

- Sherman Morrison Formula

Solving Modified Problems

- If right-hand side of linear system changes but matrix does not, then LU factorization need not be repeated to solve new system
- Only forward- and back-substitution need be repeated for new right-hand side
- This is substantial savings in work, since additional triangular solutions cost only $\mathcal{O}(n^2)$ work, in contrast to $\mathcal{O}(n^3)$ cost of factorization



Sherman-Morrison Formula

- Sometimes refactorization can be avoided even when matrix *does* change
- *Sherman-Morrison formula* gives inverse of matrix resulting from rank-one change to matrix whose inverse is already known

$$(\mathbf{A} - \mathbf{u}\mathbf{v}^T)^{-1} = \mathbf{A}^{-1} + \mathbf{A}^{-1}\mathbf{u}(1 - \mathbf{v}^T\mathbf{A}^{-1}\mathbf{u})^{-1}\mathbf{v}^T\mathbf{A}^{-1}$$

where \mathbf{u} and \mathbf{v} are n -vectors

- Evaluation of formula requires $\mathcal{O}(n^2)$ work (for matrix-vector multiplications) rather than $\mathcal{O}(n^3)$ work required for inversion



Rank-One Updating of Solution

- To solve linear system $(A - uv^T)x = b$ with new matrix, use Sherman-Morrison formula to obtain

$$\begin{aligned}x &= (A - uv^T)^{-1}b \\&= A^{-1}b + A^{-1}u(1 - v^T A^{-1}u)^{-1}v^T A^{-1}b\end{aligned}$$

which can be implemented by following steps

- Solve $Az = u$ for z , so $z = A^{-1}u$
- Solve $Ay = b$ for y , so $y = A^{-1}b$
- Compute $x = y + ((v^T y) / (1 - v^T z))z$
- If A is already factored, procedure requires only triangular solutions and inner products, so only $\mathcal{O}(n^2)$ work and no explicit inverses



Example: Rank-One Updating of Solution

- Consider rank-one modification

$$\begin{bmatrix} 2 & 4 & -2 \\ 4 & 9 & -3 \\ -2 & -1 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 8 \\ 10 \end{bmatrix}$$

(with 3, 2 entry changed) of system whose LU factorization was computed in earlier example

- One way to choose update vectors is

$$u = \begin{bmatrix} 0 \\ 0 \\ -2 \end{bmatrix} \quad \text{and} \quad v = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

Original Matrix

$$\boxed{\begin{bmatrix} 2 & 4 & -2 \\ 4 & 9 & -3 \\ -2 & -3 & 7 \end{bmatrix}}$$

so matrix of modified system is $A - uv^T$



Example, continued

- Using LU factorization of A to solve $Az = u$ and $Ay = b$,

$$z = \begin{bmatrix} -3/2 \\ 1/2 \\ -1/2 \end{bmatrix} \quad \text{and} \quad y = \begin{bmatrix} -1 \\ 2 \\ 2 \end{bmatrix}$$

- Final step computes updated solution

Q: Under what circumstances could the denominator be zero?

$$x = y + \frac{\mathbf{v}^T \mathbf{y}}{1 - \mathbf{v}^T z} z = \begin{bmatrix} -1 \\ 2 \\ 2 \end{bmatrix} + \frac{2}{1 - 1/2} \begin{bmatrix} -3/2 \\ 1/2 \\ -1/2 \end{bmatrix} = \begin{bmatrix} -7 \\ 4 \\ 0 \end{bmatrix}$$

- We have thus computed solution to modified system without factoring modified matrix



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[1] Solve $A\tilde{\mathbf{x}} = \tilde{\mathbf{b}}$:

$$A \longrightarrow LU \text{ (} O(n^3) \text{ work)}$$

$$\text{Solve } L\tilde{\mathbf{y}} = \tilde{\mathbf{b}},$$

$$\text{Solve } U\tilde{\mathbf{x}} = \tilde{\mathbf{y}} \text{ (} O(n^2) \text{ work).}$$

[2] New problem:

$$(A - \mathbf{u}\mathbf{v}^T) \mathbf{x} = \mathbf{b}. \quad (\text{different } \mathbf{x} \text{ and } \mathbf{b})$$

Key Idea:

- $(A - \mathbf{u}\mathbf{v}^T) \mathbf{x}$ differs from $A\mathbf{x}$ by only a small amount of information.
- Rewrite as: $A\mathbf{x} + \mathbf{u}\gamma = \mathbf{b}$
 $\gamma := -\mathbf{v}^T \mathbf{x} \iff \mathbf{v}^T \mathbf{x} + \gamma = 0$

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Extended system:

$$A\mathbf{x} + \gamma\mathbf{u} = \mathbf{b}$$

$$\mathbf{v}^T \mathbf{x} + \gamma = 0$$

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Extended system:

$$\begin{aligned} A\mathbf{x} + \gamma\mathbf{u} &= \mathbf{b} \\ \mathbf{v}^T \mathbf{x} + \gamma &= 0 \end{aligned}$$

In matrix form:

$$\begin{bmatrix} A & \mathbf{u} \\ \mathbf{v}^T & 1 \end{bmatrix} \begin{pmatrix} \mathbf{x} \\ \gamma \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ 0 \end{pmatrix}$$

