9. Numerical linear algebra background

- matrix structure and algorithm complexity
- solving linear equations with factored matrices
- LU, Cholesky, LDL^T factorization
- block elimination and the matrix inversion lemma
- solving underdetermined equations

Matrix structure and algorithm complexity

cost (execution time) of solving $Ax = b$ with $A \in \mathbf{R}^{n \times n}$

- for general methods, grows as n^3
- less if A is structured (banded, sparse, Toeplitz, ...)

Flop counts

- flop (floating-point operation): one addition, subtraction, multiplication, or division of two floating-point numbers
- to estimate complexity of an algorithm: express number of flops as a (polynomial) function of the problem dimensions, and simplify by keeping only the leading terms
- not an accurate predictor of computation time on modern computers
- useful as a rough estimate of complexity

Basic operations

Vector–vector operations ($x, y \in \mathbf{R}^n$)

- inner product $x^T y$: $2n - 1$ flops (or $2n$ if n is large)
- sum $x + y$, scalar multiplication αx: n flops

Matrix–vector product $y = Ax$ with $A \in \mathbf{R}^{m \times n}$

- $m(2n - 1)$ flops (or $2mn$ if n large)
- $2N$ if A is sparse with N nonzero elements
- $2p(n + m)$ if A is given as $A = UV^T$, $U \in \mathbf{R}^{m \times p}$, $V \in \mathbf{R}^{n \times p}$

Matrix–matrix product $C = AB$ with $A \in \mathbf{R}^{m \times n}$, $B \in \mathbf{R}^{n \times p}$

- $mp(2n - 1)$ flops (or $2mnp$ if n large)
- less if A and/or B are sparse
- $(1/2)m(m + 1)(2n - 1) \approx m^2 n$ if $m = p$ and C symmetric

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

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

called forward substitution

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

Linear equations that are easy to solve

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

- $2n^2$ flops to compute $x = A^T b$ for general A
- less with structure, *e.g.*, if $A = I - 2uu^T$ with $\|u\|_2 = 1$, we can compute $x = A^T b = b - 2(u^T b)u$ in $4n$ flops

Permutation matrices:

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

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

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

example:

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

The factor–solve method for solving $Ax = b$

- factor A as a product of simple matrices (usually 2 or 3):

$$A = A_1 A_2 \cdots A_k$$

  (A_i diagonal, upper or lower triangular, etc)

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

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

cost of factorization step usually dominates cost of solve step

Equations with multiple righthand sides

$$Ax_1 = b_1, \qquad Ax_2 = b_2, \qquad \ldots, \qquad Ax_m = b_m$$

cost: one factorization plus m solves

LU factorization

every nonsingular matrix A can be factored as

$$A = PLU$$

with P a permutation matrix, L lower triangular, U upper triangular

cost: $(2/3)n^3$ flops

Solving linear equations by LU factorization

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

1. *LU factorization:* factor A as $A = PLU$ ($(2/3)n^3$ flops)
2. *permutation:* solve $Pz_1 = b$ (0 flops)
3. *forward substitution:* solve $Lz_2 = z_1$ (n^2 flops)
4. *backward substitution:* solve $Ux = z_2$ (n^2 flops)

cost: $(2/3)n^3 + 2n^2 \approx (2/3)n^3$ for large n

Sparse LU factorization

$$A = P_1 L U P_2$$

- adding permutation matrix P_2 offers possibility of sparser L, U (hence, cheaper factor and solve steps)
- P_1 and P_2 chosen (heuristically) to yield sparse L, U
- choice of P_1 and P_2 depends on sparsity pattern and values of A
- cost is usually much less than $(2/3)n^3$; exact value depends in a complicated way on n, number of zeros in A, sparsity pattern

Cholesky factorization

every positive definite A can be factored as

$$A = LL^T$$

with L lower triangular

cost: $(1/3)n^3$ flops

Solving linear equations by Cholesky factorization

given: a set of linear equations $Ax = b$, with $A \in \mathbf{S}^n_{++}$
1. *Cholesky factorization:* Factor A as $A = LL^T$ ($(1/3)n^3$ flops)
2. *forward substitution:* solve $Lz_1 = b$ (n^2 flops)
3. *backward substitution:* solve $L^T x = z_1$ (n^2 flops)

cost: $(1/3)n^3 + 2n^2 \approx (1/3)n^3$ for large n

Sparse Cholesky factorization

$$A = PLL^T P^T$$

- adding permutation matrix P offers possibility of sparser L
- P chosen (heuristically) to yield sparse L
- choice of P only depends on sparsity pattern of A (unlike sparse LU)
- cost is usually much less than $(1/3)n^3$; exact value depends in a complicated way on n, number of zeros in A, sparsity pattern

