Iterative techniques in matrix algebra

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Outline

1. Norms of vectors and matrices
2. Eigenvalues and eigenvectors
3. Iterative techniques for solving linear systems
4. Error bounds and iterative refinement
5. The conjugate gradient method
Definition 1

∥·∥ : \mathbb{R}^n \rightarrow \mathbb{R} is a vector norm if

(i) \|x\| \geq 0, \forall x \in \mathbb{R}^n,
(ii) \|x\| = 0 if and only if x = 0,
(iii) \|\alpha x\| = |\alpha|\|x\| \forall \alpha \in \mathbb{R} and x \in \mathbb{R}^n,
(iv) \|x + y\| \leq \|x\| + \|y\| \forall x, y \in \mathbb{R}^n.

Definition 2

The \ell_2 and \ell_\infty norms for \( x = [x_1, x_2, \cdots, x_n]^T \) are defined by

\[
\|x\|_2 = (x^T x)^{1/2} = \left\{ \sum_{i=1}^{n} x_i^2 \right\}^{1/2}
\]

and \( \|x\|_\infty = \max_{1 \leq i \leq n} |x_i| \).

The \ell_2 norm is also called the Euclidean norm.
Theorem 3 (Cauchy-Bunyakovsky-Schwarz inequality)

For each \( x = [x_1, x_2, \cdots, x_n]^T \) and \( y = [y_1, y_2, \cdots, y_n]^T \) in \( \mathbb{R}^n \),

\[
x^T y = \sum_{i=1}^{n} x_i y_i \leq \left\{ \sum_{i=1}^{n} x_i^2 \right\}^{1/2} \left\{ \sum_{i=1}^{n} y_i^2 \right\}^{1/2} = \|x\|_2 \cdot \|y\|_2.
\]

**Proof**: If \( x = 0 \) or \( y = 0 \), the result is immediate.
Suppose \( x \neq 0 \) and \( y \neq 0 \). For each \( \alpha \in \mathbb{R} \),

\[
0 \leq \|x - \alpha y\|_2^2 = \sum_{i=1}^{n} (x_i - \alpha y_i)^2 \leq \sum_{i=1}^{n} x_i^2 - 2\alpha \sum_{i=1}^{n} x_i y_i + \alpha^2 \sum_{i=1}^{n} y_i^2,
\]

and

\[
2\alpha \sum_{i=1}^{n} x_i y_i \leq \sum_{i=1}^{n} x_i^2 + \alpha^2 \sum_{i=1}^{n} y_i^2 = \|x\|_2^2 + \alpha^2 \|y\|_2^2.
\]
Since $\|x\|_2 > 0$ and $\|y\|_2 > 0$, we can let

$$\alpha = \frac{\|x\|_2}{\|y\|_2}$$

to give

$$\left(2 \frac{\|x\|_2}{\|y\|_2}\right) \left(\sum_{i=1}^{n} x_i y_i\right) \leq \|x\|_2^2 + \frac{\|x\|_2^2}{\|y\|_2^2} \|y\|_2^2 = 2\|x\|_2^2.$$ 

Thus

$$x^T y = \sum_{i=1}^{n} x_i y_i \leq \|x\|_2 \|y\|_2.$$
For each $x, y \in \mathbb{R}^n$,

$$\|x + y\|_\infty = \max_{1 \leq i \leq n} |x_i + y_i| \leq \max_{1 \leq i \leq n} (|x_i| + |y_i|) \leq \max_{1 \leq i \leq n} |x_i| + \max_{1 \leq i \leq n} |y_i| = \|x\|_\infty + \|y\|_\infty$$

and

$$\|x + y\|_2^2 = \sum_{i=1}^{n} (x_i + y_i)^2 = \sum_{i=1}^{2} x_i^2 + 2 \sum_{i=1}^{n} x_i y_i + \sum_{i=1}^{n} y_i^2 \leq \|x\|_2^2 + 2 \|x\|_2 \|y\|_2 + \|y\|_2^2 = (\|x\|_2 + \|y\|_2)^2,$$

which gives

$$\|x + y\|_2 \leq \|x\|_2 + \|y\|_2.$$
**Definition 4**

A sequence \( \{ x^{(k)} \in \mathbb{R}^n \}_{k=1}^{\infty} \) is convergent to \( x \) with respect to the norm \( \| \cdot \| \) if \( \forall \, \varepsilon > 0, \exists \) an integer \( N(\varepsilon) \) such that

\[
\| x^{(k)} - x \| < \varepsilon, \, \forall \, k \geq N(\varepsilon).
\]

**Theorem 5**

\( \{ x^{(k)} \in \mathbb{R}^n \}_{k=1}^{\infty} \) converges to \( x \) with respect to \( \| \cdot \|_{\infty} \) if and only if

\[
\lim_{k \to \infty} x_i^{(k)} = x_i, \, \forall \, i = 1, 2, \ldots, n.
\]

**Proof:** “\( \Rightarrow \)” Given any \( \varepsilon > 0, \exists \) an integer \( N(\varepsilon) \) such that

\[
\max_{1 \leq i \leq n} | x_i^{(k)} - x_i | = \| x^{(k)} - x \|_{\infty} < \varepsilon, \, \forall \, k \geq N(\varepsilon).
\]
This result implies that

$$|x_i^{(k)} - x_i| < \varepsilon, \ \forall \ i = 1, 2, \ldots, n.$$  

Hence

$$\lim_{k \to \infty} x_i^{(k)} = x_i, \ \forall \ i.$$  

“⇐” For a given $$\varepsilon > 0$$, let $$N_i(\varepsilon)$$ represent an integer with

$$|x_i^{(k)} - x_i| < \varepsilon, \ \text{whenever} \ k \geq N_i(\varepsilon).$$  

Define

$$N(\varepsilon) = \max_{1 \leq i \leq n} N_i(\varepsilon).$$  

If $$k \geq N(\varepsilon)$$, then

$$\max_{1 \leq i \leq n} |x_i^{(k)} - x_i| = \|x^{(k)} - x\|_\infty < \varepsilon.$$  

This implies that $$\{x^{(k)}\}$$ converges to $$x$$ with respect to $$\| \cdot \|_\infty$$.  

Theorem 6

For each $x \in \mathbb{R}^n$,

$$
\|x\|_\infty \leq \|x\|_2 \leq \sqrt{n \|x\|_\infty}.
$$

Proof: Let $x_j$ be a coordinate of $x$ such that

$$
\|x\|_\infty^2 = |x_j|^2 \leq \sum_{i=1}^{n} x_i^2 = \|x\|_2^2,
$$

so $\|x\|_\infty \leq \|x\|_2$ and

$$
\|x\|_2^2 = \sum_{i=1}^{n} x_i^2 \leq \sum_{i=1}^{n} x_j^2 = n x_j^2 = n \|x\|_\infty^2,
$$

so $\|x\|_2 \leq \sqrt{n \|x\|_\infty}$. 


**Definition 7**

A matrix norm $\| \cdot \|$ on the set of all $n \times n$ matrices is a real-valued function satisfying for all $n \times n$ matrices $A$ and $B$ and all real number $\alpha$:

(i) $\| A \| \geq 0$;

(ii) $\| A \| = 0$ if and only if $A = 0$;

(iii) $\| \alpha A \| = |\alpha| \| A \|$;

(iv) $\| A + B \| \leq \| A \| + \| B \|$;

(v) $\| AB \| \leq \| A \| \| B \|$;

**Theorem 8**

*If $\| \cdot \|$ is a vector norm on $\mathbb{R}^n$, then*

$$\| A \| = \max_{\| x \| = 1} \| Ax \|$$

*is a matrix norm.*
For any \( z \neq 0 \), we have \( x = z / \| z \| \) as a unit vector. Hence

\[
\| A \| = \max_{\| x \| = 1} \| Ax \| = \max_{z \neq 0} \left\| A \left( \frac{z}{\| z \|} \right) \right\| = \max_{z \neq 0} \frac{\| Az \|}{\| z \|}.
\]

**Corollary 9**

\[
\| Az \| \leq \| A \| \cdot \| z \|.
\]

**Theorem 10**

*If \( A = [a_{ij}] \) is an \( n \times n \) matrix, then*

\[
\| A \|_{\infty} = \max_{1 \leq i \leq n} \sum_{j=1}^{n} |a_{ij}|.
\]
\textbf{Proof:} Let $x$ be an $n$-dimension vector with
\[ 1 = \|x\|_{\infty} = \max_{1 \leq i \leq n} |x_i|. \]

Then
\[
\|Ax\|_{\infty} = \max_{1 \leq i \leq n} \left| \sum_{j=1}^{n} a_{ij} x_j \right|
\]
\[ \leq \max_{1 \leq i \leq n} \sum_{j=1}^{n} |a_{ij}| \max_{1 \leq j \leq n} |x_j| = \max_{1 \leq i \leq n} \sum_{j=1}^{n} |a_{ij}|. \]

Consequently,
\[
\|A\|_{\infty} = \max_{\|x\|_{\infty}=1} \|Ax\|_{\infty} \leq \max_{1 \leq i \leq n} \sum_{j=1}^{n} |a_{ij}|.
\]

On the other hand, let $p$ be an integer with
\[
\sum_{j=1}^{n} |a_{pj}| = \max_{1 \leq i \leq n} \sum_{j=1}^{n} |a_{ij}|.
\]
and \( x \) be the vector with

\[
x_j = \begin{cases} 
1, & \text{if } a_{pj} \geq 0, \\
-1, & \text{if } a_{pj} < 0.
\end{cases}
\]

Then

\[
\|x\|_\infty = 1 \quad \text{and} \quad a_{pj}x_j = |a_{pj}|, \quad \forall \ j = 1, 2, \ldots, n,
\]

so

\[
\|Ax\|_\infty = \max_{1 \leq i \leq n} \left| \sum_{j=1}^{n} a_{ij}x_j \right| \geq \left| \sum_{j=1}^{n} a_{pj}x_j \right| = \left| \sum_{j=1}^{n} |a_{pj}| \right| = \max_{1 \leq i \leq n} \sum_{j=1}^{n} |a_{ij}|.
\]

This result implies that

\[
\|A\|_\infty = \max_{\|x\|_\infty = 1} \|Ax\|_\infty \geq \max_{1 \leq i \leq n} \sum_{j=1}^{n} |a_{ij}|.
\]

which gives

\[
\|A\|_\infty = \max_{1 \leq i \leq n} \sum_{j=1}^{n} |a_{ij}|.
\]
Definition 11 (Characteristic polynomial)

If $A$ is a square matrix, the characteristic polynomial of $A$ is defined by

$$p(\lambda) = \det(A - \lambda I).$$

Definition 12 (Eigenvalue and eigenvector)

If $p$ is the characteristic polynomial of the matrix $A$, the zeros of $p$ are eigenvalues of the matrix $A$. If $\lambda$ is an eigenvalue of $A$ and $x \neq 0$ satisfies $(A - \lambda I)x = 0$, then $x$ is an eigenvector of $A$ corresponding to the eigenvalue $\lambda$.

