Chapter 2: Systems of Equations

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Motivation

Question: Given a nonsingular square matrix A and a vector b, how to solve a linear equation $Ax = b$?

Outline

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Vectors

Definition (Vectors)

An n-dimensional **(column) vector** is of the following form

$$u = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix}.$$

Definition (Row vectors)

An n-dimensional **row vector** is of the following form

$$u = \begin{bmatrix} u_1 & u_2 & \cdots & u_n \end{bmatrix}.$$

Matrices

Definition (Matrices)

An $m \times n$ **matrix** is of the following form

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}.$$

Matrix-matrix multiplication

Definition (Matrix-matrix multiplication)

Let A be an $m \times n$ matrix, and B be $n \times p$ matrix. Then, AB, which is an $m \times p$ matrix, is defined as follows:

$$\begin{bmatrix} a_{11} & \cdots & a_{1n} \\ a_{21} & \cdots & a_{2n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1p} \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \cdots & b_{np} \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} a_{1i}b_{i1} & \sum_{i=1}^{n} a_{1i}b_{i2} & \cdots & \sum_{i=1}^{n} a_{1i}b_{ip} \\ \sum_{i=1}^{n} a_{2i}b_{i1} & \sum_{i=1}^{n} a_{2i}b_{i2} & \cdots & \sum_{i=1}^{n} a_{2i}b_{ip} \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^{n} a_{mi}b_{i1} & \sum_{i=1}^{n} a_{mi}b_{i2} & \cdots & \sum_{i=1}^{n} a_{mi}b_{ip} \end{bmatrix}.$$

Matrix form of linear equation

Definition (Matrix form)

A system of m linear equations in n unknowns can be written in **matrix form** as

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}.$$

Some basic concepts

Definition (Identity matrix)

The $n \times n$ identity matrix I_n is the matrix with $I_{ii} = 1$ for $1 \leq i \leq n$ and $I_{ij} = 0$ for $i \neq j$.

$$\begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

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Definition (Inverse)

For an $n \times n$ matrix A, the **inverse** A^{-1} of A is an $n \times n$ matrix s.t. $AA^{-1} = A^{-1}A = I_n$.

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For an $n \times n$ matrix A, the **inverse** A^{-1} of A is an $n \times n$ matrix s.t. $AA^{-1} = A^{-1}A = I_n$.

Definition (Singular)

The $n \times n$ matrix A is **nonsingular (invertible)**, if it has a inverse A^{-1}; otherwise, it is **singular (noninvertible)**.

Some basic concepts

Definition (Transpose)

The **transpose** of an $m \times n$ matrix A is the $n \times m$ matrix $A^\top$ whose entries are $A^\top_{ij} = A_{ji}$.

Some basic concepts

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Example

Let A be a 2×3 matrix as follows: $\begin{bmatrix} 1 & 1 & 3 \\ 5 & -4 & 2 \end{bmatrix}$.

Then, $A^\top$ is a 3×2 matrix as follows: $\begin{bmatrix} 1 & 5 \\ 1 & -4 \\ 3 & 2 \end{bmatrix}$.

Some basic concepts

Definition

Given a vector v,

1. p-norm: $\|v\|_p = (\sum_{i=1}^{n} |v_i|^p)^{\frac{1}{p}}$;
2. Euclidean norm (2-norm): $\|v\|_2 = \sqrt{\sum_{i=1}^{n} |v_i|^2}$;
3. Infinity norm: $\|v\|_\infty = \max\{|v_1|, \dots, |v_n|\}$;

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Proposition

1. *Non-negativity:* $\|v\|_p \geq 0$;
2. *Absolute scalability:* $\|av\|_p = |a|\|v\|_p$;
3. *Triangle inequality:* $\|v + u\|_p \leq \|v\|_p + \|u\|_p$;
4. *Separates points: If* $\|v\|_p = 0$, *then* $v = 0$.

The above propositions also hold for infinity norm.

Some basic concepts

Example

Assume that $v = (2, -1)$ and $w = (1, 3)$.

