# Iterative techniques in matrix algebra

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# Outline

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## Definition 1

$\|\cdot\|:\mathbb{R}^n\to\mathbb{R}$ 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

$$\|x\|_2=(x^Tx)^{1/2}=\left\{\sum_{i=1}^n x_i^2\right\}^{1/2} \quad \text{and} \quad \|x\|_\infty=\max_{1\leq i\leq n}|x_i|.$$

The $\ell_2$ norm is also called the Euclidean norm.

## Definition 1

$\|\cdot\| : \mathbb{R}^n \to \mathbb{R}$ 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

$$\|x\|_2 = (x^T x)^{1/2} = \left\{ \sum_{i=1}^{n} x_i^2 \right\}^{1/2} \quad \text{and} \quad \|x\|_\infty = \max_{1 \leq i \leq n} |x_i|.$$

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 $\alpha \in \mathbb{R}$,

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

and

$$2\alpha \sum_{i=1}^n x_i y_i \leq \sum_{i=1}^n x_i^2 + \alpha^2 \sum_{i=1}^n y_i^2 = \|x\|_2^2 + \alpha^2 \|y\|_2^2.$$

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Since $\|x\|_2 > 0$ and $\|y\|_2 > 0$, we can let

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

to give

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

Thus

$$x^T y = \sum_{i=1}^{n} x_i y_i \le \|x\|_2 \|y\|_2.$$

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

$$\begin{aligned} \|x+y\|_\infty &= \max_{1\le i\le n} |x_i + y_i| \le \max_{1\le i\le n} (|x_i| + |y_i|) \\ &\le \max_{1\le i\le n} |x_i| + \max_{1\le i\le n} |y_i| = \|x\|_\infty + \|y\|_\infty \end{aligned}$$

and

$$\begin{aligned} \|x+y\|_2^2 &= \sum_{i=1}^{n} (x_i + y_i)^2 = \sum_{i=1}^{2} x_i^2 + 2\sum_{i=1}^{n} x_i y_i + \sum_{i=1}^{n} y_i^2 \\ &\le \|x\|_2^2 + 2\|x\|_2\|y\|_2 + \|y\|_2^2 = (\|x\|_2 + \|y\|_2)^2, \end{aligned}$$

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## 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

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This result implies that

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

Hence

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

"$\Leftarrow$" For a given $\varepsilon > 0$, let $N_i(\varepsilon)$ represent an integer with

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

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

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

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

**Theorem 6**

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

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

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

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

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

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

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## 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)** $\|\alpha A\| = |\alpha|\|A\|$;
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- **(v)** $\|AB\| \leq \|A\|\|B\|$;

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

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

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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*

$$\|A\|_\infty = \max_{1\leq i\leq n} \sum_{j=1}^{n} |a_{ij}|.$$

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*Proof:* Let $x$ be an $n$-dimension vector with

$$1 = \|x\|_\infty = \max_{1\le i\le n} |x_i|.$$

Then

$$\begin{aligned}\|Ax\|_\infty &= \max_{1\le i\le n}\left|\sum_{j=1}^n a_{ij}x_j\right| \\ &\le \max_{1\le i\le n}\sum_{j=1}^n |a_{ij}| \max_{1\le j\le n}|x_j| = \max_{1\le i\le n}\sum_{j=1}^n |a_{ij}|.\end{aligned}$$

Consequently,

$$\|A\|_\infty = \max_{\|x\|_\infty=1}\|Ax\|_\infty \le \max_{1\le i\le n}\sum_{j=1}^n |a_{ij}|.$$

On the other hand, let $p$ be an integer with

$$\sum_{j=1}^n |a_{pj}| = \max_{1\le i\le n}\sum_{j=1}^n |a_{ij}|,$$

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$$\begin{aligned} \|Ax\|_\infty &= \max_{1\le i\le n} \left| \sum_{j=1}^n a_{ij} x_j \right| \\ &\le \max_{1\le i\le n} \sum_{j=1}^n |a_{ij}| \max_{1\le j\le n} |x_j| = \max_{1\le i\le n} \sum_{j=1}^n |a_{ij}|. \end{aligned}$$

Consequently,

$$\|A\|_\infty = \max_{\|x\|_\infty = 1} \|Ax\|_\infty \le \max_{1\le i\le n} \sum_{j=1}^n |a_{ij}|.$$

On the other hand, let $p$ be an integer with

$$\sum_{j=1}^n |a_{pj}| = \max_{1\le i\le n} \sum_{j=1}^n |a_{ij}|,$$

*Proof:* Let $x$ be an $n$-dimension vector with

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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

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

so

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

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**Exercise**

Page 441: 5, 9, 10, 11

# Eigenvalues and eigenvectors

**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

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

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**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*

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**Definition 16**

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

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

**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;*
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**Exercise**

Page 449: 11, 12, 18, 19

# Jacobi and Gauss-Siedel Iterative Techniques

- 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

$$Mx = (M - A)x + b.$$

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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.

