Convex Optimization

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Revised slides by Stephen Boyd, Lieven Vandenberghe, and Parth Nobel
B. Numerical linear algebra background
Outline

Flop counts and BLAS

Solving systems of linear equations

Block elimination
Flop count

- **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
  - simplify by keeping only the leading terms
- not an accurate predictor of computation time on modern computers, but useful as a rough estimate of complexity
Basic linear algebra subroutines (BLAS)

**vector-vector operations** \((x, y \in \mathbb{R}^n)\) (BLAS level 1)
- inner product \(x^T y\): \(2n - 1\) flops \((\approx 2n, O(n))\)
- sum \(x + y\), scalar multiplication \(\alpha x\): \(n\) flops

**matrix-vector product** \(y = Ax\) with \(A \in \mathbb{R}^{m \times n}\) (BLAS level 2)
- \(m(2n - 1)\) flops \((\approx 2mn)\)
- \(2N\) if \(A\) is sparse with \(N\) nonzero elements
- \(2p(n + m)\) if \(A\) is given as \(A = UV^T\), \(U \in \mathbb{R}^{m \times p}\), \(V \in \mathbb{R}^{n \times p}\)

**matrix-matrix product** \(C = AB\) with \(A \in \mathbb{R}^{m \times n}\), \(B \in \mathbb{R}^{n \times p}\) (BLAS level 3)
- \(mp(2n - 1)\) flops \((\approx 2mnp)\)
- less if \(A\) and/or \(B\) are sparse
- \((1/2)m(m + 1)(2n - 1) \approx m^2n\) if \(m = p\) and \(C\) symmetric
BLAS on modern computers

- there are good implementations of BLAS and variants (e.g., for sparse matrices)
- CPU single thread speeds typically 1–10 Gflops/s ($10^9$ flops/sec)
- CPU multi threaded speeds typically 10–100 Gflops/s
- GPU speeds typically 100 Gflops/s–1 Tflops/s ($10^{12}$ flops/sec)
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Block elimination
Complexity of solving linear equations

- $A \in \mathbb{R}^{n \times n}$ is invertible, $b \in \mathbb{R}^n$

- solution of $Ax = b$ is $x = A^{-1}b$

- solving $Ax = b$, i.e., computing $x = A^{-1}b$
  - almost never done by computing $A^{-1}$, then multiplying by $b$
  - for general methods, $O(n^3)$
  - (much) less if $A$ is structured (banded, sparse, Toeplitz, …)
  - e.g., for $A$ with half-bandwidth $k$ ($A_{ij} = 0$ for $|i - j| > k$, $O(k^2n)$

- it’s super useful to recognize matrix structure that can be exploited in solving $Ax = b$
Linear equations that are easy to solve

- diagonal matrices: $n$ flops; $x = A^{-1}b = (b_1/a_{11}, \ldots, b_n/a_{nn})$

- lower triangular: $n^2$ flops via **forward substitution**

  $x_1 := b_1/a_{11}$

  $x_2 := (b_2 - a_{21}x_1)/a_{22}$

  $x_3 := (b_3 - a_{31}x_1 - a_{32}x_2)/a_{33}$

  \[ \vdots \]

  $x_n := (b_n - a_{n1}x_1 - a_{n2}x_2 - \cdots - a_{n,n-1}x_{n-1})/a_{nn}$

- upper triangular: $n^2$ flops via **backward substitution**

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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: for $\pi = (\pi_1, \pi_2, \ldots, \pi_n)$ a permutation of $(1, 2, \ldots, n)$
  
  $$a_{ij} = \begin{cases} 1 & j = \pi_i \\ 0 & \text{otherwise} \end{cases}$$

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

\[
A = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, \quad A^{-1} = A^T = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}
\]
Factor-solve method for solving $Ax = b$

- factor $A$ as a product of simple matrices (usually 2–5):
  \[ A = A_1A_2 \cdots A_k \]

- e.g., $A_i$ diagonal, upper or lower triangular, orthogonal, permutation, …

- compute $x = A^{-1}b = A_k^{-1} \cdots A_2^{-1}A_1^{-1}b$ by solving $k$ ‘easy’ systems of equations
  \[ A_1x_1 = b, \quad A_2x_2 = x_1, \quad \ldots \quad A_kx = x_{k-1} \]

- cost of factorization step usually dominates cost of solve step
Solving equations with multiple righthand sides

- we wish to solve

\[ Ax_1 = b_1, \quad Ax_2 = b_2, \quad \ldots \quad Ax_m = b_m \]

- cost: one factorization plus \( m \) solves

- called factorization caching

- when factorization cost dominates solve cost, we can solve a modest number of equations at the same cost as one (!!)
LU factorization

- every nonsingular matrix $A$ can be factored as $A = PLU$ with $P$ a permutation, $L$ lower triangular, $U$ upper triangular

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

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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).

- total cost: $(2/3)n^3 + 2n^2 \approx (2/3)n^3$ for large $n$
Sparse LU factorization

- for $A$ sparse and invertible, factor as $A = P_1LUP_2$
- adding permutation matrix $P_2$ offers possibility of sparser $L$, $U$
- hence, less storage and 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
- often practical to solve very large sparse systems of equations
Cholesky factorization

- every positive definite $A$ can be factored as $A = LL^T$
- $L$ is lower triangular with positive diagonal entries
- Cholesky factorization cost: $(1/3)n^3$ flops

Solving linear equations by Cholesky factorization.

given a set of linear equations $Ax = b$, with $A \in S_{++}^n$.