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Eliminate for γ :

$$\begin{bmatrix} A & \mathbf{u} \\ 0 & 1 - \mathbf{v}^T A^{-1} \mathbf{u} \end{bmatrix} \begin{pmatrix} \mathbf{x} \\ \gamma \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ -\mathbf{v}^T A^{-1} \mathbf{b} \end{pmatrix}$$

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$$\gamma = - (1 - \mathbf{v}^T A^{-1} \mathbf{u})^{-1} \mathbf{v}^T A^{-1} \mathbf{b}$$

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$$\gamma = - (1 - \mathbf{v}^T A^{-1} \mathbf{u})^{-1} \mathbf{v}^T A^{-1} \mathbf{b}$$

$$\mathbf{x} = A^{-1} (\mathbf{b} - \mathbf{u}\gamma) = A^{-1} \left[\mathbf{b} + \mathbf{u} (1 - \mathbf{v}^T A^{-1} \mathbf{u})^{-1} \mathbf{v}^T A^{-1} \mathbf{b} \right]$$

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Extended system:

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$$\mathbf{x} = A^{-1} (\mathbf{b} - \mathbf{u}\gamma) = A^{-1} \left[\mathbf{b} + \mathbf{u} (1 - \mathbf{v}^T A^{-1} \mathbf{u})^{-1} \mathbf{v}^T A^{-1} \mathbf{b} \right]$$

$$(A - \mathbf{u}\mathbf{v}^T)^{-1} = A^{-1} + A^{-1} \mathbf{u} (1 - \mathbf{v}^T A^{-1} \mathbf{u})^{-1} \mathbf{v}^T A^{-1}.$$

Sherman Morrison: Potential Singularity

- Consider the modified system: $(A - \mathbf{u}\mathbf{v}^T) \mathbf{x} = \mathbf{b}$.
- The solution is

$$\begin{aligned}\mathbf{x} &= (A - \mathbf{u}\mathbf{v}^T)^{-1} \mathbf{b} \\ &= \left[I + A^{-1}\mathbf{u} (1 - \mathbf{v}^T A^{-1}\mathbf{u})^{-1} \mathbf{v}^T A^{-1} \right] A^{-1} \mathbf{b}.\end{aligned}$$

- If $1 - \mathbf{v}^T A^{-1}\mathbf{u} = 0$, failure.
- Why?

Sherman Morrison: Potential Singularity

- Let $\tilde{A} := (A - \mathbf{u}\mathbf{v}^T)$ and consider,

$$\begin{aligned}\tilde{A} A^{-1} &= (A - \mathbf{u}\mathbf{v}^T) A^{-1} \\ &= (I - \mathbf{u}\mathbf{v}^T A^{-1}).\end{aligned}$$

- Look at the product $\tilde{A} A^{-1} \mathbf{u}$,

$$\begin{aligned}\tilde{A} A^{-1} \mathbf{u} &= (I - \mathbf{u}\mathbf{v}^T A^{-1}) \mathbf{u} \\ &= \mathbf{u} - \mathbf{u}\mathbf{v}^T A^{-1} \mathbf{u}.\end{aligned}$$

- If $\mathbf{v}^T A^{-1} \mathbf{u} = 1$, then

$$\tilde{A} A^{-1} \mathbf{u} = \mathbf{u} - \mathbf{u} = 0,$$

which means that \tilde{A} is singular since we assume that A^{-1} exists.

- Thus, an unfortunate choice of \mathbf{u} and \mathbf{v} can lead to a singular modified matrix and this singularity is indicated by $\mathbf{v}^T A^{-1} \mathbf{u} = 1$.

