

Lecture Note 3: Stationary Iterative Methods

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1 Stationary Iterative Methods

The Gaussian elimination (or in general most direct methods) requires $O(n^3)$ computational cost, which is not acceptable when n is large. For example, let us consider the direct numerical simulation of the Navier-Stokes equation on a unit cube in 3D; we discretize the domain with N^3 cubes and compute the solutions up to $t = T$. The Navier-Stokes equation has five variables at each node, hence the solution vector is $\mathbf{u} \in \mathbb{R}^{5N^3}$. When an implicit/explicit (IMEX) method is used for the time-integration, the time step size scales with $1/N$ and the total number of time steps is $O(N)$. For each time step, there is a nonlinear equation to solve:

$$\mathbf{f}(\mathbf{u}^{n+1}) = \mathbf{g}(\mathbf{u}^n),$$

to update the solution from one time step ($\mathbf{u}^n$) to the next ($\mathbf{u}^{n+1}$). Let K be the average number of iterations in the Newton method to solve this nonlinear system, in total we need to solve a linear system $O(KN)$ times, and each such linear system is of the size $5N^3 \times 5N^3$. If a direct method is used for the linear solves, the total computational cost is:

$$O((5N^3)^3) \times O(KN) = O(KN^{10}),$$

which is prohibitive even for moderate value of N .

The target of stationary iterative methods¹ is to reduce the computational cost with linear solves to magnitudes smaller than $O(n^3)$. Particularly in solving $A\mathbf{x} = \mathbf{b}$, let us write $A = M + (A - M)$ for some matrix M and the linear system as:

$$M\mathbf{x} = -(A - M)\mathbf{x} + \mathbf{b}. \quad (1.1)$$

In an iterative method, we start with an initial guess $\mathbf{x}_0$ and try to improve the result solving for $\mathbf{x}_{k+1}$, $k = 0, 1, \dots$:

$$M\mathbf{x}_{k+1} = -(A - M)\mathbf{x}_k + \mathbf{b}, \quad \text{or equivalently} \quad \mathbf{x}_{k+1} = -M^{-1}(A - M)\mathbf{x}_k + M^{-1}\mathbf{b}. \quad (1.2)$$

Let's look at the last equation, clearly a requirement for the iterative method to make sense is that the linear system associated with M should be easy to solve in the sense that the cost is no more than $O(n^2)$. Two such choices are diagonal matrices ($\sim O(n)$) and triangular matrices ($\sim O(n^2)$). Next, we also want to make sure that if there exists a solution $\mathbf{x}$, then $\mathbf{x}_k \rightarrow \mathbf{x}$ as $k \rightarrow +\infty$. Finally, providing that $\mathbf{x}_k \rightarrow \mathbf{x}$, we hope $\|\mathbf{x}_k - \mathbf{x}\|$ to be reasonably small for only a few number of iterations. These are the questions we'd like to answer for any iterative method in this lecture.

¹Or simply "iterative methods" in this section.

Let A be non-singular and $\mathbf{x}$ solves $A\mathbf{x}=\mathbf{b}$, we first look at the convergence. Define $\boldsymbol{\varepsilon}_k = \mathbf{x}_k - \mathbf{x}$ as the error vector in the k -th iteration, then:

$$M\boldsymbol{\varepsilon}_{k+1} = M(\mathbf{x}_{k+1} - \mathbf{x}) = [-(A-M)\mathbf{x}_k + \mathbf{b}] - [-(A-M)\mathbf{x} + \mathbf{b}] = -(A-M)\boldsymbol{\varepsilon}_k,$$

or equivalently:

$$\boldsymbol{\varepsilon}_{k+1} = G\boldsymbol{\varepsilon}_k, \quad G = -M^{-1}(A-M). \quad (1.3)$$

The growth matrix G remains the same for all iterations (hence the name “stationary iterative methods”), thus we obtain an estimate on the error $\boldsymbol{\varepsilon}_k$:

$$\boldsymbol{\varepsilon}_k = G^k \boldsymbol{\varepsilon}_0 \implies \|\boldsymbol{\varepsilon}_k\| \leq \|G^k\| \|\boldsymbol{\varepsilon}_0\|. \quad (1.4)$$

Thus we have $\boldsymbol{\varepsilon}_k \rightarrow 0$ for any $\boldsymbol{\varepsilon}_0$ if $G^k \rightarrow 0$ when $k \rightarrow \infty$, for which a sufficient and necessary condition is given by Theorem 1.1.