LDL^T factorization

every nonsingular symmetric matrix A can be factored as

$$A = PLDL^T P^T$$

with P a permutation matrix, L lower triangular, D block diagonal with 1×1 or 2×2 diagonal blocks

cost: $(1/3)n^3$

- cost of solving symmetric sets of linear equations by LDL^T factorization:

$$\frac{1}{3}n^3 + 2n^2 \approx \frac{1}{3}n^3$$

- for sparse A, can choose P to yield sparse L; cost $\ll (1/3)n^3$

Equations with structured sub-blocks

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \qquad (1)$$

- variables $x_1 \in \mathbf{R}^{n_1}$, $x_2 \in \mathbf{R}^{n_2}$; blocks $A_{ij} \in \mathbf{R}^{n_i \times n_j}$
- if A_{11} is nonsingular, can eliminate x_1: $x_1 = A_{11}^{-1}(b_1 - A_{12}x_2)$
- to compute x_2, solve

$$(A_{22} - A_{21}A_{11}^{-1}A_{12})x_2 = b_2 - A_{21}A_{11}^{-1}b_1$$

Solving linear equations by block elimination

given: a nonsingular set of linear equations (1), with A_{11} nonsingular
1. form $A_{11}^{-1}A_{12}$ and $A_{11}^{-1}b_1$
2. form $S = A_{22} - A_{21}A_{11}^{-1}A_{12}$ and $\tilde{b} = b_2 - A_{21}A_{11}^{-1}b_1$
3. determine x_2 by solving $Sx_2 = \tilde{b}$
4. determine x_1 by solving $A_{11}x_1 = b_1 - A_{12}x_2$

Complexity of block elimination

Dominant terms in flop count

- step 1: $f + n_2 s$ (f is cost of factoring A_{11}; s is cost of solve step)
- step 2: $2n_2^2 n_1$ (cost dominated by product of A_{21} and $A_{11}^{-1}A_{12}$)
- step 3: $(2/3)n_2^3$

total: $f + n_2 s + 2n_2^2 n_1 + (2/3)n_2^3$

Examples

- general A_{11} ($f = (2/3)n_1^3$, $s = 2n_1^2$): no gain over standard method

$$\#\text{flops} = \frac{2}{3}n_1^3 + 2n_1^2 n_2 + 2n_2^2 n_1 + \frac{2}{3}n_2^3 = \frac{2}{3}(n_1 + n_2)^3$$

- block elimination is useful for structured A_{11} ($f \ll n_1^3$)
- for example, diagonal ($f = 0$, $s = n_1$): #flops $\approx 2n_2^2 n_1 + (2/3)n_2^3$

Structured matrix plus low rank term

$$(A + BC)x = b$$

- $A \in \mathbf{R}^{n \times n}$, $B \in \mathbf{R}^{n \times p}$, $C \in \mathbf{R}^{p \times n}$
- assume A has structure ($Ax = b$ easy to solve)

first write as

$$\begin{bmatrix} A & B \\ C & -I \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}$$

now apply block elimination: solve

$$(I + CA^{-1}B)y = CA^{-1}b,$$

then solve $Ax = b - By$

this proves the *matrix inversion lemma:* if A and $A + BC$ nonsingular,

$$(A + BC)^{-1} = A^{-1} - A^{-1}B(I + CA^{-1}B)^{-1}CA^{-1}$$

Structured matrix plus low rank term

$$(A + BC)x = b$$

Example: A diagonal, B, C dense

- method 1: form $D = A + BC$, then solve $Dx = b$

  cost: $(2/3)n^3 + 2pn^2$

- method 2 (via matrix inversion lemma): solve

$$(I + CA^{-1}B)y = CA^{-1}b, \qquad (2)$$

  then compute $x = A^{-1}b - A^{-1}By$

  total cost is dominated by (2): $2p^2n + (2/3)p^3$ (*i.e.*, linear in n)

Underdetermined linear equations

if $A \in \mathbf{R}^{p\times n}$ with $p < n$, $\mathbf{rank}\, A = p$,

$$\{x \mid Ax = b\} = \{Fz + \hat{x} \mid z \in \mathbf{R}^{n-p}\}$$

- $\hat{x}$ is (any) particular solution
- columns of $F \in \mathbf{R}^{n\times(n-p)}$ span nullspace of A
- there exist several numerical methods for computing F (QR factorization, rectangular LU factorization, ...)