Tensor Product Matrices

The tensor- (or Kronecker-) product of matrices A and B is denoted as

$$C = A \otimes B$$

and is defined as the block matrix having entries

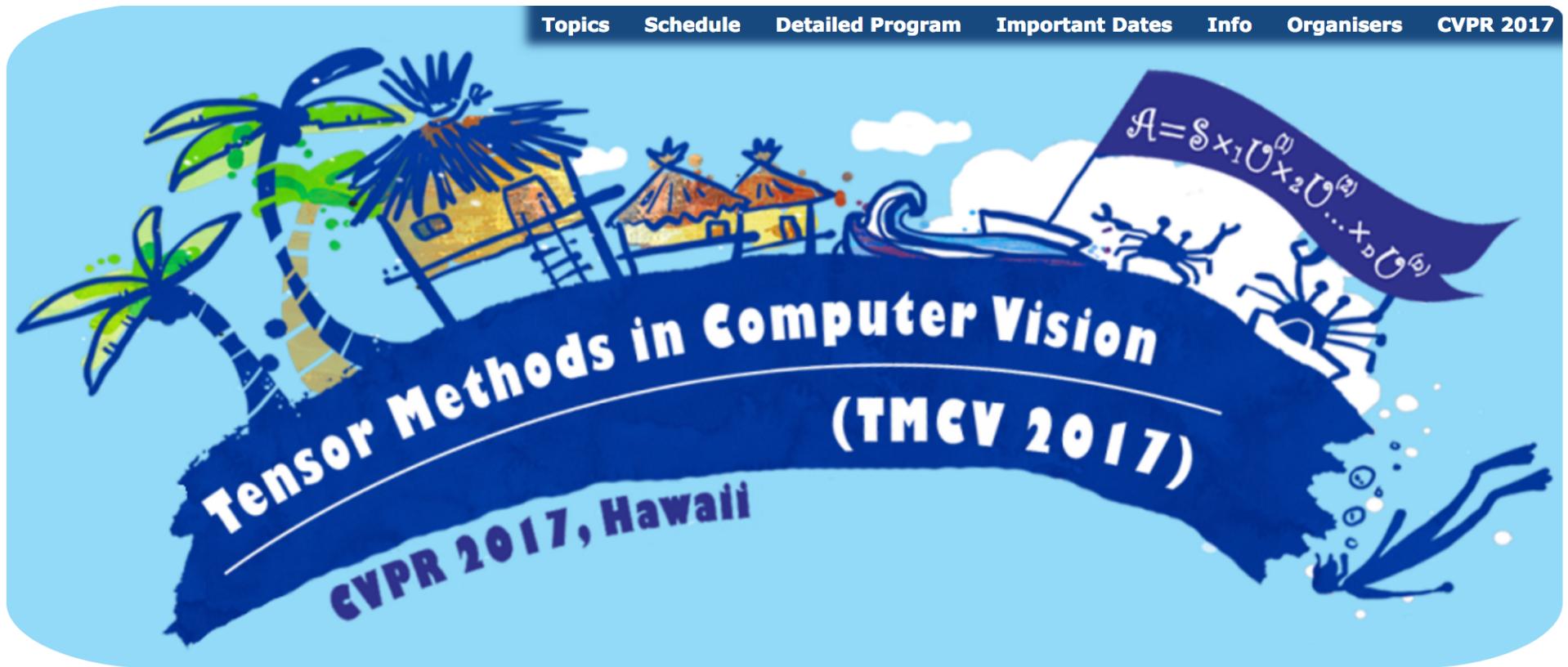
$$C := \begin{pmatrix} a_{11}B & a_{12}B & \cdots & \cdots & a_{1n}B \\ a_{21}B & a_{22}B & \cdots & \cdots & a_{2n}B \\ \vdots & \vdots & & & \vdots \\ a_{m1}B & a_{m2}B & \cdots & \cdots & a_{mn}B \end{pmatrix}.$$

Tensor-Product Matrices

- ❑ Tensor-product forms arise in many applications, including
 - ❑ Density Functional Theory (DFT) in computational chemistry (e.g., 7-dimensional tensors)
 - ❑ Partial differential equations
 - ❑ Image processing (e.g., multidimensional FFTs)
 - ❑ Machine learning (ML)
- ❑ Their importance in ML/AI applications is such that software developers and computer architects are now designing fast tensor-contraction engines to further accelerate tensor-product manipulations.

Tensor-Product Matrices

- ❑ In Computer Vision, there is even a conference series on this topic.



- Our interest here is to understand how tensor-product forms can yield very rapid direct solvers for systems of the form $A\mathbf{x} = \mathbf{b}$.
- There are two ways in which tensor-product-based matrices for the form $C = A \otimes B$ accelerate computation:
 1. They can be used to effect very fast matrix-vector products.
 2. They can be used to effect very fast matrix-matrix products.
- To begin, we focus on the matrix-matrix products, which is a bit easier to understand.

Product Rule for Tensor-Product Matrices

- Assume that the matrix pairs (D, A) and (E, B) are dimensioned such that the products DA and EB are well-defined.
- If

$$C := A \otimes B \quad \text{and} \quad F := D \otimes C,$$

then, the matrix product FC is given by

$$\begin{aligned} FC &= (D \otimes C) (A \otimes B) \\ &= DA \otimes EB. \end{aligned}$$

- This result follows from the definition of the Kronecker product, \otimes , and has many important consequences.

Uses of the Product Rule: Inverses

$$(D \otimes C) (A \otimes B) = DA \otimes EB.$$

- If $C := A \otimes B$, then

$$C^{-1} := A^{-1} \otimes B^{-1}.$$

- Specifically,

$$\begin{aligned} C^{-1}C &= (A^{-1} \otimes B^{-1}) (A \otimes B) = A^{-1}A \otimes B^{-1}B \\ &= I_A \otimes I_B = I, \end{aligned}$$

where I_A and I_B are identity matrices equal in size to A and B , respectively.

- Thus, the inverse of C is the tensor-product of two much smaller matrices, A and B .

Uses of the Product Rule: Inverses

- Example:

- Suppose A and B are full $N \times N$ matrices and $C = A \otimes B$ is $n \times n$ with $n = N^2$.
- The LU factorization of C is

$$LU = (L_A \otimes L_B)(U_A \otimes U_B).$$

- What is the cost of computing the tensor product form of LU , rather than LU directly as a function of N ?
- What is the ratio (full time over tensor-product time) when $N = 100$?

