CS 5220: Iterations and Sparse LA

David Bindel

2017-10-24

World of Linear Algebra

- Dense methods (last week)
  - Direct representation of matrices with simple data structures (no need for indexing data structure)
  - Mostly $O(n^3)$ factorization algorithms
- Sparse direct methods (Thurs)
  - Direct representation, keep only the nonzeros
  - Factorization costs depend on problem structure (1D cheap; 2D reasonable; 3D gets expensive; not easy to give a general rule, and NP hard to order for optimal sparsity)
  - Robust, but hard to scale to large 3D problems
- Iterative methods (today and Thurs)
  - Only *need* $y = Ax$ (maybe $y = A^T x$)
  - Produce successively better (?) approximations
  - Good convergence depends on *preconditioning*
  - Best preconditioners are often hard to parallelize

Linear Algebra Software: MATLAB

```
% Dense (LAPACK)
[L,U] = lu(A);
x = U\(L\b);

% Sparse direct (UMFPACK + COLAMD)
[L,U,P,Q] = lu(A);
x = Q*(U\(L\(P*b)));

% Sparse iterative (PCG + incomplete Cholesky)
tol = 1e-6;
maxit = 500;
R = cholinc(A,'0');
x = pcg(A,b,tol,maxit,R',R);
```

Linear Algebra Software: the Wider World

- Dense: LAPACK, ScaLAPACK, PLAPACK
- Sparse direct: UMFPACK, TAUCS, SuperLU, MUMPS, Pardiso, SPOOLES, ...
- Sparse iterative: too many!
- Sparse mega-libraries
  - PETSc (Argonne, object-oriented C)
  - Trilinos (Sandia, C++)
- Good references:
  - *Templates for the Solution of Linear Systems* (on Netlib)
  - Survey on “Parallel Linear Algebra Software” (Eijkhout, Langou, Dongarra – look on Netlib)
  - ACTS collection at NERSC

Software Strategies: Dense Case

Assuming you want to *use* (vs develop) dense LA code:

- Learn enough to identify right algorithm
  (e.g. is it symmetric? definite? banded? etc)
- Learn high-level organizational ideas
- Make sure you have a good BLAS
- Call LAPACK/ScaLAPACK!
- For n large: wait a while

Software Strategies: Sparse Direct Case

Assuming you want to use (vs develop) sparse LA code

- Identify right algorithm (mainly Cholesky vs LU)
- Get a good solver (often from list)
    - You *don't* want to roll your own!
- *Order your unknowns* for sparsity
    - Again, good to use someone else's software!
- For n large, 3D: get lots of memory and wait

Software Strategies: Sparse Iterative Case

Assuming you want to use (vs develop) sparse LA software…

- Identify a good algorithm (GMRES? CG?)
- Pick a good preconditioner
    - Often helps to know the application
    - … *and* to know how the solvers work!
- Play with parameters, preconditioner variants, etc…
- Swear until you get acceptable convergence?
- Repeat for the next variation on the problem

Frameworks (e.g. PETSc or Trilinos) speed experimentation.

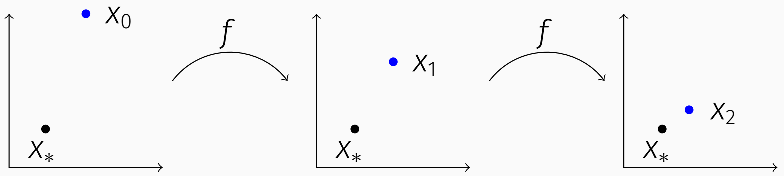
Software Strategies: Stacking Solvers

(Typical) example from a bone modeling package:

- Outer load stepping loop
- Newton method corrector for each load step
- Preconditioned CG for linear system
- Multigrid preconditioner
- Sparse direct solver for coarse-grid solve (UMFPACK)
- LAPACK/BLAS under that

First three are high level — I used a scripting language (Lua).

Iterative Idea



- f is a *contraction* if $\|f(x) - f(y)\| < \|x - y\|$.
- f has a unique *fixed point* $x_* = f(x_*)$.
- For $x_{k+1} = f(x_k)$, $x_k \to x_*$.
- If $\|f(x) - f(y)\| < \alpha\|x - y\|$, $\alpha < 1$, for all x, y, then

$$\|x_k - x_*\| < \alpha^k \|x - x_*\|$$

- Looks good *if* α not too near 1...

