Topic and contents

UNSW, School of Mathematics and Statistics

MATH2089 – Numerical Methods

Week 04 – Structured Linear Systems and Sparse Matrices

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Symmetric Matrices

Definition (Symmetric, Skew-symmetric matrices)

- A is symmetric $\iff A^T = A$
- A is skew-symmetric $\iff A^T = -A$

- A symmetric or skew-symmetric $\implies A$ square, $A \in \mathbb{R}^{n\times n}$
- A symmetric $\iff a_{ij} = a_{ji}$ for all $i, j = 1, \ldots, n$
- A symmetric $\implies$ storage $n(n+1)/2$ elements
- A skew-symmetric $\iff a_{ij} = -a_{ji}$ for all $i, j = 1, \ldots, n$
- A skew-symmetric $\implies a_{ii} = 0$ for all $i = 1, \ldots, n$

Example (Testing for symmetry)

Give MATLAB commands to determine if A is symmetric

Solution

See function M-file chksym.m

Symmetric matrices - examples

Example (Symmetric matrices)

Are the following matrices symmetric?

$$A = \begin{pmatrix} 5 & -7 & -6 \\ -7 & 13 & 2 \\ -6 & 2 & 20 \end{pmatrix}, \qquad B = \begin{pmatrix} 5 & -7 & -6 \\ -7 & 13 & 2 \\ -5 & 2 & 20 \end{pmatrix}$$

Solution

A is symmetric (why?), B is not symmetric (why?)

Example (A^TA)

Show that for any $A \in \mathbb{R}^{m\times n}$, the matrix $B = A^TA$ is symmetric.

Solution

The transpose satisfies $(UV)^T = V^TU^T$ and $(U^T)^T = U$. Thus

$$B^T = (A^TA)^T = A^T(A^T)^T = A^TA = B,$$

so $B = A^TA$ is symmetric.

Positive definite matrices

Definition (Positive-definite matrices)

Symmetric matrix $A \in \mathbb{R}^{n \times n}$ is

- positive definite $\iff$ $\mathbf{x}^T A \mathbf{x} > 0$ for all $\mathbf{x} \in \mathbb{R}^n, \mathbf{x} \neq \mathbf{0}$
- positive semi-definite $\iff$ $\mathbf{x}^T A \mathbf{x} \geq 0$ for all $\mathbf{x} \in \mathbb{R}^n$

- A is positive definite $\iff$ eigenvalues $\lambda_i(A) > 0$ for all $i = 1, \dots, n$
- A positive definite $\iff$ Cholesky factorization $A = R^T R$ exists
  - R upper triangular, $R_{ii} > 0, i = 1, \dots, n$
  - MATLAB `R = chol(A)` or `[R, p] = chol(A)`
  - No pivoting required for numerical stability
  - Flops: Cholesky $\frac{n^3}{3} + O(n^2)$ versus LU $\frac{2n^3}{3} + O(n^2)$
- $A^T A$ symmetric positive semi-definite for any $A \in \mathbb{R}^{m \times n}$

Positive definite matrices - examples

Example (Positive definite matrices)

Consider the matrices

$$A = \begin{pmatrix} 5 & -7 & -6 \\ -7 & 13 & 2 \\ -6 & 2 & 20 \end{pmatrix}, \quad B = \begin{pmatrix} 6 & -7 & -6 \\ -7 & 14 & 2 \\ -6 & 2 & 21 \end{pmatrix}, \quad C = \begin{pmatrix} 4 & -7 & -6 \\ -7 & 13 & 2 \\ -6 & 2 & 20 \end{pmatrix}.$$

Calculate, in MATLAB,

1. `S1 = A'==A, S2 = A' - A, S3 = norm(A'-A,1)`
2. The eigenvalues of A.
3. The Cholesky factorization using `[R, p] = chol(A)`

Is A symmetric? Is A positive definite?

Repeat for the matrices B and C.