The Curse of Dimensionality

- The advantage of the tensor-product representation increases with higher dimensions.
- Suppose A_j is $N \times N$, for $j = 1, \dots, d$, and

$$C = A_d \otimes A_{d-1} \otimes \cdots \otimes A_1,$$

with inverse

$$C^{-1} = A_d^{-1} \otimes A_{d-1}^{-1} \otimes \cdots \otimes A_1^{-1}.$$

- Consider $d = 7$ and $N = 10$.
- The number of nonzeros in C (*if formed*) is N^{14} , which is 800 TB and would cost you about \$10,000 in disk drives.
- The factorization cost for the tensor product form is ≈ 5000 operations. A blink of the eye on your laptop.
- Factorization of the full form will take about 10 minutes on the world's fastest computer in 2021, or about 600 years on my mac.
- Tensor-product forms are *critical* for efficient computation in many large-dimensional scientific problems.

Uses of the Product Rule: Eigenvalues

- Suppose that A is an $N \times N$ matrix with the *similarity transformation* (Chapter 4),

$$A = S\Lambda S^{-1},$$

where $S = [\mathbf{s}_1 \mathbf{s}_2 \cdots \mathbf{s}_N]$ is the (full) matrix of eigenvectors of A and $\Lambda = \text{diag}(\lambda_i)$ is the diagonal matrix of corresponding eigenvalues.

That is, $A\mathbf{s}_i = \mathbf{s}_i \lambda_i$.

- Let $T\mathcal{M}T^{-1}$ denote the similarity transformation for B , with eigenvector matrix T and eigenvalue matrix \mathcal{M} .
- Then the similarity transformation for $C = A \otimes B$ is

$$\begin{aligned} A \otimes B &= (S\Lambda S^{-1}) \otimes (T\mathcal{M}T^{-1}) \\ &= (S \otimes T) (\Lambda \otimes \mathcal{M}) (S^{-1} \otimes T^{-1}) \\ &= U\mathcal{N}U^{-1}. \end{aligned}$$

- Thus, we have diagonalized C by diagonalizing two smaller systems A and B .

Fast Matrix-Vector Products

• Evaluate $\underline{\omega} = \underline{C}\underline{u}$ $C = A \otimes B$.

• $C = A \otimes B = (A \otimes I)(I \otimes B)$

$$\underline{\omega} = \underline{C}\underline{u} = (\cancel{A \otimes I}) \cdot \underbrace{[(I \otimes B)\underline{u}]}_{=: \underline{v}} = : \underline{v}$$

$$\boxed{\begin{aligned} \underline{v} &= (I \otimes B)\underline{u} \\ \underline{\omega} &= (A \otimes I)\underline{v} \end{aligned}}$$

(2)

$$\cdot \quad V = (I \otimes B) u$$

$$I \in \mathbb{R}^{M \times N}$$

$$B \in \mathbb{R}^{N \times N} \quad n := MN$$

$$\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \\ \hline v_{N+1} \\ \vdots \\ v_{2N} \\ \hline \vdots \\ \vdots \\ v_n \end{pmatrix} = \begin{bmatrix} B & & & \\ & B & & \\ & & B & \\ & & & B \\ & & & & \ddots & & \\ & & & & & B & \\ & & & & & & \ddots & u_n \end{bmatrix}$$

The diagram illustrates the matrix-vector multiplication $V = (I \otimes B) u$. On the left, a vertical vector v is shown with entries v_1, v_2, \dots, v_N above a horizontal line, followed by v_{N+1}, \dots, v_{2N} below it, and so on down to v_n . An equals sign follows this vector. To the right of the equals sign is a large square matrix. This matrix has a block-diagonal structure where each block is a copy of matrix B . There are n such blocks along the diagonal, separated by vertical lines. The matrix is labeled with B in the top-left corner of each block. To the right of the matrix is a vertical vector u with entries u_1, u_2, \dots, u_N above a horizontal line, followed by u_{N+1}, \dots, u_{2N} below it, and so on down to u_n .

• Independent matrix-vector products! Same B!

- Independent matrix-vector products! Same B!
- RESHAPE!

$$\begin{bmatrix} v_1 & v_{1+N} & \cdots & v_{1+(M-1)N} \\ \vdots & & & \vdots \\ v_N & v_{2N} & & v_{MN} \end{bmatrix} = B \begin{bmatrix} u_1 & u_{1+N} & \cdots & u_{1+(M-1)N} \\ \vdots & \vdots & & \vdots \\ u_N & u_{2N} & & u_{MN} \end{bmatrix}$$

$\boxed{V = BU}$

Following the same logic, can show
that $\underline{w} = (\underline{A} \otimes I) \underline{v}$ has form:

$$W = VA^T$$

with

$$W = \begin{bmatrix} w_1 & w_{N+1} & \cdots \\ w_2 & w_{N+2} & \cdots \\ | & | & | \\ w_N & w_{2N} & w_{NM} \end{bmatrix}$$

So $W = BUA^T$. Very fast.

Fast Matrix-Vector Products

- Q: What is the cost of $C\mathbf{u}$, vs. the fast form for $(A \otimes B)\mathbf{u}$?

Fast Solvers: Other Systems

Fast Solvers: Other Systems

Computing $\|A\|_2$ and $\text{cond}_2(A)$.