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# 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 $x_i^{(k)}$ can be computed by

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

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**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 $k = k + 1$, $x^{(0)} = x$.
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## Example 18

Consider the linear system $Ax = b$ given by

$$
\begin{array}{rrrrrrrrrl}
E_1: & 10x_1 & - & x_2 & + & 2x_3 & & & = & 6, \\
E_2: & -x_1 & + & 11x_2 & - & x_3 & + & 3x_4 & = & 25, \\
E_3: & 2x_1 & - & x_2 & + & 10x_3 & - & x_4 & = & -11, \\
E_4: & & & 3x_2 & - & x_3 & + & 8x_4 & = & 15
\end{array}
$$

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

$$
\begin{array}{rcrrrrrrrr}
x_1 & = & & & 1/10x_2 & - & 1/5x_3 & & + & 3/5, \\
x_2 & = & 1/11x_1 & & & + & 1/11x_3 & - \; 3/11x_4 & + & 25/11, \\
x_3 & = & -1/5x_1 & + & 1/10x_2 & & & + \; 1/10x_4 & - & 11/10, \\
x_4 & = & & - & 3/8x_2 & + & 1/8x_3 & & + & 15/8.
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Then $Ax = b$ can be rewritten in the form $x = Tx + c$ with

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

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

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| k | $x_1$ | $x_2$ | $x_3$ | $x_4$ |
|---|---|---|---|---|
| 0 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 1 | 0.6000 | 2.2727 | -1.1000 | 1.8750 |
| 2 | 1.0473 | 1.7159 | -0.8052 | 0.8852 |
| 3 | 0.9326 | 2.0533 | -1.0493 | 1.1309 |
| 4 | 1.0152 | 1.9537 | -0.9681 | 0.9738 |
| 5 | 0.9890 | 2.0114 | -1.0103 | 1.0214 |
| 6 | 1.0032 | 1.9922 | -0.9945 | 0.9944 |
| 7 | 0.9981 | 2.0023 | -1.0020 | 1.0036 |
| 8 | 1.0006 | 1.9987 | -0.9990 | 0.9989 |
| 9 | 0.9997 | 2.0004 | -1.0004 | 1.0006 |
| 10 | 1.0001 | 1.9998 | -0.9998 | 0.9998 |

## 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      \n');
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('\n');
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 $x_1, \ldots, x_{i-1}$ than $x_1^{(k-1)}, \ldots, x_{i-1}^{(k-1)}$. It seems reasonable to compute $x_i^{(k)}$ using these most recently computed values. That is

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

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- 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 $k$.
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## Algorithm 2 (Gauss-Seidel Method)

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

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

End For
While $k \leq M$ and $\|x - x^{(0)}\|_2 \geq TOL$
Set $k = k + 1$, $x^{(0)} = x$.
For $i = 1, 2, \ldots, n$

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

End For
End While

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Consider the linear system $Ax = b$ given by

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E_1: & 10x_1 & - & x_2 & + & 2x_3 & & & = & 6, \\
E_2: & -x_1 & + & 11x_2 & - & x_3 & + & 3x_4 & = & 25, \\
E_3: & 2x_1 & - & x_2 & + & 10x_3 & - & x_4 & = & -11, \\
E_4: & & & 3x_2 & - & x_3 & + & 8x_4 & = & 15
\end{array}$$

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

Gauss-Seidel method gives the equation

$$\begin{aligned}
x_1^{(k)} &= \frac{1}{10}x_2^{(k-1)} - \frac{1}{5}x_3^{(k-1)} + \frac{3}{5}, \\
x_2^{(k)} &= \frac{1}{11}x_1^{(k)} + \frac{1}{11}x_3^{(k-1)} - \frac{3}{11}x_4^{(k-1)} + \frac{25}{11}, \\
x_3^{(k)} &= -\frac{1}{5}x_1^{(k)} + \frac{1}{10}x_2^{(k)} + \frac{1}{10}x_4^{(k-1)} - \frac{11}{10}, \\
x_4^{(k)} &= -\frac{3}{8}x_2^{(k)} + \frac{1}{8}x_3^{(k)} + \frac{15}{8}.
\end{aligned}$$

## Example 19

Consider the linear system $Ax = b$ given by

$$\begin{array}{lrcrcrcrcr} E_1: & 10x_1 & - & x_2 & + & 2x_3 & & & = & 6, \\ E_2: & -x_1 & + & 11x_2 & - & x_3 & + & 3x_4 & = & 25, \\ E_3: & 2x_1 & - & x_2 & + & 10x_3 & - & x_4 & = & -11, \\ E_4: & & & 3x_2 & - & x_3 & + & 8x_4 & = & 15 \end{array}$$