Stationary Iterations

Write $Ax = b$ as $A = M - K$; get fixed point of

$$Mx_{k+1} = Kx_k + b$$

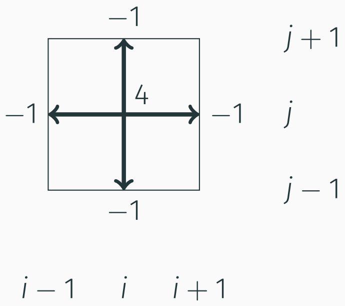
or

$$x_{k+1} = (M^{-1}K)x_k + M^{-1}b.$$

- Convergence if $\rho(M^{-1}K) < 1$
- Best case for convergence: $M = A$
- Cheapest case: $M = I$
- Realistic: choose something between

Jacobi	$M = \text{diag}(A)$
Gauss-Seidel	$M = \text{tril}(A)$

Reminder: Discretized 2D Poisson Problem



$$(Lu)_{i,j} = h^{-2}\left(4u_{i,j} - u_{i-1,j} - u_{i+1,j} - u_{i,j-1} - u_{i,j+1}\right)$$

Jacobi on 2D Poisson

Assuming homogeneous Dirichlet boundary conditions

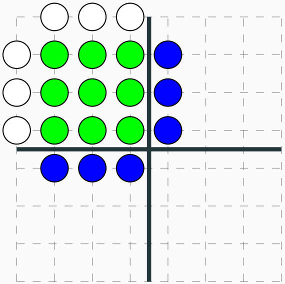
```
for step = 1:nsteps

  for i = 2:n-1
    for j = 2:n-1
      u_next(i,j) = ...
        ( u(i,j+1) + u(i,j-1) + ...
          u(i-1,j) + u(i+1,j) )/4 - ...
        h^2*f(i,j)/4;
    end
  end
  u = u_next;

end
```

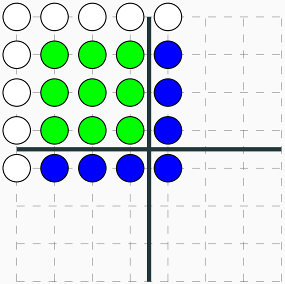
Basically do some averaging at each step.

Parallel version (5 point stencil)



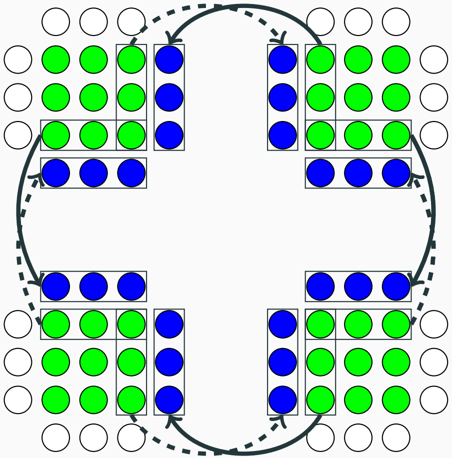
Boundary values:	white
Data on P0:	green
Ghost cell data:	blue

Parallel version (9 point stencil)



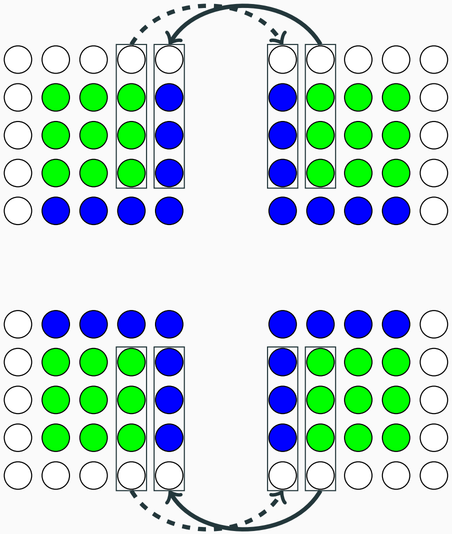
Boundary values:	white
Data on P0:	green
Ghost cell data:	blue

Parallel version (5 point stencil)



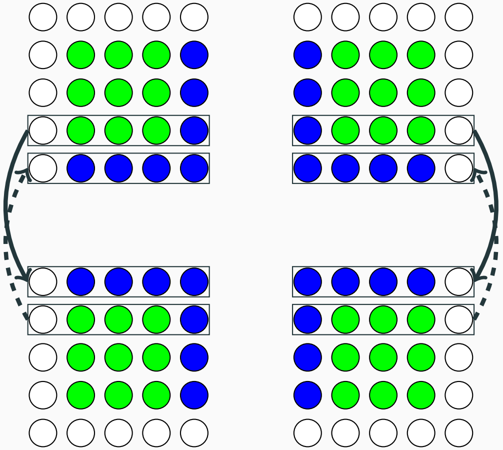
Communicate ghost cells before each step.

