Structured Matrix Computations from Structured Tensors

Lecture 5. Multiple Symmetries and Low-Rank Approximation

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Warm-Up Example: Centrosymmetry

A matrix $A \in \mathbb{R}^{n \times n}$ is *centrosymmetric* if $A = A^T$ and $A = E_n A E_n$ where

$$E_n = I_n(:, n{:}-1{:}1) \in \mathbb{R}^{n \times n}$$

E.g.,

$$E_4 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \qquad A = \begin{bmatrix} a & b & c & d \\ b & e & f & c \\ c & f & e & b \\ d & c & b & a \end{bmatrix}.$$

Symmetric about its diagonal and anti-diagonal

A Centrosymmetric Matrix is an example of a matrix that has multiple symmetries.

Warm-Up Example: Centrosymmetry

Since

$$Ax = \lambda x \qquad \Rightarrow \qquad EAEx = \lambda x \qquad \Rightarrow \qquad A(Ex) = \lambda(Ex)$$

we see that the eigenvectors come in two flavors:

$$x = Ex = \left[\begin{array}{c} x_1 \\ x_2 \\ x_3 \\ \hline x_3 \\ x_2 \\ x_1 \end{array}\right] \qquad x = -Ex = \left[\begin{array}{r} x_1 \\ x_2 \\ x_3 \\ \hline -x_3 \\ -x_2 \\ -x_1 \end{array}\right]$$

Warm-Up Example: Centrosymmetry

This means that the left and right halves of the orthogonal matrix

$$Q_E = \frac{1}{\sqrt{2}}\left[\begin{array}{c|c} I_m & I_m \\ E_m & -E_m \end{array}\right] \equiv \left[\begin{array}{c|c} Q_+ & Q_- \end{array}\right]$$

$$= \frac{1}{\sqrt{2}}\left[\begin{array}{ccc|ccc} 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 & 0 & 0 \end{array}\right]$$

define a pair of invariant subspaces.

$$EQ_+ = Q_+ \qquad EQ_- = Q_-$$

Warm-Up Example: Centrosymmetry

Thus,

$$Q_E = \frac{1}{\sqrt{2}} \left[\begin{array}{c|c} I_m & I_m \\ E_m & -E_m \end{array} \right] \equiv \left[\begin{array}{c|c} Q_+ & Q_- \end{array} \right]$$

should block diagonalize

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

if A s centrosymmetric. Indeed

$$Q_E^T A Q_E = \begin{bmatrix} A_{11} + A_{12}E_m & 0 \\ 0 & A_{11} - A_{12}E_m \end{bmatrix} \equiv \begin{bmatrix} A_+ & 0 \\ 0 & A_- \end{bmatrix}.$$

Warm-Up Example: Centrosymmetry

If A is positive definite and

$$Q_E^T A Q_E = \begin{bmatrix} A_{11} + A_{12}E_m & 0 \\ 0 & A_{11} - A_{12}E_m \end{bmatrix} \equiv \begin{bmatrix} A_+ & 0 \\ 0 & A_- \end{bmatrix}.$$

then we could solve a linear system $Ax = b$ with a pair of half-sized Cholesky factorizations

$$A_+ = G_+ G_+^T \qquad A_- = G_- G_-^T$$

Total cost = one-fourth the cost if A was just symmetric and positive definite.

If A is positive semidefinite definite and

$$Q_E^T A Q_E = \begin{bmatrix} A_{11} + A_{12}E_m & 0 \\ 0 & A_{11} - A_{12}E_m \end{bmatrix} \equiv \begin{bmatrix} A_+ & 0 \\ 0 & A_- \end{bmatrix}.$$

then we could produce a structured reduce-rank representation of A with a pair of half-sized LDL factorizations

$$P_+ A_+ P_+^T = L_+ D_+ L_+^T \qquad P_- A_- P_-^T = L_- D_- L_-^T.$$

Indeed,

$$A = \left[\; Q_+ \mid Q_- \;\right] \begin{bmatrix} A_+ & 0 \\ 0 & A_- \end{bmatrix} \left[\; Q_+ \mid Q_- \;\right]^T = Y_+ D_+ Y_+^T + Y_- D_- Y_-^T$$

where $Y_+ = Q_+ P_+^T L_+$ and $Y_- = Q_- P_-^T L_-$.

