Embedding properties of data-driven dissipative reduced order models

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1 Motivations

2 Finite-difference embedding of reduced order models
   - Stieltjes-Krein theory and finite-difference Gaussian quadratures
   - Imbedding property
   - Embedding via interpolatory-projection
   - Takeaway
   - Applications

3 Inverse problems
   - Inverse Sturm-Liouville problem

4 Beyond Stieltjes theory: Extension to Dissipative System
   - Discrete Telegrapher System

5 Conclusions
To fix idea, assume that $A$ is a PDE operator, and consider SISO ROM

$$f(s) = b^*(A + s)^{-1}b \approx f_k(s) = \tilde{b}^*(\tilde{A} + s)^{-1}\tilde{b}.$$ 

Properties of $A$ are encoded in $\tilde{A}$ via data-driven ROM $f_k$. Can we learn the state variables orthogonal to $b$ and decode those properties directly from $\tilde{A}$?

Applications: Inverse problems; manifold learning in data science; spectrally accurate FD PDE discretization; material design; etc.
Conventional structure-preserving ROMs have spectral properties similar to the one of the full scale problems, i.e., $\tilde{A}$’s spectrum or numerical range lay within the complex hull of the corresponding $A$’s counterparts.

However, this is not sufficient for embedding in the state space of the full scale problem.

We shall see how imposing a certain sparsity pattern allows us to embed $\tilde{A}$ onto state space of $A$ via connection with finite-difference schemes.
Motivations

Mathematicians enlisted to help us:

- From left to right: Thomas Joannes Stieltjes, 1856–1894; Yegor Ivanovich Zolotarev, 1847–1878; Wilhelm Cauer, 1900 – 1945; Mark Grigorievich Krein, 1907–1989
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5 Conclusions
Transfer function of Kac-Krein string

- We consider a boundary problem on $[0, L]$ for ODE

\[-(\sigma u_x)_x + \lambda \rho u = 0, \quad \sigma u_x|_{x=0} = -1, \quad u|_{x=L} = 0,\]

where $0 < L \leq \infty$, $\sigma(x)$ and $\rho(x)$ are regular enough positive functions, $\lambda \in \mathbb{C} \setminus \mathbb{R}_-$ is the Laplace frequency for parabolic problems and the square of the Laplace frequency for hyperbolic ones.

- Our data is the transfer (a.k.a. NtD map, Weyl, impedance) function

\[f(\lambda) = u|_{x=0} \in \mathbb{C}.\]

- The transfer function is Stieltjes-Markov function, e.g., for $L < \infty$ with the help of spectral decomposition it can be represented as

\[f(\lambda) = \sum_{i=1}^{\infty} \frac{r_i}{\lambda + \lambda_i},\]

where $\lambda_i \geq 0$ are eigenvalues of $-\rho^{-1}(\sigma u_x)_x$ and $r_i > 0$ are the squares of the restrictions of the eigenfunctions at $x = 0$. 
Rational approximations of transfer functions

- To **preserve structure** of the original problem consider the **ROM** via **Stieltjes** rational approximants $f_k \approx f$, that can be written in the partial fraction form as

$$f(\lambda) \approx f_k(\lambda) = \sum_{i=1}^{k} \frac{y_i}{\lambda + \theta_i}$$

with non-coinciding poles $\theta_i \geq 0$ and residues $y_i > 0$.

- $f_k$ can be computed as a Padé or multipole Padé approximant of $f$ with optimal parameters, or using control theory tools $\Rightarrow$ **spectral** (linear or super-linear) convergence!
Theorem (Thomas Joannes Stieltjes, 1893)

Any partial fraction \( f_k(\lambda) \) with positive residues \( y_i \) and non-coinciding poles \(-\theta_i \in \mathbb{R}_-\) can be equivalently presented as S-fraction

\[
\sum_{i=1}^{k} \frac{y_i}{\lambda + \theta_i} = \frac{1}{\hat{h}_1 \lambda + \frac{1}{h_1 + \frac{1}{\hat{h}_2 \lambda + \cdots + \frac{1}{h_{k-1} + \frac{1}{\hat{h}_k \lambda + \frac{1}{h_k}}}}} \]

with real positive coefficients \( \hat{h}_i, h_i, i = 1, \ldots, k \) via a \( O(k) \) direct algorithm (e.g., Lanczos).
Finite-difference realization