- Recall:

$$\text{cond}(A) := \|A^{-1}\| \cdot \|A\|,$$

$$\|A\| := \max_{\mathbf{x} \neq 0} \frac{\|A\mathbf{x}\|}{\|\mathbf{x}\|},$$

$$\|\mathbf{x}\|_2 = \left(\sum_{i=1}^n x_i^2 \right)^{\frac{1}{2}} = \sqrt{\mathbf{x}^T \mathbf{x}},$$

$$\|\mathbf{x}\|_2^2 = \mathbf{x}^T \mathbf{x}.$$

- From now on, drop the subscript “₂”.

$$\|\mathbf{x}\|^2 = \mathbf{x}^T \mathbf{x}$$

$$\|A\mathbf{x}\|^2 = (A\mathbf{x})^T (A\mathbf{x}) = \mathbf{x}^T A^T A \mathbf{x}.$$

- Matrix norm:

$$\begin{aligned}
\|A\|^2 &= \max_{\mathbf{x} \neq 0} \frac{\|\mathbf{Ax}\|^2}{\|\mathbf{x}\|^2}, \\
&= \max_{\mathbf{x} \neq 0} \frac{\mathbf{x}^T A^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}} \\
&= \lambda_{\max}(A^T A) =: \text{spectral radius of } (A^T A).
\end{aligned}$$

- The symmetric positive definite matrix $B := A^T A$ has positive eigenvalues.
- All symmetric matrices B have a complete set of orthonormal eigenvectors satisfying

$$B\mathbf{z}_j = \lambda_j \mathbf{z}_j, \quad \mathbf{z}_i^T \mathbf{z}_j = \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}.$$

- **Note:** If $\lambda_i = \lambda_j$, $i \neq j$, then can have $\mathbf{z}_i^T \mathbf{z}_j \neq 0$, but we can orthogonalize \mathbf{z}_i and \mathbf{z}_j so that $\tilde{\mathbf{z}}_i^T \tilde{\mathbf{z}}_j = 0$ and

$$\begin{aligned}
B\tilde{\mathbf{z}}_i &= \lambda_i \tilde{\mathbf{z}}_i \quad \lambda_i = \lambda_j \\
B\tilde{\mathbf{z}}_j &= \lambda_j \tilde{\mathbf{z}}_j.
\end{aligned}$$

- Assume eigenvalues are sorted with $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$.
- For any \mathbf{x} we have: $\mathbf{x} = c_1\mathbf{z}_1 + c_2\mathbf{z}_2 + \dots + c_n\mathbf{z}_n$.
- Let $\|\mathbf{x}\| = 1$.

- Want to find $\max_{\|\mathbf{x}\|=1} \frac{\mathbf{x}^T B \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \max_{\|\mathbf{x}\|=1} \mathbf{x}^T B \mathbf{x}$.

- Note:
$$\mathbf{x}^T \mathbf{x} = \left(\sum_{i=1}^n c_i \mathbf{z}_i \right)^T \left(\sum_{j=1}^n c_j \mathbf{z}_j \right)$$

$$= \sum_{i=1}^n \sum_{j=1}^n c_i c_j \mathbf{z}_i^T \mathbf{z}_j$$

$$= \sum_{i=1}^n \sum_{j=1}^n c_i c_j \delta_{ij}$$

$$= \sum_{i=1}^n c_i^2 = 1.$$

$$\implies c_1^2 = 1 - \sum_{i=2}^n c_i^2.$$

$$\begin{aligned}
\mathbf{x}^T B \mathbf{x} &= \left(\sum_{i=1}^n c_i \mathbf{z}_i \right)^T \left(\sum_{j=1}^n c_j B \mathbf{z}_j \right) \\
&= \left(\sum_{i=1}^n c_i \mathbf{z}_i \right)^T \left(\sum_{j=1}^n c_j \lambda_j \mathbf{z}_j \right) \\
&= \sum_{i=1}^n \sum_{j=1}^n c_i \lambda_j c_j \mathbf{z}_i^T \mathbf{z}_j \\
&= \sum_{i=1}^n \sum_{j=1}^n c_i \lambda_j c_j \delta_{ij} \\
&= \sum_{i=1}^n c_i^2 \lambda_i = c_1^2 \lambda_1 + c_2^2 \lambda_2 + \cdots + c_n^2 \lambda_n \\
&= \lambda_1 [c_1^2 + c_2^2 \beta_2 + \cdots + c_n^2 \beta_n], \quad 0 < \beta_i := \frac{\lambda_i}{\lambda_1} \leq 1, \\
&= \lambda_1 [(1 - c_2^2 - \cdots - c_n^2) + c_2^2 \beta_2 + \cdots + c_n^2 \beta_n] \\
&= \lambda_1 [1 - (1 - \beta_2)c_2^2 + (1 - \beta_3)c_3^2 + \cdots + (1 - \beta_n)c_n^2] \\
&= \lambda_1 [1 - \text{some positive (or zero) numbers}].
\end{aligned}$$

- Expression is maximized when $c_2 = c_3 = \cdots = c_n = 0, \implies c_1 = 1.$
- Maximum value $\mathbf{x}^T B \mathbf{x} = \lambda_{\max}(B) = \lambda_1.$
- Similarly, can show $\min \mathbf{x}^T B \mathbf{x} = \lambda_{\min}(B) = \lambda_n.$

- So, $\|A\|^2 = \max_{\lambda} \lambda(A^T A)$ = spectral radius of $A^T A$.

