Rank-structured matrices induced by dynamical systems on graphs

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Overview

The problem: what are the low-rank properties of inverses of sparse matrices?
Motivation: shortcomings of existing rank-structured representations in applications
A potential framework: GIRS matrices and their representations
GIRS representations on acyclic graphs: tree quasi-separable matrices
Conclusions & future work

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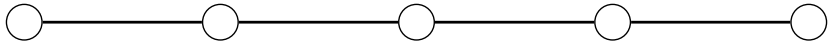
Conclusions & future work

Question: what is the algebraic structure of the inverse of a tridiagonal matrix?

$$\mathrm{A} = \begin{bmatrix} a_1 & b_1 & & & \\ c_1 & a_2 & b_2 & & \\ & c_2 & a_3 & b_3 & \\ & & c_3 & a_4 & b_4 \\ & & & c_4 & a_5 \end{bmatrix}$$

Adjacency graph $\mathbb{G}(\mathrm{A})$:



Answer: quasi-separable structure

$$
A^{-1} = \begin{bmatrix} d_1 & p_1 r_1 q_2 & p_1 r_1 r_2 q_3 & p_1 r_1 r_2 r_3 q_4 & p_1 r_1 r_2 r_3 r_4 q_5 \\ u_2 t_1 v_1 & d_2 & p_2 r_2 q_3 & p_2 r_2 r_3 q_4 & p_2 r_2 r_3 r_4 q_5 \\ u_3 t_1 v_1 & u_3 t_2 v_2 & d_3 & p_3 r_3 q_4 & p_3 r_3 r_4 q_5 \\ u_4 t_3 t_2 t_1 v_1 & u_4 t_3 t_2 v_2 & u_4 t_3 v_3 & d_4 & p_4 q_5 \\ u_5 t_4 t_3 t_2 t_1 v_1 & u_5 t_4 t_3 t_2 v_2 & u_5 t_4 t_3 v_3 & u_5 t_4 v_4 & d_5 \end{bmatrix}
$$

algebraic structure: All off-diagonal blocks are unit rank...
representation: *Quasi-separable matrices* (there are others)

Answer: quasi-separable structure

$$A^{-1} = \begin{bmatrix} d_1 & p_1 r_1 q_2 & p_1 r_1 r_2 q_3 & p_1 r_1 r_2 r_3 q_4 & p_1 r_1 r_2 r_3 r_4 q_5 \\ u_2 t_1 v_1 & d_2 & p_2 r_2 q_3 & p_2 r_2 r_3 q_4 & p_2 r_2 r_3 r_4 q_5 \\ u_3 t_1 v_1 & u_3 t_2 v_2 & d_3 & p_3 r_3 q_4 & p_3 r_3 r_4 q_5 \\ u_4 t_3 t_2 t_1 v_1 & u_4 t_3 t_2 v_2 & u_4 t_3 v_3 & d_4 & p_4 q_5 \\ u_5 t_4 t_3 t_2 t_1 v_1 & u_5 t_4 t_3 t_2 v_2 & u_5 t_4 t_3 v_3 & u_5 t_4 v_4 & d_5 \end{bmatrix}$$

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u_2 t_1 v_1 & d_2 & p_2 r_2 q_3 & p_2 r_2 r_3 q_4 & p_2 r_2 r_3 r_4 q_5 \\
u_3 t_1 v_1 & u_3 t_2 v_2 & d_3 & p_3 r_3 q_4 & p_3 r_3 r_4 q_5 \\
u_4 t_3 t_2 t_1 v_1 & u_4 t_3 t_2 v_2 & u_4 t_3 v_3 & d_4 & p_4 q_5 \\
u_5 t_4 t_3 t_2 t_1 v_1 & u_5 t_4 t_3 t_2 v_2 & u_5 t_4 t_3 v_3 & u_5 t_4 v_4 & d_5
\end{bmatrix}
$$

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algebraic structure: All off-diagonal blocks are unit rank...
representation: *Quasi-separable matrices* (there are others)

no. of parameters in the quasi-separable representation of A^{-1}

$$\approx$$

no. of nonzero entries in A

Continuous case: tridiagonal matrix A is a discretization of operator $\mathcal{A} := w(x)\frac{d^2}{dx^2}$

A simple boundary value ODE problem:

$$w(x)\frac{d^2 q(x)}{dx^2} - \lambda q(x) = 1, \quad q(0) = 0, \quad q(1) = 0, \quad w(x) = 1$$

$$\Leftrightarrow$$

Integral formulation:

$$q(x) - \lambda \int_0^1 K(x,y) q(y) \mathrm{d}y = f(x)$$

with semi-separable kernel $K(x,y) = \begin{cases} x(y-1), & 0 \le x \le y \\ y(x-1) & y \le x \le 1 \end{cases}, \quad f(x) = \frac{1}{2}x(x-1)$

Continuous case: tridiagonal matrix A is a discretization of operator $\mathcal{A} := w(x)\frac{d^2}{dx^2}$

Discretization (e.g. using Nyström's method) of

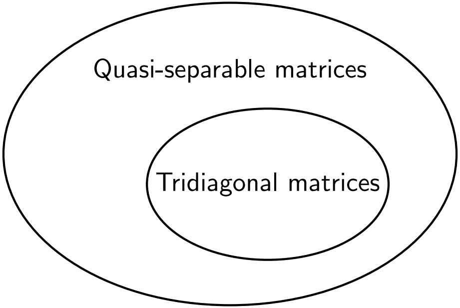
$$\int_0^1 \left(\delta(x-y) - \lambda K(x,y)\right) q(y)\mathrm{d}y = f(x)$$

yields the linear system:

$$\begin{bmatrix} d_1 & p_1 q_2 & p_1 q_3 & p_1 q_4 & p_1 q_5 \\ u_2 v_1 & d_2 & p_2 q_3 & p_2 q_4 & p_2 q_5 \\ u_3 v_1 & u_3 v_2 & d_3 & p_3 q_4 & p_3 q_5 \\ u_4 v_1 & u_4 v_2 & u_4 v_3 & d_4 & p_4 q_5 \\ u_5 v_1 & u_5 v_2 & u_5 v_3 & u_5 v_4 & d_5 \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \\ q_5 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix}$$

Quasi-separable matrices are closed under inversion!

- Closure property: The inverse of a quasi-separable matrix is *again* quasi-separable.
- Tridiagonal matrices are a *special case* of quasi-separable.
- Note: the inverse of a quasi-separable is generally *not* tridiagonal.
- Addition & products preserve "quasi-separable structures" (more later!)



Focus of this talk: what can we say for more general sparse matrices?

Given a sparse matrix $\mathrm{A} \in \mathbb{C}^{n \times n}$ with adjacency graph $\mathbb{G}(\mathrm{A})$:

1. What are the algebraic structures preserved by A^{-1}?
2. Does there exist suitable representation A^{-1} *satisfying* the closure property?