Wilhelm Cauer and Mark Krein observed that

\[ f_k = w_1, \]  

where \( w_1 \) is the Dirichlet component of the finite-difference solution

\[
\frac{1}{\hat{h}_i} \left( \frac{w_{i+1} - w_i}{h_i} - \frac{w_i - w_{i-1}}{h_{i-1}} \right) - \lambda w_i = 0, \quad i = 2, \ldots, k, \\
\left( \frac{w_1 - w_0}{h_0} \right) = -1, \quad w_{k+1} = 0.
\]
Finite-difference Gaussian quadrature rules

- Original Krein interpretation of $h$ and $\hat{h}$ was as stiffnesses and masses of a string \(^1\).

- For $\sigma = \rho(x) = 1$ they can be interpreted as respectively primary and dual steps of *staggered* three-point finite-difference scheme, as so-called ‘finite-difference Gaussian quadrature rules’, a.k.a. spectrally matched or optimal grids \(^2\).

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\(^1\) Gantmakher and Krein, 1950. Also known RC or LC interpretations by Cauer or in circuit synthesis from 1920s

\(^2\) Dr.&Knizhnerman, SINUM 2000
Examples of FD Gaussian rules with exponential convergence, $\sigma = \rho(x) = 1$

Padé for $L = 1$.\textsuperscript{3}

Optimal Zolotarev rational approximation for $L = \infty$.\textsuperscript{4}

- Observations: sharp refinement toward 0, grids *almost* centered, tend to cover the entire computational domain.

\textsuperscript{3}Dr.\&Knizhnerman, SINUM 2000
\textsuperscript{4}Ingerman, Dr., Knizhnerman, Comm. Pure\&Appl. Math., 2000
Example: plane wave propagation

\[ u_{xx} - u_{tt} = 0; \]
\[ u_x |_{x=0} = g(t), \quad u |_{x=1} = 0; \quad u |_{t<0} = 0. \]
FD Gaussian rules for 1D wave problem. II

Example: 1D wave propagation
optimal grid + 1 node

+ 1 node
Perfectly Matched Layers (PMLs) are used for reflectionless truncation of unbounded computational domains.

In non-reflecting PML waves should decay exponentially $\Rightarrow$ complex coordinate transform$^5$

The optimal rational (mod. Zolotarev) approximant yields the FD Gaussian quadr. on a complex curve.$^6$. *Optimal complex rational approximation is not unique, multiple solutions give the same results.*

$^5$Beringer, 1994; Chew, Jin, Michielsen, 1997

$^6$Dr., Guettel, Knizhnerman 2016
Rational interpolation via Loewner framework

- Interpolatory projection framework allows to construct rational interpolants by projecting PDE on the solution snapshots corresponding to the interpolation points in the form
  \[ V^T AV \tilde{u} + \lambda V^T V \tilde{u} = V^T b. \]
- We need to compute elements of \( V^T V \) and \( V^T AV \) for \( V = ((A + l_1 I)^{-1} b, \ldots, (A + l_n I)^{-1} b) \)
- Notice that 
  \[ b^T (A + l_i I)^{-1} b^T - b^T (A + l_j I)^{-1} b = (l_j - l_i) ((A + l_i I)^{-1} b)^T (A + l_j I)^{-1} b \]
- Hence, elements of \( V^T V \) are \( \frac{f(l_i) - f(l_j)}{l_j - l_i} \)
- Similarly, elements of \( V^T AV \) are \( \frac{l_i f(l_i) - l_j f(l_j)}{l_i - l_j} \).
- Time-domain counterpart is available.  

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7 Dr., Mamonov, Thaler, Zaslavsky, 2016.
8 Mayo, Antoulas, 2007; Antoulas, Beattie, Gugercin 2017
Transformation to tri-diagonal form is done via specially ordered (data-driven!) Cholesky decomposition of mass-matrix $V^T V = (R^* R)^{-1} \equiv \text{pivoted } QR \text{ of state solutions } V = QR$.\(^9\)

$Q$ is a $\approx$ sparsest basis in the range of $V$!\(^{10}\) In the figure, functions $\tilde{u}_i$ are the infinite-dimensional columns of $Q$.

