

Notes for Ma221 Lecture 12, Nov 12, 2024

Splitting Methods

Goal: given an initial guess x_0 for a solution of $Ax=b$, cheaply compute a sequence x_i converging to $A^{-1}b$.

Def: A splitting of A is a decomposition $A = M - K$ with M nonsingular

This yields the following iterative method: Write $Ax = Mx - Kx = b$, so $Mx = Kx + b$. Then compute x_{i+1} from x_i by solving $Mx_{i+1} = Kx_i + b$,

or $x_{i+1} = M^{-1}Kx_i + M^{-1}b = Rx_i + c$.

(*) $x_{i+1} = Rx_i + c$

For this to work well, we need two conditions:

(1) It should converge.

(2) Multiplying by R (i.e. solving $Mx_{i+1} = Kx_i + c$ for x_{i+1}) and

computing $c = M^{-1}b$ should be much cheaper than solving with A itself.

Lemma: Let $\|\cdot\|$ be any operator norm. Then if $\|R\| < 1$, (*) converges to $A^{-1}b$ for any x_0 .

Proof: Subtract $x = Rx + c$ from $x_{i+1} = Rx_i + c$ to get

$x_{i+1} - x = R(x_i - x)$ or

$\|x_{i+1} - x\| \leq \|R\| \|x_i - x\| \leq \dots \leq \|R\|^{i+1} \|x_0 - x\|$

which converges to zero for any x_0 if $\|R\| < 1$.

Def: The spectral radius of R is $\rho(R) = \max |\lambda|$, the largest absolute value of any eigenvalue of R

Lemma: For all operator norms, $\rho(R) \leq \|R\|$. For all R and all $\epsilon > 0$, there exists an operator norm $\|\cdot\|_*$ such that $\|R\|_* \leq \rho(R) + \epsilon$

Proof: To show $\rho(R) \leq \|R\|$, note that $\|R\| = \max_x \|R^*x\| / \|x\|$. By picking x to be an eigenvector, we see that $\|R\| \geq |\lambda|$ for any

eigenvalue λ of R . To construct $\|\cdot\|_*$, we use the Jordan Form of R :

Let $S^{-1}RS = J$ be in Jordan form, i.e. J is block diagonal with Jordan

blocks. Let $D = \text{diag}(1, \epsilon, \epsilon^2, \dots, \epsilon^{n-1})$. Then

$J_\epsilon = D^{-1}JD$ leaves the diagonal (eigenvalues) unchanged, and multiplies

each superdiagonal entry of J by ϵ , so J has eigenvalues on the diagonal,

and ϵ above the diagonal in any Jordan block. We now define a new

vector

norm by $\|x\|_* = \|(S*D)^{-1}*x\|_{\infty}$. (See Question 1.5 for the proof that

this defines a vector norm.) Then

$$\begin{aligned} \|R\|_* &= \max_x \|R*x\|_* / \|x\|_* \\ &= \max_x \|(S*D)^{-1}*R*x\|_{\infty} / \|(S*D)^{-1}*x\|_{\infty} \\ &= \max_y \|(S*D)^{-1}*R*(S*D)*y\|_{\infty} / \|y\|_{\infty} \\ &\quad \text{where } y = (S*D)^{-1}*x \\ &= \max_y \|D^{-1}*S^{-1}*R*S*D*y\|_{\infty} / \|y\|_{\infty} \\ &= \max_y \|J_{\text{eps}}*y\|_{\infty} / \|y\|_{\infty} \\ &\leq \max |\lambda| + \text{eps} \\ &= \rho(R) + \text{eps} \end{aligned}$$

Theorem: The iteration $x_{i+1} = R*x_i + c$ converges to the solution of $A*x=b$ for all starting vectors x_0 if and only if $\rho(R) < 1$.

Proof: If $\rho(R) \geq 1$, chose x_0 so that $x_0 - x$ is an eigenvector of R for

its largest eigenvalue, call it λ . Then $x_i - x = R^i*(x_0 - x) = \lambda^i*(x_0 - x)$

does not converge to zero since $|\lambda| \geq 1$.

