

Numerical Linear Algebra

Basic Iterative Solution methods

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Introduction:

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The ideas to use iterative methods for solving linear systems of equations go back to Gauss (1823), Liouville (1837) and Jacobi (1845).

After deriving an iterative procedure, in 1823, Gauss has written in a letter the following:

"... You will hardly eliminate directly anymore, at least not when you have more than two unknowns. The indirect method can be pursued while half asleep or while thinking about other things."

Before considering iterative solution methods for **linear** systems of equations, we recall how do we solve **nonlinear** problems. Let $f(x) = 0$ have to be solved and $f(x)$ is a nonlinear function in x . The usual way to approach the problem is:

$$F(x) \equiv x - f(x).$$

If x^* is the solution of $f(x) = 0$, then x^* is a stationary point for

$$x = F(x). \quad (1)$$

Then we proceed with finding the stationary point for (1) and this is done **iteratively**, namely,

$$x^{(k+1)} = F(x^{(k)}), k = 0, 1, \dots, x^{(0)} \text{ given.} \quad (2)$$

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For any initial guess $x^{(0)}$, there exists a unique fixed point x^* for $F(x)$, $x^* = \lim_{k \rightarrow \infty} x^{(k)}$ if and only if F is a contracting mapping, i.e.

$$\|F(x) - F(y)\| \leq q\|x - y\|$$

for some $q \in (0, 1)$.

Let now $f(x) \equiv Ax - b$ be linear. We use the same framework:

$$\begin{aligned} F(x) &= x - (Ax - b) \\ x^{(k+1)} &= x^{(k)} - (Ax^{(k)} - b) = x^{(k)} + r^{(k)} \end{aligned}$$

where $r^{(k)} = b - Ax^{(k)}$ is called the **residual** at iteration k .

In this way we obtain the simplest possible iterative scheme to solve

$$Ax = b,$$

namely,

$$\begin{aligned} x^{(k+1)} &= x^{(k)} - (Ax^{(k)} - b), \quad k = 0, 1, \dots \\ x^{(0)} &\text{ given.} \end{aligned}$$

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Fixed point for linear problems - when does it converge?

$$\begin{aligned} \|F(x) - F(y)\| &= \|x - (Ax - b) - y + (Ay - b)\| \\ &= \|(I - A)(x - y)\| \leq \|(I - A)\| \|x - y\| \end{aligned}$$

The simple iteration will not converge in general.

Simple iteration

For many reasons the latter form of the simple iteration is replaced by

$$x^{(k+1)} = x^{(k)} + \tau r^{(k)}, \quad (3)$$

where τ is some properly chosen method parameter.

Relation (3) defines the so-called *stationary basic iterative method of first kind*.

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If we permit τ to change from one iteration to the next, we get

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \tau_k \mathbf{r}^{(k)}, \quad (4)$$

which latter defines the so-called

non-stationary basic iterative method of first kind.

So far τ and τ_k are some scalars. Nothing prevents us to replace the method parameter by some matrix, however, if this would improve the convergence of the iterative method.

Nothing prevents us to replace the method parameter by some matrix, however, if this would improve the convergence of the iterative method. Thus, we can consider

$$\begin{aligned} \mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} + C^{-1}(\mathbf{b} - A\mathbf{x}^{(k)}) \\ \text{or} \\ \mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} + C^{-1}\mathbf{r}^{(k)}, \end{aligned} \quad (5)$$

It is easy to see that we obtain (5) by replacing $A\mathbf{x} = \mathbf{b}$ with

$$C^{-1}A\mathbf{x} = C^{-1}\mathbf{b}$$

and use the simple iteration framework.