- Now,

$$\|A^{-1}\|^2 = \max_{\mathbf{x} \neq 0} \frac{\|A^{-1}\mathbf{x}\|^2}{\|\mathbf{x}\|^2}.$$

- Let $\mathbf{x} = A\mathbf{y}$:

$$\begin{aligned} \|A^{-1}\|^2 &= \max_{\mathbf{y} \neq 0} \frac{\|A^{-1}A\mathbf{y}\|^2}{\|A\mathbf{y}\|^2} = \max_{\mathbf{y} \neq 0} \frac{\|\mathbf{y}\|^2}{\|A\mathbf{y}\|^2} = \left(\min_{\mathbf{y} \neq 0} \frac{\|A\mathbf{y}\|^2}{\|\mathbf{y}\|^2} \right)^{-1} \\ &= \frac{1}{\lambda_{\min}(A^T A)}. \end{aligned}$$

- So, $\text{cond}_2(A) = \|A^{-1}\| \cdot \|A\|$,

$$\text{cond}_2(A) = \sqrt{\frac{\lambda_{\max}(A^T A)}{\lambda_{\min}(A^T A)}}.$$

Special Types of Linear Systems

- Work and storage can often be saved in solving linear system if matrix has special properties
- Examples include
 - *Symmetric*: $A = A^T$, $a_{ij} = a_{ji}$ for all i, j
 - *Positive definite*: $x^T A x > 0$ for all $x \neq 0$
 - *Band*: $a_{ij} = 0$ for all $|i - j| > \beta$, where β is *bandwidth* of A
 - *Sparse*: most entries of A are zero



Symmetric Positive Definite (SPD) Matrices

- ❑ Very common in optimization and physical processes
- ❑ Easiest example:
 - ❑ If B is invertible, then $A := B^T B$ is SPD.
- ❑ SPD systems of the form $A \underline{x} = \underline{b}$ can be solved using
 - ❑ (stable) Cholesky factorization $A = LL^T$, or
 - ❑ iteratively with the most robust iterative solver, conjugate gradient iteration (generally with preconditioning, known as preconditioned conjugate gradients, PCG).

Cholesky Factorization and SPD Matrices.

- A is SPD: $A = A^T$ and $\mathbf{x}^T A \mathbf{x} > 0$ for all $\mathbf{x} \neq 0$.
- Seek a symmetric factorization $A = \tilde{L}\tilde{L}^T$ (not LU).
 - L *not* lower triangular but not *unit* lower triangular.
 - That is, L_{ii} not necessarily 1.
- Alternatively, seek factorization $A = LDL^T$, where L *is* unit lower triangular and D is *diagonal*.

- Start with $LDL^T = A$.
- Clearly, $LU = A$ with $U = DL^T$.
 - Follows from uniqueness of LU factorization.
 - D is a *row scaling* of L^T and thus $D_{ii} = U_{ii}$.
 - A property of SPD matrices is that all pivots are positive.
 - (Another property is that you do not need to pivot.)

- Consider standard update step:

$$\begin{aligned} a_{ij} &= a_{ij} - \frac{a_{ik} a_{kj}}{a_{kk}} \\ &= a_{ij} - \frac{a_{ik} a_{jk}}{a_{kk}} \end{aligned}$$

- Usual multiplier column entries are $l_{ik} = a_{ik}/a_{kk}$.
- Usual pivot row entries are $u_{kj} = a_{kj} = a_{jk}$.
- So, if we factor $1/d_{kk} = 1/a_{kk}$ out of U , we have:

$$\begin{aligned} d_{kk}(a_{kj}/a_{kk}) &= d_{kk}l_{kj} \\ \rightarrow U &= D(D^{-1}U) \\ &= DL^T. \end{aligned}$$

- For Cholesky, we have

$$A = LDL^T = L\sqrt{D}\sqrt{D}L^T = \tilde{L}\tilde{L}^T,$$

with $\tilde{L} = L\sqrt{D}$.

Symmetric Positive Definite Matrices

- If A is symmetric and positive definite, then LU factorization can be arranged so that $U = L^T$, which gives *Cholesky factorization*

$$A = L L^T$$

where L is lower triangular with positive diagonal entries

- Algorithm for computing it can be derived by equating corresponding entries of A and LL^T
- In 2×2 case, for example,

$$\begin{bmatrix} a_{11} & a_{21} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 \\ l_{21} & l_{22} \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} \\ 0 & l_{22} \end{bmatrix}$$

implies

$$l_{11} = \sqrt{a_{11}}, \quad l_{21} = a_{21}/l_{11}, \quad l_{22} = \sqrt{a_{22} - l_{21}^2}$$



Cholesky Factorization (Text)

Algorithm 2.7 Cholesky Factorization

```
for k = 1 to n                                { loop over columns }
     $a_{kk} = \sqrt{a_{kk}}$ 
    for i = k + 1 to n
         $a_{ik} = a_{ik}/a_{kk}$                       { scale current column }
    end
    for j = k + 1 to n
        for i = j to n
             $a_{ij} = a_{ij} - a_{ik} \cdot a_{jk}$       { from each remaining column,
                                                subtract multiple
                                                of current column }
        end
    end
end
```

*After a row scaling, this is just standard LU decomposition,
exploiting symmetry in the LU factors and A. ($U=L^T$)*