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\(^9\) Marchenko, Gel’fand, Levitan, 1950s

\(^{10}\) Borcea, Dr., Mamonov, Moskow, Zaslavsky, IP, in press
Localization of QR basis and FD Gaussian quadratures

**Figure 2.** Orthogonalized basis plotted with its corresponding finite difference grid. Stars * correspond to primary grid points and plus signs + to dual grid points. Primary grid points are color coded with corresponding basis functions. Note the masses of the basis functions are concentrated between each primary point and the next dual point.
What we learned so far

- Finite-difference Gaussian quadrature rules is a network realization of reduced order models for PDEs.
- Allow **spectral** convergence using at targeted points by optimizing finite-difference steps.
- Embeds ROM back to physical space.
- Data-driven transformation from the Loewner to network framework sparsifies projection basis functions, and make them look like finite-elements localized at the matching nodes of the finite-difference Gaussian quadratures.
Overview of applications

- Optimal discretization of perfectly matched layers (PMLs). Will be touched.\textsuperscript{11}
- Discretization of multi-scale wave propagation problems via matrix-valued networks, not in this talk\textsuperscript{12}
- Direct nonlinear solution of inverse hyperbolic problems via data-driven reduced order models. We will touch that\textsuperscript{13}
- Manifold preserving reduced order graph-Laplacians with application to cluster analysis, not in this talk.\textsuperscript{14}

\textsuperscript{12}Dr., Mamonov, Zaslavsky, SIAM MSMS, 2017
\textsuperscript{13}Dr., Mamonov, Zaslavsky, 2016 SIIMS; Dr., Mamonov, Zaslavsky, 2018 SIIMS; Borcea, Dr., Mamonov, Zaslavsky, 2019, JCP; Borcea, Dr., Mamonov, Zaslavsky, SIIMS, in press
\textsuperscript{14}Dr., Mamonov, Zaslavsky, arXive, 2020
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5 Conclusions
Continuous Sturm–Liouville inverse problem

- We consider a boundary problem on $[0, L']$ for ODE

$$-(\gamma u_{x'})_{x'} + \lambda \rho u = 0, \quad \gamma u_{x'}|_{x'=0} = -1, \quad u|_{x'=L} = 0,$$

(4)

where $0 < L < \infty$, $\sigma(x')$ and $\rho(x')$ are regular enough positive functions.

- Our data is the transfer function

$$f(\lambda) = u|_{x'=0} = \sum_{i=1}^{\infty} \frac{r_i}{\lambda + \lambda_i}.$$  

- It is impossible to find simultaneously $\gamma$, $\rho$ and $L'$ from $f$. 
Sturm–Liouville inverse problem in travel time coordinates

- Coordinate transform $dx = \frac{dx'}{c(x')}$ transforms $\gamma(x')$ to $\frac{\gamma(x)}{c(x')}$ and $\rho(x')$ to $\rho(x)c(x')$ without changing $f(\lambda)$ that’s why we can’t find simultaneously $\gamma$, $\rho$ and $L$.

- By choosing travel time coordinate with $c(x) = \sqrt{\frac{\gamma(x')}{\rho(x')}}$ (speed of wave propagation), we obtain Sturm–Liouville equation in divergence form:

$$-(\sigma u_x)_x + \lambda \sigma u = 0, \quad \sigma u_x|_{x=0} = -1, \quad u|_{x=L} = 0,$$

where $\sigma = \sqrt{\gamma(x')\rho(x')}$. is the impedance, $L = \int_0^{L'} \frac{dx'}{c(x')}$. 

- Inverse spectral problem:

$$f(\lambda) \mapsto \sigma(x).$$

Uniqueness, solvability, algorithm - Marchenko, Gel’fand, Levitan, Krein, 1950s.
Discrete inverse spectral problem, pole residues matching

- Simplest matching condition,

\[ f_k(\lambda) = \sum_{i=1}^{k} \frac{r_i}{\lambda + \theta_i} = \sum_{i=1}^{k} \frac{r_i}{\lambda + \lambda_i}, \]

i.e.,

\[ y_i = r_i, \quad \theta_i = \lambda_i, \quad i = 1, \ldots, k. \]