Definition 13 (Spectrum and Spectral Radius)

The set of all eigenvalues of a matrix $A$ is called the spectrum of $A$. The spectral radius of $A$ is

$$\rho(A) = \max\{|\lambda|; \lambda \text{ is an eigenvalue of } A\}.$$
**Theorem 14**

If $A$ is an $n \times n$ matrix, then

(i) $\|A\|_2 = \sqrt{\rho(A^T A)}$;

(ii) $\rho(A) \leq \|A\|$ for any matrix norm.

**Proof:** Proof for the second part. Suppose $\lambda$ is an eigenvalue of $A$ and $x \neq 0$ is a corresponding eigenvector such that $Ax = \lambda x$ and $\|x\| = 1$. Then

$$|\lambda| = \|\lambda\|\|x\| = \|\lambda x\| = \|Ax\| \leq \|A\|\|x\| = \|A\|,$$

that is, $|\lambda| \leq \|A\|$. Since $\lambda$ is arbitrary, this implies that $\rho(A) = \max |\lambda| \leq \|A\|$.

**Theorem 15**

For any $A$ and any $\varepsilon > 0$, there exists a matrix norm $\| \cdot \|$ such that

$$\rho(A) < \|A\| < \rho(A) + \varepsilon.$$
Definition 16

We call an $n \times n$ matrix $A$ convergent if

$$\lim_{k \to \infty} (A^k)_{ij} = 0 \quad \forall \quad i = 1, 2, \ldots, n \quad \text{and} \quad j = 1, 2, \ldots, n.$$  

Theorem 17

The following statements are equivalent.

1. $A$ is a convergent matrix;
2. $\lim_{k \to \infty} \|A^k\| = 0$ for some matrix norm;
3. $\lim_{k \to \infty} \|A^k\| = 0$ for all matrix norm;
4. $\rho(A) < 1$;
5. $\lim_{k \to \infty} A^k x = 0$ for any $x$. 

Iterative techniques for solving linear systems

- For small dimension of linear systems, it requires for direct techniques.
- For large systems, iterative techniques are efficient in terms of both computer storage and computation.

The basic idea of iterative techniques is to split the coefficient matrix $A$ into

$$A = M - (M - A),$$

for some matrix $M$, which is called the splitting matrix. Here we assume that $A$ and $M$ are both nonsingular. Then the original problem is rewritten in the equivalent form

$$Mx = (M - A)x + b.$$
This suggests an iterative process

\[ x^{(k)} = (I - M^{-1}A)x^{(k-1)} + M^{-1}b \equiv Tx^{(k-1)} + c, \]

where \( T \) is usually called the iteration matrix. The initial vector \( x^{(0)} \) can be arbitrary or be chosen according to certain conditions.

Two criteria for choosing the splitting matrix \( M \) are

- \( x^{(k)} \) is easily computed. More precisely, the system \( Mx^{(k)} = y \) is easy to solve;
- the sequence \( \{x^{(k)}\} \) converges rapidly to the exact solution.

Note that one way to achieve the second goal is to choose \( M \) so that \( M^{-1} \) approximate \( A^{-1} \).

In the following subsections, we will introduce some of the mostly commonly used classic iterative methods.
Jacobi Method

If we decompose the coefficient matrix $A$ as

$$A = L + D + U,$$

where $D$ is the diagonal part, $L$ is the strictly lower triangular part, and $U$ is the strictly upper triangular part, of $A$, and choose $M = D$, then we derive the iterative formulation for Jacobi method:

$$x^{(k)} = -D^{-1}(L + U)x^{(k-1)} + D^{-1}b.$$

With this method, the iteration matrix $T_J = -D^{-1}(L + U)$ and $c = D^{-1}b$.

Each component $x^{(k)}_i$ can be computed by

$$x^{(k)}_i = \left( b_i - \sum_{j=1}^{i-1} a_{ij} x^{(k-1)}_j - \sum_{j=i+1}^{n} a_{ij} x^{(k-1)}_j \right) / a_{ii}.$$
\[\begin{align*}
a_{11}x_1^{(k)} + a_{12}x_2^{(k-1)} + a_{13}x_3^{(k-1)} + \cdots + a_{1n}x_n^{(k-1)} &= b_1 \\
a_{21}x_1^{(k-1)} + a_{22}x_2^{(k)} + a_{23}x_3^{(k-1)} + \cdots + a_{2n}x_n^{(k-1)} &= b_2 \\
& \vdots \\
a_{n1}x_1^{(k-1)} + a_{n2}x_2^{(k-1)} + a_{n3}x_3^{(k-1)} + \cdots + a_{nn}x_n^{(k)} &= b_n.
\end{align*}\]

**Algorithm 1 (Jacobi Method)**

Given \(x^{(0)}\), tolerance \(TOL\), maximum number of iteration \(M\).
Set \(k = 1\).
While \(k \leq M\) and \(\|x - x^{(0)}\|_2 \geq TOL\)
Set \(k = k + 1, x^{(0)} = x\).
For \(i = 1, 2, \ldots, n\)
\[x_i = \left( b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(0)} - \sum_{j=i+1}^{n} a_{ij}x_j^{(0)} \right) / a_{ii} \]
End For
End While
Example 18

Consider the linear system $Ax = b$ given by

\[
E_1 : \quad 10x_1 - x_2 + 2x_3 = 6,
\]
\[
E_2 : \quad -x_1 + 11x_2 - x_3 + 3x_4 = 25,
\]
\[
E_3 : \quad 2x_1 - x_2 + 10x_3 - x_4 = -11,
\]
\[
E_4 : \quad 3x_2 - x_3 + 8x_4 = 15
\]

which has the unique solution $x = [1, 2, -1, 1]^T$.

Solving equation $E_i$ for $x_i$, for $i = 1, 2, 3, 4$, we obtain

\[
x_1 = \frac{1}{10}x_2 - \frac{1}{5}x_3 + \frac{3}{5},
\]
\[
x_2 = \frac{1}{11}x_1 + \frac{1}{11}x_3 - \frac{3}{11}x_4 + \frac{25}{11},
\]
\[
x_3 = -\frac{1}{5}x_1 + \frac{1}{10}x_2 + \frac{1}{10}x_4 - \frac{11}{10},
\]
\[
x_4 = -\frac{3}{8}x_2 + \frac{1}{8}x_3 + \frac{15}{8}.
\]
Then \( Ax = b \) can be rewritten in the form \( x = Tx + c \) with

\[
T = \begin{bmatrix}
0 & 1/10 & -1/5 & 0 \\
1/11 & 0 & 1/11 & -3/11 \\
-1/5 & 1/10 & 0 & 1/10 \\
0 & -3/8 & 1/8 & 0 \\
\end{bmatrix}
\quad \text{and} \quad
c = \begin{bmatrix}
3/5 \\
25/11 \\
-11/10 \\
15/8 \\
\end{bmatrix}
\]

and the iterative formulation for Jacobi method is

\[
x^{(k)} = Tx^{(k-1)} + c \quad \text{for} \quad k = 1, 2, \ldots.
\]

The numerical results of such iteration is list as follows:
<table>
<thead>
<tr>
<th>k</th>
<th>$x_1$</th>
<th>$x_2$</th>
<th>$x_3$</th>
<th>$x_4$</th>
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</tr>
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</table>
Matlab code of Example

clear all; delete rslt.dat; diary rslt.dat; diary on;
n = 4; xold = zeros(n,1); xnew = zeros(n,1); T = zeros(n,n);
T(1,2) = 1/10; T(1,3) = -1/5; T(2,1) = 1/11;
T(2,3) = 1/11; T(2,4) = -3/11; T(3,1) = -1/5;
T(3,2) = 1/10; T(3,4) = 1/10; T(4,2) = -3/8; T(4,3) = 1/8;
c(1,1) = 3/5; c(2,1) = 25/11; c(3,1) = -11/10; c(4,1) = 15/8;
xnew = T * xold + c; k = 0;
fprintf(' k x1 x2 x3 x4
');
while ( k <= 100 & norm(xnew-xold) > 1.0d-14 )
    xold = xnew; xnew = T * xold + c; k = k + 1;
    fprintf('%3.0f ',k);
    for jj = 1:n
        fprintf('%5.4f ',xold(jj));
    end
    fprintf('
');
end
Gauss-Seidel Method