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1. *graph-induced rank-structure (GIRS)*
2. *Rank-structured matrices induced by dynamical systems on graphs*:
   - Acyclic adjacency graphs: a *complete* answer
   - Non-acyclic adjacency graphs: a *partial* answer

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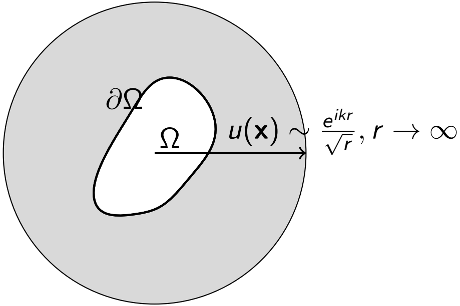
Rank-structured matrices in practice: boundary element method for BVPs

Exterior Helmholtz with Dirichlet boundary conditions

$$\nabla^2 u(\mathbf{x}) + k^2 u(\mathbf{x}) = 0, \quad \mathbf{x} \in \mathbb{R}^2 \setminus \Omega$$
$$u(\mathbf{x}) = g(\mathbf{x}), \quad \mathbf{x} \in \partial\Omega$$



Reformulate to Fredholm integral equation on $\partial\Omega$

$\downarrow$

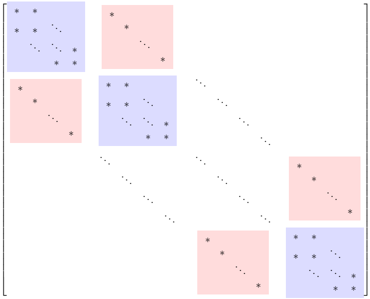
Fast multipole method (FMM): exploit low-rank structures in far-field

Rokhlin, Vladimir. "Rapid solution of integral equations of classical potential theory." Journal of computational physics 60, no. 2 (1985): 187-207.

Rank-structured matrices in practice: Schur complements in PDE discretizations

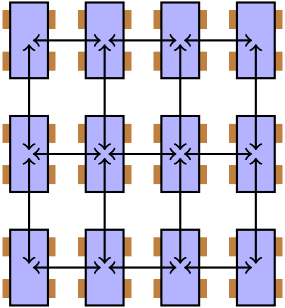
Low off-diagonal rank structure in $S_k = A_k - C_k S_{k-1}^{-1} B_k, \quad S_0 = A_0$

$$\begin{bmatrix} A_0 & B_1 & & \\ C_1 & A_1 & \ddots & \\ & \ddots & \ddots & B_{n-1} \\ & & C_{n-1} & A_{n-1} \end{bmatrix} =$$



Chandrasekaran, Shiv, Patrick Dewilde, Ming Gu, and Naveen Somasunderam. "On the numerical rank of the off-diagonal blocks of Schur complements of discretized elliptic PDEs." SIAM Journal on Matrix Analysis and Applications 31, no. 5 (2010): 2261-2290.

Rank-structured matrices in practice: optimal control of spatially distributed systems



Vehicle platoon

Vibrating string: $\frac{\partial^2 v(x,t)}{\partial t^2} = k(x)\frac{\partial^2 v(x,t)}{\partial x^2} + b(x)u(x,t)$

Low-rank structure in state-space models:

$$\dot{\boldsymbol{x}} = \mathrm{A}\boldsymbol{x} + \mathrm{B}\boldsymbol{u}$$
$$\boldsymbol{y} = \mathrm{C}\boldsymbol{x} + \mathrm{D}\boldsymbol{u}$$

Communication constraints on feedback $\boldsymbol{u} = \mathrm{F}\boldsymbol{x}$!

Rice, Justin K., and Michel Verhaegen. "Distributed control: A sequentially semi-separable approach for spatially heterogeneous linear systems." IEEE Transactions on Automatic Control 54, no. 6 (2009): 1270-1283.

Bamieh, Bassam, Fernando Paganini, and Munther A. Dahleh. "Distributed control of spatially invariant systems." IEEE Transactions on automatic control 47, no. 7 (2002): 1091-1107.

Many frameworks for efficient linear algebra with rank-structured matrices

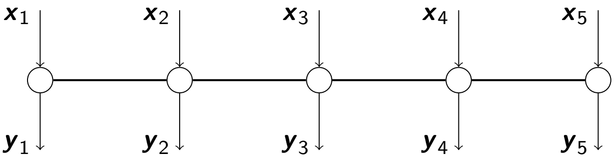
All have their benefits and special use cases:

- FMM matrices (Rokhlin & Greengard)
- Hierarchichally semi-separable (HSS) matrices (Chandrasekaran & Gu)
- Sequentially Semi-Separable (SSS) matrices (Chandrasekaran, Dewilde, van der Veen)
- HODLR
- H-matrices and H^2-matrices (Hackbusch)
- Quasi-separable matrices (Eidelman, Gohberg)
- Semi-separable matrices (Van Barel, Vandebril, Mastronardi)

Our interest:

Rank-structured matrices with closure property $\rightarrow$ direct solvers & preconditioners

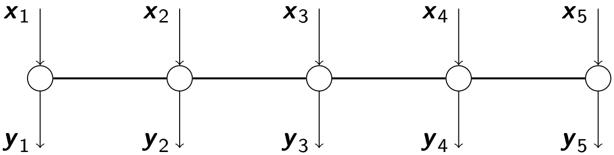
SSS matrices: input-output map of mixed linear time-variant (LTV) system



state-space dynamics:

$$
\begin{aligned}
\boldsymbol{g}_k &= \mathrm{W}_k \boldsymbol{g}_{k+1} + \mathrm{V}_k^\top \boldsymbol{x}_k, \quad \boldsymbol{g}_n = \mathrm{V}_n^\top \boldsymbol{x}_n \\
\boldsymbol{h}_k &= \mathrm{R}_k \boldsymbol{h}_{k-1} + \mathrm{Q}_k^\top \boldsymbol{x}_k, \quad \boldsymbol{h}_1 = \mathrm{Q}_1^\top \boldsymbol{x}_1 \\
\boldsymbol{y}_k &= \mathrm{U}_k \boldsymbol{g}_{k+1} + \mathrm{P}_k \boldsymbol{h}_{k-1} + \mathrm{D}_k \boldsymbol{x}_k.
\end{aligned}
$$

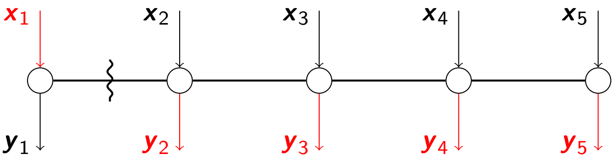
SSS matrices: input-output map of mixed linear time-variant (LTV) system



Resulting input-output relation:

$$
\begin{bmatrix}
D_1 & U_1V_2^\top & U_1W_2V_3^\top & U_1W_2W_3V_4^\top & U_1W_2W_3W_4V_5^\top \\
P_2Q_1^\top & D_2 & U_2V_3^\top & U_2W_3V_4^\top & U_2W_3W_4V_5^\top \\
P_3R_2Q_1^\top & P_3Q_2^\top & D_3 & U_3V_4^\top & U_3W_4V_5^\top \\
P_4R_3R_2Q_1^\top & P_4R_3Q_2^\top & P_4Q_3^\top & D_4 & U_4V_5^\top \\
P_5R_4R_3R_2Q_1^\top & P_5R_4R_3Q_2^\top & P_5R_4Q_3^\top & P_5Q_4^\top & D_5
\end{bmatrix}
\begin{bmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \\ \boldsymbol{x}_3 \\ \boldsymbol{x}_4 \\ \boldsymbol{x}_5 \end{bmatrix}
=
\begin{bmatrix} \boldsymbol{y}_1 \\ \boldsymbol{y}_2 \\ \boldsymbol{y}_3 \\ \boldsymbol{y}_4 \\ \boldsymbol{y}_5 \end{bmatrix}
$$