- The same Stieltjes inverse problem as discussed earlier:

\[ \sum_{i=1}^{k} \frac{y_i}{\lambda + \theta_i} \equiv \frac{1}{\gamma_1\lambda + \frac{1}{\gamma_1 + \frac{1}{\gamma_2\lambda + \ldots + \frac{1}{\gamma_{k-1} + \frac{1}{\gamma_k\lambda + \frac{1}{\gamma_k}}}}}}. \]
Discrete inverse spectral problem, pole residues matching

- But now instead of $\hat{h}_i$ and $h_i$ we have combined finite-difference stiffness & masses as $\gamma_i = \frac{h_i}{\sigma_i}$, $\hat{\gamma}_i = h_i \sigma_i$. respectively:

$$\frac{1}{\hat{\gamma}_i} \left( \frac{u_{i+1} - u_i}{\gamma_i} - \frac{u_i - u_{i-1}}{\gamma_{i-1}} \right) - Au_i = 0, \ i = 1, \ldots, k,$$

$$\left( \frac{u_1 - u_0}{\gamma_0} \right) = -1, \ u_{k+1} = 0.$$

- Can we just take some grid steps $h_i, \hat{h}_i, i = 1, \ldots, k$ and define $\sigma(x_i) \approx \frac{\hat{\gamma}_i}{\hat{h}_i}, \sigma(\hat{x}_i) \approx \frac{h_i}{\gamma_i}$, where $x_{i+1} = x_i + h_i$, $\hat{x}_i = \hat{x}_{i-1} + \hat{h}_i$?

- Depending on the grid, can get different answers for the same $\gamma, \hat{\gamma}$. So for proper embedding we need to learn the grid.
Trainable finite-difference inversion

- **Offline (training) step**: Solve the discrete inverse problem with simulated data a training model for known $\sigma = \sigma_0^{15}$ and find the grid steps $\hat{h}_i, h_i$.

- **Online step**:
  - Solve the discrete inverse problem with the measured TM data, find $\hat{\gamma}_i, \gamma_i$.
  - Using $\hat{h}_i, h_i$ obtained on the training step and $\hat{\gamma}_i, \gamma_i$ from the previous step, compute $\sigma(x_i) \approx \frac{\hat{\gamma}_i}{h_i}$, $\sigma(\hat{x}_i) \approx \frac{h_i}{\gamma_i}$.

15 E.g., $\sigma_0 = 1$
Convergence result

We assume that training and measured (validation) data are computed by matching first $k$ terms of the partial fraction expansions of corresponding transfer functions.

**Theorem (Borcea et al, CPAM 2005)**

Let us (for simplicity) assume, that the Gaussian finite-difference quadrature is computed for $\sigma(z) \equiv 1$. Then $\forall$ uniformly positive and bounded $\sigma(z)$, $\sigma(z) \in H^3[0, l]$ discrete $\sigma_i$ and $\hat{\sigma}_i$ converge to the true $\sigma(z)$ at the FD nodes **iff** the FD grid asymptotically close to the optimal one as $m \to \infty$. 
Inversion examples

**Figure:** Equidistant grid

**Figure:** FD Gaussian rule
We consider 2D inverse problem for acoustic wave eq. with an array of $m$ receivers. The shots are fired by moving the transmitter consequently at the receiver positions, so the data are the elements of the matrix-valued multi-input/multi-output (MIMO) transfer function

$$F(\lambda) = F(\lambda)^* \in \mathbb{C}^{m \times m}.$$
Multidimensional generalization of discrete inverse problem

- All SISO linear algebra is automatically extended to the MIMO case by using $m \times m$ matrix valued $h_i$ and $\hat{h}_i$ instead of scalars, i.e., instead of tridiagonal $\mathcal{T} \in \mathbb{R}^{k \times k}$ we will have block-tridiagonal matrix $\mathcal{T} \in \mathbb{R}^{mk \times mk}$ with $m \times m$ blocks, etc.