When computing $x_i^{(k)}$ for $i > 1$, $x_1^{(k)}$, $\ldots$, $x_{i-1}^{(k)}$ have already been computed and are likely to be better approximations to the exact $x_1^{(k-1)}$, $\ldots$, $x_{i-1}^{(k-1)}$. It seems reasonable to compute $x_i^{(k)}$ using these most recently computed values. That is

\[
\begin{align*}
\begin{aligned}
    a_{11}x_1^{(k)} + a_{12}x_2^{(k-1)} + a_{13}x_3^{(k-1)} + \cdots + a_{1n}x_n^{(k-1)} &= b_1 \\
    a_{21}x_1^{(k)} + a_{22}x_2^{(k)} + a_{23}x_3^{(k-1)} + \cdots + a_{2n}x_n^{(k-1)} &= b_2 \\
    a_{31}x_1^{(k)} + a_{32}x_2^{(k)} + a_{33}x_3^{(k)} + \cdots + a_{3n}x_n^{(k-1)} &= b_3 \\
    \vdots \\
    a_{n1}x_1^{(k-1)} + a_{n2}x_2^{(k-1)} + a_{n3}x_3^{(k-1)} + \cdots + a_{nn}x_n^{(k)} &= b_n.
\end{aligned}
\end{align*}
\]

This improvement induce the Gauss-Seidel method. The Gauss-Seidel method sets $M = D + L$ and defines the iteration as

\[
x^{(k)} = -(D + L)^{-1}Ux^{(k-1)} + (D + L)^{-1}b.
\]
That is, Gauss-Seidel method uses $TG = -(D + L)^{-1}U$ as the iteration matrix. The formulation above can be rewritten as

$$x^{(k)} = -D^{-1} \left( Lx^{(k)} + Ux^{(k-1)} - b \right).$$

Hence each component $x_i^{(k)}$ can be computed by

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

- For Jacobi method, only the components of $x^{(k-1)}$ are used to compute $x^{(k)}$. Hence $x_i^{(k)}$, $i = 1, \ldots, n$, can be computed in parallel at each iteration $k$.

- At each iteration of Gauss-Seidel method, since $x_i^{(k)}$ cannot be computed until $x_1^{(k)}, \ldots, x_{i-1}^{(k)}$ are available, the method is not a parallel algorithm in nature.
Algorithm 2 (Gauss-Seidel Method)

Given $x^{(0)}$, tolerance $TOL$, maximum number of iteration $M$.
Set $k = 1$.
For $i = 1, 2, \ldots, n$

$$x_i = \left( b_i - \sum_{j=1}^{i-1} a_{ij}x_j - \sum_{j=i+1}^{n} a_{ij}x_j^{(0)} \right) / a_{ii}$$
End For
While $k \leq M$ and $\|x - x^{(0)}\|_2 \geq TOL$
Set $k = k + 1$, $x^{(0)} = x$.
For $i = 1, 2, \ldots, n$

$$x_i = \left( b_i - \sum_{j=1}^{i-1} a_{ij}x_j - \sum_{j=i+1}^{n} a_{ij}x_j^{(0)} \right) / a_{ii}$$
End For
End While
Example 19

Consider the linear system $Ax = b$ given by

- $E_1 : \quad 10x_1 - x_2 + 2x_3 = 6$,
- $E_2 : \quad -x_1 + 11x_2 - x_3 + 3x_4 = 25$,
- $E_3 : \quad 2x_1 - x_2 + 10x_3 - x_4 = -11$,
- $E_4 : \quad 3x_2 - x_3 + 8x_4 = 15$

which has the unique solution $x = [1, 2, -1, 1]^T$.

Gauss-Seidel method gives the equation

\[
\begin{align*}
x^{(k)}_1 &= x^{(k)}_2 - \frac{1}{10} x^{(k-1)}_2 - \frac{1}{5} x^{(k-1)}_3 + \frac{3}{5}, \\
x^{(k)}_2 &= \frac{1}{11} x^{(k)}_1 + \frac{1}{11} x^{(k-1)}_3 - \frac{3}{11} x^{(k-1)}_4 + \frac{25}{11}, \\
x^{(k)}_3 &= -\frac{1}{5} x^{(k)}_1 + \frac{1}{10} x^{(k)}_2 + \frac{3}{10} x^{(k)}_4, \\
x^{(k)}_4 &= -\frac{3}{8} x^{(k)}_2 + \frac{1}{8} x^{(k)}_3 + \frac{15}{8}.
\end{align*}
\]
The numerical results of such iteration is list as follows:

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<td>0.9998</td>
</tr>
<tr>
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<td>1.0001</td>
<td>2.0000</td>
<td>-1.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>

- The results of Example appear to imply that the Gauss-Seidel method is superior to the Jacobi method.
- This is almost always true, but there are linear systems for which the Jacobi method converges and the Gauss-Seidel method does not.
- See Exercises 17 and 18.
Matlab code of Example

clear all; delete rslt.dat; diary rslt.dat; diary on;
n = 4; xold = zeros(n,1); xnew = zeros(n,1); A = zeros(n,n);
A(1,1)=10; A(1,2)=-1; A(1,3)=2; A(2,1)=-1; A(2,2)=11; A(2,3)=-1; A(2,4)=3; A(3,1)=2; A(3,2)=-1;
A(3,3)=10; A(3,4)=-1; A(4,2)=3; A(4,3)=-1; A(4,4)=8; b(1)=6; b(2)=25; b(3)=-11; b(4)=15;
for ii = 1:n
    xnew(ii) = b(ii);
    for jj = 1:ii-1
        xnew(ii) = xnew(ii) - A(ii,jj) * xnew(jj);
    end
    for jj = ii+1:n
        xnew(ii) = xnew(ii) - A(ii,jj) * xold(jj);
    end
    xnew(ii) = xnew(ii) / A(ii,ii);
end
k = 0; fprintf(' k x1 x2 x3 x4 
');
while ( k <= 100 & norm(xnew-xold) > 1.0d-14 )
xold = xnew; k = k + 1;
for ii = 1:n
    xnew(ii) = b(ii);
    for jj = 1:ii-1
        xnew(ii) = xnew(ii) - A(ii,jj) * xnew(jj);
    end
    for jj = ii+1:n
        xnew(ii) = xnew(ii) - A(ii,jj) * xold(jj);
    end
    xnew(ii) = xnew(ii) / A(ii,ii);
end
fprintf('%3.0f ',k);
for jj = 1:n
    fprintf('%5.4f ',xold(jj));
end
fprintf('n');
diary off
Lemma 20 (20)

If $\rho(T) < 1$, then $(I - T)^{-1}$ exists and

$$(I - T)^{-1} = \sum_{i=0}^{\infty} T^i = I + T + T^2 + \cdots.$$ 

Proof: Let $\lambda$ be an eigenvalue of $T$, then $1 - \lambda$ is an eigenvalue of $I - T$. But $|\lambda| \leq \rho(A) < 1$, so $1 - \lambda \neq 0$ and $0$ is not an eigenvalue of $I - T$, which means $(I - T)$ is nonsingular. Next we show that $(I - T)^{-1} = I + T + T^2 + \cdots$. Since

$$(I - T) \left( \sum_{i=0}^{m} T^i \right) = I - T^{m+1},$$

and $\rho(T) < 1$ implies $\|T^m\| \to 0$ as $m \to \infty$, we have

$$(I - T) \left( \lim_{m \to \infty} \sum_{i=0}^{m} T^i \right) = (I - T) \left( \sum_{i=0}^{\infty} T^i \right) = I.$$
Theorem 21

For any \( x^{(0)} \in \mathbb{R}^n \), the sequence produced by

\[
x^{(k)} = Tx^{(k-1)} + c, \quad k = 1, 2, \ldots,
\]

converges to the unique solution of \( x = Tx + c \) if and only if

\[
\rho(T) < 1.
\]

Proof: Suppose \( \rho(T) < 1 \). The sequence of vectors \( x^{(k)} \) produced by the iterative formulation are

\[
\begin{align*}
x^{(1)} &= Tx^{(0)} + c \\
x^{(2)} &= Tx^{(1)} + c = T^2x^{(0)} + (T + I)c \\
x^{(3)} &= Tx^{(2)} + c = T^3x^{(0)} + (T^2 + T + I)c \\
& \vdots
\end{align*}
\]

In general

\[
x^{(k)} = T^k x^{(0)} + (T^{k-1} + T^{k-2} + \cdots + T + I)c.
\]
Since $\rho(T) < 1$, $\lim_{k \to \infty} T^k x^{(0)} = 0$ for any $x^{(0)} \in \mathbb{R}^n$. By Lemma 20,

$$(T^{k-1} + T^{k-2} + \cdots T + I)c \to (I - T)^{-1}c, \quad \text{as} \quad k \to \infty.$$ 

Therefore

$$\lim_{k \to \infty} x^{(k)} = \lim_{k \to \infty} T^k x^{(0)} + \left(\sum_{j=0}^{\infty} T^j \right) c = (I - T)^{-1} c.$$ 

Conversely, suppose $\{x^{(k)}\} \to x = (I - T)^{-1} c$. Since

$$x - x^{(k)} = T x + c - T x^{(k-1)} - c = T (x - x^{(k-1)}) = T^2 (x - x^{(k-2)}) = \cdots = T^k (x - x^{(0)}).$$ 

Let $z = x - x^{(0)}$. Then

$$\lim_{k \to \infty} T^k z = \lim_{k \to \infty} (x - x^{(k)}) = 0.$$ 

It follows from theorem $\rho(T) < 1$. 
Theorem 22

If $\|T\| < 1$, then the sequence $x^{(k)}$ converges to $x$ for any initial $x^{(0)}$ and

1. $\|x - x^{(k)}\| \leq \|T\|^k \|x - x^{(0)}\|

2. $\|x - x^{(k)}\| \leq \frac{\|T\|^k}{1 - \|T\|} \|x^{(1)} - x^{(0)}\|.$

Proof: Since $x =Tx + c$ and $x^{(k)} = Tx^{(k-1)} + c,$

$$x - x^{(k)} = Tx + c - T x^{(k-1)} - c = T(x - x^{(k-1)}) = T^2(x - x^{(k-2)}) = \cdots \cdots = T^k(x - x^{(0)}).$$