Remark 1. *Strictly speaking, we do not need $G^k \rightarrow 0$ to deduce $\boldsymbol{\varepsilon}_k$ if we can choose $\boldsymbol{\varepsilon}_0$ carefully. In an extreme case if $\boldsymbol{\varepsilon}_0$ is in the null space of some G^{k_0} (which happens with $k_0 = 1$ in the foolish case when $M = A$), the error becomes zero after k_0 iterations.*

Theorem 1.1. $G^k \rightarrow 0$ as $k \rightarrow \infty$ if and only if $\rho(G) < 1$, where the spectral radius $\rho(G)$ is the maximum absolute value of all the eigenvalues of G .

Proof. We consider the Jordan canonical form $G = QJQ^{-1}$, where Q is invertible and J is given by:

$$J = \begin{bmatrix} J_1 & & \\ & J_2 & \\ & & \ddots \\ & & & J_m \end{bmatrix}_{n \times n}, \quad J_l = \begin{bmatrix} \lambda_l & 1 & & \\ & \lambda_l & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_l \end{bmatrix}_{n_l \times n_l} \quad . \quad l = 1, \dots, m \quad (1.5)$$

Here $\lambda_1, \dots, \lambda_m$ are the eigenvalues of G , which may not be different from each other; and $n_1 + \dots + n_m = n$.

To this end $G^k = QJ^kQ^{-1}$ and we just need to show $J^k \rightarrow 0$ if and only if $\rho(G) < 1$ or equivalently $|\lambda_l| < 1$ for all l . Because $J^k = \text{diag}(J_1^k, J_2^k, \dots, J_m^k)$, we only need to show $J_l^k \rightarrow 0$ if and only if $|\lambda_l| < 1$. The last point is straightforward as:

$$J_l^k = \begin{bmatrix} \binom{k}{k} \lambda_l^k & \binom{k}{k-1} \lambda_l^{k-1} & \binom{k}{k-2} \lambda_l^{k-2} & \dots & \binom{k}{k-n_l+1} \lambda_l^{k-n_l+1} \\ & \binom{k}{k-1} \lambda_l^k & \binom{k}{k-1} \lambda_l^{k-1} & \dots & \binom{k}{k-n_l} \lambda_l^{k-n_l} \\ & & \binom{k}{k} \lambda_l^k & \dots & \binom{k}{k-n_l-1} \lambda_l^{k-n_l-1} \\ & & & \ddots & \vdots \\ & & & & \binom{k}{k} \lambda_l^k \end{bmatrix}_{n_l \times n_l}, \quad (1.6)$$

and the fact that each entry converges to zero as $k \rightarrow \infty$. $\square$

In fact, if $G = -M^{-1}(A-M)$ has spectral radius smaller than 1, we can drop the assumption that A is non-singular (it remains true, though), as stated by the next theorem.

Theorem 1.2. *If $\rho(G) < 1$, then A is invertible.*

Proof. Because $A = M(I - G)$, we just need to show that $I - G$ is invertible for the first part. Indeed, if $(I - G)\mathbf{x} = 0$ for some vector $\mathbf{x} \in \mathbb{R}^n$, then

$$\mathbf{x} = I\mathbf{x} = G\mathbf{x} = G^2\mathbf{x} = \dots = G^k\mathbf{x} \rightarrow 0$$

by Theorem 1.1; hence the null space of $I - G$ contains only the zero vector and $I - G$ is invertible. $\square$

The condition of the preceding theorem is in general very difficult to check; and a more convenient one is based on the inequality $\|G^k\| \leq \|G\|^k$. Hence a necessary condition is given by $\|G\| < 1$ for some induced matrix norm.

