8. Numerical linear algebra background

- solving linear equations with matrix factors
- LU
- Cholesky
- eigenvalues
- null and range spaces

Linear equations that are easy to solve

diagonal matrices ($a_{ij} = 0$ if $i \neq j$): n flops

$$x = A^{-1}b = (b_1/a_{11}, \ldots, b_n/a_{nn})$$

lower triangular ($a_{ij} = 0$ if $j > i$): n^2 flops via forward substitution

$$\begin{aligned} x_1 &:= b_1/a_{11} \\ x_2 &:= (b_2 - a_{21}x_1)/a_{22} \\ x_3 &:= (b_3 - a_{31}x_1 - a_{32}x_2)/a_{33} \\ &\vdots \\ x_3 &:= (b_n - a_{n1}x_1 - a_{n2}x_2 - \cdots - a_{n,n-1}x_{n-1})/a_{nn} \end{aligned}$$

upper triangular ($a_{ij} = 0$ if $j < i$): n^2 flops via backward substitution

orthogonal matrices: $A^{-1} = A^T$

- n^2 flops to compute $x = A^T b$
- less with structure, e.g., if $A = I - 2uu^T$ with $\|u\|_2 = 1$: compute

$$x = A^T b = b - 2(u^T b)u$$

  in n flops

permutation matrices

$$a_{ij} = \begin{cases} 1 & j = \pi_i \\ 0 & \text{otherwise} \end{cases}$$

where $\pi = (\pi_1, \ldots, \pi_2)$ is a permutation of $(1, 2, \ldots, n)$

- interpretation: $Ax = (x_{\pi_1}, x_{\pi_2}, \ldots, x_{\pi_n})$
- satisfies $A^{-1} = A^T$, hence cost of solving $Ax = b$ is 0 flops

example:

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \qquad A = A^{-1} = A^T = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix}$$

Factoring matrices

- factor A as a product of k simple matrics

$$A = A_1 A_2 \cdots A_k$$

  (A_i diagonal, upper or lower triangular, orthogonal, etc)

- compute $x = A^{-1}b = A_k^{-1} \cdots A_2^{-1} A_1^{-1} b$ by solving k equations

$$A_1 x_1 = b, \qquad A_2 x_2 = x_1, \quad \cdots \quad A_k x = x_{k-1}$$

cost of factorization dominates cost of factor solves

equations with multiple right-hand sides

$$A x_1 = b_1, \qquad A x_2 = b_2, \quad \cdots \quad A x = b_m$$

cost is one factorization plus m simple solves

LU factorization

Every nonsingular matrix A can be factored as

$$PA = LU$$

with P a permutation matrix, L lower triangular, U upper triangular
cost: $(2/3)n^2$ flops

given a set of linear equations $Ax = b$, with A nonsingular
1. LU *factorization*: factor A as $A = P^T LU$ (n^3 flops)
2. *permutation*: solve $P^T z = b$ (0 flops)
3. *forward substitution*: solve $Ly = z$ (n^2 flops)
4. *backward substitution*: solve $Ux = y$ (n^2 flops)

Matlab

- `x = U\(L\b(p))`
- `x = A\b`

Cholesky factorization

The symmetric matrix A is **positive definite** if any of the following hold:

- $x^T A x > 0$ for all $x \neq 0$
- $A = FF^T$ for some nonsingular F
- $\lambda(A) > 0$
- all leading principle minors are positive