The first statement can then be derived

$$\|x - x^{(k)}\| = \|T^k(x - x^{(0)})\| \leq \|T\|^k \|x - x^{(0)}\|.$$

For the second result, we first show that

$$\|x^{(n)} - x^{(n-1)}\| \leq \|T\|^{n-1} \|x^{(1)} - x^{(0)}\| \quad \text{for any} \quad n \geq 1.$$
Since

\[ x^{(n)} - x^{(n-1)} = T x^{(n-1)} + c - T x^{(n-2)} - c \]
\[ = T (x^{(n-1)} - x^{(n-2)}) \]
\[ = T^2 (x^{(n-2)} - x^{(n-3)}) = \ldots \ldots = T^{n-1} (x^{(1)} - x^{(0)}) , \]

we have

\[ \| x^{(n)} - x^{(n-1)} \| \leq \| T \|^n \| x^{(1)} - x^{(0)} \| . \]

Let \( m \geq k \),

\[ x^{(m)} - x^{(k)} \]
\[ = \left( x^{(m)} - x^{(m-1)} \right) + \left( x^{(m-1)} - x^{(m-2)} \right) + \ldots + \left( x^{(k+1)} - x^{(k)} \right) \]
\[ = T^{m-1} (x^{(1)} - x^{(0)}) + T^{m-2} (x^{(1)} - x^{(0)}) + \ldots + T^k (x^{(1)} - x^{(0)}) \]
\[ = \left( T^{m-1} + T^{m-2} + \ldots T^k \right) (x^{(1)} - x^{(0)}) , \]
hence
\[ \|x^{(m)} - x^{(k)}\| \]
\[ \leq \left( \|T\|^{m-1} + \|T\|^{m-2} + \cdots + \|T\|^k \right) \|x^{(1)} - x^{(0)}\| \]
\[ = \|T\|^k \left( \|T\|^{m-k-1} + \|T\|^{m-k-2} + \cdots + 1 \right) \|x^{(1)} - x^{(0)}\|. \]

Since \( \lim_{m \to \infty} x^{(m)} = x \),
\[ \|x - x^{(k)}\| \]
\[ = \lim_{m \to \infty} \|x^{(m)} - x^{(k)}\| \]
\[ \leq \lim_{m \to \infty} \|T\|^k \left( \|T\|^{m-k-1} + \|T\|^{m-k-2} + \cdots + 1 \right) \|x^{(1)} - x^{(0)}\| \]
\[ = \|T\|^k \|x^{(1)} - x^{(0)}\| \lim_{m \to \infty} \left( \|T\|^{m-k-1} + \|T\|^{m-k-2} + \cdots + 1 \right) \]
\[ = \|T\|^k \frac{1}{1 - \|T\|} \|x^{(1)} - x^{(0)}\|. \]

This proves the second result.
Theorem 23

If $A$ is strictly diagonal dominant, then both the Jacobi and Gauss-Seidel methods converges for any initial vector $x^{(0)}$.

Proof: By assumption, $A$ is strictly diagonal dominant, hence $a_{ii} \neq 0$ (otherwise $A$ is singular) and

$$|a_{ii}| > \sum_{j=1, j \neq i}^{n} |a_{ij}|, \quad i = 1, 2, \ldots, n.$$ 

For Jacobi method, the iteration matrix $T_J = -D^{-1}(L + U)$ has entries

$$[T_J]_{ij} = \begin{cases} -\frac{a_{ij}}{a_{ii}}, & i \neq j, \\ 0, & i = j. \end{cases}$$

Hence

$$\|T_J\|_{\infty} = \max_{1 \leq i \leq n} \sum_{j=1, j \neq i}^{n} \left| \frac{a_{ij}}{a_{ii}} \right| = \max_{1 \leq i \leq n} \frac{1}{|a_{ii}|} \sum_{j=1, j \neq i}^{n} |a_{ij}| < 1,$$

and this implies that the Jacobi method converges.
For Gauss-Seidel method, the iteration matrix 

\[ T_G = -(D + L)^{-1}U. \]

Let \( \lambda \) be any eigenvalue of \( T_G \) and \( y, \parallel y \parallel_\infty = 1 \), is a corresponding eigenvector. Thus

\[ T_G y = \lambda y \quad \implies \quad -U y = \lambda (D + L)y. \]

Hence for \( i = 1, \ldots, n \),

\[
- \sum_{j=i+1}^{n} a_{ij} y_j = \lambda a_{ii} y_i + \lambda \sum_{j=1}^{i-1} a_{ij} y_j.
\]

This gives

\[
\lambda a_{ii} y_i = -\lambda \sum_{j=1}^{i-1} a_{ij} y_j - \sum_{j=i+1}^{n} a_{ij} y_j
\]

and

\[
|\lambda| |a_{ii}| |y_i| \leq |\lambda| \sum_{j=1}^{i-1} |a_{ij}| |y_j| + \sum_{j=i+1}^{n} |a_{ij}| |y_j|.
\]
Choose the index \( k \) such that \(|y_k| = 1 \geq |y_j|\) (this index can always be found since \( \|y\|_{\infty} = 1 \)). Then

\[
|\lambda| |a_{kk}| \leq |\lambda| \sum_{j=1}^{k-1} |a_{kj}| + \sum_{j=k+1}^{n} |a_{kj}|
\]

which gives

\[
|\lambda| \leq \frac{\sum_{j=k+1}^{n} |a_{kj}|}{|a_{kk}| - \sum_{j=1}^{k-1} |a_{kj}|} < \frac{\sum_{j=k+1}^{n} |a_{kj}|}{\sum_{j=k+1}^{n} |a_{kj}|} = 1
\]

Since \( \lambda \) is arbitrary, \( \rho(T_G) < 1 \). This means the Gauss-Seidel method converges.

- The rate of convergence depends on the spectral radius of the matrix associated with the method.
- One way to select a procedure to accelerate convergence is to choose a method whose associated matrix has minimal spectral radius.
Successive over-relaxation (SOR) method

**Definition 24**

Suppose \( \tilde{x} \in \mathbb{R}^n \) is an approximated solution of \( Ax = b \). The residual vector \( r \) for \( \tilde{x} \) is \( r = b - A\tilde{x} \).

Let the approximate solution \( x^{(k,i)} \) produced by Gauss-Seidel method be defined by

\[
x^{(k,i)} = \begin{bmatrix} x^{(k)}_1, \ldots, x^{(k)}_{i-1}, x^{(k)}_i, \ldots, x^{(k-1)}_n \end{bmatrix}^T
\]

and

\[
r^{(k)}_i = \begin{bmatrix} r^{(k)}_{1i}, r^{(k)}_{2i}, \ldots, r^{(k)}_{ni} \end{bmatrix}^T = b - Ax^{(k,i)}
\]

be the corresponding residual vector. Then the \( m \)th component of \( r^{(k)}_i \) is

\[
r^{(k)}_{mi} = b_m - \sum_{j=1}^{i-1} a_{mj} x^{(k)}_j - \sum_{j=i}^{n} a_{mj} x^{(k-1)}_j,
\]
or, equivalently,

\[ r_{mi}^{(k)} = b_m - \sum_{j=1}^{i-1} a_{mj} x_j^{(k)} - \sum_{j=i+1}^{n} a_{mj} x_j^{(k-1)} - a_{mi} x_i^{(k-1)}, \]

for each \( m = 1, 2, \ldots, n \).

In particular, the \( i \)th component of \( r_i^{(k)} \) is

\[ r_{ii}^{(k)} = b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k-1)} - a_{ii} x_i^{(k-1)}, \]

so

\[ a_{ii} x_i^{(k-1)} + r_{ii}^{(k)} = b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k-1)} \]

\[ = a_{ii} x_i^{(k)}. \]
Consequently, the Gauss-Seidel method can be characterized as choosing $x_i^{(k)}$ to satisfy

$$x_i^{(k)} = x_i^{(k-1)} + \frac{r_{ii}^{(k)}}{a_{ii}}.$$ 

Relaxation method is modified the Gauss-Seidel procedure to

$$x_i^{(k)} = x_i^{(k-1)} + \omega \frac{r_{ii}^{(k)}}{a_{ii}}$$

$$= x_i^{(k-1)} + \frac{\omega}{a_{ii}} \left[ b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k-1)} - a_{ii} x_i^{(k-1)} \right]$$

$$= (1 - \omega) x_i^{(k-1)} + \frac{\omega}{a_{ii}} \left[ b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(k)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(k-1)} \right]$$

(1)

for certain choices of positive $\omega$ such that the norm of the residual vector is reduced and the convergence is significantly faster.
These methods are called for
\[ \omega < 1: \text{ under relaxation,} \]
\[ \omega = 1: \text{ Gauss-Seidel method,} \]
\[ \omega > 1: \text{ over relaxation.} \]

Over-relaxation methods are called SOR (Successive over-relaxation). To determine the matrix of the SOR method, we rewrite (1) as

\[ a_{ii}x_i^{(k)} + \omega \sum_{j=1}^{i-1} a_{ij}x_j^{(k)} = (1 - \omega)a_{ii}x_i^{(k-1)} - \omega \sum_{j=i+1}^{n} a_{ij}x_j^{(k-1)} + \omega b_i, \]

so that if \( A = L + D + U \), then we have

\[ (D + \omega L)x^{(k)} = [(1 - \omega)D - \omega U]x^{(k-1)} + \omega b \]

or

\[ x^{(k)} = (D + \omega L)^{-1} [(1 - \omega)D - \omega U]x^{(k-1)} + \omega (D + \omega L)^{-1}b \]

\[ \equiv T_\omega x^{(k-1)} + c_\omega. \]
Example 25

The linear system $Ax = b$ given by

\begin{align*}
4x_1 + 3x_2 &= 24, \\
3x_1 + 4x_2 - x_3 &= 30, \\
-x_2 + 4x_3 &= -24,
\end{align*}

has the solution $[3, 4, -5]^T$.

