Numerical Analysis - Part II

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Lecture 17

Iterative methods for linear algebraic systems

The general *iterative* method for solving Ax = b is a rule $\mathbf{x}^{k+1} = f_k(\mathbf{x}^0, \mathbf{x}^1, \dots, \mathbf{x}^k)$. We will consider the simplest ones: *linear*, *one-step*, *stationary* iterative schemes:

$$\mathbf{x}^{k+1} = H\mathbf{x}^k + \mathbf{v}, \qquad \mathbf{x}^0, \mathbf{v} \in \mathbb{R}^n.$$
 (1)

Here one chooses H and v so that x^* , a solution of $A\mathbf{x} = \mathbf{b}$, satisfies $\mathbf{x}^* = H\mathbf{x}^* + \mathbf{v}$, i.e. it is the fixed point of the iteration (1) (if the scheme converges). Standard terminology:

the iteration matrix H, the error $\mathbf{e}^k := \mathbf{x}^* - \mathbf{x}^k$, the residual $\mathbf{r}^k := A\mathbf{e}^k$

For a given class of matrices A (e.g. positive definite matrices, or even a single particular matrix), we are interested in *convergent* methods, i.e. the methods such that $\mathbf{x}^k \to \mathbf{x}^* = A^{-1}\mathbf{b}$ for every starting value \mathbf{x}^0 . Subtracting $\mathbf{x}^* = H\mathbf{x}^* + \mathbf{v}$ from (1) we obtain

$$\mathbf{e}^{k+1} = H\mathbf{e}^k = \dots = H^{k+1}\mathbf{e}^0,\tag{2}$$

i.e., a method is convergent if $\mathbf{e}^k = H^k \mathbf{e}^0 \to 0$ for any $\mathbf{e}^0 \in \mathbb{R}^n$. (Iterative refinement). This is the scheme

$$\mathbf{x}^{k+1} = \mathbf{x}^k - S(A\mathbf{x}^k - \mathbf{b}).$$

If $S = A^{-1}$, then $\mathbf{x}^{k+1} = A^{-1}\mathbf{b} = \mathbf{x}^*$, so it is suggestive to choose S as an approximation to A^{-1} . The iteration matrix for this scheme is $H_S = I - SA$.

Solving linear systems – Splitting

(Splitting). This is the scheme

$$(A-B)\mathbf{x}^{k+1}=-B\mathbf{x}^k+\mathbf{b}\,,$$

with the iteration matrix $H = -(A - B)^{-1}B$. Any splitting can be viewed as an iterative refinement (and vice versa) because

$$(A - B)\mathbf{x}^{k+1} = -B\mathbf{x}^k + \mathbf{b} \quad \Leftrightarrow \quad (A - B)\mathbf{x}^{k+1} = (A - B)\mathbf{x}^k - (A\mathbf{x}^k - \mathbf{b})^k$$
$$\Leftrightarrow \quad \mathbf{x}^{k+1} = \mathbf{x}^k - (A - B)^{-1}(A\mathbf{x}^k - \mathbf{b}),$$

so we should seek a splitting such that $S = (A - B)^{-1}$ approximates A^{-1} .

Theorem 1 Let $H \in \mathbb{R}^{n \times n}$. Then $\lim_{k \to \infty} H^k \mathbf{z} = 0$ for any $\mathbf{z} \in \mathbb{R}^n$ if and only if $\rho(H) < 1$.

Proof. 1) Let λ be an eigenvalue of (the real) H, real or complex, such that $|\lambda| = \rho(H) \ge 1$, and let **w** be a corresponding eigenvector, i.e., $H\mathbf{w} = \lambda \mathbf{w}$. Then $H^k \mathbf{w} = \lambda^k \mathbf{w}$, and

$$\|H^{k}\mathbf{w}\|_{\infty} = |\lambda|^{k}\|\mathbf{w}\|_{\infty} \ge \|\mathbf{w}\|_{\infty} =: \gamma > 0.$$
(3)

If **w** is real, we choose $\mathbf{z} = w$, hence $\|H^k \mathbf{z}\|_{\infty} \ge \gamma$, and this cannot tend to zero.