Recall LDL with Diagonal Pivoting

If A was Symmetric and Positive Semidefinite, then we could use LDL (Cholesky) with diagonal pivoting...

$$PAP^T = LDL^T \qquad \begin{cases} P \text{ is a permutation} \\ L \in \mathbb{R}^{n^2 \times r} \text{ is unit lower triangular} \\ D = \mathrm{diag}(d_i),\ d_1 \geq d_2 \geq \cdots \geq d_r > 0 \end{cases}$$

$$PAP^T = \begin{bmatrix} \times & 0 & 0 \\ \times & \times & 0 \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix} \begin{bmatrix} d_1 & 0 & 0 \\ 0 & d_2 & 0 \\ 0 & 0 & d_3 \end{bmatrix} \begin{bmatrix} \times & \times & \times & \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times & \times & \times & \times \end{bmatrix}$$

If we want to produce a reduced rank approximation to a matrix that has multiple symmetries, then we would like the approximation to inherit those multiple symmetries.

Perfect-Shuffle Symmetry

The Two-Electron Integral Tensor (TEI)

Given a basis $\{\phi_i(\mathbf{r})\}_{i=1}^n$ of atomic orbital functions, we consider the following order-4 tensor:

$$\mathcal{A}(p,q,r,s) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\phi_p(\mathbf{r}_1)\phi_q(\mathbf{r}_1)\phi_r(\mathbf{r}_2)\phi_s(\mathbf{r}_2)}{\|\mathbf{r}_1 - \mathbf{r}_2\|} d\mathbf{r}_1 d\mathbf{r}_2.$$

The TEI tensor plays an important role in electronic structure theory and ab initio quantum chemistry.

The TEI tensor has these symmetries:

$$\mathcal{A}(p,q,r,s) \;=\; \begin{cases} \mathcal{A}(q,p,r,s) & \text{(i)} \\ \mathcal{A}(p,q,s,r) & \text{(ii)} \\ \mathcal{A}(r,s,p,q) & \text{(iii)} \end{cases}$$

We say that $\mathcal{A}$ is "((12)(34))-symmetric".

Atomic Orbital Basis $\longrightarrow$ Molecular Orbital Basis

If the molecular orbital basis functions $\{\psi_i(\mathbf{r})\}_{i=1}^n$ are defined by

$$\psi_i(\mathbf{r}) = \sum_{k=1}^n X(i,k)\phi_k(\mathbf{r}) \qquad i = 1, 2, \ldots, n$$

then the molecular orbital basis tensor

$$\mathcal{B}(p,q,r,s) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\psi_p(\mathbf{r}_1)\psi_q(\mathbf{r}_1)\psi_r(\mathbf{r}_2)\psi_s(\mathbf{r}_2)}{\|\mathbf{r}_1 - \mathbf{r}_2\|} d\mathbf{r}_1 d\mathbf{r}_2.$$

is given by...

The ((12)(34))-Symmetric Multilinear Product

$$\mathcal{B}(j_1, j_2, j_3, j_4)$$

$$=$$

$$\sum_{i_1=1}^{n} \sum_{i_2=1}^{n} \sum_{i_3=1}^{n} \sum_{i_4=1}^{n} \mathcal{A}(i_1, i_2, i_3, i_4) \cdot X(i_1, j_1) \cdot X(i_2, j_2) \cdot X(i_3, j_3) \cdot X(i_4, j_4)$$

and the tensor $\mathcal{B}$ has these symmetries...

$$\mathcal{B}(p,q,r,s) \;=\; \begin{cases} \mathcal{B}(q,p,r,s) \\ \mathcal{B}(p,q,s,r) \\ \mathcal{B}(r,s,p,q) \end{cases}$$

In other words $\mathcal{B}$ is also ((12)(34))-symmetric.