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$$\begin{array}{rcrcrcrcrcr} x_1^{(k)} & = & & & \frac{1}{10}x_2^{(k-1)} & - & \frac{1}{5}x_3^{(k-1)} & & & + & \frac{3}{5}, \\ x_2^{(k)} & = & \frac{1}{11}x_1^{(k)} & & & + & \frac{1}{11}x_3^{(k-1)} & - & \frac{3}{11}x_4^{(k-1)} & + & \frac{25}{11}, \\ x_3^{(k)} & = & -\frac{1}{5}x_1^{(k)} & + & \frac{1}{10}x_2^{(k)} & & & + & \frac{1}{10}x_4^{(k-1)} & - & \frac{11}{10}, \\ x_4^{(k)} & = & & - & \frac{3}{8}x_2^{(k)} & + & \frac{1}{8}x_3^{(k)} & & & + & \frac{15}{8}. \end{array}$$

The numerical results of such iteration is list as follows:

| k | $x_1$ | $x_2$ | $x_3$ | $x_4$ |
|---|---|---|---|---|
| 0 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| 1 | 0.6000 | 2.3273 | -0.9873 | 0.8789 |
| 2 | 1.0302 | 2.0369 | -1.0145 | 0.9843 |
| 3 | 1.0066 | 2.0036 | -1.0025 | 0.9984 |
| 4 | 1.0009 | 2.0003 | -1.0003 | 0.9998 |
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- 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.
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## 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      \n');
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');
end
```

## Lemma 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

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

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## 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*

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

$$x^{(1)} = Tx^{(0)} + c$$
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In general

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

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

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

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

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

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

The first statement can then be derived

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

For the second result, we first show that

$$\|x^{(n)} - x^{(n-1)}\| \le \|T\|^{n-1} \|x^{(1)} - x^{(0)}\| \quad \text{for any } n \ge 1.$$

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Let $m \geq k$,

$$\begin{aligned} & x^{(m)} - x^{(k)} \\ =& \left(x^{(m)} - x^{(m-1)}\right) + \left(x^{(m-1)} - x^{(m-2)}\right) + \cdots + \left(x^{(k+1)} - x^{(k)}\right) \\ =& T^{m-1}\left(x^{(1)} - x^{(0)}\right) + T^{m-2}\left(x^{(1)} - x^{(0)}\right) + \cdots + T^{k}\left(x^{(1)} - x^{(0)}\right) \\ =& \left(T^{m-1} + T^{m-2} + \cdots + T^{k}\right)\left(x^{(1)} - x^{(0)}\right), \end{aligned}$$

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**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

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

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$$T_G y = \lambda y \quad \Longrightarrow \quad -Uy = \lambda(D+L)y.$$

Hence for $i = 1, \ldots, n$,

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

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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.

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

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**Exercise**

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# Relaxation Techniques for Solving Linear Systems

**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 $\mathbf{x}^{(k,i)}$ produced by Gauss-Seidel method be defined by

$$\mathbf{x}^{(k,i)} = \left[x_1^{(k)}, \ldots, x_{i-1}^{(k)}, x_i^{(k-1)}, \ldots, x_n^{(k-1)}\right]^T$$

and

$$r_i^{(k)} = \left[r_{1i}^{(k)}, r_{2i}^{(k)}, \ldots, r_{ni}^{(k)}\right]^T = b - A\mathbf{x}^{(k,i)}$$

be the corresponding residual vector. Then the $m$th component of $r_i^{(k)}$ is

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

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for each $m = 1, 2, \ldots, n$.

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

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Consequently, the Gauss-Seidel method can be characterized as choosing $x_i^{(k)}$ to satisfy

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Relaxation method is modified the Gauss-Seidel procedure to

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

for certain choices of positive $\omega$ such that the norm of the residual vector is reduced and the convergence is significantly faster.

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These methods are called for

$\omega < 1$: under relaxation,
$\omega = 1$: Gauss-Seidel method,
$\omega > 1$: 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

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