If **w** is complex, then $\mathbf{w} = \mathbf{u} + i\mathbf{v}$ with some real vectors \mathbf{u}, \mathbf{v} . But then at least one of the sequences $(H^k \mathbf{u}), (H^k \mathbf{v})$ does not tend to zero. For if both do, then also $H^k \mathbf{w} = H^k \mathbf{u} + iH^k \mathbf{v} \to 0$, and this contradicts (3).

Proof. Cont. 2) Now, let $\rho(H) < 1$, and assume for simplicity that H possesses n linearly independent eigenvectors (\mathbf{w}_j) such that $H\mathbf{w}_j = \lambda_j \mathbf{w}_j$. Linear independence means that every $\mathbf{z} \in \mathbb{R}^n$ can be expressed as a linear combination of the eigenvectors, i.e., there exist $(c_j) \in \mathbb{C}$ such that $\mathbf{z} = \sum_{j=1}^n c_j \mathbf{w}_j$. Thus,

$$H^k \mathbf{z} = \sum_{j=1}^n c_j \lambda_j^k \mathbf{w}_j$$
,

and since $|\lambda_j| \leq \rho(H) < 1$ we have $\lim_{k \to \infty} H^k \mathbf{z} = 0$, as required. \Box

Remark 2 (Non-examinable)

The complete proof of case (2) of Theorem 1 exploits the so-called Jordan normal form of the matrix H, namely $H = SJS^{-1}$, where J is a block diagonal matrix consisting of the Jordan blocks,



To prove that $J_i^k \to 0$ if $|\lambda_i| < 1$ one should split $J_i = \lambda_i I + P$, notice that $P^m = 0$ for $m \ge n_i$, and evaluate the terms of the expansion $(\lambda_i I + P)^k = \sum_{m=0}^{n_i-1} {k \choose m} \lambda_i^{k-m} P^m$.

Solving linear systems – Convergence

Applying Theorem 1 to the error estimate (2), we arrive at the following statement.

Theorem 3

Let \mathbf{x}^* , a solution of $A\mathbf{x} = \mathbf{b}$, satisfy $\mathbf{x}^* = H\mathbf{x}^* + \mathbf{v}$ and we are given the scheme

$$\mathbf{x}^{k+1} = H\mathbf{x}^k + \mathbf{v}, \qquad \mathbf{x}^0, \mathbf{v} \in \mathbb{R}^n.$$
 (4)

Then $\mathbf{x}^k \to \mathbf{x}^*$ for any choice of \mathbf{x}^0 if and only if $\rho(H) < 1$.

Note: Of course, we would like to know not just convergence but the rate of it. For example, we achieve convergence with

$$H = \left[\begin{array}{cc} 0.99 & 10^6 \\ 0 & 0.99 \end{array} \right],$$

but it will take quite a long time. We will discuss this topic briefly later on.

Both of these methods are versions of splitting which can be applied to any A with nonzero diagonal elements. We write A as the sum of three matrices $L_0 + D + U_0$: subdiagonal (strictly lower-triangular), diagonal and superdiagonal (strictly upper-triangular) portions of A, respectively. 1) Jacobi method. We set A - B = D, the diagonal part of A, and we obtain the next iteration by solving the diagonal system

$$D\mathbf{x}^{(k+1)} = -(L_0 + U_0)\mathbf{x}^{(k)} + \mathbf{b}, \qquad H_{\mathrm{J}} = -D^{-1}(L_0 + U_0).$$

2) Gauss-Seidel method. We take $A - B = L_0 + D = L$, the lower-triangular part of A, and we generate the sequence $(\mathbf{x}^{(k)})$ by solving the triangular system

$$(L_0 + D) \mathbf{x}^{(k+1)} = -U_0 \mathbf{x}^{(k)} + \mathbf{b}, \qquad H_{GS} = -(L_0 + D)^{-1} U_0.$$

There is no need to invert $(L_0 + D)$, we calculate the components of $\mathbf{x}^{(k+1)}$ in sequence by forward substitution:

$$a_{ii}x_i^{(k+1)} = -\sum_{j < i} a_{ij}x_j^{(k+1)} - \sum_{j > i} a_{ij}x_j^{(k)} + b_i, \qquad i = 1..n.$$

As we mentioned above, the sequence $\mathbf{x}^{(k)}$ converges to the solution of $A\mathbf{x} = \mathbf{b}$ if the spectral radius of the iteration matrix,

$$H_{
m J}=-D^{-1}(L_0+U_0) ext{ or } H_{
m GS}=-(L_0+D)^{-1}U_0,$$

respectively, is less than one. Our next goal is to prove that this is the case for two important classes of matrices A:

a) diagonally dominant and b) positive definite matrices.