Concerns: I

In this case the iterative scheme takes the form

$$\begin{aligned} C\mathbf{d}^{(k)} &= \mathbf{r}^{(k)}, \\ \mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} + \mathbf{d}^{(k)} \end{aligned} \quad (6)$$

The scheme

$$\begin{aligned} C\mathbf{d}^{(k)} &= \mathbf{r}^{(k)}, \\ \mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} + \mathbf{d}^{(k)} \end{aligned}$$

has in general a higher computational complexity than (4), since a solution of a system with the matrix C is required at each iteration.

C1: Does the iteration process converge to the solution, i.e. does $\mathbf{x}^{(k)} \rightarrow \mathbf{x}^*$?

C2: If 'yes', how fast does it converge?

The number of iterations it needed for the iterative method to converge with respect to some convergence criterion, is a function of the properties of A .

Say, $it = it(n)$, where n is the size of A .

If it turns out that $it = O(n^2)$, we haven't gained anything compared to the direct solution methods.

The best one can hope for is to get $it \leq Const$, where $Const$ is independent of n .

Since the computational complexity of one iteration is in many cases proportional to n (for sparse matrices, for instance) then the complexity of the whole solution process will be $O(n)$.

C3: Is the method *robust* with respect to the method parameters (τ, τ_k) ?

C4: Is the method *robust* with respect to various problem parameters?

$$A = A(\rho, \nu, E, \dots)$$

C5: When we are using the scheme $C^{-1}Ax = C^{-1}\mathbf{b}$, it must be easy to solve systems with C .

C6: Is the method parallelizable?
Parallelization aspects become more and more important since n is XXL.

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Concerns (cont.): I

Suppose the method converges to the exact solution \mathbf{x}^* .
Then more questions arise:

C7: When do we stop the iterations?

→ We want $\|\mathbf{x}^* - \mathbf{x}^{(k)}\| \leq \varepsilon$ but \mathbf{x}^* is not known.

→ What about checking on $\mathbf{r}^{(k)}$?

→ Is it enough to have $\|\mathbf{r}^{(k)}\| \leq \tilde{\varepsilon}$?

Will the latter guarantee that $\|\mathbf{x}^* - \mathbf{x}^{(k)}\| \leq \varepsilon$?

Denote $\mathbf{e}^{(k)} = \mathbf{x}^* - \mathbf{x}^{(k)}$ (the error at iteration k). Then

$$\mathbf{r}^{(k)} = \mathbf{b} - A\mathbf{x}^{(k)} = A(\mathbf{x}^* - \mathbf{x}^{(k)}) = A\mathbf{e}^{(k)}.$$

In other words $\mathbf{e}^{(k)} = A^{-1}\mathbf{r}^{(k)}$.

Scenario: Suppose $\|A^{-1}\| = 10^8$ and $\tilde{\varepsilon} = 10^{-4}$. Then

$$\|\mathbf{e}^{(k)}\| \leq \|A^{-1}\| \|\mathbf{r}^{(k)}\| \leq 10^4, \text{ which is not very exiting.}$$

Example: Discrete Laplace Δ_h^5 :

$$\|A^{-1}\| \approx \lambda_{\min} = \frac{1}{2}(\pi h)^2 \approx 10^4 \text{ for } h = 10^{-2}.$$

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Concerns (cont.): II

C8: How do we measure (estimate) the convergence rate?

C9: How do we find good method parameters (τ, τ_k, C) , which will speed up the convergence?

We start our considerations with [C9].

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Intuitively, C has to do something with A .
 Note that if $C = A$, then $C^{-1} = A^{-1}$ and we will get convergence in one step!
 However, the computational effort to construct A^{-1} is higher than to use a direct solution method.

We try the following choice. Consider the following so-called **splitting** of A ,

$$A = C - R,$$

where C is nonsingular and R can be seen as an error matrix.

Then $C^{-1}A = C^{-1}(C - R) = I - C^{-1}R = I - B$.

- ▶ The matrix $B = C^{-1}R$ is referred to as the **iteration matrix**.
- ▶ $\|B^m\|$ is the **convergence factor for m steps**
- ▶ $(\|B^m\|)^{1/m}$ is called the **average convergence factor**.