If $\rho(R) < 1$, use the last lemma to conclude that there is an operator norm $\|R\|_*$

and an eps such that $\|R\|_* \leq \rho(R) + \text{eps} < 1$, so that $x_i - x = R^i*(x_0 - x)$ converges to zero for all x_0 .

Obviously, the smaller is $\rho(R)$, the faster is convergence. Our goal is to pick the

splitting $A = M - K$ so that multiplying by $R = \text{inv}(M)*K$ is easy, and $\rho(R)$ is small. Choosing $M = I$ and $K = I - A$ makes multiplying by R easy, but

will not generally make $\rho(R)$ small. Choosing $K = 0$ and so $R = 0$ makes convergence

immediate, but requires having the solution $c = A^{-1}*b$.

Now we can describe Jacobi, Gauss-Seidel (GS) and Successive Overrelaxation (SOR).

All share the notation $A = D - L' - U' = D*(I - L - U)$, where D is the diagonal of A ,

L' is the negative of the strictly lower triangular part, and U' is the negative of

the strictly upper triangular part of A .

Jacobi:

In words, for $j = 1$ to n , pick $x_{(i+1)}(j)$ to exactly satisfy equation j

As a loop:

for $j = 1$ to n , $x_{(i+1)}(j) = (b_j - \sum_{k \neq j} A(j,k)*x_i(k))/A(j,j)$

As a splitting: $A = D - (L'+U') = M - K$, so

$$R_J = M^{-1} * K = D^{-1} * (L'+U') = L+U$$

For the 2D Poisson equation $T_N * V + V * T_N = h^2 * F$, to get from V_i to V_{i+1} :

$$\begin{aligned} \text{for } j = 1 \text{ to } n, \text{ for } k = 1 \text{ to } n \\ V_{i+1}(j,k) = (V_i(j-1,k) + V_i(j+1,k) + V_i(j,k-1) + \\ V_i(j,k+1) \\ + h^2 * F(j,k)) / 4 \\ = \text{"average" of 4 nearest neighbors and} \end{aligned}$$

right-hand-side

Gauss-Seidel:

In words, improve on Jacobi by using most recently updated values of solution

As a loop:

$$\begin{aligned} \text{for } j = 1 \text{ to } n, x_{i+1}(j) = (b_j - \text{sum}_{\{k < j\}} A(j,k) * x_{i+1} \\ (k) \quad \dots \text{ updated } x \\ \text{components} \quad - \text{sum}_{\{k > j\}} \\ A(j,k) * x_i(k)) / A(j,j) \\ \quad \dots \text{ older } x \\ \text{components} \end{aligned}$$

As a splitting: $A = (D-L') - U'$, so

$$R_{GS} = (D-L')^{-1} * U' = (D * (I - D^{-1} * L'))^{-1} * U' = (I - L)^{-1} * U$$

Note that the order in which we update entries matters in GS (unlike Jacobi).

For 2D Poisson there are two orders to consider:

natural order (rowwise or columnwise update of $V(i,j)$)

Red-Black (RB) ordering: color the entries in the 2D mesh like a checkerboard,

and number the Reds before all the Blacks. Note that each Red node only has

Black neighbors, and vice-versa. Thus when updating Red nodes, we can

update them in any order, since all the Black neighbors have old data.

Then when we update the Black nodes, we can update them in any order,

because all the Red neighbors have new data.

For all (j,k) nodes that are Red ($j+k$ even)

$$\begin{aligned} V_{i+1}(j,k) = (V_i(j-1,k) + V_i(j+1,k) + V_i(j,k-1) + \\ V_i(j,k+1) \\ + h^2 * F(j,k)) / 4 \quad \dots \text{ only use old data} \end{aligned}$$

For all (j,k) nodes that are Black ($j+k$ odd)

$$\begin{aligned} V_{i+1}(j,k) = (V_{i+1}(j-1,k) + V_{i+1}(j+1,k) + \\ V_{i+1}(j,k-1) \\ + V_{i+1}(j,k+1) \\ + h^2 * F(j,k)) / 4 \quad \dots \text{ only use new data} \end{aligned}$$

SOR: In words: This depends on a parameter w : We let the result of SOR be

a weighted combination of the old (x_i) and new ($x_{(i+1)}$) solutions

that GS would have computed:

$$x^{\text{SOR}(w)}_{(i+1)}(j) = (1-w)x_i(j) + w x^{\text{GS}}_{(i+1)}(j)$$

When $w=1$, SOR(1) is just GS. When $w < 1$ we would call this underrelaxation,

and when $w > 1$, we call it overrelaxation. We prefer to "overrelax" with the

intuition that if moving in the direction from x_i to $x_{(i+1)}$ was a good idea,

moving even farther in the same direction is better.

