Tutorial 8: Sparse linear algebra in MATLAB

COMP5930M Scientific Computation

Today

MATLAB sparse matrix handling

Creating sparse matrices

Experiments with real-world matrices

Direct solvers: fill-in and reordering

Indirect solvers: Jacobi and Gauss-Seidel

Sparse matrices in MATLAB

- MATLAB uses sparse column-major format
- We do not need to access it in that form
- Most MATLAB operations on matrices, eg. multiplication or $\backslash$, also work automatically on sparse matrices
- Main difference in eigenvalue computations; for dense matrices use `eig`, for sparse matrices use `eigs`

Creating and accessing sparse matrices

- Creation: A = spalloc(n,n,nnz)
  `A` is an `n` × `n` sparse matrix with space for `nnz` non-zeros
- Access: A(i,j)=c or c=A(i,j)
  Direct, simple access through normal matrix notation
  (no need to use the sparse column data structure)
- Visualisation: spy(A)
  Plots a graph of the sparse structure

Finding challenging linear problems to solve

- Matrix market: `https://math.nist.gov/MatrixMarket/`
- Download matrices arising from real-world problems:
  - flow dynamics
  - structural engineering
  - electrical circuit simulation
  - economics
  - quantum physics
  - etc.
- Useful resource for testing linear albegra algorithms

Direct solution by LU-factorisation

```
function x = directLU(A,b)
    [L,U,P] = lu(A);
    z = forwardSubstitution(L, P*b, size(b,1));
    x = backSubstitution(U, z, size(z,1));
end
```

Note: The decomposition $PA = LU$ implies solving two systems:

1. $Lz = Pb$
2. $Ux = z$

The first problem is solved using forward-substitution and the second problem back-substitution. Both have $O(n^2)$ complexity.

Back-substitution

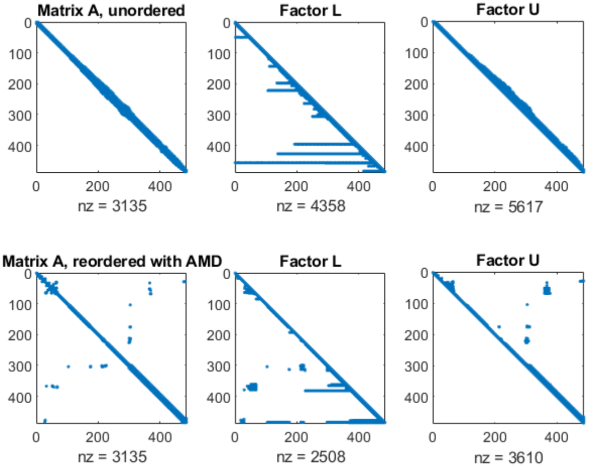
```
function x = backSubstitution(U,b,n)

x = zeros(n,1);
for j = n : -1 : 1
    if (U(j,j)==0) error('Matrix is singular!'); end;
    x(j) = b(j) / U(j,j);
    b(1:j-1) = b(1:j-1) - U(1:j-1,j) * x(j);
end
```

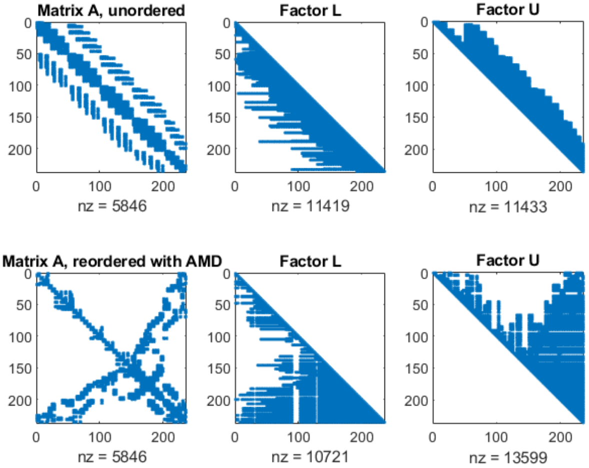
Forward-substitution

```
function x = forwardSubstitution(L,b,n)

x = zeros(n,1);
for j = 1 : n
    if (L(j,j)==0) error('Matrix is singular!'); end;
    x(j)=b(j)/L(j,j);
    b(j+1:n)=b(j+1:n)-L(j+1:n,j)*x(j);
end
```



For very sparse matrices, AMD reduces fill-in of L, U factors



For more complex matrices there can be little reduction in fill-in

Jacobi and Gauss-Seidel iteration

```
% Split the matrix A = D + E
D = diag(diag(A)); % Jacobi
D = triu(A,0);     % Gauss-Seidel
E = A - D;

Bfun = @(X)(-D\(E*X)); % Function to evaluate B * x
z = D \ b;

while ( norm(r)/norm(x0) > tol && k < maxIter )
    x = Bfun(x0) + z;
    x0 = x;
    r = b - A*x0;
    k = k + 1;
end
```

Example: Comparison of basic iterative methods

The matrix

$$A = \begin{bmatrix} 14 & 0 & 5 & 2 & 1 \\ 0 & 8 & -3 & 1 & -2 \\ 5 & -3 & 12 & 2 & 5 \\ 2 & 1 & 2 & 6 & 1 \\ 1 & -2 & 5 & 1 & 8 \end{bmatrix}$$

is symmetric, positive definite but not strictly diagonally dominant.

Jacobi: $\rho(B) \approx 0.916$ method converges in 21 iterations

Gauss-Seidel: $\rho(B) \approx 0.262$ method converges in 7 iterations