2 Jacobi Method

A simplest iterative method is given by choosing M as the diagonal part of A , this is called the *Jacobi method*. Let $A = L + D + U$, where L , D , and U are the lower-tridiagonal part, diagonal part, and upper-tridiagonal part, respectively (not to be confused with the LU or LDU decomposition!). Then in the Jacobi method, $M = D$ and (1.2) reduces to:

$$\mathbf{x}_{k+1} = -D^{-1}(L + U)\mathbf{x}_k + D^{-1}\mathbf{b}. \quad (2.1)$$

The growth matrix $G = -D^{-1}(L + U)$ is:

$$G = - \begin{bmatrix} \frac{1}{a_{11}} & & & \\ & \frac{1}{a_{22}} & & \\ & & \ddots & \\ & & & \frac{1}{a_{nn}} \end{bmatrix} \begin{bmatrix} 0 & a_{12} & \dots & a_{1n} \\ a_{21} & 0 & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & 0 \end{bmatrix} = - \begin{bmatrix} 0 & \frac{a_{12}}{a_{11}} & \dots & \frac{a_{1n}}{a_{11}} \\ \frac{a_{21}}{a_{22}} & 0 & \dots & \frac{a_{2n}}{a_{22}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{a_{n1}}{a_{nn}} & \frac{a_{n2}}{a_{nn}} & \dots & 0 \end{bmatrix}. \quad (2.2)$$

If the diagonal elements of A are sufficiently large, say:

$$|a_{ii}| > \sum_{j \neq i} |a_{ij}|, \quad \forall i = 1, 2, \dots, n, \quad (2.3)$$

then we have $\|G\|_\infty < 1$. By the argument at the end of Section 1, we see that the Jacobi method converges if A is *diagonally dominant*, i.e., if A satisfies (2.3).

(2.3) actually provides a way to estimate the number of iterations needed in order to achieve certain accuracy. Let:

$$\rho_{\text{jac}} = \max_i \frac{\sum_{j \neq i} |a_{ij}|}{|a_{ii}|} < 1, \quad (2.4)$$

then by (1.4) $\|\epsilon_k\|_\infty \leq \rho_{\text{jac}}^k \|\epsilon_0\|_\infty$.

To see an example of diagonal-dominate linear systems, we consider the implicit method to solve the system of ordinary differential equations:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}).$$

Let $\mathbf{x}_m$ and $\mathbf{x}_{m+1}$ be the solutions at t_m and $t_{m+1} = t_m + \Delta t_m$, respectively; then we update the solution from $\mathbf{x}_m$ to $\mathbf{x}_{m+1}$ by:

$$\frac{\mathbf{x}_{m+1} - \mathbf{x}_m}{\Delta t_m} = \mathbf{f}(\mathbf{x}_m) + \frac{\partial \mathbf{f}(\mathbf{x}_m)}{\partial \mathbf{x}} (\mathbf{x}_{m+1} - \mathbf{x}_m),$$

which involves the linear system with $A_m = I + \Delta t_m \frac{\partial \mathbf{f}(\mathbf{x}_m)}{\partial \mathbf{x}}$. Thus we can always find a diagonal-dominant matrix A_m by choosing a small Δt_m .

3 Gauss-Seidel Method

The Jacobi method can be written component-by-component as:

$$\text{for } i = 1, 2, \dots, n : \quad (3.1)$$

$$x_{k+1;i} = \frac{1}{a_{ii}} \left(- \sum_{j \neq i} a_{ij} x_{k;j} + b_j \right).$$

Here we denote $\mathbf{x}_k = [x_{k;i}]$. One argument about the Jacobi method is that we're not using the most updated information in the solution, i.e. it is always the components of $\mathbf{x}_k$ that appear on the right hand side of the updating formula.