- Numerical results of Gauss-Seidel method with $x^{(0)} = [1, 1, 1]^T$:

<table>
<thead>
<tr>
<th>k</th>
<th>$x_1$</th>
<th>$x_2$</th>
<th>$x_3$</th>
</tr>
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</tr>
<tr>
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<td>3.8125000</td>
<td>-5.0468750</td>
</tr>
<tr>
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<td>-5.0292969</td>
</tr>
<tr>
<td>3</td>
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<td>-5.0183105</td>
</tr>
<tr>
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<td>-5.0114441</td>
</tr>
<tr>
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<td>3.0343323</td>
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<td>-5.0071526</td>
</tr>
<tr>
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<td>3.9821186</td>
<td>-5.0044703</td>
</tr>
<tr>
<td>7</td>
<td>3.0134110</td>
<td>3.9888241</td>
<td>-5.0027940</td>
</tr>
</tbody>
</table>
Numerical results of SOR method with $\omega = 1.25$ and $x^{(0)} = [1, 1, 1]^T$:

<table>
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<tr>
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<th>$x_1$</th>
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<th>$x_3$</th>
</tr>
</thead>
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<td>1.0000000</td>
<td>1.0000000</td>
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<tr>
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<td>-4.6004238</td>
</tr>
<tr>
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<td>-5.0966863</td>
</tr>
<tr>
<td>4</td>
<td>2.9570512</td>
<td>4.0074838</td>
<td>-4.9734897</td>
</tr>
<tr>
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<td>-5.0057135</td>
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<tr>
<td>6</td>
<td>2.9963276</td>
<td>4.0009262</td>
<td>-4.9982822</td>
</tr>
<tr>
<td>7</td>
<td>3.0000498</td>
<td>4.0002586</td>
<td>-5.0003486</td>
</tr>
</tbody>
</table>
Numerical results of SOR method with $\omega = 1.6$ and $x^{(0)} = [1, 1, 1]^T$:

<table>
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<td>7</td>
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</tbody>
</table>
Matlab code of SOR

clear all; delete rslt.dat; diary rslt.dat; diary on;
n = 3; xold = zeros(n,1); xnew = zeros(n,1); A = zeros(n,n); DL = zeros(n,n); DU = zeros(n,n);
A(1,1)=4; A(1,2)=3; A(2,1)=3; A(2,2)=4; A(2,3)=-1; A(3,2)=-1; A(3,3)=4;
b(1,1)=24; b(2,1)=30; b(3,1)=-24; omega=1.25;

for ii = 1:n
    DL(ii,ii) = A(ii,ii);
    for jj = 1:ii-1
        DL(ii,jj) = omega * A(ii,jj);
    end
    DU(ii,ii) = (1-omega)*A(ii,ii);
    for jj = ii+1:n
        DU(ii,jj) = -omega * A(ii,jj);
    end
end

c = omega * (DL \ b); xnew = DL \ ( DU * xold ) + c;
k = 0; fprintf(' k x1 x2 x3 
');
while ( k <= 100 & norm(xnew-xold) > 1.0d-14 )
    xold = xnew; k = k + 1; xnew = DL \ ( DU * xold ) + c;
    fprintf('%3.0f ',k);
    for jj = 1:n
        fprintf('%5.4f ',xold(jj));
    end
    fprintf(' 
');
end

diary off
Theorem 26 (Kahan)

If \( a_{ii} \neq 0 \), for each \( i = 1, 2, \ldots, n \), then \( \rho(T_\omega) \geq |\omega - 1| \). This implies that the SOR method can converge only if \( 0 < \omega < 2 \).

Theorem 27 (Ostrowski-Reich)

If \( A \) is positive definite and the relaxation parameter \( \omega \) satisfying \( 0 < \omega < 2 \), then the SOR iteration converges for any initial vector \( x^{(0)} \).

Theorem 28

If \( A \) is positive definite and tridiagonal, then \( \rho(T_G) = [\rho(T_J)]^2 < 1 \) and the optimal choice of \( \omega \) for the SOR iteration is

\[
\omega = \frac{2}{1 + \sqrt{1 - [\rho(T_J)]^2}}.
\]

With this choice of \( \omega \), \( \rho(T_\omega) = \omega - 1 \).
Example 29

The matrix

\[
A = \begin{bmatrix}
4 & 3 & 0 \\
3 & 4 & -1 \\
0 & -1 & 4 \\
\end{bmatrix},
\]

given in previous example, is positive definite and tridiagonal.

Since

\[
T_J = -D^{-1}(L + U) = \begin{bmatrix}
\frac{1}{4} & 0 & 0 \\
0 & \frac{1}{4} & 0 \\
0 & 0 & \frac{1}{4} \\
\end{bmatrix} \begin{bmatrix}
0 & -3 & 0 \\
-3 & 0 & 1 \\
0 & 1 & 0 \\
\end{bmatrix}
\]

\[
= \begin{bmatrix}
0 & -0.75 & 0 \\
-0.75 & 0 & 0.25 \\
0 & 0.25 & 0 \\
\end{bmatrix},
\]
we have

\[ T_J - \lambda I = \begin{bmatrix} -\lambda & -0.75 & 0 \\ -0.75 & -\lambda & 0.25 \\ 0 & 0.25 & -\lambda \end{bmatrix}, \]

so

\[ \det(T_J - \lambda I) = -\lambda(\lambda^2 - 0.625). \]

Thus,

\[ \rho(T_J) = \sqrt{0.625} \]

and

\[ \omega = \frac{2}{1 + \sqrt{1 - [\rho(T_J)]^2}} = \frac{2}{1 + \sqrt{1 - 0.625}} \approx 1.24. \]

This explains the rapid convergence obtained in previous example when using \( \omega = 0.125 \).
Symmetric Successive Over Relaxation (SSOR) Method

Let $A$ be symmetric and $A = D + L + L^T$. The idea is in fact to implement the SOR formulation twice, one forward and one backward, at each iteration. That is, SSOR method defines

$$\begin{align*}
(D + \omega L)x^{(k-\frac{1}{2})} &= [(1 - \omega)D - \omega L^T]x^{(k-1)} + \omega b, \
(D + \omega L^T)x^{(k)} &= [(1 - \omega)D - \omega L]x^{(k-\frac{1}{2})} + \omega b.
\end{align*}$$

Define

$$\begin{align*}
M_\omega &:= D + \omega L, \\
N_\omega &:= (1 - \omega)D - \omega L^T.
\end{align*}$$

Then from the iterations (2) and (3), it follows that

$$\begin{align*}
x^{(k)} &= (M_\omega^{-T}N_\omega^TN_\omega^{-1}N_\omega)x^{(k-1)} + \omega (M_\omega^{-T}N_\omega^T M_\omega^{-1} + M_\omega^{-T})b, \\
&\equiv T(\omega)x^{(k-1)} + M(\omega)^{-1}b.
\end{align*}$$
But

\[
((1 - \omega)D - \omega L) (D + \omega L)^{-1} + I
= (-\omega L - D - \omega D + 2D)(D + \omega L)^{-1} + I
= -I + (2 - \omega)D(D + \omega L)^{-1} + I
= (2 - \omega)D(D + \omega L)^{-1}.
\]

Thus

\[
M(\omega)^{-1} = \omega \left( D + \omega L^T \right)^{-1} (2 - \omega)D(D + \omega L)^{-1},
\]

then the splitting matrix is

\[
M(\omega) = \frac{1}{\omega(2 - \omega)}(D + \omega L)D^{-1} \left( D + \omega L^T \right).
\]

The iteration matrix is

\[
T(\omega) = (D + \omega L^T)^{-1} \left[ (1 - \omega)D - \omega L \right] (D + \omega L)^{-1} \left[ (1 - \omega)D - \omega L^T \right].
\]
Error bounds and iterative refinement

Example 30

The linear system $Ax = b$ given by

$$
\begin{bmatrix}
1 & 2 \\
1.0001 & 2
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2
\end{bmatrix} =
\begin{bmatrix}
3 \\
3.0001
\end{bmatrix}
$$

has the unique solution $x = [1, 1]^T$.

The poor approximation $\tilde{x} = [3, 0]^T$ has the residual vector

$$
r = b - A\tilde{x} =
\begin{bmatrix}
3 \\
3.0001
\end{bmatrix} -
\begin{bmatrix}
1 & 2 \\
1.0001 & 2
\end{bmatrix}
\begin{bmatrix}
3 \\
0
\end{bmatrix} =
\begin{bmatrix}
0 \\
-0.0002
\end{bmatrix},
$$

so $\|r\|_\infty = 0.0002$. Although the norm of the residual vector is small, the approximation $\tilde{x} = [3, 0]^T$ is obviously quite poor; in fact, $\|x - \tilde{x}\|_\infty = 2$. 
The solution of above example represents the intersection of the lines

\[ \ell_1 : x_1 + 2x_2 = 3 \quad \text{and} \quad \ell_2 : 1.0001x_1 + 2x_2 = 3.0001. \]

\( \ell_1 \) and \( \ell_2 \) are nearly parallel. The point \((3, 0)\) lies on \( \ell_1 \) which implies that \((3, 0)\) also lies close to \( \ell_2 \), even though it differs significantly from the intersection point \((1, 1)\).
Theorem 31

Suppose that $\tilde{x}$ is an approximate solution of $Ax = b$, $A$ is nonsingular matrix and $r = b - A\tilde{x}$. Then

$$\|x - \tilde{x}\| \leq \|r\| \cdot \|A^{-1}\|$$

and if $x \neq 0$ and $b \neq 0$,

$$\frac{\|x - \tilde{x}\|}{\|x\|} \leq \|A\| \cdot \|A^{-1}\| \frac{\|r\|}{\|b\|}.$$  

Proof: Since

$$r = b - A\tilde{x} = Ax - A\tilde{x} = A(x - \tilde{x})$$

and $A$ is nonsingular, we have

$$\|x - \tilde{x}\| = \|A^{-1}r\| \leq \|A^{-1}\| \cdot \|r\|. \quad (4)$$

Moreover, since $b = Ax$, we have

$$\|b\| \leq \|A\| \cdot \|x\|. $$
It implies that

\[ \frac{1}{\|x\|} \leq \frac{\|A\|}{\|b\|}. \quad (5) \]

Combining Equations (4) and (5), we have

\[ \frac{\|x - \tilde{x}\|}{\|x\|} \leq \frac{\|A\| \cdot \|A^{-1}\|}{\|b\|} \|r\|. \]

**Definition 32 (Condition number)**

The condition number of nonsingular matrix \( A \) is

\[ \kappa(A) = \|A\| \cdot \|A^{-1}\|. \]

For any nonsingular matrix \( A \),

\[ 1 = \|I\| = \|A \cdot A^{-1}\| \leq \|A\| \cdot \|A^{-1}\| = \kappa(A). \]
Definition 33

A matrix $A$ is **well-conditioned** if $\kappa(A)$ is close to 1, and is **ill-conditioned** when $\kappa(A)$ is significantly greater than 1.