The ranks of the so-called Hankel blocks dictate the state dimension sizes

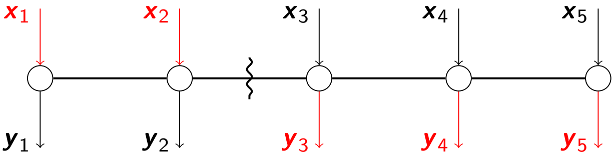


state dimension of $\boldsymbol{h}_1 \Leftrightarrow$ rank H_1

$$\left[\begin{array}{c|cccc} \mathrm{A}_{11} & \mathrm{A}_{12} & \mathrm{A}_{13} & \mathrm{A}_{14} & \mathrm{A}_{15} \\ \hline \mathrm{A}_{21} & \mathrm{A}_{22} & \mathrm{A}_{23} & \mathrm{A}_{24} & \mathrm{A}_{25} \\ \mathrm{A}_{31} & \mathrm{A}_{32} & \mathrm{A}_{33} & \mathrm{A}_{34} & \mathrm{A}_{35} \\ \mathrm{A}_{41} & \mathrm{A}_{42} & \mathrm{A}_{43} & \mathrm{A}_{44} & \mathrm{A}_{45} \\ \mathrm{A}_{51} & \mathrm{A}_{52} & \mathrm{A}_{53} & \mathrm{A}_{54} & \mathrm{A}_{55} \end{array}\right] \left[\begin{array}{c} \boldsymbol{x}_1 \\ \hline \boldsymbol{x}_2 \\ \boldsymbol{x}_3 \\ \boldsymbol{x}_4 \\ \boldsymbol{x}_5 \end{array}\right] = \left[\begin{array}{c} \boldsymbol{y}_1 \\ \hline \boldsymbol{y}_2 \\ \boldsymbol{y}_3 \\ \boldsymbol{y}_4 \\ \boldsymbol{y}_5 \end{array}\right]$$

Notice how the cuts correspond to the Hankel blocks

The ranks of the so-called Hankel blocks dictate the state dimension sizes



state dimension of $\boldsymbol{h}_2 \Leftrightarrow$ rank H_2

$$\left[\begin{array}{cc|ccc} \mathrm{A}_{11} & \mathrm{A}_{12} & \mathrm{A}_{13} & \mathrm{A}_{14} & \mathrm{A}_{15} \\ \mathrm{A}_{21} & \mathrm{A}_{22} & \mathrm{A}_{23} & \mathrm{A}_{24} & \mathrm{A}_{25} \\ \hline \mathrm{A}_{31} & \mathrm{A}_{32} & \mathrm{A}_{33} & \mathrm{A}_{34} & \mathrm{A}_{35} \\ \mathrm{A}_{41} & \mathrm{A}_{42} & \mathrm{A}_{43} & \mathrm{A}_{44} & \mathrm{A}_{45} \\ \mathrm{A}_{51} & \mathrm{A}_{52} & \mathrm{A}_{53} & \mathrm{A}_{54} & \mathrm{A}_{55} \end{array}\right] \left[\begin{array}{c} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \\ \hline \boldsymbol{x}_3 \\ \boldsymbol{x}_4 \\ \boldsymbol{x}_5 \end{array}\right] = \left[\begin{array}{c} \boldsymbol{y}_1 \\ \boldsymbol{y}_2 \\ \hline \boldsymbol{y}_3 \\ \boldsymbol{y}_4 \\ \boldsymbol{y}_5 \end{array}\right]$$

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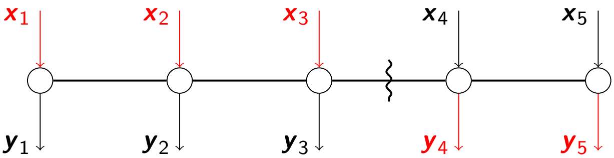
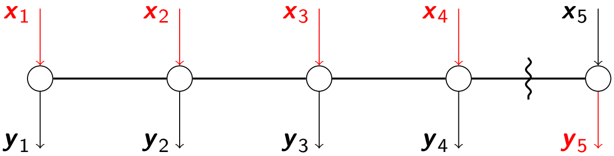


state dimension of $\boldsymbol{h}_3 \Leftrightarrow$ rank H_3

$$\left[\begin{array}{ccc|cc} \mathrm{A}_{11} & \mathrm{A}_{12} & \mathrm{A}_{13} & \mathrm{A}_{14} & \mathrm{A}_{15} \\ \mathrm{A}_{21} & \mathrm{A}_{22} & \mathrm{A}_{23} & \mathrm{A}_{24} & \mathrm{A}_{25} \\ \mathrm{A}_{31} & \mathrm{A}_{32} & \mathrm{A}_{33} & \mathrm{A}_{34} & \mathrm{A}_{35} \\ \hline \mathrm{A}_{41} & \mathrm{A}_{42} & \mathrm{A}_{43} & \mathrm{A}_{44} & \mathrm{A}_{45} \\ \mathrm{A}_{51} & \mathrm{A}_{52} & \mathrm{A}_{53} & \mathrm{A}_{54} & \mathrm{A}_{55} \end{array}\right] \left[\begin{array}{c} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \\ \boldsymbol{x}_3 \\ \hline \boldsymbol{x}_4 \\ \boldsymbol{x}_5 \end{array}\right] = \left[\begin{array}{c} \boldsymbol{y}_1 \\ \boldsymbol{y}_2 \\ \boldsymbol{y}_3 \\ \hline \boldsymbol{y}_4 \\ \boldsymbol{y}_5 \end{array}\right]$$

Notice how the cuts correspond to the Hankel blocks

The ranks of the so-called Hankel blocks dictate the state dimension sizes



state dimension of $\boldsymbol{h}_4 \Leftrightarrow$ rank H_4

$$\left[\begin{array}{cccc|c} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{21} & A_{22} & A_{23} & A_{24} & A_{25} \\ A_{31} & A_{32} & A_{33} & A_{34} & A_{35} \\ A_{41} & A_{42} & A_{43} & A_{44} & A_{45} \\ \hline A_{51} & A_{52} & A_{53} & A_{54} & A_{55} \end{array}\right] \left[\begin{array}{c} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \\ \boldsymbol{x}_3 \\ \boldsymbol{x}_4 \\ \hline \boldsymbol{x}_5 \end{array}\right] = \left[\begin{array}{c} \boldsymbol{y}_1 \\ \boldsymbol{y}_2 \\ \boldsymbol{y}_3 \\ \boldsymbol{y}_4 \\ \hline \boldsymbol{y}_5 \end{array}\right]$$

Notice how the cuts correspond to the Hankel blocks

It is quite easy to write down the SSS representation for the tridiagonal matrix!

$$\left[\begin{array}{cc|ccc} a_1 & b_1 & 0 & 0 & 0 \\ c_1 & a_2 & b_2 & 0 & 0 \\ \hline \color{red}{0} & \color{red}{c_2} & a_3 & b_3 & 0 \\ \color{red}{0} & \color{red}{0} & c_3 & a_4 & b_4 \\ \color{red}{0} & \color{red}{0} & 0 & c_4 & a_5 \end{array}\right] \left[\begin{array}{c} \color{red}{x_1} \\ \color{red}{x_2} \\ \hline x_3 \\ x_4 \\ x_5 \end{array}\right] = \left[\begin{array}{c} y_1 \\ y_2 \\ \hline \color{red}{y_3} \\ \color{red}{y_4} \\ \color{red}{y_5} \end{array}\right]$$