MATLAB `pdex1.m`

Banded matrices

Definition (Banded matrices)

$A \in \mathbb{R}^{m \times n}$ has

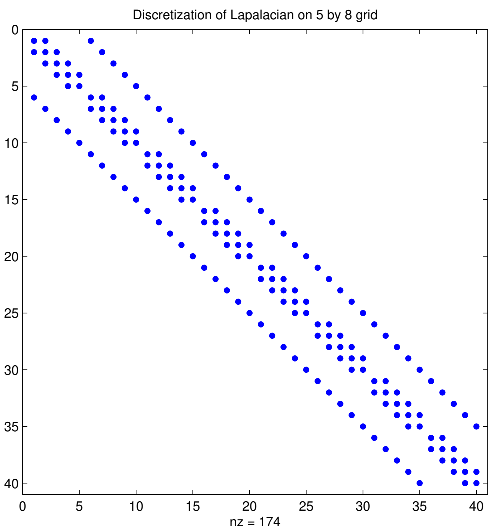
- upper bandwidth m_u $\iff$ $a_{ij} = 0 \quad \forall j > i + m_u$
- lower bandwidth m_l $\iff$ $a_{ij} = 0 \quad \forall i > j + m_l$
- total bandwidth $m_l + m_u + 1$

- L lower triangular $\iff$ upper bandwidth $m_u = 0$
- U upper triangular $\iff$ lower bandwidth $m_l = 0$
- D diagonal $\iff$ lower bandwidth $m_l = 0$, upper bandwidth $m_u = 0$
- MATLAB spy plots: pattern of non-zero elements in matrix

Proposition (Factorization of banded matrices)

Banded matrix A, lower bandwidth m_l and upper bandwidth m_u $\implies$ LU factorization of A: L lower bandwidth m_l, U upper bandwidth m_u

Banded matrix – Example



Example

Spy plot: non-zero elements in A: give size, upper, lower and total bandwidth, number of non-zero elements

Solution

- *size(A) = [40 40]*
- *Upper bandwidth* $m_u = 5$
- *Lower bandwidth* $m_l = 5$
- *Bandwidth* 11
- *nnz(A) = 174*

Fill-in

Definition (Fill-in)

Fill-in: creation of non-zero elements where original elements were zero

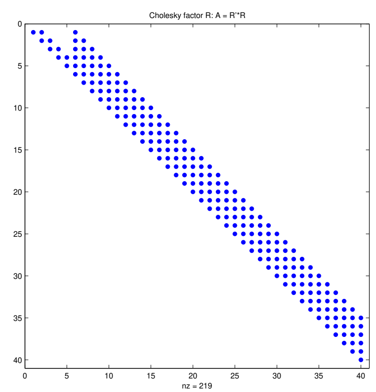
- Row operations can cause fill-in

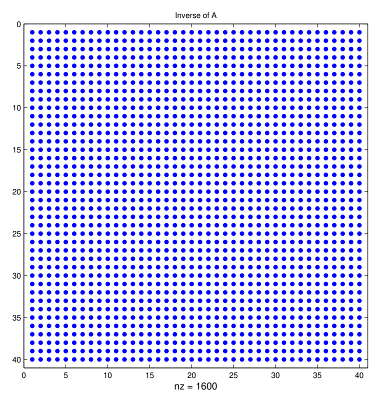
$$\begin{bmatrix} x & x & x & x & x & x & x & \\ & x & x & x & & x & & \\ & & x & x & x & x & x & \\ & & & x & x & x & x & x \\ & & & x & & & & \\ & & & x & & & & \\ & & & x & & & & \\ & & & x & & & & \end{bmatrix} \underset{\text{op}}{\overset{\text{row}}{\longrightarrow}} \begin{bmatrix} x & x & x & x & x & x & x & \\ & x & x & x & & x & & \\ & & x & x & x & x & x & \\ & & & x & x & x & x & x \\ & & & 0 & y & y & y & y \\ & & & 0 & y & y & y & y \\ & & & 0 & y & y & y & y \\ & & & 0 & y & y & y & y \end{bmatrix}$$

- Matrix multiplication can cause fill-in

Banded matrices – fill-in

- Banded matrix: fill-in during factorization only occurs within bands
- Inverse A^{-1} can get lot of fill-in $\Longrightarrow$ avoid explicitly calculating A^{-1}