A modification that always use the most recent data and saves some storage is the following:

$$\text{for } i = 1, 2, \dots, n : \quad (3.2)$$

$$x_{k+1;i} = \frac{1}{a_{ii}} \left(- \sum_{j < i} a_{ij} x_{k+1;j} - \sum_{j > i} a_{ij} x_{k;j} + b_j \right).$$

This algorithm is known as the *Gauss-Seidel method*; and it is equivalent to the choice $M = D + L$:

$$\mathbf{x}_{k+1} = -(D + L)^{-1} (U \mathbf{x}_k - \mathbf{b}). \quad (3.3)$$

The Gauss-Seidel method also guarantees convergence for arbitrary initial data for diagonally dominant matrices. Particularly, similar to (2.4) we can derive a decay rate:

$$\rho_{\text{gs}} = \max_i \frac{\sum_{j > i} |a_{ij}|}{|a_{ii}| - \sum_{j < i} |a_{ij}|}. \quad (3.4)$$

We prove in the exercises $\|-(D + L)^{-1}U\|_{\infty} \leq \rho_{\text{gs}}$ and hence deduce that $\|\boldsymbol{\epsilon}_k\|_{\infty} \leq \rho_{\text{gs}}^k \|\boldsymbol{\epsilon}_0\|_{\infty}$. Comparing (2.4) and (3.4) we see for the same diagonally dominant matrix A , $\rho_{\text{gs}} \leq \rho_{\text{jac}}$; hence the Gauss-Seidel method in general converges faster than the Jacobi method, at the cost of solving a triangular system instead of a diagonal one at each iteration.

Because solving the linear system $L + D$ involves forward substitution, the method described before is also called the *forward Gauss-Seidel method*. Similarly, we can choose $M = D + U$ and establishing similar convergent result for diagonally dominant matrices; and this method is called the *backward Gauss-Seidel method*.

Finally, we show the convergence of the forward Gauss-Seidel method for another type of very important matrices, namely the symmetric positive-definite ones. This is a direct result of the following theorem and Theorem 1.1.

Theorem 3.1. *Let A be symmetric positive-definite, then $G = -(L+D)^{-1}L^t$ satisfies $\rho(G) < 1$.*

Proof. Clearly D has all its diagonal entries positive and it is non-singular; thus we may write:

$$-G = [D^{\frac{1}{2}}(D^{-\frac{1}{2}}LD^{-\frac{1}{2}} + I)D^{\frac{1}{2}}]^{-1}L^t = D^{-\frac{1}{2}}(\tilde{L} + I)^{-1}\tilde{L}^t D^{\frac{1}{2}}, \quad \text{where} \quad \tilde{L} = D^{-\frac{1}{2}}LD^{-\frac{1}{2}}.$$

Let $\lambda \in \mathbb{C}$ be any eigenvalue of $-G$, since:

$$(\tilde{L} + I)^{-1}\tilde{L}^t = -D^{\frac{1}{2}}GD^{-\frac{1}{2}},$$

λ is also an eigenvalue of $-\tilde{G} = (\tilde{L} + I)^{-1}\tilde{L}^t$. Choose $\mathbf{z} \in \mathbb{C}^n$ as a unit eigenvector of $-\tilde{G}$ corresponding to λ , i.e.

$$\tilde{L}^t \mathbf{z} = \lambda(\tilde{L} + I)\mathbf{z}.$$

Define $\tilde{A} = \tilde{L} + I + \tilde{L}^t = D^{-\frac{1}{2}}(L + D + L^t)D^{-\frac{1}{2}} = D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$, then $\tilde{A}$ is also symmetric positive-definite. Let us define $\alpha = \mathbf{z}^* \tilde{L} \mathbf{z}$ and denote $\alpha = a + ib$, $a, b \in \mathbb{R}$; we also denote $\mathbf{z} = \mathbf{x} + i\mathbf{y}$ where $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$. Then we have:

$$\bar{\alpha} = \alpha^* = \mathbf{z}^* \tilde{L}^t \mathbf{z} = \lambda \mathbf{z}^* (\tilde{L} + I) \mathbf{z} = \lambda(1 + \alpha),$$

where we used the assumption $\mathbf{z}^* \mathbf{z} = 1$.