The w's and r's are zero for the mixed LTV system:

$$\begin{aligned} g_k &= 0 \cdot g_{k+1} + 1 \cdot x_k, \quad g_n = 1 \cdot x_n \\ h_k &= 0 \cdot h_{k-1} + 1 \cdot x_k, \quad h_1 = 1 \cdot x_1 \\ y_k &= b_k \cdot g_{k+1} + c_k \cdot h_{k-1} + a_k x_k. \end{aligned}$$

Square partitions: Hankel block ranks are preserved during inversion

Lemma

Let $\begin{bmatrix} \mathrm{B}_{11} & \mathrm{B}_{12} \\ \mathrm{B}_{21} & \mathrm{B}_{22} \end{bmatrix} = \begin{bmatrix} \mathrm{A}_{11} & \mathrm{A}_{12} \\ \mathrm{A}_{21} & \mathrm{A}_{22} \end{bmatrix}^{-1} \in \mathbb{F}^{(n_1+n_2)\times(n_1+n_2)}$ *with square* $A_{11} \in \mathbb{F}^{n_1 \times n_1}$. *Then,*

$$\operatorname{rank} \mathrm{B}_{21} = \operatorname{rank} \mathrm{A}_{21}, \qquad \operatorname{rank} \mathrm{B}_{12} = \operatorname{rank} \mathrm{A}_{12}.$$

The inverse of the tridiagonal is also described by a mixed LTV system:

$$\begin{aligned} g_k &= w_k \cdot g_{k+1} + v_k \cdot x_k, \\ h_k &= r_k \cdot h_{k-1} + q_k \cdot x_k, \\ y_k &= b_k \cdot g_{k+1} + c_k \cdot h_{k-1} + a_k x_k. \end{aligned}$$

but w's and r's will *no longer* zero!

Algebraic properties of SSS: *closure* under sums, products, and inverses!

- Inverse of an SSS matrix (with square partitions) is again an SSS matrix of the same state dimensions.
- Sums of SSS matrices are SSS, but with a *doubling* of the state dimensions.
- Products of SSS matrices are also SSS with a *doubling* of the state dimensions.

From mat-vec to solving $Ax = b$: matrix representation of state-space equations

$$
\left[\begin{array}{cccc|cccc|ccccc}
I & -W_2 & & & & & & & & -V_2^T & & & \\
 & I & -W_3 & & & & & & & & -V_3^T & & \\
 & & I & -W_4 & & & & & & & & -V_4^T & \\
 & & & I & & & & & & & & & -V_5^T \\
\hline
 & & & & I & & & & -Q_1^T & & & & \\
 & & & & -R_2 & I & & & & -Q_2^T & & & \\
 & & & & & -R_3 & I & & & & -Q_3^T & & \\
 & & & & & & -R_4 & I & & & & -Q_4^T & \\
\hline
U_1 & & & & & & & & D_1 & & & & \\
 & U_2 & & & P_2 & & & & & D_2 & & & \\
 & & U_3 & & & P_3 & & & & & D_3 & & \\
 & & & U_4 & & & P_4 & & & & & D_4 & \\
 & & & & & & & P_5 & & & & & D_5
\end{array}\right]
\left[\begin{array}{c}
g_2 \\ g_3 \\ g_4 \\ g_5 \\ \hline h_1 \\ h_2 \\ h_3 \\ h_4 \\ \hline x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5
\end{array}\right]
=
\left[\begin{array}{c}
0 \\ 0 \\ 0 \\ 0 \\ \hline 0 \\ 0 \\ 0 \\ 0 \\ \hline b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5
\end{array}\right]
$$

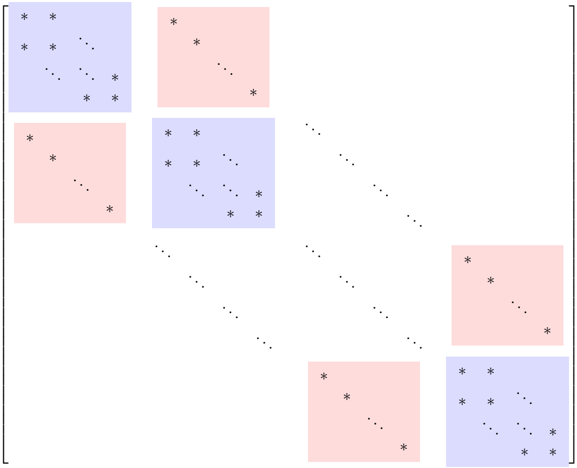
From mat-vec to solving $Ax = b$: re-ordering yields a fast solver

Block-sparsity pattern *matches* the underlying graph!

$$
\left[\begin{array}{cc|ccc|ccc|ccc|cc}
I & -Q_1^T & & & & & & & & & & & \\
 & D_1 & U_1 & & & & & & & & & & \\
\hline
 & & I & & -V_2^T & -W_2 & & & & & & & \\
-R_2 & & & I & -Q_2^T & & & & & & & & \\
P_2 & & & & D_2 & U_2 & & & & & & & \\
\hline
 & & & & & I & & -V_3^T & -W_3 & & & & \\
 & & & -R_3 & & & I & -Q_3^T & & & & & \\
 & & & P_3 & & & & D_3 & U_3 & & & & \\
\hline
 & & & & & & & & I & & -V_4^T & -W_4 & \\
 & & & & & & -R_4 & & & I & -Q_4^T & & \\
 & & & & & & P_4 & & & & D_4 & U_4 & \\
\hline
 & & & & & & & & & & & I & -V_5^T \\
 & & & & & & & & & P_5 & & & D_5
\end{array}\right]
\left[\begin{array}{c}
h_1 \\ x_1 \\ \hline g_2 \\ h_2 \\ x_2 \\ \hline g_3 \\ h_3 \\ x_3 \\ \hline g_4 \\ h_4 \\ x_4 \\ \hline g_5 \\ x_5
\end{array}\right]
=
\left[\begin{array}{c}
0 \\ b_1 \\ \hline 0 \\ 0 \\ b_2 \\ \hline 0 \\ 0 \\ b_3 \\ \hline 0 \\ 0 \\ b_4 \\ \hline 0 \\ b_5
\end{array}\right]
$$

Recall: Line graphs have a *perfect* elimination order!

SSS matrices not suitable for 2D Laplacians: Hankel ranks grow with $O(\sqrt{n})$



with $\sqrt{n}$-by-$\sqrt{n}$ block partitioning $\rightarrow$ approx. $n^{1.5}$ parameters

Overview

The problem: what are the low-rank properties of inverses of sparse matrices?