Using the splitting $A = C - R$ we obtain the following equivalent form of the iterative procedure:

$$\begin{aligned} A = C - R &\longrightarrow R = C - A \\ \mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} + C^{-1}(\mathbf{b} - A\mathbf{x}^{(k)}) \\ &= \mathbf{x}^{(k)} + C^{-1}\mathbf{b} - C^{-1}(C - R)\mathbf{x}^{(k)} \\ &= C^{-1}\mathbf{b} + C^{-1}R\mathbf{x}^{(k)} \\ C\mathbf{x}^{(k+1)} &= R\mathbf{x}^{(k)} + \mathbf{b} \end{aligned} \quad (7)$$

The matrix C is called a **preconditioner** to A . Its general purpose is to improve the properties of A in order to achieve a better (faster) convergence of the method.

Theorem

The sequence $\{\mathbf{x}^{(k)}\}$ from $C\mathbf{x}^{(k+1)} = R\mathbf{x}^{(k)} + \mathbf{b}$ converges to the solution \mathbf{x}^* of $A\mathbf{x} = \mathbf{b}$ for any initial guess $\mathbf{x}^{(0)}$ if and only if there holds

$$\rho(B) \equiv \rho(C^{-1}R) < 1$$

where $\rho(\dots)$ denotes the spectral radius.

Proof.

Let $\mathbf{e}^{(k)} = \mathbf{x}^* - \mathbf{x}^{(k)}$, $A = C - R$. Then

$$\begin{aligned} C\mathbf{x}^* &= R\mathbf{x}^* + \mathbf{b} \\ C\mathbf{x}^{(k)} &= R\mathbf{x}^{(k-1)} + \mathbf{b} \\ C\mathbf{e}^{(k)} &= R\mathbf{e}^{(k-1)} \\ \mathbf{e}^{(k)} &= B\mathbf{e}^{(k-1)} = B^2\mathbf{e}^{(k-2)} = \dots = B^k\mathbf{e}^{(0)}. \end{aligned}$$

If $\rho(C^{-1}R) < 1$ then $\lim_{k \rightarrow \infty} B^k = 0$ and $\mathbf{e}^{(k)} \rightarrow 0$. □

Let $\lambda_i = \text{eig}(B)$ and $\rho(B) = |\lambda_j|$ i.e., λ_j is the eigenvalue of B , such that $\rho(B) = |\lambda_j|$. Let \mathbf{v}^j be the corresponding eigenvector. Then $(\mathbf{v}^j)^m = B^m \mathbf{v}^j = \lambda_j^m \mathbf{v}^j \rightarrow 0$.

$$\mathbf{e}^{(0)} = \sum_{k=1}^n \beta_k \mathbf{v}^k = \beta_j \mathbf{v}^j + \dots$$

$$B^m \mathbf{e}^{(0)} = \tilde{\beta}_j B^m \mathbf{v}^j + \dots$$

and at least one component of $\mathbf{e}^{(m)}$ does not converge to zero.

The basic argument in the latter proof is that if $\rho(B) < 1$ then $B^k \rightarrow 0$. This can be shown in the following way.

Lemma

Let T be a nonsingular matrix and let $\|\mathbf{x}\|_T = \|T\mathbf{x}\|_\infty$. Let $\|A\|_T = \sup_{\mathbf{x} \neq \mathbf{0}} \frac{\|A\mathbf{x}\|_T}{\|\mathbf{x}\|_T}$ be the induced matrix norm. Then.

- (a) $\|A\|_T = \|TAT^{-1}\|_\infty$
- (b) For any $\varepsilon > 0$ and matrix A , there exists a nonsingular matrix T such that $\|A\|_T \leq \rho(A) + \varepsilon$.
In other words, there exist matrix norms, which are arbitrary close to the spectral radius of a given matrix.

Proof.

