Welcome to Ma221! Lecture 14, Sep 25

Gaussian Elim. for matrices w. structure

Symmetric Pos. def (s.p.d.) (real case only)

A s.p.d iff $A = A^T$ and $x^T A x > 0 \ \forall x \neq 0$

Lemma:

1) X nonsingular $\Rightarrow$ A s.p.d. $\Leftrightarrow$ $X^T A X$ s.p.d.

2) A s.p.d, $H = A(i:j, i:j)$ "principal submatrix"

$\Rightarrow$ H s.p.d

3) A s.p.d. iff $A = A^T$, all evals $\lambda_i > 0$

pf: $A = A^T \Rightarrow AQ = Q\Lambda \quad \Lambda = \text{diag}(\lambda_i)$

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

A s.p.d iff $\Lambda = \text{diag}(\lambda_i)$ s.p.d iff

$\sum_{i=1}^{n} \lambda_i x_i^2 > 0 \ \forall x \neq 0$ iff $\lambda_i > 0$

4) A s.p.d $\Rightarrow A(i,i) > 0$ and

$$\max_{i,j} |A(i,j)| = \max_i |A(i,i)|$$

pf. $x = e_i \Rightarrow x^T A x = A(i,i) > 0$

Suppose $|A(i,j)|$ $i \neq j$ were largest

x = all zeroes except $x_i = 1$, $x_j = -\text{sign}(A(i,j))$

$x^T A x = A(i,i) + A(j,j) - 2|A(i,j)| < 0$ contradiction

5) Basis of Cholesky

A s.p.d. iff $A = L \cdot L^T$

L lower triangular $L_{ii} > 0$

pf. induction on n, show

Schur complement is s.p.d

$$A = \begin{array}{c|c} & \begin{array}{cc} 1 & n-1 \end{array} \\ \begin{array}{c} 1 \\ n-1 \end{array} & \left[\begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array}\right] \end{array} = \left[\begin{array}{c|c} \sqrt{A_{11}} & 0 \\ \hline \frac{A_{21}}{\sqrt{A_{11}}} & I \end{array}\right] \cdot \left[\begin{array}{c|c} \sqrt{A_{11}} & \frac{A_{12}}{\sqrt{A_{11}}} \\ \hline 0 & S \end{array}\right]$$

$$S = A_{22} - \frac{A_{21} \cdot A_{12}}{A_{11}}$$

$$= \left[\begin{array}{c|c} \sqrt{A_{11}} & 0 \\ \hline \frac{A_{21}}{\sqrt{A_{11}}} & I \end{array}\right] \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & S \end{array}\right] \left[\begin{array}{c|c} \sqrt{A_{11}} & A_{12}/\sqrt{A_{11}} \\ \hline 0 & I \end{array}\right]$$

$$= X \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & S \end{array}\right] X^T$$

$\Rightarrow \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & S \end{array}\right]$ s.p.d. $\Rightarrow S$ s.p.d.

$\Rightarrow$ by induction $S = L_s \cdot L_s^T$

$$A = \left[\begin{array}{c|c} \sqrt{A_{11}} & 0 \\ \hline \frac{A_{21}}{\sqrt{A_{11}}} & I \end{array}\right] \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & L_s \end{array}\right] \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & L_s^T \end{array}\right] \left[\begin{array}{c|c} \sqrt{A_{11}} & A_{12}/\sqrt{A_{11}} \\ \hline 0 & I \end{array}\right]$$

$$= \left[\begin{array}{c|c} \sqrt{A_{11}} & 0 \\ \hline \frac{A_{21}}{\sqrt{A_{11}}} & L_s \end{array}\right] \cdot \left[\begin{array}{c|c} \sqrt{A_{11}} & A_{12}/\sqrt{A_{11}} \\ \hline 0 & L_s^T \end{array}\right] = L \cdot L^T$$

QED

Def: A s.p.d then $A = LL^T$, L lowertriang.
$L_{ii} > 0$ called Cholesky factorization

Relationship to GE without pivoting
if A s.p.d $A = LU$ $L_{ii} = 1$
no pivoting

Let $D(i,i) = \sqrt{U(i,i)}$ diagonal
$A = (LD)(D^{-1}U) = L_s \cdot L_s^T$ is
Cholesky factorization
proof: HW

Fact suggests that any LU alg can
be modified to do Cholesky
with $\frac{1}{2}$ flops, $\frac{1}{2}$ memory

Simplest version:
for $j = 1:n$
$L(j,j) = \left(A(j,j) - \sum_{i=1}^{j-1} L(j,i)^2 \right)^{1/2}$
$L(j+1:n,j) = (A(j+1:n,j) - L(j+1:n, 1:j-1) \cdot L(j,1:j-1)^T) / L(j,j)$

All idea for speeding up GE:
blocking, recursion, comm. lower bounds
apply to Cholesky

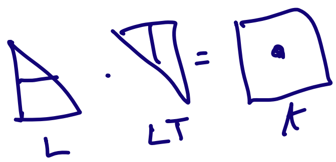
Error Analysis: Same approach as GE!

$$(A+E)(x+\delta x) = b$$

$$|E| \le 3 \cdot n \cdot \varepsilon \, |L| \cdot |L^T|$$

But no pivoting, how do we bound this?