In previous example,

$$A = \begin{bmatrix} 1 & 2 \\ 1.0001 & 2 \end{bmatrix}.$$

Since

$$A^{-1} = \begin{bmatrix} -10000 & 10000 \\ 5000.5 & -5000 \end{bmatrix},$$

we have

$$\kappa(A) = \| A \|_\infty \cdot \| A^{-1} \|_\infty = 3.0001 \times 20000 = 60002 \gg 1.$$
How to estimate the effective condition number in $t$-digit arithmetic without having to invert the matrix $A$?

- If the approximate solution $\tilde{x}$ of $Ax = b$ is being determined using $t$-digit arithmetic and Gaussian elimination, then

$$\|r\| = \|b - A\tilde{x}\| \approx 10^{-t}\|A\| \cdot \|\tilde{x}\|.$$ 

- All the arithmetic operations in Gaussian elimination technique are performed using $t$-digit arithmetic, but the residual vector $r$ are done in double-precision (i.e., $2t$-digit) arithmetic.

- Use the Gaussian elimination method which has already been calculated to solve

$$Ay = r.$$ 

Let $\tilde{y}$ be the approximate solution.
Then
\[ \tilde{y} \approx A^{-1}r = A^{-1}(b - A\tilde{x}) = x - \tilde{x} \]
and
\[ x \approx \tilde{x} + \tilde{y}. \]

Moreover,
\[
\|\tilde{y}\| \approx \|x - \tilde{x}\| = \|A^{-1}r\| \\
\leq \|A^{-1}\| \cdot \|r\| \approx \|A^{-1}\|(10^{-t}\|A\| \cdot \|\tilde{x}\|) = 10^{-t}\|\tilde{x}\|\kappa(A). \\
\]

It implies that
\[ \kappa(A) \approx \frac{\|\tilde{y}\|}{\|\tilde{x}\|} 10^t. \]

Iterative refinement

In general, \( \tilde{x} + \tilde{y} \) is a more accurate approximation to the solution of \( Ax = b \) than \( \tilde{x} \).
Algorithm 3 (Iterative refinement)

Given tolerance $TOL$, maximum number of iteration $M$, number of digits of precision $t$.

Solve $Ax = b$ by using Gaussian elimination in $t$-digit arithmetic.

Set $k = 1$

while ($k \leq M$)

    Compute $r = b - Ax$ in $2t$-digit arithmetic.

    Solve $Ay = r$ by using Gaussian elimination in $t$-digit arithmetic.

    If $\|y\|_\infty < TOL$, then stop.

    Set $k = k + 1$ and $x = x + y$.

End while
Example 34

The linear system given by

\[
\begin{bmatrix}
3.3330 & 15920 & -10.333 \\
2.2220 & 16.710 & 9.6120 \\
1.5611 & 5.1791 & 1.6852
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3
\end{bmatrix}
= 
\begin{bmatrix}
15913 \\
28.544 \\
8.4254
\end{bmatrix}
\]

has the exact solution \( x = [1, 1, 1]^T \).

Using Gaussian elimination and five-digit rounding arithmetic leads successively to the augmented matrices

\[
\begin{bmatrix}
3.3330 & 15920 & -10.333 & 15913 \\
0 & -10596 & 16.501 & -10580 \\
0 & -7451.4 & 6.5250 & -7444.9
\end{bmatrix}
\]

and

\[
\begin{bmatrix}
3.3330 & 15920 & -10.333 & 15913 \\
0 & -10596 & 16.501 & -10580 \\
0 & 0 & -5.0790 & -4.7000
\end{bmatrix}
\]
The approximate solution is

\[ \tilde{x}^{(1)} = [1.2001, 0.99991, 0.92538]^T. \]

The residual vector corresponding to \( \tilde{x} \) is computed in double precision to be

\[
\begin{align*}
r^{(1)} & = b - A\tilde{x}^{(1)} \\
& = \begin{bmatrix}
15913 \\
28.544 \\
8.4254
\end{bmatrix} - \begin{bmatrix}
3.3330 & 15920 & -10.333 \\
2.2220 & 16.710 & 9.6120 \\
1.5611 & 5.1791 & 1.6852
\end{bmatrix} \begin{bmatrix}
1.2001 \\
0.99991 \\
0.92538
\end{bmatrix} \\
& = \begin{bmatrix}
15913 \\
28.544 \\
8.4254
\end{bmatrix} - \begin{bmatrix}
15913.00518 \\
28.26987086 \\
8.611560367
\end{bmatrix} \\
& = \begin{bmatrix}
-0.00518 \\
0.27412914 \\
-0.186160367
\end{bmatrix}.
\end{align*}
\]

Hence the solution of \( Ay = r^{(1)} \) to be

\[ \tilde{y}^{(1)} = [-0.20008, 8.9987 \times 10^{-5}, 0.074607]^T \]

and the new approximate solution \( x^{(2)} \) is

\[ x^{(2)} = x^{(1)} + \tilde{y}^{(1)} = [1.0000, 1.0000, 0.99999]^T. \]
Using the suggested stopping technique for the algorithm, we compute $r^{(2)} = b - A\tilde{x}^{(2)}$ and solve the system $Ay^{(2)} = r^{(2)}$, which gives

$$\tilde{y}^{(2)} = [1.5002 \times 10^{-9}, 2.0951 \times 10^{-10}, 1.0000 \times 10^{-5}]^T.$$ 

Since

$$\|\tilde{y}^{(2)}\|_\infty \leq 10^{-5},$$

we conclude that

$$\tilde{x}^{(3)} = \tilde{x}^{(2)} + \tilde{y}^{(2)} = [1.0000, 1.0000, 1.0000]^T$$

is sufficiently accurate.

In the linear system

$$Ax = b,$$

$A$ and $b$ can be represented exactly. Realistically, the matrix $A$ and vector $b$ will be perturbed by $\delta A$ and $\delta b$, respectively, causing the linear system

$$(A + \delta A)x = b + \delta b$$

to be solved in place of $Ax = b$. 
Theorem 35
Suppose $A$ is nonsingular and
\[ \| \delta A \| < \frac{1}{\| A^{-1} \|} . \]
Then the solution $\tilde{x}$ of $(A + \delta A)\tilde{x} = b + \delta b$ approximates the solution $x$ of $Ax = b$ with the error estimate
\[ \frac{\| x - \tilde{x} \|}{\| x \|} \leq \frac{\kappa(A)}{1 - \kappa(A)(\| \delta A \|/\| A \|)} \left( \frac{\| \delta b \|}{\| b \|} + \frac{\| \delta A \|}{\| A \|} \right) . \]

- If $A$ is well-conditioned, then small changes in $A$ and $b$ produce correspondingly small changes in the solution $x$.
- If $A$ is ill-conditioned, then small changes in $A$ and $b$ may produce large changes in $x$. 
The conjugate gradient method

Consider the linear systems

\[ Ax = b \]

where \( A \) is large sparse and symmetric positive definite. Define the inner product notation

\[ \langle x, y \rangle = x^T y \text{ for any } x, y \in \mathbb{R}^n. \]

**Theorem 36**

Let \( A \) be symmetric positive definite. Then \( x^* \) is the solution of \( Ax = b \) if and only if \( x^* \) minimizes

\[ g(x) = \langle x, Ax \rangle - 2 \langle x, b \rangle. \]
**Proof:**

(“⇒”) Rewrite $g(x)$ as

\[
g(x) = \langle x - x^*, A(x - x^*) \rangle + \langle x, Ax^* \rangle + \langle x^*, Ax \rangle \\
- \langle x^*, Ax^* \rangle - 2 \langle x, b \rangle \\
= \langle x - x^*, A(x - x^*) \rangle - \langle x^*, Ax^* \rangle \\
+ 2 \langle x, Ax^* \rangle - 2 \langle x, b \rangle \\
= \langle x - x^*, A(x - x^*) \rangle - \langle x^*, Ax^* \rangle + 2 \langle x, Ax^* - b \rangle.
\]

Suppose that $x^*$ is the solution of $Ax = b$, i.e., $Ax^* = b$. Then

\[
g(x) = \langle x - x^*, A(x - x^*) \rangle - \langle x^*, Ax^* \rangle
\]

which minimum occurs at $x = x^*$. 
("\Leftarrow") Fixed vectors \( x \) and \( v \), for any \( \alpha \in \mathbb{R} \),

\[
f(\alpha) \equiv g(x + \alpha v)
\]

\[
= \langle x + \alpha v, Ax + \alpha Av \rangle - 2 \langle x + \alpha v, b \rangle
\]

\[
= \langle x, Ax \rangle + \alpha \langle v, Ax \rangle + \alpha \langle x, Av \rangle + \alpha^2 \langle v, Av \rangle - 2 \langle x, b \rangle - 2\alpha \langle v, b \rangle
\]

\[
= \langle x, Ax \rangle - 2 \langle x, b \rangle + 2\alpha \langle v, Ax \rangle - 2\alpha \langle v, b \rangle + \alpha^2 \langle v, Av \rangle
\]

\[
= g(x) + 2\alpha \langle v, Ax - b \rangle + \alpha^2 \langle v, Av \rangle.
\]