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$$\begin{aligned} x^{(k)} &= (D+\omega L)^{-1}[(1-\omega)D - \omega U]\, x^{(k-1)} + \omega(D+\omega L)^{-1} b \\ &= T_\omega x^{(k-1)} + c_\omega. \end{aligned}$$

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## Example 25

The linear system $Ax = b$ given by

$$\begin{array}{rcrcrcr} 4x_1 & + & 3x_2 & & & = & 24, \\ 3x_1 & + & 4x_2 & - & x_3 & = & 30, \\ & - & x_2 & + & 4x_3 & = & -24, \end{array}$$

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

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

| k | $x_1$ | $x_2$ | $x_3$ |
|---|---|---|---|
| 0 | 1.0000000 | 1.0000000 | 1.0000000 |
| 1 | 5.2500000 | 3.8125000 | -5.0468750 |
| 2 | 3.1406250 | 3.8828125 | -5.0292969 |
| 3 | 3.0878906 | 3.9267578 | -5.0183105 |
| 4 | 3.0549316 | 3.9542236 | -5.0114441 |
| 5 | 3.0343323 | 3.9713898 | -5.0071526 |
| 6 | 3.0214577 | 3.9821186 | -5.0044703 |
| 7 | 3.0134110 | 3.9888241 | -5.0027940 |

- Numerical results of SOR method with $\omega = 1.25$ and $x^{(0)} = [1, 1, 1]^T$:

| k | $x_1$ | $x_2$ | $x_3$ |
|---|---|---|---|
| 0 | 1.0000000 | 1.0000000 | 1.0000000 |
| 1 | 6.3125000 | 3.5195313 | -6.6501465 |
| 2 | 2.6223145 | 3.9585266 | -4.6004238 |
| 3 | 3.1333027 | 4.0102646 | -5.0966863 |
| 4 | 2.9570512 | 4.0074838 | -4.9734897 |
| 5 | 3.0037211 | 4.0029250 | -5.0057135 |
| 6 | 2.9963276 | 4.0009262 | -4.9982822 |
| 7 | 3.0000498 | 4.0002586 | -5.0003486 |

- Numerical results of SOR method with $\omega = 1.6$ and $x^{(0)} = [1, 1, 1]^T$:

| k | $x_1$ | $x_2$ | $x_3$ |
|---|---|---|---|
| 0 | 1.0000000 | 1.0000000 | 1.0000000 |
| 1 | 7.8000000 | 2.4400000 | -9.2240000 |
| 2 | 1.9920000 | 4.4560000 | -2.2832000 |
| 3 | 3.0576000 | 4.7440000 | -6.3324800 |
| 4 | 2.0726400 | 4.1334400 | -4.1471360 |
| 5 | 3.3962880 | 3.7855360 | -5.5975040 |
| 6 | 3.0195840 | 3.8661760 | -4.6950272 |
| 7 | 3.1488384 | 4.0236774 | -5.1735127 |

## 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        \n');
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('\n');
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 $\omega$, $\rho(T_\omega) = \omega - 1$.*

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## 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

$$\begin{aligned} T_J &= -D^{-1}(L+U) = \begin{bmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{4} \end{bmatrix} \begin{bmatrix} 0 & -3 & 0 \\ -3 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \\ &= \begin{bmatrix} 0 & -0.75 & 0 \\ -0.75 & 0 & 0.25 \\ 0 & 0.25 & 0 \end{bmatrix}, \end{aligned}$$

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 $\omega = 0.125$

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# 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

$$(D+\omega L)x^{(k-\frac{1}{2})} = \left[(1-\omega)D - \omega L^T\right] x^{(k-1)} + \omega b, \quad (2)$$

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Define

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

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

$$\begin{aligned} x^{(k)} &= \left(M_\omega^{-T} N_\omega^T M_\omega^{-1} N_\omega\right) x^{(k-1)} + \omega \left(M_\omega^{-T} N_\omega^T M_\omega^{-1} + M_\omega^{-T}\right) b \\ &= T(\omega) x^{(k-1)} + M(\omega)^{-1} b. \end{aligned}$$

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But

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&((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}.
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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

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

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**Exercise**

Page 467: 2, 8

# 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, $\|x - \tilde{x}\|_\infty = 2$.

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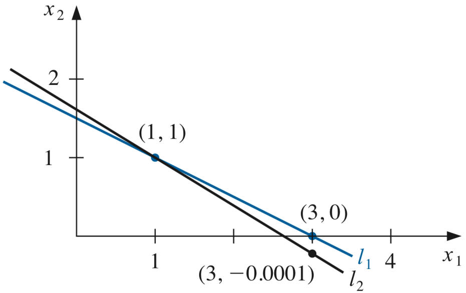
The solution of above example represents the intersection of the lines

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

$\ell_1$ 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 $(1, 1)$.



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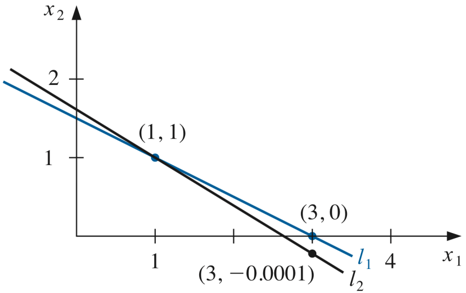

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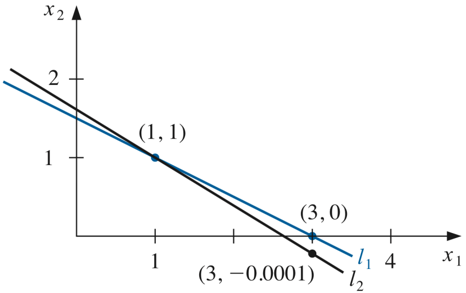

**Theorem 31**

*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

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**Definition 32 (Condition number)**

The condition number of nonsingular matrix $A$ is

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

For any nonsingular matrix $A$,

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$$1 = \|I\| = \|A \cdot A^{-1}\| \leq \|A\| \cdot \|A^{-1}\| = \kappa(A).$$

**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

$$\kappa(A) = \|A\|_\infty \cdot \|A^{-1}\|_\infty = 3.0001 \times 20000 = 60002 \gg 1.$$