(a) $\|\mathbf{x}\|_T$ is a vector norm and T^{-1} exists.

$$\begin{aligned} \|A\|_T &= \sup_{\mathbf{x} \neq \mathbf{0}} \frac{\|A\mathbf{x}\|_T}{\|\mathbf{x}\|_T} = \sup_{\mathbf{x} \neq \mathbf{0}} \frac{\|TA\mathbf{x}\|_\infty}{\|T\mathbf{x}\|_\infty} \\ &= \sup_{\mathbf{y} \neq \mathbf{0}} \frac{\|TAT^{-1}\mathbf{y}\|_\infty}{\|\mathbf{y}\|_\infty} = \|TAT^{-1}\|_\infty. \end{aligned}$$



(b) We use Schur's lemma: There exists a unitary matrix U , such that

$$UAU^{-1} = W = \begin{bmatrix} w_{11} & * & * & \dots & * \\ 0 & w_{22} & * & \dots & * \\ & & \ddots & \dots & \vdots \\ & & & & w_{nn} \end{bmatrix},$$

where $w_{ii} = \lambda_i \in S(A)$; $S(A)$ denotes the spectrum of A . Let $\delta > 0$ and define $D = D(\delta) = \text{diag}\{\delta^{-1}, \delta^{-2}, \dots, \delta^{-n}\}$. Then DWD^{-1} is also

upper triangular and $(DWD^{-1})_{ij} = \begin{cases} 0, & j < i \\ w_{ii}, & j = i \\ w_{ij}\delta^{j-i}, & j > i. \end{cases}$

$$\Rightarrow \|DWD^{-1}\|_\infty \leq \max_i \left\{ |w_{ii}| + n \max_{j>i} |w_{ij}| \delta^{j-i} \right\}.$$

We see that for any given $\varepsilon > 0$ we can choose $\delta > 0$ small enough so that $n \max_{j>i} |w_{ij}| \delta^{j-1} < \varepsilon$. Hence,

$$\begin{aligned} \|DWD^{-1}\|_{\infty} &\leq \rho(A) + \varepsilon \\ \|A\|_T &= \|TAT^{-1}\|_{\infty} = \|DUAU^{-1}D^{-1}\|_{\infty} \\ &= \|DWD^{-1}\|_{\infty} \leq \rho(A) + \varepsilon. \end{aligned}$$

(for $T = DU$, nonsingular).

Lemma

For any square matrix there holds

- (a) $\lim_{k \rightarrow \infty} A^k = 0 \Leftrightarrow \rho(A) < 1$,
- (b) If $\rho(A) < 1$ then $(I - A)^{-1} = I + A + A^2 + \dots$ is convergent.

Proof.

(a) \Rightarrow : If $\rho(A) < 1$ then choose $\varepsilon > 0$: $\rho(A) + \varepsilon < 1$. Then there exists a nonsingular T (which depends on A), such that $\|A\|_T \leq \rho(A) + \varepsilon < 1$.

$$\Rightarrow \|A^k\|_T \leq \|A\|_T^k \rightarrow 0 \Rightarrow \lim_{k \rightarrow \infty} A^k = 0$$

(a) \Leftarrow : If $\lim_{k \rightarrow \infty} A^k = 0$, let $\{\lambda, \mathbf{v}\}$ be an eigensolution of A , then

$\lambda^k \mathbf{v} = A^k \mathbf{v} \rightarrow 0$. This is true for all eigenvalues, thus $\rho(A) = \max |\lambda| < 1$.

(b) $(I - A)(I + A + A^2 + \dots) = I - A^{k+1}$. If $\rho(A) < 1$ then $A^k \rightarrow 0 \Rightarrow$ (b) follows. □

Theorem 1 shows both convergence and rate of convergence ($\mathbf{e}^{(k)} = B^k \mathbf{e}^{(0)}$). The latter is difficult to compute. Also the convergence may not be monotone.