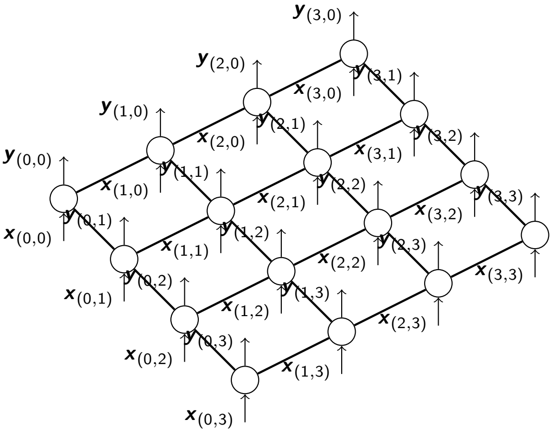
Motivation: shortcomings of existing rank-structured representations in applications

A potential framework: GIRS matrices and their representations

GIRS representations on acyclic graphs: tree quasi-separable matrices

Conclusions & future work

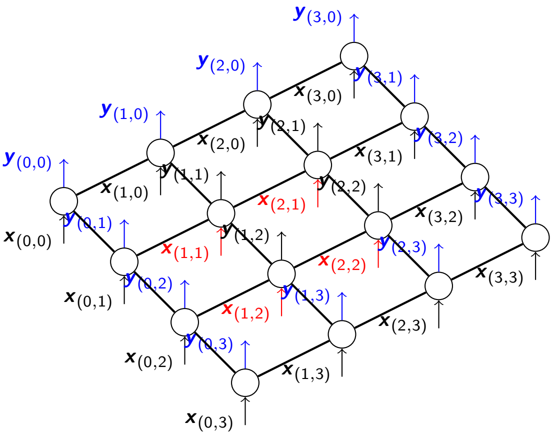
Graph-partitioned matrices: associate a directed graph with a block-partitioned matrix



Associate $\mathbb{G} = (\mathbb{V}, \mathbb{E})$ with a block-partitioned matrix

$$\boldsymbol{y}_i = \sum_{j \in \mathbb{V}} \mathrm{T}\{i, j\} \boldsymbol{x}_j, \quad i \in \mathbb{V}.$$

Hankel blocks induced by graph cuts



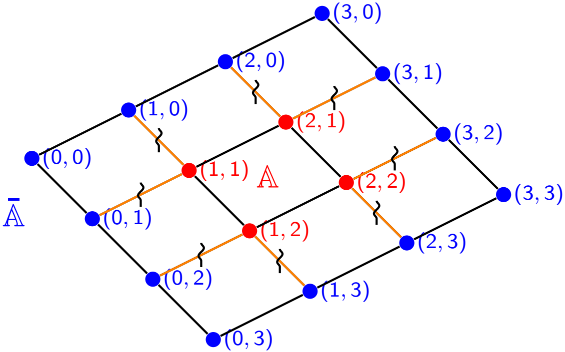
Let $\mathbb{A} \subset \mathbb{V}$ and $\bar{\mathbb{A}} = \mathbb{V} \setminus \mathbb{A}$ so that

$$\Pi_1 \mathrm{T} \Pi_2 = \begin{bmatrix} \mathrm{T}\{\mathbb{A}, \mathbb{A}\} & \mathrm{T}\{\mathbb{A}, \bar{\mathbb{A}}\} \\ \mathrm{T}\{\bar{\mathbb{A}}, \mathbb{A}\} & \mathrm{T}\{\bar{\mathbb{A}}, \bar{\mathbb{A}}\} \end{bmatrix}.$$

Call $\mathrm{T}\{\bar{\mathbb{A}}, \mathbb{A}\}$ as the *Hankel block induced by* $\mathbb{A}$.

This generalizes the Hankel blocks from earlier!

GIRS: a full characterization of all low-rank structures in $(\mathrm{T}, \mathbb{G})$



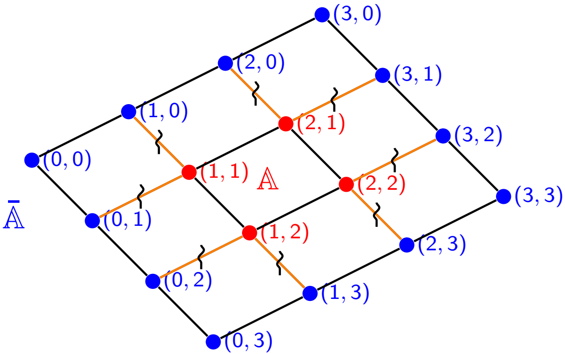
Definition (GIRS property)

$(\mathrm{T}, \mathbb{G})$ satisfies the *graph-induced rank structure* for a constant $c \geq 0$ if $\forall \mathbb{A} \subset \mathbb{V}$,

$$\operatorname{rank} \mathrm{T}\{\bar{\mathbb{A}}, \mathbb{A}\} \leq c \cdot \mathcal{E}(\mathbb{A}),$$

where $\mathcal{E}(\mathbb{A})$ the number of border edges.

The GIRS property is an invariant under inversion



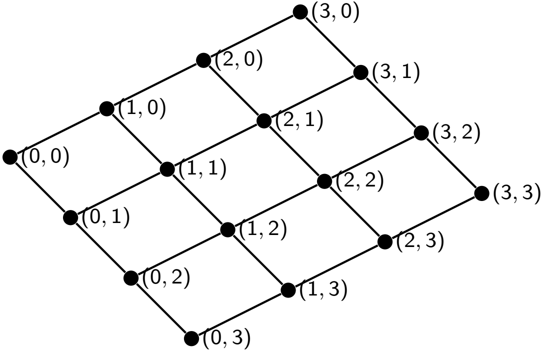
Theorem (GIRS property)

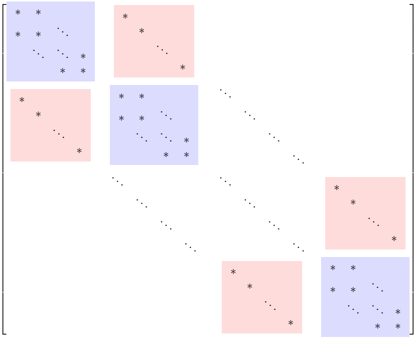
If $(\mathrm{T}, \mathbb{G})$ satisfies the graph-induced rank structure for a constant $c \geq 0$, then so does $(\mathrm{T}^{-1}, \mathbb{G})$.

Proof.

Recall the lemma from earlier... □

The 2D-Laplacian satisfies the GIRS property for $c = 1$ if $\mathbb{G}$ is the adjacency graph

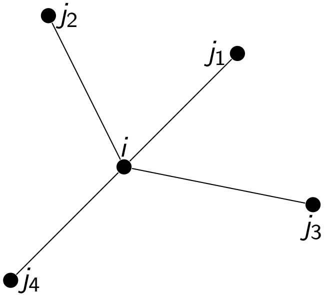




In fact, all sparse matrices are GIRS with $c = 1$ w.r.t. their adjacency graph...

GIRS representations: run "LTV systems" on arbitrary graphs

Associate with every edge $(i,j) \in \mathbb{E}$ the state vector $\boldsymbol{h}_{(i,j)} \in \mathbb{F}^{\rho(i,j)}$.