Later we will show how to pick w optimally for the model problem.

As a loop:

$$\text{for } j = 1 \text{ to } n, \quad x_{(i+1)}(j) = (1-w)x_i(j) + w*(b_j - \text{sum}_{\{k < j\}}$$

$A(j,k)x_{(i+1)}(k)$

... updated x

components

$$- \text{sum}_{\{k > j\}}$$

$A(j,k)x_i(k) \text{)} / A(j,j)$

... older x

components

As a splitting multiply through by D to get

$$(D-w*L')x_{(i+1)} = ((1-w)*D + w*U')x_i + w*b$$

and then divide by w to get the splitting

$$A = (D/w - L') - (D/w - D + U')$$

or

$$R_{\text{SOR}}(w) = (D/w - L')^{-1} * (D/w - D + U') = (I - w*L)^{-1} * ((1-w)*I + w*U)$$

For 2D Poisson with Red-Black Ordering:

For all (j,k) nodes that are Red

$$V_{(i+1)}(j,k) = (1-w)V_i(j,k) + w*(V_i(j-1,k) + V_i(j+1,k) + V_i(j,k-1) +$$

$V_i(j,k+1)$

$+ h^2 * F(j,k)) / 4$... only use old data

For all (j,k) nodes that are Black

$$V_{(i+1)}(j,k) = (1-w)V_i(j,k) + w*(V_{(i+1)}(j-1,k) + V_{(i+1)}(j+1,k) +$$

$V_{(i+1)}(j,k-1)$

$+ V_{(i+1)}(j,k+1)$

$+ h^2 * F(j,k)) / 4$... use new data

Now we analyze the convergence of these basic methods, in general and for the

Model Problem (2D Poisson) in particular.

Jacobi's method for the Model problem is easy to analyze, since in the

splitting

$T_{n \times n} = M - K = 4I - (4I - T_{n \times n})$, so $R = M^{-1}K = I - T_{n \times n}/4$, so the eigenvalues of R are $1 - (\lambda_i + \lambda_j)/4$ for all pairs of eigenvalues $\lambda_i = 2(1 - \cos(i\pi/(n+1)))$ and λ_j of T_n , and so the spectral radius $\rho(R)$ of R is

$1 - \lambda_{\min}/2 = 1 - (1 - \cos(\pi/(n+1))) = \cos(\pi/(n+1)) \sim 1 - \pi^2/2(n+1)^2$

which gets closer to 1 as n grows, i.e. Jacobi converges more slowly.

Since the error after m steps is multiplied by $\rho(R)^m$, we estimate the speed of convergence by computing how many steps m are needed to reduce the error by a constant factor. Setting $\rho(R) = 1 - x$ and solving $(1-x)^m = \exp(-1)$ for simplicity, we get

$$(1-x)^m = (1-x)^{[(1/x)*m*x]} \sim \exp(-m*x) = \exp(-1)$$

or $m = 1/x = 2(n+1)^2/\pi^2 = O(n^2) = O(N)$ steps, where $N=n^2$ is the number of unknowns. Note that $\text{cond}(T_{n \times n}) \sim 4N/\pi^2$ is also $O(N)$.

So the number of iterations grows proportionally to the dimension N , and to the condition number. So to reduce the error by any constant factor costs $O(N)$ iterations * $O(N)$ flops_per_iteration, or $O(N^2)$ overall, explaining the entry in the table above. This is typical for many iterative methods: the number of iterations grows with the condition number (multigrid is an important exception!).