Cholesky Factorization

- One way to write resulting general algorithm, in which Cholesky factor L overwrites original matrix A , is

```
for  $j = 1$  to  $n$ 
    for  $k = 1$  to  $j - 1$ 
        for  $i = j$  to  $n$ 
             $a_{ij} = a_{ij} - a_{ik} \cdot a_{jk}$ 
        end
    end
     $a_{jj} = \sqrt{a_{jj}}$ 
    for  $k = j + 1$  to  $n$ 
         $a_{kj} = a_{kj}/a_{jj}$ 
    end
end
```



Cholesky Factorization, continued

- Features of Cholesky algorithm for symmetric positive definite matrices
 - All n square roots are of positive numbers, so algorithm is well defined
 - No pivoting is required to maintain numerical stability
 - Only lower triangle of A is accessed, and hence upper triangular portion need not be stored
 - Only $n^3/6$ multiplications and similar number of additions are required
- Thus, Cholesky factorization requires only about half work and **half storage** compared with LU factorization of general matrix by Gaussian elimination, and also avoids need for pivoting



Linear Algebra Very Short Summary

Main points:

- ❑ Conditioning of matrix $\text{cond}(A)$ bounds our expected accuracy.
 - ❑ e.g., if $\text{cond}(A) \sim 10^5$ we expect at most 11 significant digits in \underline{x} .
 - ❑ Why?
 - ❑ We start with IEEE double precision – 16 digits. We lose 5 because condition $(A) \sim 10^5$, so we have $11 = 16-5$.
- ❑ Stable algorithm (i.e., pivoting) important to realizing this bound.
 - ❑ Some systems don't need pivoting (e.g., SPD, diagonally dominant)
 - ❑ Unstable algorithms can sometimes be rescued with iterative refinement.
- ❑ Costs:
 - ❑ Full matrix $\rightarrow O(n^2)$ storage, $O(n^3)$ work (wall-clock time)
 - ❑ Sparse or banded matrix, substantially less.

- ❑ The following slides present the book's derivation of the LU factorization process.
- ❑ I'll highlight a few of them that show the equivalence between the outer product approach and the elementary elimination matrix approach.

Example: Triangular Linear System

$$\begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 8 \end{bmatrix}$$

- Using back-substitution for this upper triangular system, last equation, $4x_3 = 8$, is solved directly to obtain $x_3 = 2$
- Next, x_3 is substituted into second equation to obtain $x_2 = 2$
- Finally, both x_3 and x_2 are substituted into first equation to obtain $x_1 = -1$



Elimination

- To transform general linear system into triangular form, we need to replace selected nonzero entries of matrix by zeros
- This can be accomplished by taking linear combinations of rows
- Consider 2-vector $a = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$
- If $a_1 \neq 0$, then

$$\begin{bmatrix} 1 & 0 \\ -a_2/a_1 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} a_1 \\ 0 \end{bmatrix}$$



Elementary Elimination Matrices

- More generally, we can annihilate *all* entries below k th position in n -vector a by transformation

$$M_k a = \begin{bmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & -m_{k+1} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & -m_n & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_k \\ a_{k+1} \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_k \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

where $m_i = a_i/a_k$, $i = k + 1, \dots, n$

- Divisor a_k , called *pivot*, must be nonzero



Elementary Elimination Matrices, continued

- Matrix M_k , called *elementary elimination matrix*, adds multiple of row k to each subsequent row, with *multipliers* m_i chosen so that result is zero
- M_k is unit lower triangular and nonsingular
- $M_k = I - m_k e_k^T$, where $m_k = [0, \dots, 0, m_{k+1}, \dots, m_n]^T$ and e_k is k th column of identity matrix
- $M_k^{-1} = I + m_k e_k^T$, which means $M_k^{-1} = :L_k$ is same as M_k except signs of multipliers are reversed



Elementary Elimination Matrices, continued

- If M_j , $j > k$, is another elementary elimination matrix, with vector of multipliers m_j , then

$$\begin{aligned} M_k M_j &= \mathbf{I} - m_k e_k^T - m_j e_j^T + m_k e_k^T m_j e_j^T \\ &= \mathbf{I} - m_k e_k^T - m_j e_j^T \end{aligned}$$

which means product is essentially “union,” and similarly for product of inverses, $L_k L_j$



Comment on update step and $\underline{m}_k \underline{e}^T_k$

- Recall, $\underline{v} = C \underline{w} \in \text{span}\{C\}$.
- $\therefore V = (\underline{v}_1 \underline{v}_2 \dots \underline{v}_n) = C (\underline{w}_1 \underline{w}_2 \dots \underline{w}_n) \in \text{span}\{C\}$.

- If $C = \underline{c}$, i.e., C is a column vector and therefore of rank 1, then V is in $\text{span}\{C\}$ and is of rank 1.

- All columns of V are multiples of \underline{c} .

- Thus, $W = \underline{c} \underline{r}^T$ is an $n \times n$ matrix of rank 1.
 - All columns are multiples of the first column and
 - All rows are multiples of the first row.