We start with recalling the simple, but very useful Gershgorin theorem.

All eigenvalues of an $n \times n$ matrix A are contained in the union of the Gershgorin discs in the complex plane:

$$\sigma(A) \subset \cup_{i=1}^n \Gamma_i, \quad \Gamma_i := \{ z \in \mathbb{C} : |z - a_{ii}| \le r_i \}, \quad r_i := \sum_{j \ne i} |a_{ij}|.$$

Definition 4 (Strictly diagonally dominant matrices)

A matrix A is called strictly diagonally dominant by rows (resp. by columns) if

$$|\mathbf{a}_{ii}| > \sum_{j \neq i} |\mathbf{a}_{ij}|, \quad i = 1..n$$
 (resp. $|\mathbf{a}_{jj}| > \sum_{i \neq j} |\mathbf{a}_{ij}|, \quad j = 1..n$).

From Gershgorin theorem, it follows that strictly diagonally dominant matrices are nonsingular.

Convergence of iterations

Theorem 5

If A is strictly diagonally dominant, then both the Jacobi and the Gauss-Seidel methods converge.

Proof. For the Gauss-Seidel method, the eigenvalues of the iteration matrix $H_{\rm GS} = -(L_0 + D)^{-1}U_0$ satisfy the equation

$$\det[H_{\mathrm{GS}} - \lambda I] = \det[-(L_0 + D)^{-1}U_0 - \lambda I] = 0.$$

Moreover,

$$\det[-(L_0+D)^{-1}U_0-\lambda I]=0 \ \Rightarrow \ \det[A_\lambda]:=\det[U_0+\lambda D+\lambda L_0]=0.$$

It is easy to see that if $A = L_0 + D + U_0$ is strictly diagonally dominant, then for $|\lambda| \ge 1$ the matrix $A_{\lambda} = \lambda L_0 + \lambda D + U_0$ is strictly diagonally dominant too, hence it is nonsingular, and therefore the equality det $[A_{\lambda}] = 0$ is impossible. Thus $|\lambda| < 1$, hence convergence. The proof for the Jacobi method is the same. \Box

Theorem 6 (The Householder–John theorem)

If A and B are real matrices such that both A and $A-B-B^{T}$ are symmetric positive definite, then the spectral radius of $H = -(A - B)^{-1}B$ is strictly less than one.

Proof. Let λ be an eigenvalue of H, so $H\mathbf{w} = \lambda \mathbf{w}$ holds, where $\mathbf{w} \neq \mathbf{0}$ is an eigenvector. (Note that both λ and \mathbf{w} may have nonzero imaginary parts when H is not symmetric, e.g. in the Gauss-Seidel method.) The definition of H provides equality $-B\mathbf{w} = \lambda(A - B)\mathbf{w}$, and we note that $\lambda \neq 1$ since otherwise A would be singular (which it is not). Thus, we deduce

$$\overline{\mathbf{w}}^{\mathsf{T}} B \mathbf{w} = \frac{\lambda}{\lambda - 1} \overline{\mathbf{w}}^{\mathsf{T}} A \mathbf{w}, \tag{5}$$

where the bar means complex conjugation.

The Householder–John theorem

Proof. Cont. Moreover, writing $\mathbf{w} = \mathbf{u} + i\mathbf{v}$, where \mathbf{u} and \mathbf{v} are real, we find (for $C = C^T$) the identity $\overline{\mathbf{w}}^T C \mathbf{w} = \mathbf{u}^T C \mathbf{u} + \mathbf{v}^T C \mathbf{v}$, so symmetric positive definiteness in the assumption implies $\overline{\mathbf{w}}^T A \mathbf{w} > 0$ and $\overline{\mathbf{w}}^T (A - B - B^T) \mathbf{w} > 0$. In the latter inequality, we use relation (5) and its conjugate transpose to obtain

$$0 < \overline{\mathbf{w}}^T A \mathbf{w} - \overline{\mathbf{w}}^T B \mathbf{w} - \overline{\mathbf{w}}^T B^T \mathbf{w} = \left(1 - \frac{\lambda}{\lambda - 1} - \frac{\overline{\lambda}}{\overline{\lambda} - 1}\right) \overline{\mathbf{w}}^T A \mathbf{w}$$
$$= \frac{1 - |\lambda|^2}{|\lambda - 1|^2} \overline{\mathbf{w}}^T A \mathbf{w}.$$