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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

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Let $\tilde{y}$ be the approximate solution.

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Then

$$\tilde{y} \approx A^{-1}r = A^{-1}(b - A\tilde{x}) = x - \tilde{x}$$

and

$$x \approx \tilde{x} + \tilde{y}.$$

Moreover,

$$\begin{aligned} \|\tilde{y}\| &\approx \|x - \tilde{x}\| = \|A^{-1}r\| \\ &\leq \|A^{-1}\| \cdot \|r\| \approx \|A^{-1}\|(10^{-t}\|A\| \cdot \|\tilde{x}\|) = 10^{-t}\|\tilde{x}\|\kappa(A). \end{aligned}$$

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 $\tilde{x}$.

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**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

$$\left[\begin{array}{ccc|c} 3.3330 & 15920 & -10.333 & 15913 \\ 0 & -10596 & 16.501 & -10580 \\ 0 & -7451.4 & 6.5250 & -7444.9 \end{array}\right]$$

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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

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

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

$$x^{(2)} = x^{(1)} + \tilde{y}^{(1)} = [1.0000, 1.0000, 0.99999]^T.$$

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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

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

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

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

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## 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 $x$.

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**Exercise**

Page 476: 2, 4, 7, 8

# The conjugate gradient method

Consider the linear systems

$$Ax = b$$

where $A$ is large sparse and symmetric positive definite. Define the inner product notation

$$< x, y >= x^T y \quad \text{for any} \quad x, y \in \mathbb{R}^n.$$

**Theorem 36**

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

$$g(x) =< x, Ax > -2 < x, b > .$$

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## Proof:

(" $\Rightarrow$") Rewrite $g(x)$ as

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\begin{aligned}
g(x) &= <x-x^*, A(x-x^*)> + <x, Ax^*> + <x^*, Ax> \\
&\quad - <x^*, Ax^*> -2<x, b> \\
&= <x-x^*, A(x-x^*)> - <x^*, Ax^*> \\
&\quad +2<x, Ax^*> -2<x, b> \\
&= <x-x^*, A(x-x^*)> - <x^*, Ax^*> +2<x, Ax^*-b> .
\end{aligned}
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Suppose that $x^*$ is the solution of $Ax=b$, i.e., $Ax^*=b$. Then

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("$\Leftarrow$") Fixed vectors $x$ and $v$, for any $\alpha \in \mathbb{R}$,

$$
\begin{aligned}
& f(\alpha) \equiv g(x + \alpha v) \\
= & < x + \alpha v, Ax + \alpha Av > -2 < x + \alpha v, b > \\
= & < x, Ax > + \alpha < v, Ax > + \alpha < x, Av > + \alpha^2 < v, Av > \\
& - 2 < x, b > -2\alpha < v, b > \\
= & < x, Ax > -2 < x, b > +2\alpha < v, Ax > -2\alpha < v, b > + \alpha^2 < v, Av > \\
= & g(x) + 2\alpha < v, Ax - b > + \alpha^2 < v, Av > .
\end{aligned}
$$

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

$$f'(\alpha) = 2 < v, Ax - b > + 2\alpha < v, Av >,$$

the minimum occurs at

$$\hat{\alpha} = -\frac{< v, Ax - b >}{< v, Av >} = \frac{< v, b - Ax >}{< v, Av >}.$$

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\begin{aligned}
& f(\alpha) \equiv g(x + \alpha v) \\
= & < x + \alpha v, Ax + \alpha Av > -2 < x + \alpha v, b > \\
= & < x, Ax > + \alpha < v, Ax > + \alpha < x, Av > + \alpha^2 < v, Av > \\
& - 2 < x, b > -2\alpha < v, b > \\
= & < x, Ax > -2 < x, b > + 2\alpha < v, Ax > -2\alpha < v, b > + \alpha^2 < v, Av > \\
= & g(x) + 2\alpha < v, Ax - b > + \alpha^2 < v, Av > .
\end{aligned}
$$

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

$$f'(\alpha) = 2 < v, Ax - b > + 2\alpha < v, Av >,$$

the minimum occurs at

$$\hat{\alpha} = -\frac{< v, Ax - b >}{< v, Av >} = \frac{< v, b - Ax >}{< v, Av >}.$$

("$\Leftarrow$") Fixed vectors $x$ and $v$, for any $\alpha \in \mathbb{R}$,

$$\begin{aligned} & f(\alpha) \equiv g(x+\alpha v) \\ = & < x+\alpha v, Ax+\alpha Av > -2 < x+\alpha v, b > \\ = & < x, Ax > +\alpha < v, Ax > +\alpha < x, Av > +\alpha^2 < v, Av > \\ & -2 < x, b > -2\alpha < v, b > \\ = & < x, Ax > -2 < x, b > +2\alpha < v, Ax > -2\alpha < v, b > +\alpha^2 < v, Av > \\ = & g(x) + 2\alpha < v, Ax-b > +\alpha^2 < v, Av > . \end{aligned}$$

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and

$$\begin{aligned} g(x+\hat{\alpha}v) &= f(\hat{\alpha}) = g(x) - 2\frac{< v, b - Ax >}{< v, Av >} < v, b - Ax > \\ &\quad + \left(\frac{< v, b - Ax >}{< v, Av >}\right)^2 < v, Av > \\ &= g(x) - \frac{< v, b - Ax >^2}{< v, Av >}. \end{aligned}$$