Because \( f \) is a quadratic function of \( \alpha \) and \( \langle v, Av \rangle \) is positive, \( f \) has a minimal value when \( f'(\alpha) = 0 \). Since

\[
f'(\alpha) = 2 \langle v, Ax - b \rangle + 2\alpha \langle v, Av \rangle,
\]

the minimum occurs at

\[
\hat{\alpha} = -\frac{\langle v, Ax - b \rangle}{\langle v, Av \rangle} = \frac{\langle v, b - Ax \rangle}{\langle v, Av \rangle}.
\]
and

$$g(x + \hat{\alpha}v) = f(\hat{\alpha}) = g(x) - 2 \frac{\langle v, b - Ax \rangle}{\langle v, Av \rangle} \langle v, b - Ax \rangle$$

$$+ \left( \frac{\langle v, b - Ax \rangle}{\langle v, Av \rangle} \right)^2 \langle v, Av \rangle$$

$$= g(x) - \frac{\langle v, b - Ax \rangle^2}{\langle v, Av \rangle}.$$

So, for any nonzero vector $v$, we have

$$g(x + \hat{\alpha}v) < g(x) \text{ if } \langle v, b - Ax \rangle \neq 0 \quad (6)$$

and

$$g(x + \hat{\alpha}v) = g(x) \text{ if } \langle v, b - Ax \rangle = 0. \quad (7)$$

Suppose that $x^*$ is a vector that minimizes $g$. Then

$$g(x^* + \hat{\alpha}v) \geq g(x^*) \text{ for any } v. \quad (8)$$
From (6), (7) and (8), we have

\[ < v, b - Ax^* > = 0 \quad \text{for any} \quad v, \]

which implies that \( Ax^* = b. \)

Let

\[ r = b - Ax. \]

Then

\[ \alpha = \frac{< v, b - Ax >}{< v, Av >} = \frac{< v, r >}{< v, Av >}. \]

If \( r \neq 0 \) and if \( v \) and \( r \) are not orthogonal, then

\[ g(x + \alpha v) < g(x) \]

which implies that \( x + \alpha v \) is closer to \( x^* \) than is \( x. \)
Let \( x^{(0)} \) be an initial approximation to \( x^* \) and \( v^{(1)} \neq 0 \) be an initial search direction. For \( k = 1, 2, 3, \ldots, \) we compute

\[
\alpha_k = \frac{\langle v^{(k)}, b - Ax^{(k-1)} \rangle}{\langle v^{(k)}, Av^{(k)} \rangle},
\]

\[
x^{(k)} = x^{(k-1)} + \alpha_k v^{(k)}
\]

and choose a new search direction \( v^{(k+1)} \).

**Question:** How to choose \( \{v^{(k)}\} \) such that \( \{x^{(k)}\} \) converges rapidly to \( x^* \)?

Let \( \Phi : \mathbb{R}^n \to \mathbb{R} \) be a differential function on \( x \). Then it holds

\[
\frac{\Phi(x + \varepsilon p) - \Phi(x)}{\varepsilon} = \nabla \Phi(x)^T p + O(\varepsilon).
\]

The right hand side takes minimum at

\[
p = -\frac{\nabla \Phi(x)}{\|\nabla \Phi(x)\|} \quad \text{(i.e., the largest descent)}
\]

for all \( p \) with \( \|p\| = 1 \) (neglect \( O(\varepsilon) \)).
Denote $x = [x_1, x_2, \ldots, x_n]^T$. Then

$$g(x) = \langle x, Ax \rangle - 2 \langle x, b \rangle = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} x_i x_j - 2 \sum_{i=1}^{n} x_i b_i.$$ 

It follows that

$$\frac{\partial g}{\partial x_k}(x) = 2 \sum_{i=1}^{n} a_{ki} x_i - 2b_k, \text{ for } k = 1, 2, \ldots, n.$$ 

Therefore, the gradient of $g$ is

$$\nabla g(x) = \left[ \frac{\partial g}{\partial x_1}(x), \frac{\partial g}{\partial x_2}(x), \ldots, \frac{\partial g}{\partial x_n}(x) \right]^T = 2(Ax - b) = -2r.$$
Steepest descent method (gradient method)

Given an initial $x_0 \neq 0$.
For $k = 1, 2, \ldots$

$$r_{k-1} = b - Ax_{k-1}$$

If $r_{k-1} = 0$, then stop;
else $\alpha_k = \frac{r_{k-1}^T r_k}{r_{k-1}^T Ar_{k-1}}$, $x_k = x_{k-1} + \alpha_k r_{k-1}$.
End for

Theorem 37

If $x_k, x_{k-1}$ are two approximations of the steepest descent method for solving $Ax = b$ and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n > 0$ are the eigenvalues of $A$, then it holds:

$$\|x_k - x^*\|_A \leq \left(\frac{\lambda_1 - \lambda_n}{\lambda_1 + \lambda_n}\right) \|x_{k-1} - x^*\|_A,$$

where $\|x\|_A = \sqrt{x^T Ax}$. Thus the gradient method is convergent.
If the condition number of $A (\lambda_1 / \lambda_n)$ is large, then
\[ \frac{\lambda_1 - \lambda_n}{\lambda_1 + \lambda_n} \approx 1. \]
The gradient method converges very slowly. Hence this method is not recommendable.

It is favorable to choose that the search directions $\{v^{(i)}\}$ as mutually $A$-conjugate, where $A$ is symmetric positive definite.

**Definition 38**

Two vectors $p$ and $q$ are called $A$-conjugate ($A$-orthogonal), if $p^T A q = 0$. 
Lemma 39

Let \( v_1, \ldots, v_n \neq 0 \) be pairwisely \( A\)-conjugate. Then they are linearly independent.

Proof: From

\[
0 = \sum_{j=1}^{n} c_j v_j
\]

follows that

\[
0 = (v_k)^T A \left( \sum_{j=1}^{n} c_j v_j \right) = \sum_{j=1}^{n} c_j (v_k)^T A v_j = c_k (v_k)^T A v_k,
\]

so \( c_k = 0 \), for \( k = 1, \ldots, n \).
Theorem 40

Let $A$ be symm. positive definite and $v_1, \ldots, v_n \in \mathbb{R}^n \setminus \{0\}$ be pairwisely $A$-orthogonal. Give $x_0$ and let $r_0 = b - Ax_0$. For $k = 1, \ldots, n$, let

$$\alpha_k = \frac{\langle v_k, b - Ax_{k-1} \rangle}{\langle v_k, Av_k \rangle} \quad \text{and} \quad x_k = x_{k-1} + \alpha_k v_k.$$

Then $Ax_n = b$ and

$$\langle b - Ax_k, v_j \rangle \geq 0, \quad \text{for each} \quad j = 1, 2, \ldots, k - 1.$$

Proof: Since, for each $k = 1, 2, \ldots, n$,

$$x_k = x_{k-1} + \alpha_k v_k,$$

we have

$$Ax_n = Ax_{n-1} + \alpha_n Av_n = (Ax_{n-2} + \alpha_{n-1} Av_{n-1}) + \alpha_n Av_n = \cdots$$

$$= Ax_0 + \alpha_1 Av_1 + \alpha_2 Av_2 + \cdots + \alpha_n Av_n.$$
It implies that

\[
< Ax_n - b, v_k > \\
= < Ax_0 - b, v_k > + \alpha_1 < Av_1, v_k > + \cdots + \alpha_n < Av_n, v_k > \\
= < Ax_0 - b, v_k > + \alpha_1 < v_1, Av_k > + \cdots + \alpha_n < v_n, Av_k > \\
= < Ax_0 - b, v_k > + \alpha_k < v_k, Av_k > \\
= < Ax_0 - b, v_k > + \frac{< v_k, b - Ax_{k-1} >}{< v_k, Av_k >} < v_k, Av_k > \\
= < Ax_0 - b, v_k > + < v_k, b - Ax_{k-1} > \\
= < Ax_0 - b, v_k > \\
+ < v_k, b - Ax_0 + Ax_0 - Ax_1 + \cdots - Ax_{k-2} + Ax_{k-2} - Ax_{k-1} > \\
= < Ax_0 - b, v_k > + < v_k, b - Ax_0 > + < v_k, Ax_0 - Ax_1 > \\
+ \cdots + < v_k, Ax_{k-2} - Ax_{k-1} > \\
= < v_k, Ax_0 - Ax_1 > + \cdots + < v_k, Ax_{k-2} - Ax_{k-1} > .
\]
For any $i$

$$x_i = x_{i-1} + \alpha_i v_i \quad \text{and} \quad Ax_i = Ax_{i-1} + \alpha_i Av_i,$$

we have

$$Ax_{i-1} - Ax_i = -\alpha_i Av_i.$$ 

Thus, for $k = 1, \ldots, n$,

$$< Ax_n - b, v_k > = -\alpha_1 < v_k, Av_1 > - \cdots - \alpha_{k-1} < v_k, Av_{k-1} > = 0$$

which implies that $Ax_n = b$.