The Block Matrix Product Formulation

If $A = (A_{rs})$ and $B = (B_{rs})$ are n-by-n block matrices with n-by-n blocks and

$$\mathcal{A}(p,q,r,s) \;\;\leftrightarrow\;\; [\, A_{rs} \,]_{pq}$$

$$\mathcal{B}(p,q,r,s) \;\;\leftrightarrow\;\; [\, B_{rs} \,]_{pq}$$

then the ((12)(34))-symmetric multilinear product is equivalent to

$$B \;=\; (X \otimes X)^T A (X \otimes X)$$

The matrix A (and B) is special...

A "Inherits" $\mathcal{A}$'s Structure

Since

$$\mathcal{A}(p,q,r,s) \;\leftrightarrow\; [\,A_{rs}\,]_{pq}$$

and

$$\mathcal{A}(p,q,r,s) \;=\; \begin{cases} \mathcal{A}(q,p,r,s) & \text{(i)} \\ \mathcal{A}(p,q,s,r) & \text{(ii)} \\ \mathcal{A}(r,s,p,q) & \text{(iii)} \end{cases}$$

it follows that

(i) The blocks of A are symmetric ($A_{rs}^T = A_{rs}$) because of (i).

(ii) A is symmetric as a block matrix ($A_{rs} = A_{sr}$) because (ii).

Time to Talk About Unfoldings

The tensor $\mathcal{A} \in \mathbb{R}^{n\times n\times n\times n}$ can be unfolded several ways.

- We have depicted the $[1,3] \times [2,4]$ unfolding $A = \mathcal{A}_{[1,3]\times[2,4]}$ defined by

$$\mathcal{A}(i_1, i_2, i_3, i_4) \;\rightarrow\; A(i_1 + (i_3 - 1)n, i_2 + (i_4 - 1)n)$$

- Also of interest is the $[1,2] \times [3,4]$ unfolding $A = \mathcal{A}_{[1,2]\times[3,4]}$ defined by

$$\mathcal{A}(i_1, i_2, i_3, i_4) \;\rightarrow\; A(i_1 + (i_2 - 1)n, i_3 + (i_4 - 1)n)$$

If $\mathcal{A}$ is ((12)(34))-symmetric, these two unfoldings display different multiple symmetries...

If $A = \mathcal{A}_{[1,3]\times[2,4]}$, then (as we have seen) A is block symmetric with symmetric blocks.

$$A = \left[\begin{array}{ccc|ccc|ccc} 11 & 12 & 13 & 12 & 17 & 18 & 13 & 18 & 22 \\ 12 & 14 & 15 & 17 & 19 & 20 & 18 & 23 & 24 \\ 13 & 15 & 16 & 18 & 20 & 21 & 22 & 24 & 25 \\ \hline 12 & 17 & 18 & 14 & 19 & 23 & 15 & 20 & 24 \\ 17 & 19 & 20 & 19 & 26 & 27 & 20 & 27 & 29 \\ 18 & 20 & 21 & 23 & 27 & 28 & 24 & 29 & 30 \\ \hline 13 & 18 & 22 & 15 & 20 & 24 & 16 & 21 & 25 \\ 18 & 23 & 24 & 20 & 27 & 29 & 21 & 28 & 30 \\ 22 & 24 & 25 & 24 & 29 & 30 & 25 & 30 & 31 \end{array}\right].$$

The $[1,2]\times[3,4]$ Unfolding of a ((12)(34)) Symmetric $\mathcal{A}$

If $A = \mathcal{A}_{[1,2]\times[3,4]}$, then A is symmetric and (among other things) is "perfect shuffle" symmetric.

