Sparse Systems and Iterative Methods

Paul Heckbert

Computer Science Department
Carnegie Mellon University

PDE's and Sparse Systems

- A system of equations is *sparse* when there are few nonzero coefficients, e.g. O(*n*) nonzeros in an *n*x*n* matrix.
- **Partial Differential Equations generally yield sparse systems of equations.**
- Integral Equations generally yield dense (non-sparse) systems of equations.
- Sparse systems come from other sources besides PDE's.

Example: PDE Yielding Sparse System

- Laplace's Equation in 2-D: $\nabla^2 u = u_{xx} + u_{yy} = 0$
  - domain is unit square $[0,1]^2$
  - value of function $u(x,y)$ specified on boundary
  - solve for $u(x,y)$ in interior

Sparse Matrix Storage

- Brute force: store nxn array, O(n^2) memory
  - but most of that is zeros – wasted space (and time)!
- Better: use data structure that stores only the nonzeros

```
col 1   2   3   4   5   6   7   8   9  10...
val 0   1   0   0   1  -4   1   0   0   1...
16 bit integer indices:  2, 5, 6, 7,10
32 bit floats:           1, 1,-4, 1, 1
```

- Memory requirements, if *kn* nonzeros:
  - brute force: $4n^2$ bytes, sparse data struc: $6kn$ bytes

An Iterative Method: Gauss-Seidel

- System of equations $Ax=b$
- Solve ith equation for x_i:
- Pseudocode:

```
until x stops changing
   for i = 1 to n
      x[i] ← (b[i]-sum{j≠i}{a[i,j]*x[j]})/a[i,i]
```

- modified x values are fed back in immediately
- converges if A is symmetric positive definite

Variations on Gauss-Seidel

- Jacobi's Method:
  - Like Gauss-Seidel except two copies of x vector are kept, "old" and "new"
  - No feedback until a sweep through n rows is complete
  - Half as fast as Gauss-Seidel, stricter convergence requirements
- Successive Overrelaxation (SOR)
  - extrapolate between old x vector and new Gauss-Seidel x vector, typically by a factor ω between 1 and 2.
  - Faster than Gauss-Seidel.

Conjugate Gradient Method

- Generally for symmetric positive definite, only.

- Convert linear system $Ax=b$
- into optimization problem: minimize x^TAx-x^Tb
  - a parabolic bowl

- Like gradient descent
  - but search in conjugate directions
  - not in gradient direction, to avoid zigzag problem
- Big help when bowl is elongated (cond(A) large)

Conjugate Directions

Convergence of Conjugate Gradient Method

- If $K = \text{cond}(A) = \lambda_{max}(A)/ \lambda_{min}(A)$
- then conjugate gradient method converges linearly with coefficient (sqrt(K)-1)/(sqrt(K)+1) worst case.
- often does much better: without roundoff error, if A has m distinct eigenvalues, converges in m iterations!