Lecture 21
Sparse Matrix Algorithms

MIT 18.335J / 6.337J

Introduction to Numerical Methods

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Sparse vs. Dense Matrices

- A *sparse matrix* is a matrix with enough zeros that it is worth taking advantage of them [Wilkinson]

$$\begin{bmatrix} \bullet & & \bullet & \bullet & \bullet \\ & \bullet & & & \\ \bullet & & \bullet & & \\ \bullet & & & \bullet & \\ \bullet & & & & \bullet \end{bmatrix}$$

- A *structured matrix* has enough structure that it is worthwhile to use it (e.g. Toeplitz)

$$\begin{bmatrix} a & b & c & d & e \\ b & a & b & c & d \\ c & b & a & b & c \\ d & c & b & a & b \\ e & d & c & b & a \end{bmatrix}$$

- A *dense matrix* is neither sparse nor structured

$$\begin{bmatrix} \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \end{bmatrix}$$

MATLAB Sparse Matrices: Design Principles

- Most operations should give the same results for sparse and full matrices
- Sparse matrices are never created automatically, but once created they propagate
- Performance is important – but usability, simplicity, completeness, and robustness are more important
- Storage for a sparse matrix should be $O(\mathrm{nonzeros})$
- Time for a sparse operation should be close to $O(\mathrm{flops})$

Data Structures for Matrices

Full:

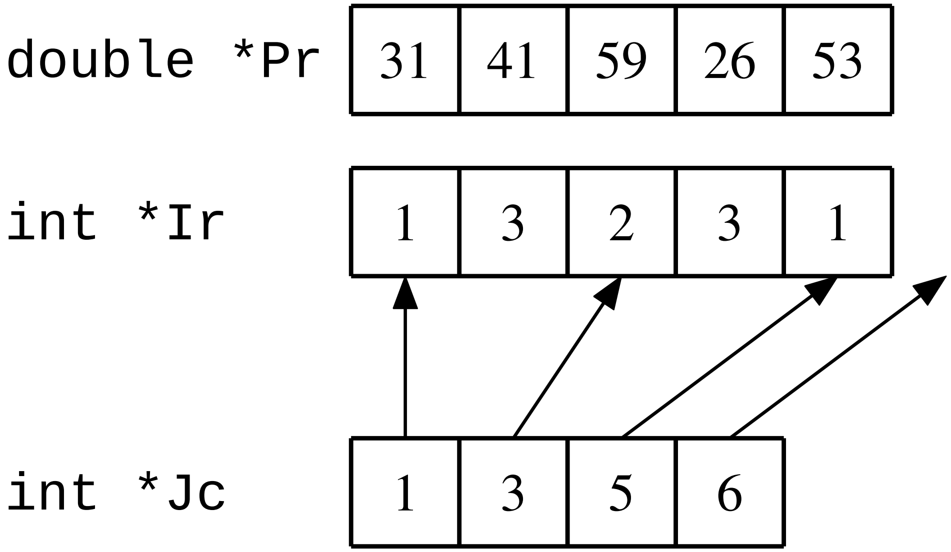
- Storage: Array of real (or complex) numbers
- Memory: `nrows*ncols`

31	0	53
0	59	0
41	26	0

`double *A`

Sparse:

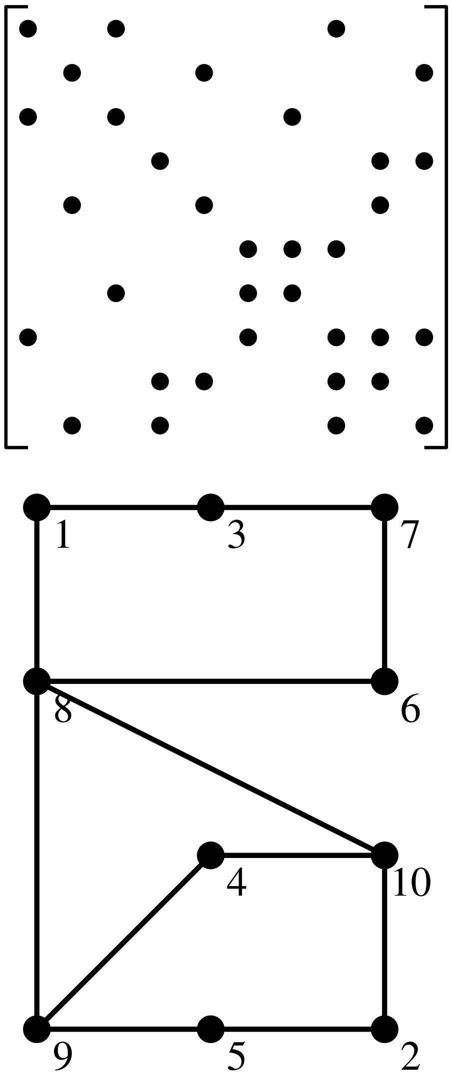
- Compressed column storage
- Memory: About `1.5*nnz+.5*ncols`