- Trick: $m \times m$ matrix valued continued fraction

$$\frac{1}{\hat{h}_1 \lambda + \frac{1}{h_1 + \frac{1}{\hat{h}_2 \lambda + \ldots \frac{1}{h_{k-1} + \frac{1}{\hat{h}_k \lambda + \frac{1}{h_k}}}}}}$$

does not rely on commuting of matrix Stieltjes parameters $h_i \in \mathbb{R}^{m \times m}$, $\hat{h}_i \in \mathbb{R}^{m \times m}$. 
Imaging hydraulic fractures

- Important application: acoustic monitoring of hydraulic fracturing
- Multiple thin fractures (down to 1 cm in width, here 10 cm)
- Very high contrasts: $c = 4500 \text{m/s}$ in the surrounding rock, $c = 1500 \text{m/s}$ in the fluid inside fractures
Imaging hydraulic fractures

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Summary: compress and embed

- We consider large-scale multi-input/multi-output problems for hyperbolic and parabolic linear-time invariant dynamical systems that can be described by Stieltjes theory.
- We approximate these problems by reduced order problems (ROMs) via Stieltjes continued fractions that can be realized via sparse networks with scalar as well as matrix weights, mimicking discretization of the underlying continuous problems.
- The ROM weights are chosen via rigorous learning algorithms, and can be interpreted as finite-difference grid steps or discretized media parameters.
- Thus compressed by ROM data are imbedded back to physical space and allow to image PDE coefficients.
- Embedding is particularly important for solution of inverse scattering problems with strong multi-scattering effects (e.g. multiple echoes), when conventional linearized (Born) inversion is not applicable. More in Jörn Zimmerling’s poster today.
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5. Conclusions
Quadratic second order problem and Telegrapher System

- By adding damping term to the second order problem in travel time coordinates we obtain quadratic problem

\[ -(\sigma u_x)_x + s\gamma u - s^2 \sigma u = 0, \quad \sigma u_x|_{x=0} = -1, \quad u|_{x=L} = 0, \]

where \( s = \sqrt{-\lambda} \).

- However we will use a more general Telegrapher or transmission line system, that in first order form can be written as

\[
\begin{align*}
    r(x)u(x, s) + \sigma(x) \frac{d}{dx}v(x, s) &= -su(x, s), \\
    \frac{1}{\sigma(x)} \frac{d}{dx}u(x, s) + \hat{r}(x)v(x, s) &= -sv(x, s), \\
    v(0) &= -1, \quad u(L) = 0.
\end{align*}
\]

(5)

- The Telegrapher system is equivalent to the quadratic problem when \( r = \frac{\gamma(x)}{\sigma(x)} \) and \( \hat{r} = 0 \).
Passive ROM of dissipative systems.

- We define transfer function:
  \[ \tilde{f}(s) = u|_{x=0}. \]

- For \( r, \hat{r} \geq 0 \) the Telegrapher system is port-Hamiltonian, and \( \tilde{f} \) is passive.

- Assuming that we can construct passive ROM \( \tilde{f}_k(s) \approx \tilde{f}^{16} \) in the form
  \[ \tilde{f}_k(s) = \sum_{i=1}^{k} \frac{y_i}{s + \theta_i} \]

  such that \( \tilde{f}_k(s) = \overline{\tilde{f}_k(s)} \), we want to match \( \tilde{f}_k(s) \) by the transfer function of the discrete Telegrapher system.

\(^{16}\text{Questions to Beattie, Gugercin, Mehrmann - :)\)
ROM realization of dissipative systems.

The discrete Telegrapher system with tri-diagonal matrix

\[
\begin{align*}
    r_j u_j + \frac{v_j - v_{j-1}}{\hat{h}_j/\sigma_j} &= -su_j, \\
    \frac{u_{j+1} - u_j}{\hat{\sigma}_j h_j} + \hat{r}_j v_j &= -sv_j,
\end{align*}
\]

\[j = 1, \ldots, k,\]
\[v_0 = -1, \quad u_{k+1} = 0,\]

where

\[u_1 = \tilde{f}_k(s).\]
Ladder RCL realization

- Equivalent realization in terms of the ladder RCL network \( \equiv \) discrete telegrapher system.

- The ROM parameters correspond to capacitors \( \hat{H}_j = \hat{h}_j/\sigma_j \), inductors \( H_j = \hat{\sigma}_j h_j \), primary conductors \( R_j = r_i \) and dual conductors \( \hat{R}_j = \hat{r}_i \).