Now $\lambda \neq 1$ implies $|\lambda - 1|^2 > 0$. Hence, recalling that $\overline{\mathbf{w}}^T A \mathbf{w} > 0$, we see that $1 - |\lambda|^2$ is positive. Therefore $|\lambda| < 1$ occurs for every eigenvalue of H as required.

Corollary 7

- 1) If A is symmetric positive definite, then the Gauss-Seidel method converges.
- 2) If both A and 2D-A are symmetric positive definite, then the Jacobi method converges.

Proof. 1) For the Gauss-Seidel method, we take $A - B = L_0 + D$, thus $B = U_0$ is the superdiagonal part of symmetric A, hence $A - B - B^T$ is equal to D, the diagonal part of A, and if A is positive definite, then D is positive definite too (this is the first part of the Exercise 23 from Example Sheets). 2) For the Jacobi method, we have B = A - D, and if A is symmetric, then $A - B - B^T = 2D - A$. (The latter matrix is the same as A except that the signs of the off-diagonal elements are reversed.) As we have seen in the previous sections linear systems $A\mathbf{x} = \mathbf{b}$, where A is a real symmetric positive (negative) definite matrix, frequently occur in numerical methods for solving elliptic partial differential equations.

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A typical example we already encountered is Poisson's equation on a square where the *five-point formula* approximation yields an $n \times n$ system of linear equations with $n = m^2$ unknowns $u_{p,q}$:

$$u_{p-1,q} + u_{p+1,q} + u_{p,q-1} + u_{p,q+1} - 4u_{p,q} = h^2 f(ph,qh)$$
(6)

In the *natural ordering*, when the grid points are arranged by columns, A is the following block tridiagonal matrix:

$$A = \begin{bmatrix} B & I & & \\ I & B & I & \\ & \ddots & \ddots & \ddots & \\ & I & B & I \\ & & & I & B \end{bmatrix}, \qquad B = \begin{bmatrix} -4 & 1 & & \\ 1 & -4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -4 & 1 \\ & & & 1 & -4 \end{bmatrix}.$$
(7)

Lemma 8

For any ordering of the grid points, the matrix A of the system (6) is symmetric and negative definite.

Proof II

Proof. Let *U* be any linear operator changing the grid ordering. Then *U* is clearly unitary $(||Ux||_2 = ||x||_2 \text{ for any } x)$. Note that any matrix \tilde{A} representing the the system of equations (6) can be written as $\tilde{A} = UAU^*$ for some unitary matrix *U*, where *A* is as in (7). Self-adjointness is preserved by unitary operators, and so is the spectrum. Thus, \tilde{A} is self-adjoint (symmetric as it is real). Moreover, $\sigma(A)$ does not intersect the positive half plane by the Gershgorin theorem, so we only need to show that $0 \notin \sigma(A)$. If Ax = 0 then, by the definition of *A*, *x* must have elements of equal modulus, however, then the definition of *B* (that gives *A*) implies that x = 0.

Note that when p or q is equal to 1 or m, then the values $u_{0,q}$, $u_{p,0}$ or $u_{p,m+1}$, $u_{m+1,q}$ are known boundary values and they should be moved to the right-hand side, thus leaving fewer unknowns on the left.

For any ordering of the grid points (ph, qh) we have shown in Lemma 8 that the matrix A of this linear system is symmetric and negative definite.

Corollary 9

For the linear system (6), for any ordering of the grid, both Jacobi and Gauss-Seidel methods converge.

Proof. By Lemma 8, *A* is symmetric and negative definite, hence convergence of Gauss-Seidel. To prove convergence of the Jacobi method, we need negative definiteness of the matrix 2D - A, and that follows by the same arguments as in Lemma 8: recall that the proof operates with the modulus of the off-diagonal elements and does not depend on their sign.