Suppose that

$$< r_{k-1}, v_j >= 0 \quad \text{for} \quad j = 1, 2, \ldots, k - 1. \quad (9)$$

By the result

$$r_k = b - Ax_k = b - A(x_{k-1} + \alpha_k v_k) = r_{k-1} - \alpha_k Av_k$$
it follows that

\[ < r_k, v_k > = < r_{k-1}, v_k > - \alpha_k < Av_k, v_k > \]

\[ = < r_{k-1}, v_k > - \frac{< v_k, b - Ax_{k-1} >}{< v_k, Av_k >} < Av_k, v_k > \]

\[ = 0. \]

From assumption (9) and \( A \)-orthogonality, for \( j = 1, \ldots, k - 1 \)

\[ < r_k, v_j > = < r_{k-1}, v_j > - \alpha_k < Av_k, v_j > = 0 \]

which is completed the proof by the mathematic induction.

\[ \square \]

Method of conjugate directions:

Let \( A \) be symmetric positive definite, \( b, x_0 \in \mathbb{R}^n \). Given

\( v_1, \ldots, v_n \in \mathbb{R}^n \backslash \{0\} \) pairwisely \( A \)-orthogonal.

\[ r_0 = b - Ax_0, \]

For \( k = 1, \ldots, n, \)

\[ \alpha_k = \frac{< v_k, r_{k-1} >}{< v_k, Av_k >}, \]

\[ x_k = x_{k-1} + \alpha_k v_k, \]

\[ r_k = r_{k-1} - \alpha_k Av_k = b - Ax_k. \]
Practical Implementation

- In $k$-th step a direction $v_k$ which is $A$-orthogonal to $v_1, \ldots, v_{k-1}$ must be determined.
- It allows for orthogonalization of $r_k$ against $v_1, \ldots, v_k$.
- Let $r_k \neq 0$, $g(x)$ decreases strictly in the direction $-r_k$. For $\varepsilon > 0$ small, we have $g(x_k - \varepsilon r_k) < g(x_k)$.

If $r_{k-1} = b - Ax_{k-1} \neq 0$, then we use $r_{k-1}$ to generate $v_k$ by

$$v_k = r_{k-1} + \beta_{k-1} v_{k-1}. \quad (10)$$

Choose $\beta_{k-1}$ such that

$$0 = < v_{k-1}, Av_k > = < v_{k-1}, Ar_{k-1} + \beta_{k-1} Av_{k-1} >$$

$$= < v_{k-1}, Ar_{k-1} > + \beta_{k-1} < v_{k-1}, Av_{k-1} > .$$
That is

\[ \beta_{k-1} = -\frac{\langle v_{k-1}, Ar_{k-1} \rangle}{\langle v_{k-1}, Av_{k-1} \rangle}. \]  

(11)

**Theorem 41**

Let \( v_k \) and \( \beta_{k-1} \) be defined in (10) and (11), respectively. Then \( r_0, \ldots, r_{k-1} \) are mutually orthogonal and

\[ \langle v_k, Av_i \rangle = 0, \quad \text{for } i = 1, 2, \ldots, k-1. \]

That is \( \{v_1, \ldots, v_k\} \) is an A-orthogonal set.

Having chosen \( v_k \), we compute

\[
\alpha_k = \frac{\langle v_k, r_{k-1} \rangle}{\langle v_k, Av_k \rangle} = \frac{\langle r_{k-1} + \beta_{k-1}v_{k-1}, r_{k-1} \rangle}{\langle v_k, Av_k \rangle} = \frac{\langle r_{k-1}, r_{k-1} \rangle + \beta_{k-1} \langle v_{k-1}, r_{k-1} \rangle}{\langle v_k, Av_k \rangle} = \frac{\langle r_{k-1}, r_{k-1} \rangle}{\langle v_k, Av_k \rangle}.
\]  

(12)
Since

\[ r_k = r_{k-1} - \alpha_k A v_k, \]

we have

\[ \langle r_k, r_k \rangle = \langle r_{k-1}, r_k \rangle - \alpha_k \langle A v_k, r_k \rangle = -\alpha_k \langle r_k, A v_k \rangle. \]

Further, from (12),

\[ \langle r_{k-1}, r_{k-1} \rangle = \alpha_k \langle v_k, A v_k \rangle, \]

so

\[ \beta_k = -\frac{\langle v_k, A r_k \rangle}{\langle v_k, A v_k \rangle} = -\frac{\langle r_k, A v_k \rangle}{\langle v_k, A v_k \rangle} = \frac{(1/\alpha_k) \langle r_k, r_k \rangle}{(1/\alpha_k) \langle r_{k-1}, r_{k-1} \rangle} = \frac{\langle r_k, r_k \rangle}{\langle r_{k-1}, r_{k-1} \rangle}. \]
Algorithm 4 (Conjugate Gradient method (CG-method))

Let $A$ be s.p.d., $b \in \mathbb{R}^n$, choose $x_0 \in \mathbb{R}^n$, $r_0 = b - Ax_0 = v_0$. If $r_0 = 0$, then $N = 0$ stop, otherwise for $k = 0, 1, \ldots$

(a). $\alpha_k = \frac{\langle r_k, r_k \rangle}{\langle v_k, Av_k \rangle}$,

(b). $x_{k+1} = x_k + \alpha_k v_k$,

(c). $r_{k+1} = r_k - \alpha_k Av_k$,

(d). If $r_{k+1} = 0$, let $N = k + 1$, stop.

(e). $\beta_k = \frac{\langle r_{k+1}, r_{k+1} \rangle}{\langle r_k, r_k \rangle}$,

(f). $v_{k+1} = r_{k+1} + \beta_k v_k$.

- Theoretically, the exact solution is obtained in $n$ steps.
- If $A$ is well-conditioned, then approximate solution is obtained in about $\sqrt{n}$ steps.
- If $A$ is ill-conditioned, then the number of iterations may be greater than $n$. 
Select a nonsingular matrix $C$ so that
\[ \tilde{A} = C^{-1}AC^{-T} \]
is better conditioned.
Consider the linear system
\[ \tilde{A}\tilde{x} = \tilde{b}, \]
where
\[ \tilde{x} = C^Tx \quad \text{and} \quad \tilde{b} = C^{-1}b. \]
Then
\[ \tilde{A}\tilde{x} = (C^{-1}AC^{-T})(C^Tx) = C^{-1}Ax. \]
Thus,
\[ Ax = b \iff \tilde{A}\tilde{x} = \tilde{b} \quad \text{and} \quad x = C^{-T}\tilde{x}. \]
Since
\[ \tilde{x}_k = C^T x_k, \]
we have
\[ \tilde{r}_k = \tilde{b} - \tilde{A}\tilde{x}_k = C^{-1}b - (C^{-1}AC^{-T}) C^T x_k \]
\[ = C^{-1}(b - Ax_k) = C^{-1}r_k. \]

Let
\[ \tilde{v}_k = C^T v_k \quad \text{and} \quad w_k = C^{-1}r_k. \]

Then
\[ \tilde{\beta}_k = \frac{\langle \tilde{r}_k, \tilde{r}_k \rangle}{\langle \tilde{r}_{k-1}, \tilde{r}_{k-1} \rangle} = \frac{\langle C^{-1}r_k, C^{-1}r_k \rangle}{\langle C^{-1}r_{k-1}, C^{-1}r_{k-1} \rangle} \]
\[ = \frac{\langle w_k, w_k \rangle}{\langle w_{k-1}, w_{k-1} \rangle}. \]
Thus,
\[
\tilde{\alpha}_k = \frac{\langle \tilde{r}_{k-1}, \tilde{r}_{k-1} \rangle}{\langle \tilde{v}_k, \tilde{A} \tilde{v}_k \rangle} = \frac{\langle C^{-1}r_{k-1}, C^{-1}r_{k-1} \rangle}{\langle C^T v_k, C^{-1} AC^{-T} CT v_k \rangle}
\]
\[
= \frac{\langle w_{k-1}, w_{k-1} \rangle}{\langle C^T v_k, C^{-1} Av_k \rangle}
\]
and, since
\[
\langle C^T v_k, C^{-1} Av_k \rangle = (v_k)^T CC^{-1} Av_k = (v_k)^T Av_k
\]
\[
= \langle v_k, Av_k \rangle,
\]
we have
\[
\tilde{\alpha}_k = \frac{\langle w_{k-1}, w_{k-1} \rangle}{\langle v_k, Av_k \rangle}.
\]
Further,
\[
\tilde{x}_k = \tilde{x}_{k-1} + \tilde{\alpha}_k \tilde{v}_k, \quad \text{so} \quad C^T x_k = C^T x_{k-1} + \tilde{\alpha}_k C^T v_k
\]
and
\[
x_k = x_{k-1} + \tilde{\alpha}_k v_k.
\]
Continuing,

\[ \tilde{r}_k = \tilde{r}_{k-1} - \tilde{\alpha}_k \tilde{A} \tilde{v}_k, \]

so

\[ C^{-1} r_k = C^{-1} r_{k-1} - \tilde{\alpha}_k C^{-1} AC^{-T} C^T v_k \]

and

\[ r_k = r_{k-1} - \tilde{\alpha}_k A v_k. \]

Finally,

\[ \tilde{v}_{k+1} = \tilde{r}_k + \tilde{\beta}_k \tilde{v}_k \quad \text{and} \quad C^T v_{k+1} = C^{-1} r_k + \tilde{\beta}_k C^T v_k, \]

so

\[ v_{k+1} = C^{-T} C^{-1} r_k + \tilde{\beta}_k v_k = C^{-T} w_k + \tilde{\beta}_k v_k. \]
Algorithm 5 (Preconditioned CG-method (PCG-method))

Choose $C$ and $x_0$.

Set $r_0 = b - Ax_0$, solve $Cw_0 = r_0$ and $C^Tv_1 = w_0$.

If $r_0 = 0$, then $N = 0$ stop, otherwise for $k = 1, 2, \ldots$

(a). $\alpha_k = < w_{k-1}, w_{k-1} > / < v_k, Av_k >$,
(b). $x_k = x_{k-1} + \alpha_k v_k$,
(c). $r_k = r_{k-1} - \alpha_k Av_k$,
(d). If $r_k = 0$, let $N = k + 1$, stop.

Otherwise, solve $Cw_k = r_k$ and $C^Tz_k = w_k$,
(e). $\beta_k = < w_k, w_k > / < w_{k-1}, w_{k-1} >$,
(f). $v_{k+1} = z_k + \beta_k v_k$. 