Cholesky factorization every symmetric positive definite matrix A can be factored as

$$A = R^T R$$

with R upper triangular
cost: $(1/3)n^3$ flops

inductive definition of Cholesky

$$
\begin{aligned}
A = \begin{pmatrix} a_{11} & w^T \\ w & K \end{pmatrix} &= \underbrace{\begin{pmatrix} \alpha & \\ w/\alpha & I \end{pmatrix}}_{R_1^T} \underbrace{\begin{pmatrix} 1 & \\ & K - ww^T/\alpha \end{pmatrix}}_{A_1} \underbrace{\begin{pmatrix} \alpha & w^T/\alpha \\ & I \end{pmatrix}}_{R_1} \\
&= \begin{pmatrix} \alpha & \\ w/\alpha & I \end{pmatrix} \begin{pmatrix} 1 & \\ & R_2^T R_2 \end{pmatrix} \begin{pmatrix} \alpha & w^T/\alpha \\ & I \end{pmatrix} \\
&= \begin{pmatrix} \alpha & \\ w/\alpha & R_2^T \end{pmatrix} \begin{pmatrix} 1 & \\ & I \end{pmatrix} \begin{pmatrix} \alpha & w^T/\alpha \\ & R_2 \end{pmatrix}
\end{aligned}
$$

where

- $\alpha = \sqrt{a_{11}}$
- $K - ww^T/\alpha = R_2^T R_2$, R_2 upper triangular

solving with the Cholesky factorization

given a set of linear equations $Ax = b$, with A symmetric

1. *Cholesky factorization*: factor A as $A = R^TR$ (n^3 flops)
2. *forward substitution*: solve $R^Ty = b$ (n^2 flops)
3. *backward substitution*: solve $Rx = y$ (n^2 flops)

Matlab

- `x = R\(R'\b)`
- `x = A\b`

QR factorization

Every $m \times n$ matrix A ($m \geq n$) can be factorized as

$$A = QR = \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} \begin{pmatrix} R_1 \\ 0 \end{pmatrix}$$

with

- Q orthogonal (i.e., $Q^TQ = I$ and square)
- Q_1, Q_2 orthonormal (i.e., $Q_1^TQ_1 = I$)
- R_1 upper triangular

orthogonal transformations are rotations:

$$\|Qx\|^2 = (x^TQ^T)(Qx) = x^T(Q^TQ)x = x^Tx = \|x\|^2$$

solving linear least-squares problems

$$\|Ax-b\|^2 = \|Q^T(Ax-b)\|^2 = \left\| \begin{pmatrix} R \\ 0 \end{pmatrix} x - \begin{pmatrix} Q_1^T b \\ Q_2^T b \end{pmatrix} \right\|^2 = \|Rx - Q_1^T b\|^2 + \|Q_2^T b\|^2$$

leasts-square solution is then solution to

$$Rx = Q_1^T b$$

Matlab

- `[Q,R] = qr(A,0); % "thin" QR of A`
- `x = R\(Q'*b)`
- `x = A\b`

Eigenvalue decomposition

A square, $n \times n$

eigenvalue-eigenvector pair (λ, x) (with $x \neq 0$)

$$Ax = \lambda x \qquad \text{ie,} \qquad AX = X\Lambda \quad \text{with } \Lambda \text{ diagonal}$$

A is **diagonalizable** if X is nonsingular:

$$A = X\Lambda X^{-1}$$

A is **unitarily diagonalizable** if $X = Q$ is orthogonal:

$$A = Q\Lambda Q^T$$

symmetric matrices

- are unitarily diagonalizable
- have real eigenvalues

Null and range space

$$A \text{ is } m \times n,\ m \le n$$

nullspace of A are the vectors orthogonal to its rows:

- $\operatorname{null}(A) = \{p \in \mathbf{R}^n \mid Ap = 0\}$
- $\dim \operatorname{null}(A) = n - \operatorname{rank}(A)$
- Z is a basis for $\operatorname{null}(A)$ if any $q \in \operatorname{null}(A)$ can be written as

$$q = Zw \qquad \text{for some } w$$

range of A^T are the vectors spanned by the rows of A:

- $\operatorname{range}(A^T) = \{q \in \mathbf{R}^n \mid q = A^T y \text{ for some } y \in \mathbf{R}^m\}$
- $\dim \operatorname{range}(A^T) = \operatorname{rank}(A)$

orthogonal subspaces

- $\operatorname{null}(A) \perp \operatorname{range}(A^T)$