Numerical Analysis II
Iterative techniques in matrix algebra

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[1] These slides are based on Prof. Tsung-Ming Huang(NTNU)'s original slides

Outline

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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

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Definition

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

The ℓ_2 and ℓ_∞ norms for $x = [x_1, x_2, \cdots, x_n]^T$ are defined by

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

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Theorem (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 $x \neq 0$ or $y \neq 0$. 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

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

Thus

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

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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

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which gives

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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

$$\|x^{(k)} - x\| < \varepsilon,\ \forall\ k \ge N(\varepsilon).$$

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

Proof: "$\Rightarrow$" Given any $\varepsilon > 0$, $\exists$ an integer $N(\varepsilon)$ such that

$$\max_{1\le i\le n} |x_i^{(k)} - x_i| = \|x^{(k)} - x\|_\infty < \varepsilon, \ \forall\, k \ge N(\varepsilon).$$

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

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

Define

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

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

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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

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

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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 α:

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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

$$\|Az\| \leq \|A\| \cdot \|z\|.$$

Theorem

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

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Proof: Let x be an n-dimension vector with

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

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

Then

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

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Eigenvalues and eigenvectors

Definition (Characteristic polynomial)

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

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

Definition (Eigenvalue and eigenvector)

If p is the characteristic polynomial of the matrix A, the zeros of p are eigenvalues of the matrix A. If λ 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 λ.

Definition (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

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Theorem

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 λ is an eigenvalue of A and $x \neq 0$ is a corresponding eigenvector such that $Ax = \lambda x$ and $\|x\| = 1$. Then

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

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

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

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The following statements are equivalent.

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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.

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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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If we decompose the coefficient matrix A as

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Example

Consider the linear system $Ax = b$ given by

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

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}{lcrcrcrcrcr}
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, \\
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Then $Ax = b$ can be rewritten in the form $x = Tx + c$ with

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

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:

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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

$$\begin{array}{rcl}
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

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

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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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\begin{array}{lclcrcrcrcr}
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}
$$

Example

Consider the linear system $Ax = b$ given by

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

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

Gauss-Seidel method gives the equation

$$
\begin{array}{lclclclclcl}
x_1^{(k)} & = & & & \frac{1}{10}x_2^{(k-1)} & - & \frac{1}{5}x_3^{(k-1)} & & & + & \frac{3}{5}, \\
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$$

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
5	1.0001	2.0000	-1.0000	1.0000

- 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
diary off
```

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 λ be an eigenvalue of T, then $1 - \lambda$ is an eigenvalue of $I - T$. But $|\lambda| \le \rho(A) < 1$, so $1 - \lambda \ne 0$ 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

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

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Theorem

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

$$\begin{aligned} x^{(1)} &= Tx^{(0)} + c \\ x^{(2)} &= Tx^{(1)} + c = T^2 x^{(0)} + (T + I)c \\ x^{(3)} &= Tx^{(2)} + c = T^3 x^{(0)} + (T^2 + T + I)c \\ &\vdots \end{aligned}$$

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Theorem

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 $x^{(k)} = Tx^{(k-1)} + c$,

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

The first statement can then be derived

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

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Theorem

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

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Successive over-relaxation (SOR) method

Definition

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 mth 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 ith component of $r_i^{(k)}$ is

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Relaxation method is modified the Gauss-Seidel procedure to

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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

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so that if $A = L + D + U$, then we have

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Example

The linear system $Ax = b$ given by

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

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

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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 (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 (Ostrowski-Reich)

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

Theorem

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

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

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Example

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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This explains the rapid convergence obtained in previous example when using $\omega = 0.125$

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

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

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

then the splitting matrix is

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Error bounds and iterative refinement

Example

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

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

ℓ_1 and ℓ_2 are nearly parallel. The point $(3, 0)$ lies on ℓ_1 which implies that $(3, 0)$ also lies close to ℓ_2, even though it differs significantly from the intersection point $(1, 1)$.

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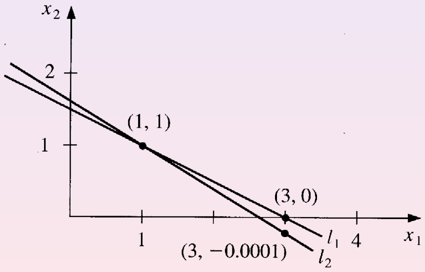

Theorem

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* $b \neq 0$,

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Proof: Since

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

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

□

Definition (Condition number)

The condition number of nonsingular matrix A is

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

For any nonsingular matrix A,

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

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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

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

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

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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

$$Ay = r.$$

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

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

and

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

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

- 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

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

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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 (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

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

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

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 δA and δb, respectively, causing the linear system

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

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Theorem

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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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

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

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

So, for any nonzero vector v, we have

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

and

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

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

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

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g(x+\hat{\alpha}v) &= f(\hat{\alpha}) = g(x) - 2\frac{< v, b-Ax >}{< v, Av >} < v, b-Ax > \\
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&= g(x) - \frac{< v, b-Ax >^2}{< v, Av >}.
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So, for any nonzero vector v, we have

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

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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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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

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:

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

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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

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

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Lemma

Let $v_1, \ldots, v_n \neq 0$ be pairwise 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 $k = 1, \ldots, n$.

Lemma

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

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Theorem

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

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

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Theorem

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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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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\end{aligned}
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For any i

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

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Suppose that

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

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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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- 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 β_{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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Theorem

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

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

Since

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

we have

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

Further, from (12),

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

so

$$\begin{aligned} \beta_k &= -\frac{< v_k, A r_k >}{< v_k, A v_k >} = -\frac{< r_k, A v_k >}{< v_k, A v_k >} \\ &= \frac{(1/\alpha_k) < r_k, r_k >}{(1/\alpha_k) < r_{k-1}, r_{k-1} >} = \frac{< r_k, r_k >}{< r_{k-1}, r_{k-1} >}. \end{aligned}$$

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

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

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

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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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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,

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

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

Thus,

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Since

$$\tilde{x}_k = C^T x_k,$$

we have

$$\begin{aligned} \tilde{r}_k &= \tilde{b} - \tilde{A}\tilde{x}_k = C^{-1}b - \left(C^{-1}AC^{-T}\right) C^T x_k \\ &= C^{-1}(b - Ax_k) = C^{-1} r_k. \end{aligned}$$

Let

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

Then

$$\begin{aligned} \tilde{\beta}_k &= \frac{< \tilde{r}_k, \tilde{r}_k >}{< \tilde{r}_{k-1}, \tilde{r}_{k-1} >} = \frac{< C^{-1}r_k, C^{-1}r_k >}{< C^{-1}r_{k-1}, C^{-1}r_{k-1} >} \\ &= \frac{< w_k, w_k >}{< w_{k-1}, w_{k-1} >}. \end{aligned}$$

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Thus,

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and, since

$$\begin{aligned}< C^T v_k, C^{-1} A v_k > &= (v_k)^T C C^{-1} A v_k = (v_k)^T A v_k \\ &= < v_k, A v_k >,\end{aligned}$$

we have

$$\tilde{\alpha}_k = \frac{< w_{k-1}, w_{k-1} >}{< v_k, A v_k >}.$$

Further,

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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,

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so

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and

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Finally,

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Finally,

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Algorithm (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). $r_k = r_{k-1} - \alpha_k A v_k$,

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