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

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

and

$$g(x+\hat{\alpha}v) = g(x) \text{ if } < v, b - Ax >= 0. \tag{7}$$

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

$$g(x^* + \hat{\alpha}v) \geq g(x^*) \text{ for any } v. \tag{8}$$

and

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From (6), (7) and (8), we have

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

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

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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

$$\begin{aligned} \alpha_k &= \frac{< v^{(k)}, b - Ax^{(k-1)} >}{< v^{(k)}, Av^{(k)} >}, \\ x^{(k)} &= x^{(k-1)} + \alpha_k v^{(k)} \end{aligned}$$

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 $O(\varepsilon)$).

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

It follows that

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

Therefore, the gradient of $g$ is

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

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## 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 $\alpha_k = \frac{r_{k-1}^T r_{k-1}}{r_{k-1}^T A r_{k-1}}$, $x_k = x_{k-1} + \alpha_k r_{k-1}$.

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 $\|x\|_A = \sqrt{x^T A x}$. Thus the gradient method is convergent.*

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- 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 $p^TAq=0$.

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## 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 $k = 1, \ldots, n$. ∎

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## Theorem 40

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

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

*Then $Ax_n = b$ and*

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

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

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

we have

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**Theorem 40**

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

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

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

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It implies that

$$
\begin{aligned}
& < Ax_n - b, v_k > \\
= & < Ax_0 - b, v_k > + \alpha_1 < Av_1, v_k > + \cdots + \alpha_n < Av_n, v_k > \\
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= & < Ax_0 - b, v_k > + < v_k, b - Ax_{k-1} > \\
= & < Ax_0 - b, v_k > \\
& + < v_k, b - Ax_0 + Ax_0 - Ax_1 + \cdots - Ax_{k-2} + Ax_{k-2} - Ax_{k-1} > \\
= & < Ax_0 - b, v_k > + < v_k, b - Ax_0 > + < v_k, Ax_0 - Ax_1 > \\
& + \cdots + < v_k, Ax_{k-2} - Ax_{k-1} > \\
= & < v_k, Ax_0 - Ax_1 > + \cdots + < v_k, Ax_{k-2} - Ax_{k-1} > .
\end{aligned}
$$

For any $i$

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

we have

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

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

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

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Suppose that

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

By the result

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

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

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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.

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## 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

$$v_k = r_{k-1} + \beta_{k-1} v_{k-1}. \tag{10}$$

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

$$\begin{aligned} 0 &= < v_{k-1}, Av_k >=< v_{k-1}, Ar_{k-1} + \beta_{k-1} Av_{k-1} > \\ &= < v_{k-1}, Ar_{k-1} > + \beta_{k-1} < v_{k-1}, Av_{k-1} > . \end{aligned}$$

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That is

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**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*

$$< v_k, Av_i >= 0, \quad \text{for } i = 1, 2, \ldots, k-1.$$

*That is $\{v_1, \ldots, v_k\}$ is an $A$-orthogonal set.*

Having chosen $v_k$, we compute

$$\begin{aligned} \alpha_k &= \frac{< v_k, r_{k-1} >}{< v_k, Av_k >} = \frac{< r_{k-1} + \beta_{k-1} v_{k-1}, r_{k-1} >}{< v_k, Av_k >} \\ &= \frac{< r_{k-1}, r_{k-1} >}{< v_k, Av_k >} + \beta_{k-1} \frac{< v_{k-1}, r_{k-1} >}{< v_k, Av_k >} \\ &= \frac{< r_{k-1}, r_{k-1} >}{< v_k, Av_k >}. \end{aligned} \tag{12}$$

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That is

$$\beta_{k-1} = -\frac{< v_{k-1}, Ar_{k-1} >}{< v_{k-1}, Av_{k-1} >}. \tag{11}$$