$$(|L| \cdot |L^T|)_{ij} = \sum_k |L_{ik}| \cdot |L_{jk}|$$



$$\le \|L(i,:)\|_2 \cdot \|L(j,:)\|_2$$

$$= \sqrt{A(i,i)} \cdot \sqrt{A(j,j)}$$

$\le$ largest entry in A (which is on diagonal)

$\Rightarrow$ numerically stable without pivoting

$\Rightarrow$ can choose any pivot from diagonal, will do so later to maximize sparsity

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Symmetric Indefinite A

Still possible to save $\frac{1}{2}$ flops, $\frac{1}{2}$ memory but more complicated

Ex: $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ can't choose a diagonal pivot

Bunch Kaufman pivoting

$$A = (\Pi L_i P_i) D (\quad)^T \qquad L_i = \begin{bmatrix} 1 & & & 0 \\ & \ddots & & \\ & \vdots & 1 & \\ & & & 1 \end{bmatrix}$$

P_i swaps 1 or 2 rows+cols

D blockdiagonal with 1x1 and 2x2 blocks

more complicated to use BLAS3
see LAPACK ssytrf

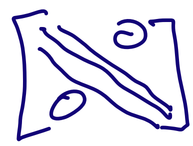
Rook pivoting: variant on Bunch-Kaufman
searches for good pivot more completely,
better backward error bound
ssytrf_rk ssytrf_rook

Aasen Factorization: can hit comm lowerbound

$$A = P L T L^T P^T \qquad P = \text{perm}$$

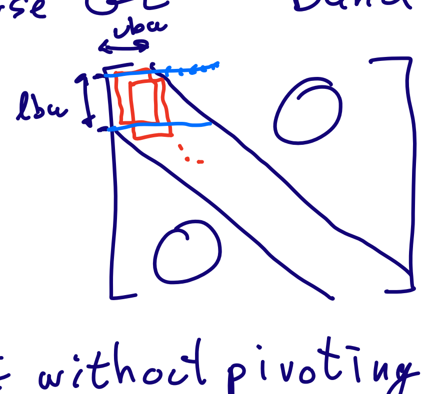
$$L = \triangle$$

T = tridiagonal



see notes for details ssytrf_aa

Sparse GE: Band Matrices



GE without pivoting: each step of GE
costs lbw · ubw mults and adds

$\Rightarrow$ total cost $= 2n \cdot lbw \cdot ubw + n \cdot lbw$
$= O(n)$ for small lbw, ubw

GE with pivoting: $ubw(U) = ubw(A) + lbw(A)$

"$lbw(L)$" $= lbw(A)$ but nonzeroes in each col of L not adjacent

$\sim$ same cost

LAPACK: sgbtrf

Where band matrices arise:

from discretizing D.E.s:

each unknown only depends on nearest neighbors

$\Rightarrow$ banded

Ex. Sturm-Liouville problem

$$-y''(x) + q(x)\cdot y(x) = r(x) \qquad x \in [0,1]$$

$$y(0)=\alpha, \quad y(1)=\beta \qquad q(x) \geq \bar{q} > 0$$

discretize at $x(i) = i \cdot h$ $\qquad h = \frac{1}{N+1}$

unknowns $y(i) = y(x(i))$ for $i = 1, \dots N$

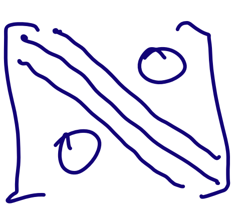
approximate $y''(i) = \dfrac{y(i+1) - 2\cdot y(i) + y(i-1)}{h^2}$

$$q(i) = q(x(i)), \quad r(i) = r(x(i))$$

$$\frac{-(y(i+1) - 2\cdot y(i) + y(i-1))}{h^2} + q(i)\cdot y(i) = r(i)$$

$i = 1 .. N$

or $Ay = r$ $\quad N \times N$



$$A = \mathrm{diag}\left(\frac{2}{h^2} + q(i)\right)$$

$+ \mathrm{diag}\left(\frac{-1}{h^2}, 1\right)$ above diagonal

$+\mathrm{diag}\left(\frac{-1}{h^2}, -1\right)$ below diagonal

Show A is s.p.d.

Gershgorin's Thm: All evals of A lie in n circles in complex plane: circle i has center $A(i,i)$ and radius $\sum_{\substack{j=1\\ j\neq i}}^{n} |A(i,j)|$

proof: $Ax = \lambda x$, $|x(i)|$ largest entry in x

$$(A(i,i)-\lambda)x(i) = \sum_{\substack{j=1\\ j\neq i}}^{n} A(i,j)\cdot x(j)$$

$$\frac{|A(i,i)-\lambda|\cdot|x(i)|}{|x(i)|} \le \sum_{\substack{j=1\\ j\neq i}}^{n} |A(i,j)|\cdot \underbrace{\frac{|x(j)|}{|x(i)|}}_{\le 1}$$

$$|A(i,i)-\lambda| \le \sum_{\substack{j=1\\ j\neq i}}^{n} |A(i,j)| \quad \text{QED}$$

Apply to Sturm-Liouville:

circles centered at $\frac{2}{h^2} + q(i)$ with radii $\frac{2}{h^2}$, since $q(i) \ge \bar{q} > 0$ these circles in right half plane $\Rightarrow$ eigenvalues $> 0 \Rightarrow A$ s.p.d.