$$A = \left[\begin{array}{ccc|ccc|ccc} 11 & 12 & 13 & 12 & 14 & 15 & 13 & 15 & 16 \\ 12 & 17 & 18 & 17 & 19 & 20 & 18 & 20 & 21 \\ 13 & 18 & 22 & 18 & 23 & 24 & 22 & 24 & 25 \\ \hline 12 & 17 & 18 & 17 & 19 & 20 & 18 & 20 & 21 \\ 14 & 19 & 23 & 19 & 26 & 27 & 23 & 27 & 28 \\ 15 & 20 & 24 & 20 & 27 & 29 & 24 & 29 & 30 \\ \hline 13 & 18 & 22 & 18 & 23 & 24 & 22 & 24 & 25 \\ 15 & 20 & 24 & 20 & 27 & 29 & 24 & 29 & 30 \\ 16 & 21 & 25 & 21 & 28 & 30 & 25 & 30 & 31 \end{array}\right]$$

Each column reshapes into a 3x3 symmetric matrix, e.g., $A(:,)$ reshapes to

$$\left[\begin{array}{ccc} 11 & 12 & 13 \\ 12 & 14 & 15 \\ 13 & 15 & 16 \end{array}\right]$$

What is perfect shuffle symmetry?

Perfect Shuffle Symmetry

An n^2-by-n^2 matrix A has perfect shuffle symmetry if

$$A = \Pi_{n,n} A \Pi_{n,n}$$

where

$$\Pi_{n,n} \; = \; I_{n^2}(:, v), \qquad v \; = \; [\, 1{:}n{:}n^2 \mid 2{:}n{:}n^2 \mid \; \cdots \; \mid n{:}n{:}n^2 \,].$$

e.g.,

$$\Pi_{3,3} \; = \; \left[\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right]$$

The Perfect Shuffle Π_{nn}

Because $\Pi_{n,n}$ is symmetric it has just two eigenvalues: $+1$ and -1.

$$\Pi_{3,3} = \left[\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right] \left[\begin{array}{c} x_{11} \\ x_{21} \\ x_{31} \\ \mathbf{x_{12}} \\ x_{22} \\ x_{32} \\ x_{13} \\ x_{23} \\ x_{33} \end{array}\right] = \pm \left[\begin{array}{c} x_{11} \\ x_{12} \\ x_{13} \\ \mathbf{x_{21}} \\ x_{22} \\ x_{23} \\ x_{31} \\ x_{32} \\ x_{33} \end{array}\right]$$

If $\Pi_{n,n}x = x$, then $\texttt{reshape}(x, n, n)$ is symmetric.

If $\Pi_{n,n}x = -x$, then $\texttt{reshape}(x, n, n)$ is skew-symmetric.

Low-Rank PS-Symmetric Approximation

PS-Symmetry

Definition

The n^2-by-n^2 matrix A is *PS-symmetric* if $A \;=\; A^T \;=\; \Pi_{n,n} A \Pi_{n,n}$.

PS Fact 1

If A is PS-Symmetric, then so is $B \;=\; (X \otimes X)^T A (X \otimes X)$.

PS Fact 2

If $\mathcal{A}$ is ((12)(34))-symmetric and $A = \mathcal{A}_{[1,2]\times[3,4]}$ then

$$\Pi_{n,n} A = A \qquad A \Pi_{n,n} = A$$

and so (of course) A is PS-symmetric.

What we have:

A (cheap) positive definite PS-symmetric matrix $A \in \mathbb{R}^{n^2 \times n^2}$ where $\text{rank}(A) \approx n$ and $X \in \mathbb{R}^{n \times n}$.

What we Want

A low rank positive semidefinite approximation $\tilde{B}$ to

$$B = (X \otimes X)^T A (X \otimes X)$$

that is also PS-Symmetric

Solution Framework:

1. Closed-form block diagonalization with a special highly-structured orthogonal $Q = [Q_1 \; Q_2]$:

$$Q^T A Q \; = \; \begin{bmatrix} A_1 & 0 \\ 0 & A_2 \end{bmatrix}$$

2. Compute half-sized rank-revealing LDL factorizations:

$$P_i A_i P_i^T \; \approx \; L_i D_i L_i^T \, , \quad i = 1, 2$$

3. Set

$$\tilde{A} \; = \; Y_1 D_1 Y_1^T \; + \; Y_2 D_2 Y_2^T$$

where $Y_i = Q_i P_i^T L_i$.