It is often possible to improve the efficiency of the splitting method by *relaxation*. Specifically, instead of letting $(A - B)\mathbf{x}^{(k+1)} = -B\mathbf{x}^{(k)} + \mathbf{b}$, we let

 $(A-B)\widehat{\mathbf{x}}^{(k+1)} = -B\mathbf{x}^{(k)} + \mathbf{b}$, and then $\mathbf{x}^{(k+1)} = \omega \widehat{\mathbf{x}}^{(k+1)} + (1-\omega)\mathbf{x}^{(k)}$

where ω is a real constant called the *relaxation parameter*.

Note that $\omega = 1$ corresponds to the standard "unrelaxed" iteration. Good choice of ω leads to a smaller spectral radius of the iteration matrix (compared with the "unrelaxed" method), and the smaller the spectral radius, the faster the iteration converges.

Relaxation

To this end, let us express the relaxation iteration matrix H_{ω} in terms of $H = -(A - B)^{-1}B$. We have

$$\widehat{\mathbf{x}}^{(k+1)} = H\mathbf{x}^{(k)} + \mathbf{v} \quad \Rightarrow \quad \begin{aligned} \mathbf{x}^{(k+1)} &= \omega \widehat{\mathbf{x}}^{(k+1)} + (1-\omega)\mathbf{x}^{(k)} \\ &= \omega H\mathbf{x}^{(k)} + (1-\omega)\mathbf{x}^{(k)} + \omega \mathbf{v}, \end{aligned}$$

hence

$$H_{\omega} = \omega H + (1 - \omega)I.$$

It follows that the spectra of H_{ω} and H are related by the rule $\lambda_{\omega} = \omega \lambda + (1 - \omega)$, therefore one may try to choose $\omega \in \mathbb{R}$ to minimize

$$\rho(H_{\omega}) = \max \{ |\omega\lambda + (1-\omega)| : \lambda \in \sigma(H) \}.$$

In general, $\sigma(H)$ is unknown, but often we have some information about it which can be utilized to find a "good" (rather than "best") value of ω . For example, suppose that it is known that $\sigma(H)$ is real and resides in the interval $[\alpha, \beta]$ where $-1 < \alpha < \beta < 1$. In that case we seek ω to minimize

$$\max \left\{ \left| \omega \lambda + (1 - \omega) \right| : \lambda \in [\alpha, \beta] \right\}.$$

It is readily seen that, for a fixed $\lambda < 1$, the function $f(\omega) = \omega \lambda + (1 - \omega)$ is decreasing, therefore, as ω increases (decreases) from 1 the spectrum of H_{ω} moves to the left (to the right) of the spectrum of H. It is clear that the optimal location of the spectrum $\sigma(H_{\omega})$ (or of the interval $[\alpha_{\omega}, \beta_{\omega}]$ that contains $\sigma(H_{\omega})$) is the one which is centralized around the origin:

The speed of convergence of some iterative methods (Jacobi with relaxation, Gauss–Seidel, etc.) can be increased drastically within the context of solving linear equations that originate in the discretization of PDEs. Herewith we analyse (with a great deal of hand-waving) the system $A\mathbf{u} = \mathbf{b}$ originated from the 5-point formula for the Poisson equation on an $m \times m$ square grid Ω_h , being solved by the *damped* Jacobi iteration.

The damped Jacobi iteration

This is the Jacobi method with a relaxation parameter ω :

$$\widehat{\mathbf{u}}^{(\nu+1)} = -D^{-1}(A-D)\mathbf{u}^{(\nu)} + D^{-1}\mathbf{b} = (I-D^{-1}A)\mathbf{u}^{(\nu)} + D^{-1}\mathbf{b} \mathbf{u}^{(\nu+1)} = \omega \widehat{\mathbf{u}}^{(\nu+1)} + (1-\omega)\mathbf{u}^{(\nu)} = (I-\omega D^{-1}A)\mathbf{u}^{(\nu)} + \omega D^{-1}\mathbf{b} .$$