Theorem

Consider $C\mathbf{x}^{(k+1)} = R\mathbf{x}^{(k)} + \mathbf{b}$, $B = C^{-1}R$ and let $\rho(B) < 1$. Then

$$\|\mathbf{x}^* - \mathbf{x}^{(k)}\| \leq \frac{\|B\|}{1 - \|B\|} \|\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)}\|$$

Proof.

$\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)} = B(\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)})$ and $\mathbf{x}^{(k+m+1)} - \mathbf{x}^{(k+m)} = B^{m+1}(\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)})$. We have

$$\begin{aligned} \|\mathbf{x}^{(k+s)} - \mathbf{x}^{(k)}\| &= \left\| \sum_{j=0}^{s-1} (\mathbf{x}^{(k+j+1)} - \mathbf{x}^{(k+j)}) \right\| \leq \\ &\|\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}\| + \|\mathbf{x}^{(k+2)} - \mathbf{x}^{(k+1)}\| + \dots \end{aligned}$$

Therefore

$$\|\mathbf{x}^{(k+m+1)} - \mathbf{x}^{(k+m)}\| \leq \sum_{j=0}^m \|B^j\| \|\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)}\| = \frac{\|B\| - \|B\|^{m+1}}{1 - \|B\|} \|\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)}\|$$

We let now $m \rightarrow \infty$, i.e., $\mathbf{x}^{k+m} \rightarrow \mathbf{x}^*$, $\|B\|^m \rightarrow 0$.

$$\Rightarrow \|\mathbf{x}^* - \mathbf{x}^{(k)}\| \leq \frac{\|B\|}{1 - \|B\|} \|\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)}\|.$$

Stopping tests:

Theorem 4 can be used to get information whether the iteration error $\mathbf{e}^{(k)} = \mathbf{x}^* - \mathbf{x}^{(k)}$ is small enough.

In practice, most used stopping tests are:

(S1) $\|\mathbf{r}^{(k)}\| \leq \varepsilon$, residual based, absolute

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(S3) $\|\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)}\| \leq \varepsilon$

(S4) $\|\mathbf{x}^* - \mathbf{x}^{(k)}\| \leq \varepsilon_0 \|\mathbf{x}^* - \mathbf{x}^{(0)}\|$.

If the latter is wanted, then we must check on (S3) and choose ε such that $\varepsilon \leq \frac{\|B\|}{1-\|B\|} \varepsilon_0 \|\mathbf{x}^* - \mathbf{x}^{(0)}\|$.

Either estimate of $\|A^{-1}\|$ or of $\|B\|$ is required.

Choice 'J'

Let $A = D - L - U$, where D is diagonal, U is strictly upper triangular and L is strictly lower triangular.

Let $C \equiv D$, $R = L + U$. The iterative scheme is known as **Jacobi** iteration:

$$D\mathbf{x}^{(k+1)} = (L + U)\mathbf{x}^{(k)} + \mathbf{b}$$

Entry-wise $x_i^{k+1} = \frac{1}{a_{ii}} \left(b_i - \sum_{j \neq i} a_{ij}x_j \right) ..$

For the method to converge: $B = D^{-1}(L + U)$

$$\rho(B) \leq \|D^{-1}(L + U)\|_{\infty} = \max_{1 \leq i \leq n} \sum_{j=1, j \neq i}^n \left| \frac{a_{ij}}{a_{ii}} \right|$$

We want $\rho(B) < 1$. One class of matrices, for which Jacobi method converges is when A is strictly diagonally dominant.