Diagonals

Definition (Diagonals)

Diagonal k of $A \in \mathbb{R}^{m\times n} \iff a_{ij} : j - i = k$

- Diagonal $0 \iff j - i = 0 \iff i = j$ main diagonal
- Diagonal $1 \iff j - i = 1 \iff j = i + 1$ super-diagonal
- Diagonal $-1 \iff j - i = -1 \iff j = i - 1$ sub-diagonal
- MATLAB command diag

Example (MATLAB diag command)

Give the results of

```
u = [2 1 0 -1 2];
A = diag(u), B = diag(u,1), C = diag(u,-1)
X = [11 12 13; 21 22 23; 31 32 33]
diag(X), diag(diag(X))
```

Solution (MATLAB M-file diagex1.m)

Tridiagonal matrices

Definition (Tridiagonal matrix)

A tridiagonal $\iff$ upper bandwidth $m_u = 1$ and lower bandwidth $m_l = 1$

- Tridiagonal matrix

$$A = \begin{bmatrix} b_1 & c_1 & 0 & \cdots & 0 & 0 \\ a_2 & b_2 & c_2 & 0 & \cdots & 0 \\ 0 & a_3 & b_3 & c_3 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & a_{n-1} & b_{n-1} & c_{n-1} \\ 0 & 0 & \cdots & 0 & a_n & b_n \end{bmatrix}$$

- Storage $n + 2(n-1) = 3n - 2$ elements
- Thomas algorithm
  - Gaussian elimination/ back-substitution exploiting structure
  - MATLAB function M-file tridiag.m
  - $8n + O(1)$ flops

Thomas algorithm

test_thomas.m

```
>> a = [-2 -1 0 1];
>> b = [1 2 2 4 1];
>> c = [6 4 8 6];
>> d = [8 16 32 32 8];
>> x = tridiag(a,b,c,d)
>> x = x'
x =
 -28   6  -13   8   0
```

$$\begin{bmatrix} 1 & 6 & 0 & 0 & 0 \\ -2 & 2 & 4 & 0 & 0 \\ 0 & -1 & 2 & 8 & 0 \\ 0 & 0 & 0 & 4 & 6 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = \begin{bmatrix} 8 \\ 16 \\ 32 \\ 32 \\ 8 \end{bmatrix}$$

Sparse matrices

Definition (Sparse matrix)

- A sparse $\iff$ zero elements in A can be exploited to improve efficiency (storage, time)
- Sparsity of $A \in \mathbb{R}^{m\times n}$ is number of non-zero elements in A divided by total number of elements (mn) in A (express as %)

Example (Sparsity)

Give the sparsity of $A \in \mathbb{R}^{n\times n}$ where A is diagonal, tridiagonal, triangular

Solution

- *Diagonal matrix: sparsity* $= 100n/n^2 \approx 100/n\%$
- *Tridiagonal matrix: sparsity* $= 100(3n-2)/n^2 \approx 300/n\%$
- *Triangular matrix: sparsity* $= 100n(n+1)/(2n^2) \approx 50\%$

Sparse matrices – storage

- A sparse $\implies$ only store non-zero elements of A
  - Row index i, column index j, element a_{ij}
  - More efficient, more complicated sparse storage schemes
- MATLAB M-file `spex1.m`
  - number of non-zero elements `nnz(A)`
  - sparsity `100*nnz(A)/numel(A)`
  - `sparse`, `full` commands
  - `speye`
  - sparse diagonals `spdiags`
- Fill-in during matrix operations
  - Reorder rows and columns to reduce fill-in
  - Conflict with reordering for numerical stability, except Cholesky
  - A symmetric apply same reordering to rows, columns
  - MATLAB functions `amd`, `colamd`, `symamd`, `symrcm`

Reordering to reduce fill-in

- Chemical Engineering plant simulation:
  `http://math.nist.gov/MatrixMarket/data/Harwell-Boeing/chemwest/chemwest.html`
- Column reordering: `q = colamd(A); x = A(:,q) \ b`
- Symmetric reordering: `p = symrcm(A); y = A(p,p) \ b(p)`
- MATLAB M-file `west.m`