Next, we compute $\mathbf{z}^* \tilde{A} \mathbf{z}$:

$$\mathbf{z}^* \tilde{A} \mathbf{z} = \mathbf{z}^* (\tilde{L} + I + \tilde{L}^t) \mathbf{z} = (1 + \lambda) \mathbf{z}^* (\tilde{L} + I) \mathbf{z} = (1 + \lambda)(1 + \alpha) = 1 + \alpha + \bar{\alpha} = 1 + 2a.$$

However, by the positive definiteness of $\tilde{A}$, we have:

$$\mathbf{z}^* \tilde{A} \mathbf{z} = (\mathbf{x}^t - i\mathbf{y}^t) \tilde{A} (\mathbf{x} + i\mathbf{y}) = \mathbf{x}^t \tilde{A} \mathbf{x} + \mathbf{y}^t \tilde{A} \mathbf{y} > 0 \quad \Rightarrow \quad 1 + 2a > 0.$$

Thus by $\lambda = \bar{\alpha}/(1 + \alpha)$ we have:

$$|\lambda|^2 = \left| \frac{a - ib}{1 + a + ib} \right|^2 = \frac{a^2 + b^2}{1 + 2a + a^2 + b^2} < 1.$$

The proof is completed by noting that $\rho(G) = \rho(-G)$ and the choice of λ is arbitrary. $\square$

4 SOR Method

The successive over-relaxation method (SOR) takes a “linear combination” of the Jacobi method and the Gauss-Seidel method to provide more control over the convergence rate. Particularly, we choose $M = M_\omega = \frac{1}{\omega}D + L$ for some $\omega > 0$ – Letting $\omega = \infty$ the method tends to the Jacobi method and setting $\omega = 1$ the method corresponds to the forward Gauss-Seidel.

For the SOR with $\omega > 0$, we have:

$$G = G_\omega = -\left(\frac{1}{\omega}D + L\right)^{-1} \left(\frac{\omega - 1}{\omega}D + U\right).$$

It can be shown that if A is symmetric positive-definite and $0 < \omega < 2$, then the SOR method converges. The proof is similar to that of Theorem 3.1, and the details are left as an exercise.

Note that due to a theorem of by Kahan [1], $\rho(G_\omega) \geq |\omega - 1|$; hence a necessary condition for the SOR method to converge is also $0 < \omega < 2$.

A major purpose of the SOR method is that it allows people to tune ω in order to minimize $\rho(G_\omega)$ for some special matrices. For example, if A is symmetric positive-definite and also tridiagonal, then $\rho(G_{\text{gs}}) = \rho(G_{\text{jac}})^2 < 1$ and the optimal choice for SOR is:

$$\omega = \frac{2}{1 + \sqrt{1 - \rho(G_{\text{jac}})^2}}.$$

In this case, $\rho(G_\omega) = \omega - 1$, which is optimal by the Kahan theorem.

5 Related Topics: Acceleration and Preconditioners

The acceleration technique tries to improve the convergence of an existing iterative method. Suppose we obtained $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k$ from the standard iterative method, then the plan is to compute a linear combination:

$$\mathbf{y}_k = \sum_{i=0}^k \nu_i(k) \mathbf{x}_i, \quad (5.1)$$

so that $\mathbf{y}_k$ represents a better approximation to the exact solution. Note that a natural condition on the coefficients is $\sum_{i=0}^k \nu_i(k) = 1$, so that if all iterates are exact, so is $\mathbf{y}_k$. If we define a polynomial:

$$p_k(x) = \nu_0(k) + \nu_1(k)x + \dots + \nu_k(k)x^k \quad (5.2)$$

and extend its definition to matrices naturally, we have:

$$\mathbf{y}_k - \mathbf{x} = p_k(G)\boldsymbol{\varepsilon}_0,$$

where $\mathbf{x}$ is the exact solution. Hence the target is to minimize $\|p_k(G)\|$ in a certain norm.

The Chebyshev semi-iterative method for symmetric matrices makes use of the fact that the eigenvalues of $p_k(G)$ are $p_k(\lambda)$, where λ is any eigenvalue of G . Knowing that any eigenvalue of G lies between -1 and 1 , the method utilizes the Chebyshev polynomials $c_k(x)$ defined recursively by $c_0(x) = 1$, $c_1(x) = x$, and $c_{k+1}(x) = 2xc_k(x) - c_{k-1}(x)$, and define:

$$p_k(x) = \frac{1}{c_k(\mu)} c_k\left(-1 + 2 \frac{x - \lambda_{\min}}{\lambda_{\max} - \lambda_{\min}}\right),$$

where $\mu = -1 + 2 \frac{1 - \lambda_{\min}}{\lambda_{\max} - \lambda_{\min}}$, $-1 < \lambda_{\min} < \lambda_{\max} < 1$ are the smallest and largest eigenvalues of G , respectively.