Elementary Elimination Matrices, continued

- Matrix M_k , called *elementary elimination matrix*, adds multiple of row k to each subsequent row, with *multipliers* m_i chosen so that result is zero
- M_k is unit lower triangular and nonsingular
- $M_k = I - m_k e_k^T$, where $m_k = [0, \dots, 0, m_{k+1}, \dots, m_n]^T$ and e_k is k th column of identity matrix
- $M_k^{-1} = I + m_k e_k^T$, which means $M_k^{-1} = :L_k$ is same as M_k except signs of multipliers are reversed



Example: Elementary Elimination Matrices

- For $\mathbf{a} = \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix}$,

$$\mathbf{M}_1 \mathbf{a} = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}$$

and

$$\mathbf{M}_2 \mathbf{a} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1/2 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 0 \end{bmatrix}$$



Example, continued

- Note that

$$\mathbf{L}_1 = \mathbf{M}_1^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix}, \quad \mathbf{L}_2 = \mathbf{M}_2^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1/2 & 1 \end{bmatrix}$$

and

$$\mathbf{M}_1 \mathbf{M}_2 = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & 1/2 & 1 \end{bmatrix}, \quad \mathbf{L}_1 \mathbf{L}_2 = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & -1/2 & 1 \end{bmatrix}$$



Gaussian Elimination

- To reduce general linear system $Ax = b$ to upper triangular form, first choose M_1 , with a_{11} as pivot, to annihilate first column of A below first row
 - System becomes $M_1 A x = M_1 b$, but solution is unchanged
- Next choose M_2 , using a_{22} as pivot, to annihilate second column of $M_1 A$ below second row
 - System becomes $M_2 M_1 A x = M_2 M_1 b$, but solution is still unchanged
- Process continues for each successive column until all subdiagonal entries have been zeroed



Gaussian Elimination

- To reduce general linear system $Ax = b$ to upper triangular form, first choose M_1 , with a_{11} as pivot, to annihilate first column of A below first row
 - System becomes $M_1 Ax = M_1 b$, but solution is unchanged
- Next choose M_2 , using a_{22} as pivot, to annihilate second column of $M_1 A$ below second row
 - System becomes $M_2 M_1 Ax = M_2 M_1 b$, but solution is still unchanged
- *Technically, this should be a'_{22} , the 2-2 entry in $A' := M_1 A$. Thus, we don't know all the pivots in advance.*



Gaussian Elimination, continued

- Resulting upper triangular linear system

$$\begin{aligned} M_{n-1} \cdots M_1 A x &= M_{n-1} \cdots M_1 b \\ M A x &= M b \end{aligned}$$

can be solved by back-substitution to obtain solution to original linear system $Ax = b$

- Process just described is called *Gaussian elimination*



LU Factorization

- Product $L_k L_j$ is unit lower triangular if $k < j$, so

$$L = M^{-1} = M_1^{-1} \cdots M_{n-1}^{-1} = L_1 \cdots L_{n-1}$$

is unit lower triangular

- By design, $U = MA$ is upper triangular
- So we have

$$A = LU$$

with L unit lower triangular and U upper triangular

- Thus, Gaussian elimination produces *LU factorization* of matrix into triangular factors



LU Factorization, continued

- Having obtained LU factorization, $\mathbf{A}\mathbf{x} = \mathbf{b}$ becomes $\mathbf{L}\mathbf{U}\mathbf{x} = \mathbf{b}$, and can be solved by forward-substitution in lower triangular system $\mathbf{L}\mathbf{y} = \mathbf{b}$, followed by back-substitution in upper triangular system $\mathbf{U}\mathbf{x} = \mathbf{y}$
- Note that $\mathbf{y} = \mathbf{M}\mathbf{b}$ is same as transformed right-hand side in Gaussian elimination
- Gaussian elimination and LU factorization are two ways of expressing same solution process



Example: Gaussian Elimination

- Use Gaussian elimination to solve linear system

$$\mathbf{A}\mathbf{x} = \begin{bmatrix} 2 & 4 & -2 \\ 4 & 9 & -3 \\ -2 & -3 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 8 \\ 10 \end{bmatrix} = \mathbf{b}$$

- To annihilate subdiagonal entries of first column of \mathbf{A} ,

$$M_1 \mathbf{A} = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 4 & -2 \\ 4 & 9 & -3 \\ -2 & -3 & 7 \end{bmatrix} = \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 1 & 5 \end{bmatrix},$$

$$M_1 \mathbf{b} = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 8 \\ 10 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 12 \end{bmatrix}$$



Example, continued

- To annihilate subdiagonal entry of second column of $M_1 A$,

$$M_2 M_1 A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 1 & 5 \end{bmatrix} = \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 4 \end{bmatrix} = U,$$

$$M_2 M_1 b = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ 12 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 8 \end{bmatrix} = Mb$$



Example, continued

- We have reduced original system to equivalent upper triangular system

$$U\mathbf{x} = \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 8 \end{bmatrix} = M\mathbf{b}$$

which can now be solved by back-substitution to obtain

$$\mathbf{x} = \begin{bmatrix} -1 \\ 2 \\ 2 \end{bmatrix}$$



Example, continued

- To write out LU factorization explicitly,

$$L_1 L_2 = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 1 & 1 \end{bmatrix} = L$$

so that

$$A = \begin{bmatrix} 2 & 4 & -2 \\ 4 & 9 & -3 \\ -2 & -3 & 7 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 4 \end{bmatrix} = LU$$