1. Choice GS-B Choose $C \equiv D - U$, $R = L$

Backward Gauss-Seidel $(D - U)\mathbf{x}^{(k+1)} = L\mathbf{x}^{(k)} + \mathbf{b}$

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2. Choice GS-F Choose $C \equiv D - L$, $R = U$

Forward Gauss-Seidel $(D - L)\mathbf{x}^{(k+1)} = U\mathbf{x}^{(k)} + \mathbf{b}$

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3. G-S is convergent for s.p.d. matrices.
4. make it more fancy: $A = D - L - U$. Then

$$\omega A = \omega D - \omega L - \omega U + D - D \leftarrow \text{overrelaxation}$$

$$= (D - \omega L) - (\omega U + (1 - \omega)D)$$
 Choose $C \equiv D - \omega L, R = \omega U + (1 - \omega)D$:
 SOR $(D - \omega L)\mathbf{x}^{(k+1)} = [\omega U + (1 - \omega)D]\mathbf{x}^{(k)} + \omega \mathbf{b}$

One can see SOR as a generalization of G-S ($\omega = 1$). Rewrite
 $(D - \omega L)\mathbf{x}^{(k+1)} = [\omega U + (1 - \omega)D]\mathbf{x}^{(k)} + \omega \mathbf{b}$
 as $(\frac{1}{\omega}D - L)\mathbf{x}^{(k+1)} = [(\frac{1}{\omega} - 1)D + U]\mathbf{x}^{(k)} + \mathbf{b}$
 For the iteration matrix $B_\omega = (\frac{1}{\omega}D - L)^{-1} [(\frac{1}{\omega} - 1)D + U]$
 One can show that $\rho(B_\omega) < 1$ for $0 < \omega < 2$. Furthermore, there is
 an optimal value of ω , for which $\rho(B_\omega)$ is minimized:

$$\omega_{opt} = \frac{2}{1 + \sqrt{1 - \rho(\hat{B})^2}}, \quad \hat{B} = I - D_A^{-1}A.$$

Rate of convergence: Let $\lambda_i = \text{eig}(B_\omega)$.
 $\left| \prod_{i=1}^n \lambda_i \right| = |\det((1 - \omega)I + \omega D^{-1}U)| = |1 - \omega|^n. \Rightarrow$ at least one
 $\lambda_i \geq |1 - \omega|.$
 $\Rightarrow \rho(B_\omega) \geq |1 - \omega|.$
 We want $\rho(B_\omega) < 1$, i.e. $|1 - \omega| \leq \rho(B_\omega) < 1, \Rightarrow 0 < \omega < 2.$

Let $A, C, R \in \mathbf{R}^{n \times n}$ and consider $A = C - R$. A splitting of A is called

- ▶ **regular** if C is monotone and $R \geq 0$ (elementwise)
- ▶ **weak regular** if C is monotone and $C^{-1}R \geq 0$
- ▶ **nonnegative** if C^{-1} exists and $C^{-1}R \geq 0$
- ▶ **convergent** if $\rho(C^{-1}R) < 1$.

Recall: A matrix is called *monotone* if $Ax > 0$ implies $x > 0$.

Theorem: A - monotone $\Leftrightarrow A^{-1} \geq 0$.

Let A be symmetric matrix.

$$\begin{aligned} \mathbf{x}_0 \text{ given, } \quad \mathbf{x}_1 &= \mathbf{x}_0 + \frac{1}{2}\beta_0\mathbf{r}_0 \\ \text{For } k = 0, 1, \dots \text{ until convergence} \\ \mathbf{x}_{k+1} &= \alpha_k\mathbf{x}_k + (1 - \alpha_k)\mathbf{x}_{k-1} + \beta_k\mathbf{r}_k. \\ \mathbf{r}_k &= \mathbf{b} - A\mathbf{x}_k. \end{aligned}$$

$$\alpha_k = \frac{a+b}{2}\beta_k, \quad \frac{1}{\beta_k} = \frac{a+b}{2} - \left(\frac{b-a}{4}\right)^2 \beta_{k-1}, \quad \beta_0 = \frac{4}{a+b}.$$

Note that $\alpha_k > 1, k \geq 1$.

Modifications for nonsymmetric matrices exist.