**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*

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we have

$$< r_k, r_k > = < r_{k-1}, r_k > -\alpha_k < Av_k, r_k > = -\alpha_k < r_k, Av_k > .$$

Further, from (12),

$$< r_{k-1}, r_{k-1} > = \alpha_k < v_k, Av_k >,$$

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## 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). $\alpha_k = \frac{<r_k, r_k>}{<v_k, Av_k>}$,
(b). $x_{k+1} = x_k + \alpha_k v_k$,
(c). $r_{k+1} = r_k - \alpha_k A v_k$,
(d). If $r_{k+1} = 0$, let $N = k + 1$, stop.
(e). $\beta_k = \frac{<r_{k+1}, r_{k+1}>}{<r_k, r_k>}$,
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- Theoretically, the exact solution is obtained in $n$ steps.
- If $A$ is well-conditioned, then approximate solution is obtained in about $\sqrt{n}$ steps.
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## Theorem 42

*CG-method satisfies the following error estimate*

$$\|x_k - x^*\|_A \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^k \|x_0 - x^*\|_A,$$

*where* $\kappa = \frac{\lambda_1}{\lambda_n}$ *and* $\lambda_1 \geq \cdots \geq \lambda_n > 0$ *are the eigenvalues of* $A$*.*

## Remark 1 (Compare with Gradient method)

Let $x_k^G$ be the $k$th iterate of Gradient method. Then

$$\|x_k^G - x^*\|_A \leq \left|\frac{\lambda_1 - \lambda_n}{\lambda_1 + \lambda_n}\right|^k \|x_0 - x^*\|_A.$$

But

$$\frac{\lambda_1 - \lambda_n}{\lambda_1 + \lambda_n} = \frac{\kappa - 1}{\kappa + 1} > \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1},$$

because in general $\sqrt{\kappa} \ll \kappa$. Therefore the CG-method is much better than Gradient method.

Select a nonsingular matrix $C$ so that

$$\tilde{A} = C^{-1} A C^{-T}$$

is better conditioned.

Consider the linear system

$$\tilde{A}\tilde{x} = \tilde{b},$$

where

$$\tilde{x} = C^T x \quad \text{and} \quad \tilde{b} = C^{-1} b.$$

Then

$$\tilde{A}\tilde{x} = (C^{-1} A C^{-T})(C^T x) = C^{-1} A x.$$

Thus,

$$Ax = b \;\Leftrightarrow\; \tilde{A}\tilde{x} = \tilde{b} \;\text{ and }\; x = C^{-T}\tilde{x}.$$

Select a nonsingular matrix $C$ so that

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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

$$C^{-1} r_k = C^{-1} r_{k-1} - \tilde{\alpha}_k C^{-1} A C^{-T} C^T v_k$$

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

$$v_{k+1} = C^{-T} C^{-1} r_k + \tilde{\beta}_k v_k = C^{-T} w_k + \tilde{\beta}_k v_k.$$

Continuing,

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

so

$$C^{-1} r_k = C^{-1} r_{k-1} - \tilde{\alpha}_k C^{-1} A C^{-T} C^T v_k$$

and

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

Finally,

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

so

$$v_{k+1} = C^{-T} C^{-1} r_k + \tilde{\beta}_k v_k = C^{-T} w_k + \tilde{\beta}_k v_k.$$

Continuing,

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

so

$$C^{-1} r_k = C^{-1} r_{k-1} - \tilde{\alpha}_k C^{-1} A C^{-T} C^T v_k$$

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

$$v_{k+1} = C^{-T} C^{-1} r_k + \tilde{\beta}_k v_k = C^{-T} w_k + \tilde{\beta}_k v_k.$$

Continuing,

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

so

$$C^{-1} r_k = C^{-1} r_{k-1} - \tilde{\alpha}_k C^{-1} A C^{-T} C^T v_k$$

and

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

Finally,

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

so

$$v_{k+1} = C^{-T} C^{-1} r_k + \tilde{\beta}_k v_k = C^{-T} w_k + \tilde{\beta}_k v_k.$$

Continuing,

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

so

$$C^{-1} r_k = C^{-1} r_{k-1} - \tilde{\alpha}_k C^{-1} A C^{-T} C^T v_k$$

and

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

Finally,

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

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 $C^T v_1 = w_0$.
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 $C^T z_k = w_k$,
(e). $\beta_k =< w_k, w_k > / < w_{k-1}, w_{k-1} >$,
(f). $v_{k+1} = z_k + \beta_k v_k$.

*Simplification:* Let

$$r_k = CC^T z_k \equiv M z_k.$$

Then

$$\begin{aligned}
\tilde{\beta}_k &= \frac{< \tilde{r}_k, \tilde{r}_k >}{< \tilde{r}_{k-1}, \tilde{r}_{k-1} >} = \frac{< C^{-1} r_k, C^{-1} r_k >}{< C^{-1} r_{k-1}, C^{-1} r_{k-1} >} \\
&= \frac{< z_k, r_k >}{< z_{k-1}, r_{k-1} >}, \\
\tilde{\alpha}_k &= \frac{< \tilde{r}_{k-1}, \tilde{r}_{k-1} >}{< \tilde{v}_k, \tilde{A}\tilde{v}_k >} = \frac{< C^{-1} r_{k-1}, C^{-1} r_{k-1} >}{< C^T v_k, C^{-1} A C^{-T} C^T v_k >} \\
&= \frac{< z_{k-1}, r_{k-1} >}{< v_k, A v_k >}, \\
v_{k+1} &= C^{-T} C^{-1} r_k + \tilde{\beta}_k v_k = z_k + \tilde{\beta}_k v_k.
\end{aligned}$$

## Algorithm: CG-method with preconditioner $M$

**Input:** Given $x_0$ and $r_0 = b - Ax_0$, solve $Mz_0 = r_0$. Set $v_1 = z_0$ and $k = 1$.

