J. Dölz, H. Egger, M. Schlottbom: A model reduction approach for inverse problems with operator valued data <https://arxiv.org/abs/2004.11827>)]