In MIMO setting these parameters, as well as electric variables \( U_j(t) \) and magnetic variables \( V_j(t) \) are matrix-valued to account for “lateral” (relative to the transmission line), cross-range electromagnetic propagation.
Extended Stieltjes String:

In the figure we show the spring-mass-damper realization. Consistent with original Stieltjes string when \( \hat{m}_j = \hat{h}_j / \sigma_j \) and \( k_j = 1 / (\hat{\sigma}_j h_j) \). The damping coefficients are given by \( c_j = r_j \) and \( \hat{c}_j = 1 / \hat{r}_j \). Note that if \( r_j = 0 \) and \( \hat{r}_j = 0 \) recovers the original Stieltjes.
Discrete inverse problem via J-Hermitian Lanczos

- Assume weakly damped systems ($\Im(\theta \neq 0)$, $k$ even, $\theta_{2i} = \bar{\theta}_{2i+1}$, $y_{2i} = \bar{y}_{2i+1}$, $i = 1, \ldots, k/2$).

- 2$k$ complex spectral data $\theta_{2i}$ $y_{2i}$, $i = 1, \ldots, k/2$

2$k$ steps of J-symmetric Lanczos $\mapsto$

4$k$ real parameters $\hat{\sigma}_j h_j$, $\hat{h}_j/\sigma_j$, $r_i$ and $\hat{r}_i$, $i = 1, \ldots, k$.  


Finite-difference inversion of dissipative problems, first try

- Offline (training) step: Obtain grid $h_i, \hat{h}_i$ from training via the same non-damped problem $(r(x) = \hat{r}(x) = 0)$ as before.
- Online step:
  - Solve the discrete inverse problem via J-Hermitian Lanczos with the measured damped data $\tilde{f}(s)$, find $\hat{h}_j/\sigma_j, \hat{\sigma}_j h_j, r_i, \hat{r}_i$.
  - Using grid obtained from offline step compute $\sigma(x_i) = \sigma_i, \hat{\sigma}(\hat{x}_i) = \hat{\sigma}_i, r(\hat{x}_i) = r_i, \hat{r}(x_i) = \hat{r}_i$. 
Inversion results, first try

- $\sigma$ is as good as for the non damped problem.
- However $r_i$ does not match $r(x)$ and $\hat{r}_i$ even negative for this passive problem, i.e., the ladder realization is not in port-Hamiltonian form, counterintuitively. There are no positivity results as in the Stieltjes case. Known artifact in network synthesis.
Need one more stretching

- Let us consider frequency dependent stretching

\[ dx = \frac{dx''}{1 + \frac{\lambda(x'')}{s}}. \]

- In the Fourier domain when \( s \) is imaginary, this transform becomes famous non-reflective complex PML stretching.

- In new coordinates (omitting lower order term \( O(\frac{||\lambda||}{s}) \)).

\[
[r(x'') - \lambda(x'')] u(x'', s) + \sigma(x'') \frac{d}{dx''} v(x'', s) = -su(x'', s),
\]

\[
\frac{1}{\sigma(x'')} \frac{d}{dx''} u(x'', s) + [\hat{r}(x'') - \lambda(x'')] v(x'', s) = -sv(x'', s). \quad (7)
\]
Inversion results constrained by PML stretching.

- In the classical Sturm-Liouville problem we could not find two coefficients simultaneously and used travel the time transform to get rid of one. Similarly, here we can not find both $r$ and $\hat{r}$, need to do the same, i.e., use prior. Here it is triviality of dual losses $[\hat{r}(x'') - \lambda(x'')] = 0$, that yields primary loss $\approx [\hat{r}(x'') + r(x'')]$. 
Inversion results constrained by PML stretching.

- Assumption of model independent grid becomes inaccurate for strong damping due to neglected $O\left(\frac{\|\lambda\|}{s}\right)$ term. Need to train grid for damped problems, work in progress.
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5. Conclusions
Summary: compress, transform, stretch and embed

- We approximate transfer functions by data-driven ROMs that can be realized via sparse networks with scalar as well as matrix weights, mimicking discretization of the underlying continuous problems.
- The ROM weights are chosen via rigorous learning algorithms, and can be interpreted as finite-difference grid steps or discretized media parameters, thus embedding data-driven ROMs back to physical space.
- Extending invariant coordinate stretching from continuous to discrete settings is a key.
- Applications to inverse problems, PDE discretization etc.
To do:

- Nonlinear problems (known connection of Krein theory with and nonlinear PDEs); MIMO dissipative problems; optimal sponge layers for anisotropic wave problems; cloaking design; graph-convolution NN.
- You are welcome to our team!