"State-space" dynamics:

$$\begin{bmatrix} \boldsymbol{h}_{(i,j_1)} \\ \vdots \\ \boldsymbol{h}_{(i,j_p)} \\ \hline \boldsymbol{y}_i \end{bmatrix} = \left[\begin{array}{ccc|c} \mathrm{A}^i_{j_1,j_1} & \cdots & \mathrm{A}^i_{j_1,j_p} & \mathrm{B}^i_{j_1} \\ \vdots & \ddots & \vdots & \vdots \\ \mathrm{A}^i_{j_p,j_1} & \cdots & \mathrm{A}^i_{j_p,j_p} & \mathrm{B}^i_{j_p} \\ \hline \mathrm{C}^i_{j_1} & \cdots & \mathrm{C}^i_{j_p} & \mathrm{D}^i \end{array}\right] \begin{bmatrix} \boldsymbol{h}_{(j_1,i)} \\ \vdots \\ \boldsymbol{h}_{(j_p,i)} \\ \hline \boldsymbol{x}_i \end{bmatrix}$$

GIRS representations generalize SSS matrices

$$S^1 = \left[\begin{array}{c|c} 0 & B^i_{i+1} \\ \hline C^i_{i+1} & D^i \end{array}\right] \qquad S^n = \left[\begin{array}{c|c} 0 & B^i_{i-1} \\ \hline C^i_{i-1} & D^i \end{array}\right]$$

$$S^i = \left[\begin{array}{cc|c} 0 & A^i_{i+1,i-1} & B^i_{i+1} \\ A^i_{i-1,i+1} & 0 & B^i_{i-1} \\ \hline C^i_{i+1} & C^i_{i-1} & D^i \end{array}\right]$$

Line graph: diagonal edge-to-edge operators can be set to zero *without* loss-of-generality!

$\Downarrow$

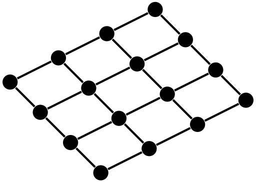
Decouples dynamics in *upstream* & downstream flow!

GIRS representation allow for linear parametrizations of 2D Laplacians

Edge-to-edge operators again zero (similar to tridiagonal matrices):

$$
\mathrm{S}^{(i,j)} = \begin{array}{c|cccc|c}
 & (i{+}1,j) & (i{-}1,j) & (i,j{+}1) & (i,j{-}1) & x_{(i,j)} \\
(i{+}1,j{+}1) & 0 & 0 & 0 & 0 & * \\
(i{-}1,j{+}1) & 0 & 0 & 0 & 0 & * \\
(i{+}1,j{-}1) & 0 & 0 & 0 & 0 & * \\
(i{-}1,j{-}1) & 0 & 0 & 0 & 0 & * \\
\hline
y_{(i,j)} & * & * & * & * & *
\end{array}
$$

Using a scalar partitioning $\rightarrow$ approx. $5^2 \cdot n$ parameters



For general GIRS representation, Gauss elimination is needed for mat-vec operation!

$$\begin{aligned} \boldsymbol{h}_{(i,j)} - \sum_{w \in \mathcal{N}(i)} \mathrm{A}^i_{j,w} \boldsymbol{h}_{(w,i)} - \mathrm{B}^i_j \boldsymbol{x}_i &= 0, \quad (i,j) \in \mathbb{E} \\ \sum_{i \in \mathcal{N}(j)} \mathrm{C}^j_i \boldsymbol{h}_{(i,j)} + \mathrm{D}^j \boldsymbol{x}_i &= \boldsymbol{y}_j, \quad j \in \mathbb{V}. \end{aligned}$$

$$\downarrow$$

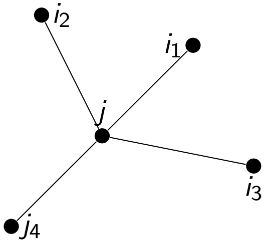
$$\begin{bmatrix} \mathrm{I} - \mathrm{A} & \mathrm{B} \\ \mathrm{C} & \mathrm{D} \end{bmatrix} \begin{bmatrix} \boldsymbol{h} \\ \boldsymbol{x} \end{bmatrix} = \begin{bmatrix} 0 \\ \boldsymbol{y} \end{bmatrix}$$

$$\downarrow$$

Solve $(\mathrm{I} - \mathrm{A})\boldsymbol{h} = -\mathrm{B}\boldsymbol{x}$ to find $\boldsymbol{h}$ first!

One needs to be cautious that $\mathrm{I} - \mathrm{A}$ is not singular!

GIRS representations admit fast solvers through the sparse embedding trick!



Conditions for a fast solver:

1. state dimensions $\rho_{(i,j)}$ are small,
2. degrees of the nodes are small,
3. $\mathbb{G}$ is a good elimination order.

$$
\begin{aligned}
\boldsymbol{h}_{(i,j)} - \sum_{w \in \mathcal{N}(i)} \mathrm{A}^i_{j,w} \boldsymbol{h}_{(w,i)} - \mathrm{B}^i_j \boldsymbol{x}_i &= 0, \quad (i,j) \in \mathbb{E} \\
\sum_{i \in \mathcal{N}(j)} \mathrm{C}^j_i \boldsymbol{h}_{(i,j)} + \mathrm{D}^j \boldsymbol{x}_i &= \boldsymbol{y}_j, \quad j \in \mathbb{V}.
\end{aligned}
$$

$\downarrow$

Group adjoining variables:

$\boldsymbol{\theta}_j = (\boldsymbol{h}_{(i_1,j)}, \ldots, \boldsymbol{h}_{(i_p,j)}, \boldsymbol{x}_j)$ and $\boldsymbol{\gamma}_j = (0, \ldots, 0, \boldsymbol{y}_j)$

$\downarrow$

Block-sparsity pattern of $\Xi \boldsymbol{\theta} = \boldsymbol{\gamma}$ satisfies
$\Xi_{ij} = 0$ if $(i,j) \notin \mathbb{E}$.

Example: 2-by-3 mesh

$$
\left[\begin{array}{ccc|cccc|ccc|ccc|cccc|ccc}
A^1_{2,2} & A^1_{2,4} & B^1_2 & -I & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
A^1_{4,2} & A^1_{4,4} & B^1_4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -I & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
C^1_2 & C^1_4 & D^1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
-I & 0 & 0 & A^2_{1,1} & A^2_{1,3} & A^2_{1,5} & B^2_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & A^2_{3,1} & A^2_{3,3} & A^2_{3,5} & B^2_3 & -I & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & A^2_{5,1} & A^2_{5,3} & A^2_{5,5} & B^2_5 & 0 & 0 & 0 & 0 & 0 & 0 & -I & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & C^2_1 & C^2_3 & C^2_5 & D^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & -I & 0 & 0 & A^3_{2,2} & A^3_{2,6} & B^3_2 & 0 & 0 & 0 & 0 & 0 & 0 & & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & A^3_{6,2} & A^3_{6,6} & B^3_6 & 0 & 0 & 0 & 0 & 0 & 0 & & -I & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & C^3_2 & C^3_6 & D^3 & 0 & 0 & 0 & 0 & 0 & 0 & & 0 & 0 & 0 \\
\hline
0 & -I & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & A^4_{1,1} & A^4_{1,5} & B^4_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & A^4_{5,1} & A^4_{5,5} & B^4_5 & 0 & -I & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & C^4_1 & C^4_5 & D^4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & -I & 0 & 0 & 0 & 0 & 0 & 0 & 0 & A^5_{2,2} & A^5_{2,4} & A^5_{2,6} & B^5_1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -I & 0 & A^5_{4,2} & A^5_{4,4} & A^5_{4,6} & B^5_3 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & A^5_{6,2} & A^5_{6,4} & A^5_{6,6} & B^5_5 & 0 & -I & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & C^5_2 & C^5_4 & C^5_6 & D^5 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -I & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & A^6_{3,3} & A^6_{3,5} & B^6_3 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -I & 0 & A^6_{5,3} & A^6_{5,5} & B^6_5 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & C^6_3 & C^6_5 & D^6
\end{array}\right]
\left[\begin{array}{c}
\mathbf{h}_{(2,1)} \\ \mathbf{h}_{(4,1)} \\ \mathbf{x}_1 \\ \hline
\mathbf{h}_{(1,2)} \\ \mathbf{h}_{(3,2)} \\ \mathbf{h}_{(5,2)} \\ \mathbf{x}_2 \\ \hline
\mathbf{h}_{(2,3)} \\ \mathbf{h}_{(6,3)} \\ \mathbf{x}_3 \\ \hline
\mathbf{h}_{(1,4)} \\ \mathbf{h}_{(5,4)} \\ \mathbf{x}_4 \\ \hline
\mathbf{h}_{(2,5)} \\ \mathbf{h}_{(4,5)} \\ \mathbf{h}_{(6,5)} \\ \mathbf{x}_5 \\ \hline
\mathbf{h}_{(3,6)} \\ \mathbf{h}_{(5,6)} \\ \mathbf{x}_6
\end{array}\right]
=
\left[\begin{array}{c}
0 \\ 0 \\ \mathbf{y}_1 \\ \hline
0 \\ 0 \\ 0 \\ \mathbf{y}_2 \\ \hline
0 \\ 0 \\ \mathbf{y}_3 \\ \hline
0 \\ 0 \\ \mathbf{y}_4 \\ \hline
0 \\ 0 \\ 0 \\ \mathbf{y}_5 \\ \hline
0 \\ 0 \\ \mathbf{y}_6
\end{array}\right]
$$