4. $B \; \approx \; \tilde{B} \; = \; (X \otimes X)^T \tilde{A} (X \otimes X)$

The Block Diagonalization

Recall that if S is a symmetric matrix and $v = \texttt{reshape}(S, n^2, 1)$ then $\Pi_{n,n} v \;=\; v$.

A basis for the invariant subspace:

$$\left\{ \begin{bmatrix} 1\\0\\0\\0\\0\\0\\0\\0\\0 \end{bmatrix}, \begin{bmatrix} 0\\1\\0\\0\\0\\0\\0\\0\\0 \end{bmatrix}, \begin{bmatrix} 0\\0\\1\\0\\0\\0\\0\\0\\0 \end{bmatrix}, \begin{bmatrix} 0\\1\\0\\1\\0\\0\\0\\0\\0 \end{bmatrix}, \begin{bmatrix} 0\\0\\1\\0\\0\\0\\1\\0\\0 \end{bmatrix}, \begin{bmatrix} 0\\0\\0\\0\\0\\1\\0\\1\\0 \end{bmatrix} \right\}$$

The span of these vectors is invariant for a PS-symmetric matrix A:

$$\Pi_{n,n} v = v \quad \Rightarrow Av = (\Pi_{n,n} A \Pi_{n,n}) v = \Pi_{n,n}(A \Pi_{n,n} v) = \Pi_{n,n}(Av)$$

The Block Diagonalization

Recall that if S is a skew-symmetric matrix and $v = \texttt{reshape}(S, n^2, 1)$ then $\Pi_{n,n} v \;=\; -v$.

A basis for the invariant subspace:

$$\left\{ \begin{bmatrix} 0 \\ 1 \\ 0 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ -1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ -1 \\ 0 \end{bmatrix} \right\}$$

The span of these vectors is invariant for a PS-symmetric matrix A:

$$\Pi_{n,n} v = v \quad \Rightarrow Av = (\Pi_{n,n} A \Pi_{n,n}) v = \Pi_{n,n}(A \Pi_{n,n} v) = \Pi_{n,n}(Av)$$

The Orthogonal Matrix $Q_{n,n}$

$$Q_{3,3} = \frac{1}{\sqrt{2}} \left[\begin{array}{cccccc|ccc} \sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 & -1 \\ 0 & 0 & \sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right] = [\ Q_{\text{sym}} \mid Q_{\text{skew}}\ ]$$

$$Q_{3,3}(:,4) \equiv \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad Q_{3,3}(:,7) \equiv \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Block Diagonalization

If $A \in \mathbb{R}^{n^2 \times n^2}$ is PS-symmetric then

$$Q_{n,n}^T A Q_{n,n} = \left[\begin{array}{cccccc|ccc} \times & \times & \times & \times & \times & \times & 0 & 0 & 0 \\ \times & \times & \times & \times & \times & \times & 0 & 0 & 0 \\ \times & \times & \times & \times & \times & \times & 0 & 0 & 0 \\ \times & \times & \times & \times & \times & \times & 0 & 0 & 0 \\ \times & \times & \times & \times & \times & \times & 0 & 0 & 0 \\ \times & \times & \times & \times & \times & \times & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & 0 & 0 & \times & \times & \times \end{array}\right] = \left[\begin{array}{cc} A_{\text{sym}} & 0 \\ 0 & A_{\text{skew}} \end{array}\right]$$

But there is more...

$A_{\text{skew}} = 0$!

Suppose $\mathcal{A}$ is ((12)(34)) symmetric and $A = \mathcal{A}_{[1,2]\times[3,4]}$.

Recall that the rows of A are reshaped symmetric matrices, i.e., $A = A\Pi_{n,n}$.

Thus

$$
\begin{aligned}
A_{\text{skew}} &= Q_{\text{skew}}^T A Q_{\text{skew}} \\
&= Q_{\text{skew}}^T (A\Pi_{n,n}) Q_{\text{skew}} \\
&= Q_{\text{skew}}^T A (\Pi_{n,n} Q_{\text{skew}}) \\
&= -Q_{\text{skew}}^T A Q_{\text{skew}} \;=\; -A_{\text{skew}}
\end{aligned}
$$

So $A_{\text{skew}} = 0$.