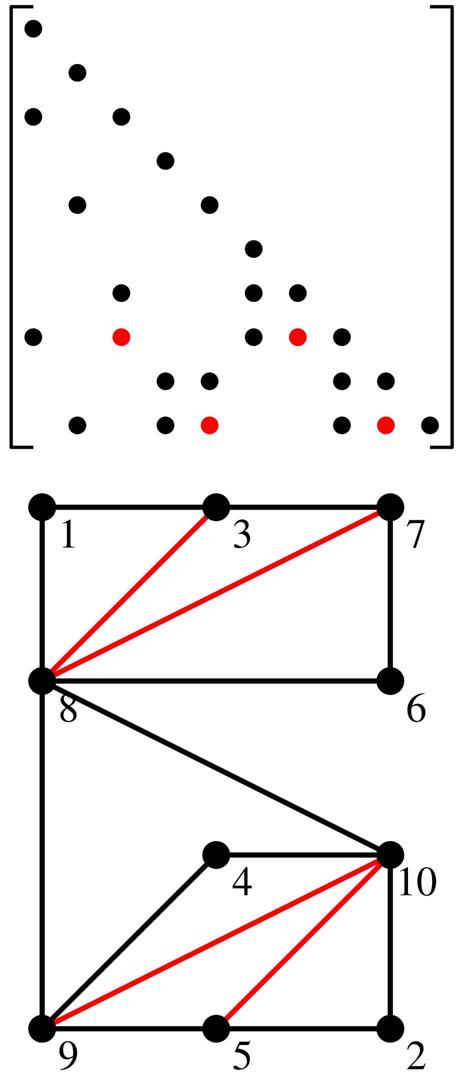
Compressed Column Format - Observations

- Element look-up: $O(\log \text{#elements in column})$ time
- Insertion of new nonzero very expensive
- Sparse vector = Column vector (not Row vector)

Graphs and Sparsity: Cholesky Factorization



$G(A)$



$G^{+}(A)$

Fill: New nonzeros in factor

Symmetric Gaussian Elimination:

for $j = 1$ **to** N

Add edges between j's higher-numbered neighbors

Permutations of the 2-D Model Problem

- 2-D Model Problem: Poisson's Equation on $n \times n$ finite difference grid
- Total number of unknowns $n^2 = N$
- Theoretical results for the fill-in:
  - With natural permutation: $O(N^{3/2})$ fill
  - With any permutation: $\Omega(N \log N)$ fill
  - With a *nested dissection* permutation: $O(N \log N)$ fill

Nested Dissection Ordering

- A *separator* in a graph G is a set S of vertices whose removal leaves at least two connected components
- A *nested dissection* ordering for an N-vertex graph G numbers its vertices from 1 to N as follows:
  - Find a separator S, whose removal leaves connected components $T_1, T_2, \ldots, T_k$
  - Number the vertices of S from $N - |S| + 1$ to N
  - Recursively, number the vertices of each component: T_1 from 1 to $|T_1|$, T_2 from $|T_1| + 1$ to $|T_1| + |T_2|$, etc
  - If a component is small enough, number it arbitrarily
- It all boils down to finding good separators!

Heuristic Fill-Reducing Matrix Permutations

- Banded orderings (Reverse Cuthill-McKee, Sloan, etc):
  - Try to keep all nonzeros close to the diagonal
  - Theory, practice: Often wins for “long, thin” problems
- Minimum degree:
  - Eliminate row/col with fewest nonzeros, add fill, repeat
  - Hard to implement efficiently – current champion is “Approximate Minimum Degree” [Amestoy, Davis, Duff]
  - Theory: Can be suboptimal even on 2-D model problem
  - Practice: Often wins for medium-sized problems

Heuristic Fill-Reducing Matrix Permutations

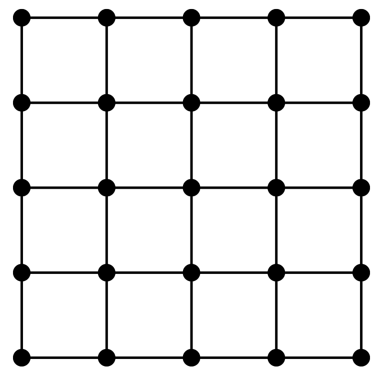
- Nested dissection:
  - Find a separator, number it *last*, proceed recursively
  - Theory: Approximately optimal separators $\Longrightarrow$ approximately optimal fill and flop count
  - Practice: Often wins for very large problems
- The best modern general-purpose orderings are ND/MD hybrids

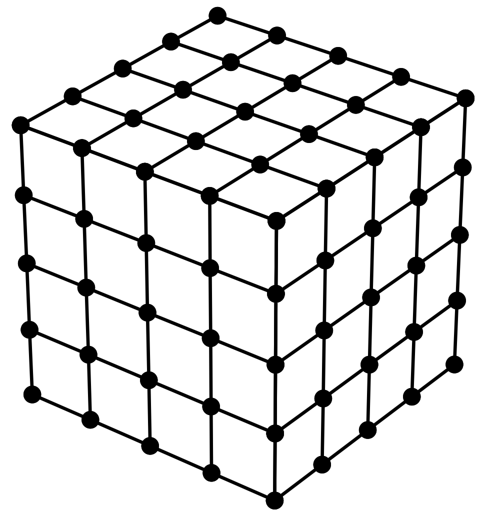
Fill-Reducing Permutations in Matlab

- Reverse Cuthill-McKee:
  - `p=symrcm(A);`
  - Symmetric permutation: `A(p,p)` often has smaller bandwidth than A
- Symmetric approximate minimum degree:
  - `p=symamd(A);`
  - Symmetric permutation: `chol(A(p,p))` sparser than `chol(A)`
- Nonsymmetric approximate minimum degree:
  - `p=colamd(A);`
  - Column permutation: `lu(A(:,p))` sparser than lu(A)
- Symmetric nested dissection:
  - Not built into MATLAB, several versions in the MESHPART toolbox

Complexity of Direct Methods

- Time and space to solve any problem on any well-shaped finite element mesh with N nodes:





	1-D	2-D	3-D
Space (fill):	$O(N)$	$O(N \log N)$	$O(N^{4/3})$
Time (flops):	$O(N)$	$O(N^{3/2})$	$O(N^2)$