GIRS representations (generically) satisfy the closure property

$$\begin{bmatrix} \mathrm{I}-\mathrm{A} & \mathrm{B} \\ \mathrm{C} & \mathrm{D} \end{bmatrix} \begin{bmatrix} \boldsymbol{h} \\ \boldsymbol{x} \end{bmatrix} = \begin{bmatrix} 0 \\ \boldsymbol{y} \end{bmatrix}$$

$$\downarrow$$

$$\begin{bmatrix} \mathrm{I}-(\mathrm{A}-\mathrm{B}\mathrm{D}^{-1}\mathrm{C}) & \mathrm{B}\mathrm{D}^{-1} \\ \mathrm{D}^{-1}\mathrm{C} & \mathrm{D}^{-1} \end{bmatrix} \begin{bmatrix} \boldsymbol{h} \\ \boldsymbol{y} \end{bmatrix} = \begin{bmatrix} 0 \\ \boldsymbol{x} \end{bmatrix}$$

$$\downarrow$$

$$\mathrm{S}^{i} = \left[\begin{array}{ccc|c} \mathrm{A}^{i}_{j_1,j_1} - \mathrm{B}^{i}_{j_1}\,\mathrm{inv}(\mathrm{D}^{i})\mathrm{C}^{i}_{j_1} & \cdots & \mathrm{A}^{i}_{j_1,j_p} - \mathrm{B}^{i}_{j_1}\,\mathrm{inv}(\mathrm{D}^{i})\mathrm{C}^{i}_{j_p} & \mathrm{B}^{i}_{j_1}\,\mathrm{inv}(\mathrm{D}^{i}) \\ \vdots & \ddots & \vdots & \vdots \\ \mathrm{A}^{i}_{j_p,j_1} - \mathrm{B}^{i}_{j_p}\,\mathrm{inv}(\mathrm{D}^{i})\mathrm{C}^{i}_{j_1} & \cdots & \mathrm{A}^{i}_{j_p,j_p} - \mathrm{B}^{i}_{j_p}\,\mathrm{inv}(\mathrm{D}^{i})\mathrm{C}^{i}_{j_p} & \mathrm{B}^{i}_{j_p}\,\mathrm{inv}(\mathrm{D}^{i}) \\ \hline \mathrm{inv}(\mathrm{D}^{i})\mathrm{C}^{i}_{j_1} & \cdots & \mathrm{inv}(\mathrm{D}^{i})\mathrm{C}^{i}_{j_p} & \mathrm{inv}(\mathrm{D}^{i}) \end{array}\right]$$

Also, addition and product have nice formulas

SSS inverse and GIRS representation inverse: a subtle difference

The formula in the previous slide gives:

$$
\mathrm{S}^i = \left[\begin{array}{cc|c}
-\mathrm{B}^i_{i+1}\mathrm{inv}(\mathrm{D}^i)\mathrm{C}^i_{i+1} & \mathrm{A}^i_{i+1,i-1} - \mathrm{B}^i_{i+1}\mathrm{inv}(\mathrm{D}^i)\mathrm{C}^i_{i-1} & \mathrm{B}^i_{i+1}\mathrm{inv}(\mathrm{D}^i) \\
\mathrm{A}^i_{i-1,i+1} - \mathrm{B}^i_{i-1}\mathrm{inv}(\mathrm{D}^i)\mathrm{C}^i_{i+1} & -\mathrm{B}^i_{i-1}\mathrm{inv}(\mathrm{D}^i)\mathrm{C}^i_{i-1} & \mathrm{B}^i_{i-1}\mathrm{inv}(\mathrm{D}^i) \\
\hline
\mathrm{inv}(\mathrm{D}^i)\mathrm{C}^i_{i+1} & \mathrm{inv}(\mathrm{D}^i)\mathrm{C}^i_{i-1} & \mathrm{inv}(\mathrm{D}^i)
\end{array}\right]
$$

SSS theory guarantees more! A realization of form:

$$
\mathrm{S}^i = \left[\begin{array}{cc|c}
0 & \mathrm{A}^i_{i+1,i-1} & \mathrm{B}^i_{i+1} \\
\mathrm{A}^i_{i-1,i+1} & 0 & \mathrm{B}^i_{i-1} \\
\hline
\mathrm{C}^i_{i+1} & \mathrm{C}^i_{i-1} & \mathrm{D}^i
\end{array}\right]
$$

The latter requires *no* Gauss elimination for mat-vec!

GIRS representations satisfy the GIRS property by construction

Theorem

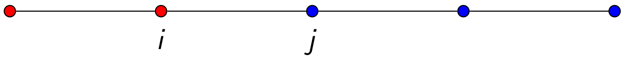
A GIRS representation with rank-profile $\{\rho_e\}_{e \in \mathbb{E}}$ *of a graph-partitioned matrix* $(\mathbb{T}, \mathbb{G})$ *satisfies the GIRS-property for*

$$c = \max_{e \in \mathbb{E}} \rho_e.$$

Proof.

A proof of this theorem was given in a talk in CAM23 at Selva di Fasano by Shiv Chandrasekaran. □

SSS matrices: the result can be extended in the other as well.



A one-to-one relationship between Hankel block ranks and state dimensions:

$$\rho_{(i,j)} = \text{rank}\, \mathrm{H}_{(i,j)} := \text{rank}\, \mathrm{T}\{\bar{\mathbb{A}}, \mathbb{A}\}$$

Stronger result: Implication is in both directions:

$$\rho_{(i,j)} < c \qquad \Leftrightarrow \qquad \mathrm{T} \text{ is GIRS-}c$$

Can the implication be in both directions in general?

Conjecture

A graph-partitioned matrix $(\mathbb{T}, \mathbb{G})$ is GIRS-c if, and only if, there exists GIRS representation for $(\mathbb{T}, \mathbb{G})$ with $\rho_e < c$ for all $e \in \mathbb{E}$.

Small GIRS constant implies compact GIRS representation!

This conjecture is intimately tied to the construction/realization problem!