More on $\tilde{B}$

Since

$$\tilde{A} \;=\; YDY^T \;=\; \sum_{k=1}^{r} d_k y_k y_k^T$$

where $Y = [y_1 \mid \cdots \mid y_r\,]$, it follows that

$$\tilde{B} \;=\; (X \otimes X)^T \tilde{A}(X \otimes X) \;=\; \sum_{k=1}^{r} d_k w_k w_k^T$$

where $w_k \;=\; (X \otimes X)y_k,\; k = 1{:}r$.

The rank-1 matrices $w_k w_k^T$ are PS-symmetric.

$O(rn^3)$ instead of $O(n^5)$

Representing $\tilde{\mathcal{B}}$

We have shown this:

$$\tilde{\mathcal{B}}_{[1,2]\times[3,4]} = \sum_{k=1}^{r} d_k w_k w_k^T$$

It is not hard to show this

$$\tilde{\mathcal{B}}_{[1,3]\times[2,4]} = \sum_{k=1}^{r} d_k W_k \otimes W_k$$

where $W_k = \text{reshape}(w_k, n, n)$ is symmetric.

The Kronecker product expansion is an LDL-based version of a truncated Kronecker Product SVD of B:

$$B = \sum_{k=1}^{n^2} \sigma_i U_i \otimes V_i \qquad V_i = U_i = U_i^T$$

A Comment On LDL

The integrals that define the entries in ((12)(34))-symmetric $\mathcal{A}$ may be expensive to evaluate.

If $A = \mathcal{A}_{[1,2]\times[3,4]}$ has rank r then LDL costs $O(n^2r^2)$.

It would be unfortunate if we had to compute all the entries in A: $O(n^4)$ integrals.

Solution: Lazy LDL.

$PAP^T = LDL^T$ (Lazy Evaluation Version)

At the start of step 4:

$$
PAP^T = \left[\begin{array}{ccc|ccccc}
\mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\mathbf{x} & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 \\
\mathbf{x} & \mathbf{x} & \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\
\hline
\mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{1} & 0 & 0 & 0 & 0 \\
\mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & \mathbf{1} & 0 & 0 & 0 \\
\mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & 0 & \mathbf{1} & 0 & 0 \\
\mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & 0 & 0 & \mathbf{1} & 0 \\
\mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & 0 & 0 & 0 & \mathbf{1}
\end{array}\right]
\left[\begin{array}{ccc|ccccc}
\mathbf{d} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \mathbf{d} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \mathbf{d} & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & \mathbf{x} & \times & \times & \times & \times \\
0 & 0 & 0 & \times & \mathbf{x} & \times & \times & \times \\
0 & 0 & 0 & \times & \times & \mathbf{x} & \times & \times \\
0 & 0 & 0 & \times & \times & \times & \mathbf{x} & \times \\
0 & 0 & 0 & \times & \times & \times & \times & \mathbf{x}
\end{array}\right]
\left[\begin{array}{ccc|ccccc}
\mathbf{1} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\
0 & \mathbf{1} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\
0 & 0 & \mathbf{1} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\
\hline
0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1}
\end{array}\right]
$$

$PAP^T = LDL^T$ (Lazy Evaluation Version)

Find the largest remaining diagonal entry:

$$PAP^T = \left[\begin{array}{ccc|ccccc} \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\ \hline \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{1} & 0 & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & \mathbf{1} & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & 0 & \mathbf{1} & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & 0 & 0 & \mathbf{1} & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & 0 & 0 & 0 & \mathbf{1} \end{array}\right] \left[\begin{array}{ccc|ccccc} \mathbf{d} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{d} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{d} & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & \mathbf{x} & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \mathbf{x} & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \blacksquare & \times & \times \\ 0 & 0 & 0 & \times & \times & \times & \mathbf{x} & \times \\ 0 & 0 & 0 & \times & \times & \times & \times & \mathbf{x} \end{array}\right] \left[\begin{array}{ccc|ccccc} \mathbf{1} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ 0 & \mathbf{1} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ 0 & 0 & \mathbf{1} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \hline 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} \end{array}\right]$$