There are two benefits of using the Chebyshev polynomials. First, $c_k(x)$ satisfies $|c_k(x)| \leq 1$ on $[-1, 1]$ and it grows rapidly off this interval; thus the following estimate expects to be small:

$$\|\mathbf{y}_k - \mathbf{x}\|_2 \leq \frac{1}{|c_k(\mu)|} \|\boldsymbol{\varepsilon}_0\|_2.$$

Secondly, the recursive relation in the Chebyshev polynomials enables the following algorithm that completely removes the need to compute the iterates $\mathbf{x}_k$ but calculate $\mathbf{y}_k$ directly:

$$\begin{aligned} \mathbf{y}_{k+1} &= \omega_{k+1}(\mathbf{y}_k - \mathbf{y}_{k-1} + \gamma \mathbf{z}_k) + \mathbf{y}_{k-1}, \\ M\mathbf{z}_k &= \mathbf{b} - A\mathbf{y}_k, \end{aligned}$$

where $\gamma = \frac{2}{2-\lambda_{\min}-\lambda_{\max}}$, $\omega_{k+1} = 2 \frac{2-\lambda_{\min}-\lambda_{\max}}{\lambda_{\max}-\lambda_{\min}} \frac{c_k(\mu)}{c_{k+1}(\mu)}$.

Another use of the iterative methods is to construct preconditioners. A (left) preconditioner P modifies the original equation $A\mathbf{x} = \mathbf{b}$ to:

$$PA\mathbf{x} = P\mathbf{b}. \quad (5.3)$$

In general, the preconditioner depends highly on the problems to be solved, such as the low-Mach preconditioner for low-speed aerodynamic problems.

From a pure linear algebra point of view, though, the iterative method provides a class of preconditioners given by $P = M^{-1}$. In this case, we still need to solve a non-trivial system with $M^{-1}A$, but the hope is that $M^{-1}A$ will be better conditioned than A itself. Corresponding to the previous methods, we have the following preconditioners:

$$P_{\text{jac}} = D^{-1}, \quad P_{\text{gs}} = (L + D)^{-1}, \quad P_{\text{sor}} = (L + \omega^{-1}D)^{-1}.$$

Exercises

Exercise 1. Use mathematical induction to show (1.6) in the case $n_l = 3$.

Exercise 2. Let A be diagonally dominant and we want to complete the proof that the Gauss-Seidel method converges. Particularly let $G = -(L + D)^{-1}U$, show that $\|G\|_{\infty} \leq \rho_{\text{gs}}$, which is given by (3.4).

Hint: Use the definition of induced matrix norms, we just need to show that for all $\|\mathbf{x}\|_{\infty} = 1$, there is $\|\mathbf{y}\|_{\infty} \leq \rho_{\text{gs}}$, where $\mathbf{y} = G\mathbf{x}$. And for this purpose, use $D\mathbf{y} = -L\mathbf{y} - U\mathbf{x}$.

Exercise 3. Show that if A is symmetric, diagonally dominant, and all its diagonal elements are positive, then A is positive definite.

Hint: Show that $\mathbf{x}^t A \mathbf{x} \geq 0$ and derive the condition for the equality to hold. For this purpose, use the inequality $a_{ij}x_i y_j \geq -\left(\frac{1}{2}|a_{ij}|x_i^2 + \frac{1}{2}|a_{ji}|x_j^2\right)$.

Exercise 4. Prove that if A is symmetric positive definite, then the SOR method with $0 < \omega < 2$ converges.

Exercise 5. Let us consider the SOR method with $\omega > 0$, show that:

$$|\det G_{\omega}| = |1 - \omega|^n.$$

Then deduce that $\rho(G_{\omega}) \geq |1 - \omega|$, the Kahan theorem.

Hint: The determinant of a matrix A is the product of all the eigenvalues of A .

References

- [1] William Morton Kahan. Gauss-Seidel methods of solving large systems of linear equations. PhD thesis, University of Toronto, 1958.