Provided the variables are updated in the appropriate order for 2D Poisson, we get

$\rho(R_{GS}) = \rho(R_J)^2$, i.e. one step of Gauss-Seidel reduces the error as much as

two Jacobi steps; this is better but the overall complexity $O(N^2)$ is the same.

Then, again with the right update order, and the right choice of overrelaxation parameter w , $SOR(w)$ for 2D Poisson is much faster with

$$\rho(R_{SOR}(w_{opt})) \sim 1 - 2\pi/n$$

for large n , which is close to 1 but much farther away than $\rho(R_J)$, and takes only $O(n) = O(\sqrt{N})$ steps to reduce the error by a constant

factor, for an overall cost of $O(N^{3/2})$ as opposed to $O(N^2)$.

Now we present (and prove some of!) the general theory of these three methods applied to $Ax=b$.

Thm 1: If A is strictly row diagonally dominant:

$$|A_{ii}| > \sum_{j \neq i} |A_{ij}|$$

then both Jacobi and GS converge, and GS is at least as fast as Jacobi in the sense that $\|R_{GS}\|_{\infty} \leq \|R_J\|_{\infty} < 1$

Proof: (just for Jacobi; see Thm 6.2 in text for full proof):

$$\text{Split } A = D - (D - A) \text{ so } R_J = D^{-1}(D-A) = I - D^{-1}A$$

$$\text{So } \sum_i |R_J(j,i)|$$

$$= |1 - A(j,j)/A(j,j)| + \sum_{i \neq j} |A(j,i)|/|A(j,j)|$$
$$= (\sum_{i \neq j} |A(j,i)|) / |A(j,j)|$$

< 1 by strict row diagonal dominance
so $\|R_J\|_\infty < 1$ and Jacobi converges

The model problem is not strictly row diagonally dominant, since the diagonal equals the negative sum of the off diagonals in most rows. We call a matrix where

$$|A_{ii}| \geq \sum_{j \neq i} |A_{ij}|$$

in all rows, with strict inequality at least once, weakly row diagonally

dominant. This alone is not enough for convergence: consider

$$A = \begin{bmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \text{ and}$$

$$R = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \text{ whose powers do not converge.}$$

So we need one more condition:

Def: A matrix A is irreducible if there is no permutation P such that $P^*A^*P^T$ is block triangular. Equivalently, the (directed) graph corresponding to entries of A is "strongly connected", i.e. there is a path from every vertex to every other vertex.

The model problem satisfies this definition, since a mesh is strongly connected. And for the vertices next to a boundary of the mesh, $|A_{ii}| > \sum_{j \neq i} |A_{ij}|$, yielding

Thm 2: If A is weakly row diagonally dominant and irreducible (like the model problem) then $\rho(R_{GS}) < \rho(R_J) < 1$, so both Jacobi and GS converge, and GS is faster. (Thm 6.3 in text; see reference [249] in text for proof)

Now we come to SOR(w):

Thm 3: If A is spd, then SOR(w) converges if and only if $0 < w < 2$. In particular SOR(1) = GS converges. (see Thm 6.5 in text for proof)

The previous results describe the most general situations in which we can prove convergence of splitting methods.

To analyze the convergence of SOR(w) on the model problem we need to use another graph theoretic property of the matrix:

Def: A matrix has Property A if there is a permutation P such that $P^*A^*P^T = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$ has the property that A_{11} and A_{22} are diagonal. In graph theoretic terms, the vertices V of the graph can be broken into two disjoint sets $V = V_1 \cup V_2$, where there are no edges between pairs of vertices in V_1 , or between pairs of vertices in V_2 . Such a graph is called bipartite.

Ex: For a model problem on a 1D mesh, let the odd numbered nodes be V_1 and the even numbered be V_2 ; since there are only edges connecting even and odd nodes, the matrix has property A.

Ex: For a model problem on a 2D mesh, think of the vertices forming a checkerboard so they are either Red or Black. Then the edges only connect Red to Black, so the matrix has Property A. Another way to say this is to put vertices v_{ij} with $i+j$ odd in V_1 and $i+j$ even in V_2 . This works for the 3D model problem and in higher dimensions.