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Motivation: shortcomings of existing rank-structured representations in applications

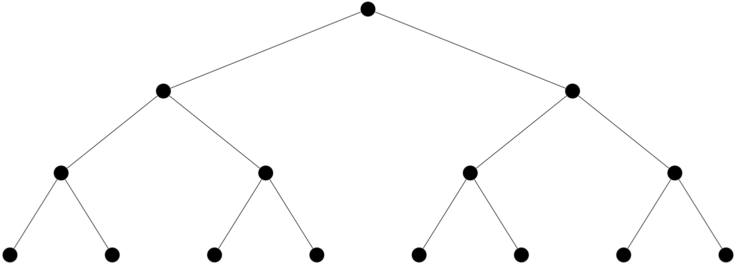
A potential framework: GIRS matrices and their representations

GIRS representations on acyclic graphs: tree quasi-separable matrices

Conclusions & future work

A partial verification of the GIRS conjecture

Acyclic graphs: *tree* interpretation



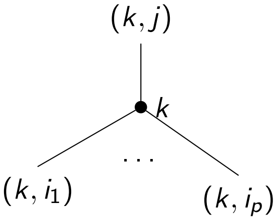
chordal structure $\rightarrow$ "fast" solvers through elimination of leaf nodes

Theorem

The GIRS conjecture holds for acyclic graphs, i.e., graphs with no cycles.

Proving GIRS conjecture: a special tree quasi-separable (TQS) realization always exists

Node k with parent j and children $i_1, \ldots, i_p$:



$$
\mathrm{S}^k = \left[\begin{array}{cccc|c}
0 & \cdots & \mathrm{A}^k_{i_1,i_p} & \mathrm{A}^k_{i_1,j} & \mathrm{B}^k_{i_1} \\
\vdots & \ddots & \vdots & \vdots & \vdots \\
\mathrm{A}^k_{i_p,i_1} & \cdots & 0 & \mathrm{A}^k_{i_p,j} & \mathrm{B}^k_{i_p} \\
\mathrm{A}^k_{j,i_i} & \cdots & \mathrm{A}^k_{j,i_p} & 0 & \mathrm{B}^k_{j} \\
\hline
\mathrm{C}^k_{i_1} & \cdots & \mathrm{C}^k_{i_p} & \mathrm{C}^k_{j} & \mathrm{D}^k
\end{array}\right]
$$

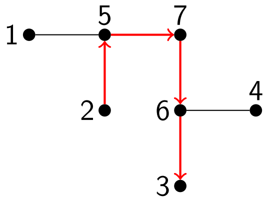
Tree graph: Diagonal edge-to-edge operators are set to zero!

$\Downarrow$

Decouples dynamics into an explicit flow starting from the leaves!

Proving GIRS conjecture: a special tree quasi-separable (TQS) realization always exists

Entries Node k with parent j and children $i_1, \ldots, i_p$:



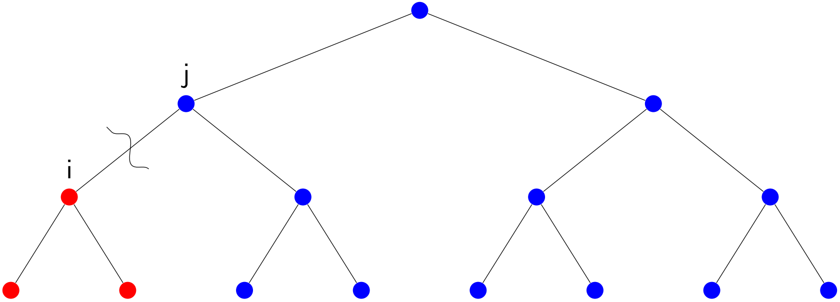
$$\mathrm{T}\{3,2\} = \mathrm{C}_6^3 \mathrm{A}_{3,7}^6 \mathrm{A}_{6,5}^7 \mathrm{A}_{7,2}^5 \mathrm{B}_5^2$$

Tree graph: Diagonal edge-to-edge operators are set to zero!

$\Downarrow$

Decouples dynamics into an explicit flow starting from the leaves!

SSS generalization: Hankel block ranks specify dimensions of minimal TQS representation



$$\rho_{(i,j)} = \text{rank}\, \mathrm{H}_{(i,j)} := \text{rank}\, \mathrm{T}\{\bar{\mathbb{A}}, \mathbb{A}\}$$

Construction from a finite number of low-rank factorizations:

Govindarajan, N., Chandrasekaran, S., Dewilde, P. (2024). Tree quasi-separable matrices: a simultaneous generalization of sequentially and hierarchically semi-separable representations. arXiv preprint.

TQS is a strict generalization of SSS and HSS

- TQS reduces to SSS if $\mathbb{G}$ is the line graph.
- TQS reduces to HSS if $\mathbb{G}$ is a binary tree with *empty* non-leaf nodes.
- In all other cases, it is neither SSS nor HSS.

Many of the algorithms for SSS and HSS *generalize* to TQS:

development of more flexible and powerful code possible!

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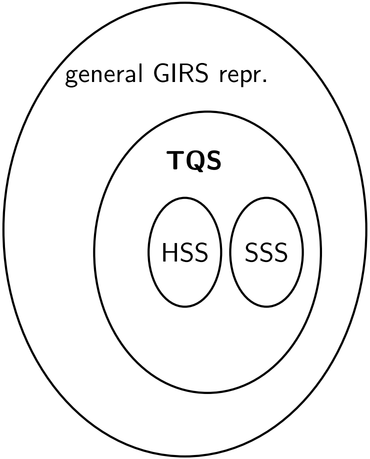
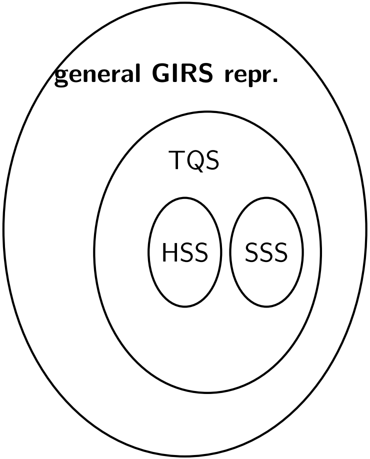
The state of affairs: *acyclic* graph-partitioned matrices



- *GIRS conjecture:* solved and true!
- Construction: TQS realizations is possible in finite number of low-rank factorizations.
- *Special realizations:* A special TQS realization always exists that decouples dynamics into an explicit flow.
- *Algebraic properties:* closed under sums, products, and inverses.
- *Fast solvers:* chordal structure ensures good elimination order.

The state of affairs: *general* graph-partitioned matrices



- *GIRS conjecture:* yet to be answered!
- *Construction:* no general algorithm for constructing realizations.
- *Special realizations:* not known when realizations exist that simplify the dynamics.
- *Algebraic properties:* closure under sums, products, and inverses.
- *Fast solvers:* contingent on existence of good elimination orders.

Future work

1. Develop formulas, factorization algorithms, software for TQS, e.g.:
   - Inner-outer
   - (Pseudo-)inverse
   - LU / Cholesky
   - ULV
2. Applications of TQS, e.g.:
   - Exterior Helmholtz problems on "branchy" domains
   - Distributed control on acyclic graphs
3. Theoretical work: proving GIRS conjecture for cycle graphs?
4. Construction of more general GIRS representations using optimization-based techniques?

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