$PAP^T = LDL^T$ (Lazy Evaluation Version)

Permute into the lead diagonal position:

$$PAP^T = \left[\begin{array}{ccc|ccccc} \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\ \hline \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{1} & 0 & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & \mathbf{1} & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & 0 & \mathbf{1} & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & 0 & 0 & \mathbf{1} & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & 0 & 0 & 0 & \mathbf{1} \end{array}\right] \left[\begin{array}{ccc|ccccc} \mathbf{d} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{d} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{d} & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & \blacksquare & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \mathbf{x} & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \mathbf{x} & \times & \times \\ 0 & 0 & 0 & \times & \times & \times & \mathbf{x} & \times \\ 0 & 0 & 0 & \times & \times & \times & \times & \mathbf{x} \end{array}\right] \left[\begin{array}{ccc|ccccc} \mathbf{1} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ 0 & \mathbf{1} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ 0 & 0 & \mathbf{1} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \hline 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} \end{array}\right]$$

$PAP^T = LDL^T$ (Lazy Evaluation Version)

Evaluate the entries in the subcolumn:

$$PAP^T = \left[\begin{array}{ccc|ccccc} \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\ \hline \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{1} & 0 & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & \mathbf{1} & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & 0 & \mathbf{1} & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & 0 & 0 & \mathbf{1} & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & 0 & 0 & 0 & \mathbf{1} \end{array}\right] \left[\begin{array}{ccc|ccccc} \mathbf{d} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{d} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{d} & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & \blacksquare & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ 0 & 0 & 0 & \mathbf{x} & \mathbf{x} & \times & \times & \times \\ 0 & 0 & 0 & \mathbf{x} & \times & \mathbf{x} & \times & \times \\ 0 & 0 & 0 & \mathbf{x} & \times & \times & \mathbf{x} & \times \\ 0 & 0 & 0 & \mathbf{x} & \times & \times & \times & \mathbf{x} \end{array}\right] \left[\begin{array}{ccc|ccccc} \mathbf{1} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ 0 & \mathbf{1} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ 0 & 0 & \mathbf{1} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \hline 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} \end{array}\right]$$

$PAP^T = LDL^T$ (Lazy Evaluation Version)

Get the next L-column and update remaining diagonal entries...

$$PAP^T = \left[\begin{array}{cccc|cccc} \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{1} & 0 & 0 & 0 & 0 \\ \hline \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{1} & 0 & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & \mathbf{1} & 0 & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & 0 & \mathbf{1} & 0 \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & 0 & 0 & 0 & \mathbf{1} \end{array}\right] \left[\begin{array}{cccc|cccc} \mathbf{d} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \mathbf{d} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbf{d} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbf{d} & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \mathbf{x} & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \mathbf{x} & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times & \mathbf{x} & \times \\ 0 & 0 & 0 & 0 & \times & \times & \times & \mathbf{x} \end{array}\right] \left[\begin{array}{cccc|cccc} \mathbf{1} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ 0 & \mathbf{1} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ 0 & 0 & \mathbf{1} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ 0 & 0 & 0 & \mathbf{1} & \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \hline 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} \end{array}\right]$$

Conclusions

- Tensor problems with multiple symmetries lead to matrix problems with multiple symmetries.
- This talk revolved around an order-4 tensor and matrices with two symmetries.
- Current methods do not fully exploit PS-Symmetry.
- Anticipate more dramatic savings if we pursue this methodology on higher-order problems with numerous symmetries.

Optional "Fun" Problems

Problem E5. How would you compute the Schur Decomposition of a PS-symmetric matrix?

Problem A5. If a matrix is symmetric, the work involved in solving $Ax = b$ is halved. If a matrix is centrosymmetric, then the work involved is reduced by a factor of 4. If a matrix has 3 types of symmetry then work should be reduced by a factor of ????