```
repeat
    Compute α_k = z_{k-1}^T r_{k-1} / v_k^T A v_k;
    Compute x_k = x_{k-1} + α_k v_k;
    Compute r_k = r_{k-1} - α_k A v_k;
    if r_k = 0 then
        Stop;
    else
        Solve M z_k = r_k;
        Compute β_k = z_k^T r_k / z_{k-1}^T r_{k-1};
        Compute v_{k+1} = z_k + β_k v_k;
    end if
    Set k = k + 1;
until r_k = 0
```

**Choices of $M$ (Criterion):**

**(i)** cond$(M^{-1/2}AM^{-1/2})$ is nearly by 1, i.e., $M^{-1/2}AM^{-1/2} \approx I, A \approx M$.

**(ii)** The linear system $Mz = r$ must be easily solved. e.g. $M = LL^T$.

**(iii)** $M$ is symmetric positive definite.

**(i) Jacobi method:** $A = D - (L + R), \quad M = D$

$$\begin{aligned} x_{k+1} &= x_k + D^{-1} r_k \\ &= x_k + D^{-1}(b - Ax_k) \\ &= D^{-1}(L + R)x_k + D^{-1}b \end{aligned}$$

**(ii) Gauss-Seidel:** $A = (D - L) - R, \quad M = D - L$

$$\begin{aligned} x_{k+1} &= x_k + z_k \\ &= x_k + (D - L)^{-1}(b - Ax_k) \\ &= (D - L)^{-1} R x_k + (D - L)^{-1} b. \end{aligned}$$

**(iii) SOR-method:** Write

$$\omega A = (D - \omega L) - ((1-\omega)D + \omega R) \equiv M - N.$$

Then we have

$$\begin{aligned} x_{k+1} &= (D-\omega L)^{-1}(\omega R + (1-\omega)D)x_k + (D-\omega L)^{-1}\omega b \\ &= (D-\omega L)^{-1}((D-\omega L) - \omega A)x_k + (D-\omega L)^{-1}\omega b \\ &= (I - (D-\omega L)^{-1}\omega A)x_k + (D-\omega L)^{-1}\omega b \\ &= x_k + (D-\omega L)^{-1}\omega(b - Ax_k) \\ &= x_k + \omega M^{-1} r_k. \end{aligned}$$

**(iv) SSOR:** $A = D - L - L^T$. Let

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

Then

$$\begin{aligned} x_{i+1} &= \left(M_\omega^{-T} N_\omega^T M_\omega^{-1} N_\omega\right) x_i + \tilde{b} \\ &\equiv G x_i + M(\omega)^{-1} b \end{aligned}$$

with

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