Thm 4: Suppose matrix A has Property A, and we do SOR(w) updating all the vertices in V_1 before all the vertices in V_2 . Then the eigenvalues μ of R_J and λ of $R_{SOR}(w)$ are related by

$$(*) \quad (\lambda + w - 1)^2 = \lambda w^2 \mu^2$$

In particular, if $w=1$, then $\lambda = \mu^2$, so $\rho(R_{SOR}(1)) = \rho(R_{GS}) = \rho(R_J)^2$, and GS converges twice as fast as Jacobi. (This appears as Thm 6.6 in the text.)

Proof: Assuming we number all vertices in V_1 before the vertices in V_2 , matrix A will look like $A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$ where A_{11} and A_{22} are diagonal, since property A tells us there are no edges connected vertices in V_1 to V_1 or V_2 to V_2 .

For Poisson this means $T = 4I + \begin{bmatrix} 0 & 0 \\ A_{21} & 0 \end{bmatrix} + \begin{bmatrix} 0 & A_{12} \\ 0 & 0 \end{bmatrix} = D - L' - U'$.

Now since λ is an eigenvalue of $R_{SOR}(w)$ we get

$$\begin{aligned} 0 &= \det(\lambda I - R_{SOR}(w)) \\ &= \det(\lambda I - (I - wL)^{-1}((1-w)I + wU)) \\ &= \det((I - wL) * \begin{pmatrix} \lambda I - (1-w)I - wU \\ (I - wL)^{-1} \end{pmatrix}) \\ &= \det(\lambda I - \lambda wL - (1-w)I - wU) \\ &= \det((\lambda - 1 + w)I - \lambda wL - wU) \\ &= \det(\sqrt{\lambda} w * \\ &\quad * [(\lambda - 1 + w)/(\sqrt{\lambda} w)I - \sqrt{\lambda}L - U/ \\ &\quad \sqrt{\lambda}]) \\ &= (\sqrt{\lambda} w)^n * \\ &\quad \det((\lambda - 1 + w)/(\sqrt{\lambda} w)I - \sqrt{\lambda}L - U/ \\ &\quad \sqrt{\lambda}) \end{aligned}$$

Because of the sparsity of L and U , we can let $D = \begin{bmatrix} I & 0 \\ 0 & I/\sqrt{\lambda} \end{bmatrix}$

and note that $D * (\sqrt{\lambda} L) * \text{inv}(D) = L$, and $D * (U/\sqrt{\lambda}) * \text{inv}(D) = U$.

so we can premultiply the matrix inside $\det(\)$ by D and postmultiply by $\text{inv}(D)$,

without changing the determinant, to get

$$\begin{aligned} 0 &= \det((\lambda - 1 + w)/(\sqrt{\lambda} w)I - L - U) \\ &= \det((\lambda - 1 + w)/(\sqrt{\lambda} w)I - R_J) \end{aligned}$$

i.e. $(\lambda - 1 + w)/(\sqrt{\lambda} w)$ is an eigenvalue μ of the Jacobi matrix R_J .

More generally, since we know all eigenvalues μ of R_J for the model problem, we

can use (*) to figure out all eigenvalues λ of $R_{SOR}(w)$, then
then pick w_{opt}
to minimize $\rho(R_{SOR}(w_{opt}))$. This yields

Thm 5: Suppose A has property A, we do SOR(w) updating vertices in V_1
before V_2 as
before, all eigenvalues of R_J are real, and $\mu = \rho(R_J) < 1$ (as in the
model problem).

Then

$$w_{opt} = 2/(1+\sqrt{1-\mu^2})$$

$$\rho(R_{SOR}(w_{opt})) = w_{opt} - 1 = \mu^2 / (1+\sqrt{1-\mu^2})^2$$

In particular, for the 2D model problem on an $n \times n$ grid

$$w_{opt} = 2/(1+\sin(\pi/(n+1))) \sim 2$$

$$\rho(R_{SOR}(w_{opt})) = \cos^2(\pi/(n+1))/(1+\sin(\pi/(n+1)))^2 \sim 1 -$$

$2\pi/(n+1)$

The proof follows by solving (*) for λ (see Thm 6.7 in the text).