Sparse Matrix Algorithms

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 $O(\text{nonzeros})$.
- Time for a sparse operation should be close to $O(\text{flops})$.

Data Structures for Matrices

Full:
- Storage: Array of real (or complex) numbers
- Memory: $n\text{rows}*n\text{cols}$

Sparse:
- Compressed column storage
- Memory: About $1.5*\text{nnz}+.5*\text{ncols}$

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

Fill: New nonzeros in factor
- Symmetric Gaussian
- Elimination:
  - for $j = 1$ to $N$
  - Add edges between $j$'s higher-numbered neighbors

Sparse vs. Dense Matrices

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

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

- A dense matrix is neither sparse nor structured
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 \( \implies \) 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:
  - \( p = \	ext{symrcm}(A) \);
  - Symmetric permutation: \( A(p, p) \) often has smaller bandwidth than \( A \)
- Symmetric approximate minimum degree:
  - \( p = \text{symamd}(A) \);
  - Symmetric permutation: \( \text{chol}(A(p, p)) \) sparser than \( \text{chol}(A) \)
- Nonsymmetric approximate minimum degree:
  - \( p = \text{colamd}(A) \);
  - Column permutation: \( \text{lu}(A(:, p)) \) sparser than \( \text{lu}(A) \)
- 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:

<table>
<thead>
<tr>
<th></th>
<th>1-D</th>
<th>2-D</th>
<th>3-D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Space (fill)</td>
<td>( O(N) )</td>
<td>( O(N \log N) )</td>
<td>( O(N^{4/3}) )</td>
</tr>
<tr>
<td>Time (flops)</td>
<td>( O(N) )</td>
<td>( O(N^{3/2}) )</td>
<td>( O(N^2) )</td>
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