Parallel version (9 point stencil)



Communicate in two phases (EW, NS) to get corners.

Parallel version (9 point stencil)



Communicate in two phases (EW, NS) to get corners.

Gauss-Seidel on 2D Poisson

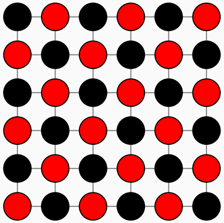
```
for step = 1:nsteps

  for i = 2:n-1
    for j = 2:n-1
      u(i,j) = ...
        ( u(i,j+1) + u(i,j-1) + ...
          u(i-1,j) + u(i+1,j) )/4 - ...
        h^2*f(i,j)/4;
    end
  end

end
```

Bottom values depend on top; how to parallelize?

Red-Black Gauss-Seidel



Red depends only on black, and vice-versa.

Generalization: multi-color orderings

Red black Gauss-Seidel step

```
for i = 2:n-1
  for j = 2:n-1
    if mod(i+j,2) == 0
      u(i,j) = ...
    end
  end
end

for i = 2:n-1
  for j = 2:n-1
    if mod(i+j,2) == 1,
    u(i,j) = ...
  end
end
```

Parallel red-black Gauss-Seidel sketch

At each step

- Send black ghost cells
- Update red cells
- Send red ghost cells
- Update black ghost cells

More Sophistication

- Successive over-relaxation (SOR): extrapolate Gauss-Seidel direction
- Block Jacobi: let M be a block diagonal matrix from A
    - Other block variants similar
- Alternating Direction Implicit (ADI): alternately solve on vertical lines and horizontal lines
- Multigrid

These are mostly just the opening act for...

Krylov Subspace Methods

What if we only know how to multiply by A?
About all you can do is keep multiplying!

$$\mathcal{K}_k(A, b) = \operatorname{span}\left\{b, Ab, A^2b, \ldots, A^{k-1}b\right\}.$$

Gives surprisingly useful information!

Example: Conjugate Gradients

If A is symmetric and positive definite, $Ax = b$ solves a minimization:

$$\begin{aligned} \phi(x) &= \frac{1}{2}x^T Ax - x^T b \\ \nabla\phi(x) &= Ax - b. \end{aligned}$$

Idea: Minimize $\phi(x)$ over $\mathcal{K}_k(A, b)$.
Basis for the *method of conjugate gradients*

Example: GMRES

Idea: Minimize $\|Ax - b\|^2$ over $\mathcal{K}_k(A, b)$.
Yields *Generalized Minimum RESidual* (GMRES) method.

Convergence of Krylov Subspace Methods

- KSPs are *not* stationary (no constant fixed-point iteration)
- Convergence is surprisingly subtle!
- CG convergence upper bound via *condition number*
    - Large condition number iff form $\phi(x)$ has long narrow bowl
    - Usually happens for Poisson and related problems
- *Preconditioned* problem $M^{-1}Ax = M^{-1}b$ converges faster?
- Whence M?
    - From a stationary method?
    - From a simpler/coarser discretization?
    - From approximate factorization?

PCG

```
Compute $r^{(0)} = b - Ax$
for $i = 1, 2, \ldots$
    solve $Mz^{(i-1)} = r^{(i-1)}$
    $\rho_{i-1} = (r^{(i-1)})^T z^{(i-1)}$
    if $i == 1$
        $p^{(1)} = z^{(0)}$
    else
        $\beta_{i-1} = \rho_{i-1}/\rho_{i-2}$
        $p^{(i)} = z^{(i-1)} + \beta_{i-1} p^{(i-1)}$
    endif
    $q^{(i)} = Ap^{(i)}$
    $\alpha_i = \rho_{i-1}/(p^{(i)})^T q^{(i)}$
    $x^{(i)} = x^{(i-1)} + \alpha_i p^{(i)}$
    $r^{(i)} = r^{(i-1)} - \alpha_i q^{(i)}$
end
```

Parallel work:

- Solve with M
- Product with A
- Dot products
- Axpys

Overlap comm/comp.

PCG bottlenecks

Key: fast solve with M, product with A

- Some preconditioners parallelize better!
  (Jacobi vs Gauss-Seidel)
- Balance speed with performance.
  - Speed for set up of M?
  - Speed to apply M after setup?
- Cheaper to do two multiplies/solves at once...
  - Can't exploit in obvious way — lose stability
  - Variants allow multiple products — Hoemmen's thesis
- Lots of fiddling possible with M; matvec with A?