The error decay is expressed in terms of the iteration matrix H_{ω} :

$$\mathbf{e}^{(\nu)} = [H_\omega]^{
u} \mathbf{e}^{(0)}, \qquad H_\omega = I - \omega D^{-1} A = I + \frac{1}{4} \omega A,$$

and it follows from the results of Lecture 2 that the eigenvectors and the eigenvalues of H_{ω} are

$$\mathbf{w}^{k,\ell} = (\sin ix \sin jy), \qquad \lambda_{k,\ell}(\omega) = 1 - \omega \left(\sin^2 \frac{x}{2} + \sin^2 \frac{y}{2}\right),$$
$$x = \frac{k\pi}{m+1}, \quad y = \frac{\ell\pi}{m+1}.$$

We see that $\rho(H_{\omega}) < 1$ for any ω in (0, 1], guaranteeing convergence, although a very slow one. In particular, for the "pure" Jacobi iteration (with $\omega = 1$) we have $\rho(H_J) = 1 - 2\sin^2 \frac{\pi}{2(m+1)} \approx 1 - \frac{\pi^2}{2m^2}$, and for $\omega < 1$ the spectral radius is even closer to 1.

The damped Jacobi iteration

However, expanding the error with respect to the (orthogonal) eigenvectors we obtain

$$\mathbf{e}^{(\nu)} = \sum_{k,\ell} a_{k,\ell}^{(\nu)} \mathbf{w}^{k,\ell}, \quad \mathbf{e}^{(\nu)} = [H_{\omega}]^{\nu} \mathbf{e}^{(0)} \quad \Rightarrow \quad |a_{k,\ell}^{(\nu)}| = |\lambda_{k,\ell}(\omega)|^{\nu} |a_{k,\ell}^{(0)}|,$$

i.e. the components of $\mathbf{e}^{(\nu)}$ (with respect to the basis of eigenvectors) decay at a different rate for different frequences (k, ℓ) . To this end, we define

 Ω_h -low frequences (LF):

$$\mathbf{w}^{(k,\ell)} = (\sin \pi k \phi \sin \pi \ell \psi) \big|_{\Omega_h}$$
 with both k and ℓ from $[1, \frac{m+1}{2})$,

 Ω_h -high frequences (HF):

$$\mathbf{w}^{(k,\ell)} = (\sin \pi k \phi \sin \pi \ell \psi) \big|_{\Omega_h}$$
 with either k or ℓ from $[\frac{m+1}{2}, m]$.

Let us determine the least factor $\mu(\omega)$ by which the amplitudes of HF components are damped per iteration. We have

$$\begin{split} \mu(\omega) &= \max \left\{ \left| \lambda_{k,\ell}(\omega) \right| : \quad \frac{m+1}{2} \le k \le m, \quad 1 \le \ell \le m \right\} \\ &= \max \left\{ \left| 1 - \omega \left(\sin^2 \frac{x}{2} + \sin^2 \frac{y}{2} \right) \right| : \quad \frac{\pi}{2} \le x \le \pi, \quad 0 \le y \le \pi \right\} \\ &= \max \left\{ \left| 1 - \frac{1}{2} \omega \right|, |1 - 2\omega| \right\}, \end{split}$$

and it is seen that the optimal factor μ_* is attained when $1 - \frac{1}{2}\omega = -(1 - 2\omega)$, i.e. for $\omega_* = \frac{4}{5}$, and its value is $\mu_* = \frac{3}{5}$.

Therefore, for the coefficients at the HF components of $\mathbf{e}^{(\nu)}$ we obtain

$$|a_{k,\ell}^{(
u)}| \leq |\mu_*|^
u |a_{k,\ell}^{(0)}| = \left(rac{3}{5}
ight)^
u |a_{k,\ell}^{(0)}| \ll |a_{k,\ell}^{(0)}|\,,$$

i.e. the damped Jacobi method converges fast for high frequencies. For the remaining Ω_h -low frequences we notice that

$$k, \ell \in [1, \frac{m+1}{2}) = [1, \frac{1}{2h}) \implies \\ \{ \mathbf{w}_{h}^{(k,\ell)} = (\sin \pi k\phi \sin \pi \ell \psi) \big|_{\Omega_{h}} \} \approx \{ \mathbf{w}_{2h}^{(k,\ell)} = (\sin \pi k\phi \sin \pi \ell \psi) \big|_{\Omega_{2h}} \} \\ \overbrace{\Omega_{h}\text{-low frequences}}$$