Sparse matrix data structure

- Typically either
  Compressed Sparse Row (CSR)
  or
  Compressed Sparse Column (CSC)
  - Informally “ia-ja” format
  - CSR is better for matrix-vector multiplies; CSC can be better for factorization
- CSR:
  - Array of all values, row by row
  - Array of all column indices, row by row
  - Array of pointers to start of each row

Direct Solvers

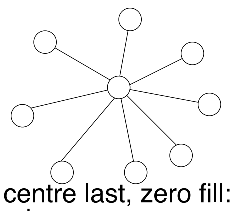
- We’ll just peek at Cholesky factorization of SPD matrices: $A=LL^T$
  - In particular, pivoting not required!
- Modern solvers break Cholesky into three phases:
  - Ordering: determine order of rows/columns
  - Symbolic factorization: determine sparsity structure of L in advance
  - Numerical factorization: compute values in L
- Allows for much greater optimization…

Graph model of elimination

- Take the graph whose adjacency matrix matches A
- Choosing node “i” to eliminate next in row-reduction:
  - Subtract off multiples of row i from rows of neighbours
  - In graph terms: unioning edge structure of i with all its neighbours
  - A is symmetric -> connecting up all neighbours of i into a “clique”
- New edges are called “fill”
  (nonzeros in L that are zero in A)
- Choosing a different sequence can result in different fill

Extreme fill

- The star graph



- If you order centre last, zero fill:
  O(n) time and memory
- If you order centre first, $O(n^2)$ fill:
  $O(n^3)$ time and $O(n^2)$ memory

Fill-reducing orderings

- Finding minimum fill ordering is NP-hard
- Two main heuristics in use:
  - Minimum Degree: (greedy incremental) choose node of minimum degree first
    - Without many additional accelerations, this is too slow, but now very efficient: e.g. AMD
  - Nested Dissection: (divide-and-conquer) partition graph by a node separator, order separator last, recurse on components
    - Optimal partition is also NP-hard, but very good/fast heuristic exist: e.g. Metis
    - Great for parallelism: e.g. ParMetis

A peek at Minimum Degree

- See George & Liu, “The evolution of the minimum degree algorithm”
  - A little dated now, but most of key concepts explained there
- Biggest optimization: don’t store structure explicitly
  - Treat eliminated nodes as “quotient nodes”
  - Edge in L
    = path in A via zero or more eliminated nodes

A peek at Nested Dissection

- Core operation is graph partitioning
- Simplest strategy: breadth-first search
- Can locally improve with Kernighan-Lin
- Can make this work fast by going multilevel

Theoretical Limits

- In 2D (planar or near planar graphs), Nested Dissection is within a constant factor of optimal:
  - O(n log n) fill (n=number of nodes - think s^2)
  - O($n^{3/2}$) time for factorization
  - Result due to Lipton & Tarjan…
- In 3D asymptotics for well-shaped 3D meshes is worse:
  - O($n^{5/3}$) fill (n=number of nodes - think s^3)
  - O(n^2) time for factorization
- Direct solvers are very competitive in 2D, but don't scale nearly as well in 3D

Symbolic Factorization

- Given ordering, determining L is also just a graph problem
- Various optimizations allow determination of row or column counts of L in nearly O(nnz(A)) time
  - Much faster than actual factorization!
- One of the most important observations: good orderings usually results in **supernodes**: columns of L with identical structure
- Can treat these columns as a single block column

Numerical Factorization

- Can compute L column by column with left-looking factorization
- In particular, compute a supernode (block column) at a time
  - Can use BLAS level 3 for most of the numerics
  - Get huge performance boost, near "optimal"

Software

- See Tim Davis's list at www.cise.ufl.edu/research/sparse/codes/

- Ordering: AMD and Metis becoming standard
- Cholesky: PARDISO, CHOLMOD, …
- General: PARDISO, UMFPACK, …