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 $L^Tx = z_1$ ($n^2$ flops).

- total cost: $(1/3)n^3 + 2n^2 \approx (1/3)n^3$ for large $n$
Sparse Cholesky factorization

- for sparse positive define $A$, factor as $A = PLL^T P^T$
- adding permutation matrix $P$ offers possibility of sparser $L$
- same as
  - permuting rows and columns of $A$ to get $\tilde{A} = P^T AP$
  - then finding Cholesky factorization of $\tilde{A}$
- $P$ 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
Example

- Sparse $A$ with upper arrow sparsity pattern
  \[
  A = \begin{bmatrix}
    \ast & \ast & \ast & \ast & \ast \\
    \ast & \ast & \ast & \ast & \ast \\
    \ast & \ast & \ast & \ast & \ast \\
    \ast & \ast & \ast & \ast & \ast \\
    \ast & \ast & \ast & \ast & \ast 
  \end{bmatrix}
  \]

- $L$ is full, with $O(n^2)$ nonzeros; solve cost is $O(n^2)$

- Reverse order of entries (i.e., permute) to get lower arrow sparsity pattern
  \[
  \tilde{A} = \begin{bmatrix}
    \ast & \ast & \ast & \ast & \ast \\
    \ast & \ast & \ast & \ast & \ast \\
    \ast & \ast & \ast & \ast & \ast \\
    \ast & \ast & \ast & \ast & \ast \\
    \ast & \ast & \ast & \ast & \ast 
  \end{bmatrix}
  \]

- $L$ is sparse with $O(n)$ nonzeros; cost of solve is $O(n)$
**LDL^T factorization**

- every nonsingular symmetric matrix $A$ can be factored as

$$A = PLDL^TP^T$$

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

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

- cost of solving linear equations with symmetric $A$ by LDL^T factorization:

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

- for sparse $A$, can choose $P$ to yield sparse $L$; cost $\ll (1/3)n^3$
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Block elimination
Equations with structured sub-blocks

- express $Ax = b$ in blocks as

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

with $x_1 \in \mathbb{R}^{n_1}$, $x_2 \in \mathbb{R}^{n_2}$; blocks $A_{ij} \in \mathbb{R}^{n_i \times n_j}$

- assuming $A_{11}$ is nonsingular, can eliminate $x_1$ as

$$x_1 = A_{11}^{-1} (b_1 - A_{12} x_2)$$

- to compute $x_2$, solve

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

- $S = A_{22} - A_{21} A_{11}^{-1} A_{12}$ is the Shur complement
Bock elimination method

Solving linear equations by block elimination.

given a nonsingular set of linear equations with $A_{11}$ nonsingular.

1. Form $A^{-1}_{11}A_{12}$ and $A^{-1}_{11}b_1$.
2. Form $S = A_{22} - A_{21}A^{-1}_{11}A_{12}$ and $\tilde{b} = b_2 - A_{21}A^{-1}_{11}b_1$.
3. Determine $x_2$ by solving $Sx_2 = \tilde{b}$.
4. Determine $x_1$ by solving $A_{11}x_1 = b_1 - A_{12}x_2$.

dominant terms in flop count

- step 1: $f + n_2s$ ($f$ is cost of factoring $A_{11}$; $s$ is cost of solve step)
- step 2: $2n_2^2n_1$ (cost dominated by product of $A_{21}$ and $A^{-1}_{11}A_{12}$)
- step 3: $(2/3)n_2^3$

total: $f + n_2s + 2n_2^2n_1 + (2/3)n_2^3$
Examples

- for general $A_{11}, f = (2/3)n_1^3, s = 2n_1^2$
  
  $$
  \text{#flops} = (2/3)n_1^3 + 2n_1^2n_2 + 2n_2^2n_1 + (2/3)n_2^3 = (2/3)(n_1 + n_2)^3
  $$
  
  so, no gain over standard method

- block elimination is useful for structured $A_{11}$ ($f \ll n_1^3$)

- for example, $A_{11}$ diagonal ($f = 0, s = n_1$): \#flops $\approx 2n_2^2n_1 + (2/3)n_2^3$
Structured plus low rank matrices

- we wish to solve \((A + BC)x = b\), \(A \in \mathbb{R}^{n \times n}\), \(B \in \mathbb{R}^{n \times p}\), \(C \in \mathbb{R}^{p \times n}\)
- assume \(A\) has structure (i.e., \(Ax = b\) easy to solve)
- first uneliminate to write as block equations with new variable \(y\)

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

- 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 \(A + BC\) are nonsingular,

\[(A + BC)^{-1} = A^{-1} - A^{-1}B(I + CA^{-1}B)^{-1}CA^{-1}\]
Example: Solving diagonal plus low rank equations

- with $A$ diagonal, $p \ll n$, $A + BC$ is called **diagonal plus low rank**
- for covariance matrices, called a **factor model**

- method 1: form $D = A + BC$, then solve $Dx = b$
  - storage $n^2$
  - solve cost $(2/3)n^3 + 2pn^2$ (**cubic** in $n$)

- method 2: solve $(I + CA^{-1}B)y = CA^{-1}b$, then compute $x = A^{-1}b - A^{-1}By$
  - storage $O(np)$
  - solve cost $2p^2n + (2/3)p^3$ (**linear** in $n$)