- $\|v\|_2 = \sqrt{|2|^2 + |-1|^2} = \sqrt{5}$ and $\|v\|_\infty = \max\{|2|, |-1|\} = 2$;
- $\|w\|_2 = \sqrt{|1|^2 + |3|^2} = \sqrt{10}$ and $\|w\|_\infty = \max\{|1|, |3|\} = 3$;

Some basic concepts

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- $\|2v\|_2 = \sqrt{|2 \times 2|^2 + |2 \times (-1)|^2} = 2\sqrt{5}$;
- $\|3v\|_\infty = \max\{|3 \times 2|, |3 \times (-1)|\} = 6 = 3 \times 2$;

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- $\|v + w\|_2 = \sqrt{|2 + 1|^2 + |-1 + 3|^2} = \sqrt{13} < \sqrt{5} + \sqrt{10} = \|v\|_2 + \|w\|_2$;
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- $\|v + w\|_\infty = \max\{|2+1|, |-1+3|\} = 3 < 2 + 3 = \|v\|_\infty + \|w\|_\infty$;
- $\|0\|_2 = 0$ and $\|0\|_\infty = 0$.

Linear Subspace

Definition

Let $v_1, \cdots, v_m$ be n-dimensional vectors.
The subspace of V: $\{v_1, \cdots, v_m\}$ is $\{x \mid x = a_1 v_1 + \cdots + a_m v_m\}$.
A point $y \in R^n$ is in V, if $y \in V$ (*i.e.*, there is a vector of $a_1, \cdots, a_m$ s.t. $y = a_1 v_1 + \cdots + a_m v_m$.)

Example (Orthonormal sets)

1. $\{(1,1)\}$ (Figure ??)
2. $\{(1,0,0),(0,1,0)\}$; (Figures ??)

Linear Subspace

Definition

Let V and V' be two subspaces. We say V is a subspace of V', denoted by $V \subseteq V'$, if every point of V is in V'.

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Lemma

Let $V : \{v_1, \cdots, v_m\}$ and $V' : \{v'_1, \cdots, v'_n\}$ be two subspaces. Then, $V \subseteq V'$ iff $v_i \in V'$ for $1 \leq i \leq n$.

Linear Subspace

Proof.

($\Leftarrow$): Let $v \in V$.

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($\Leftarrow$): Let $v \in V$.
Then, $v = a_1 v_1 + \cdots + a_m v_m$.
By the assumption, $v_i = b_{1i} v'_1 + \cdots + b_{ni} v'_n$ for $1 \leq i \leq m$.

Linear Subspace

Proof.

($\Leftarrow$): Let $v \in V$.
Then, $v = a_1 v_1 + \cdots + a_m v_m$.
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$$v = a_1 v_1 + \cdots + a_m v_m$$

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By the assumption, $v_i = b_{1i} v_1' + \cdots + b_{ni} v_n'$ for $1 \leq i \leq m$.

$$\begin{aligned} v &= a_1 v_1 + \cdots + a_m v_m \\ &= a_1 (b_{11} v_1' + \cdots + b_{n1} v_n') + \cdots + a_m (b_{1m} v_1' + \cdots + b_{nm} v_n') \end{aligned}$$

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$$\begin{aligned} v &= a_1 v_1 + \cdots + a_m v_m \\ &= a_1(b_{11} v_1' + \cdots + b_{n1} v_n') + \cdots + a_m(b_{1m} v_1' + \cdots + b_{nm} v_n') \\ &= [\Sigma_{i=1}^{m}(a_i \cdot b_{1i}) v_1'] + \cdots + [\Sigma_{i=1}^{m}(a_i \cdot b_{1n}) v_n']. \end{aligned}$$

Linear Subspace

Proof.

($\Leftarrow$): Let $v \in V$.
Then, $v = a_1 v_1 + \cdots + a_m v_m$.
By the assumption, $v_i = b_{1i} v'_1 + \cdots + b_{ni} v'_n$ for $1 \leq i \leq m$.

$$\begin{aligned} v &= a_1 v_1 + \cdots + a_m v_m \\ &= a_1(b_{11} v'_1 + \cdots + b_{n1} v'_n) + \cdots + a_m(b_{1m} v'_1 + \cdots + b_{nm} v'_n) \\ &= [\Sigma_{i=1}^m (a_i \cdot b_{1i}) v'_1] + \cdots + [\Sigma_{i=1}^m (a_i \cdot b_{1n}) v'_n]. \end{aligned}$$

($\Rightarrow$): Each v_i is also a point of V. By the assumption that $V \subseteq V'$, we get that $v_i \in V'$.

Orthonormal sets

Definition

A **unit** vector is a vector whose Euclidean norm is 1, *i.e.*, $\sum_{i=1}^{n} v_i^2 = 1$.

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Example (Orthonormal sets)

1. $\{(1,0,0),(0,1,0),(0,0,1)\}$;
2. $\{(\frac{\sqrt{2}}{2},\frac{\sqrt{2}}{2}),(\frac{\sqrt{2}}{2},-\frac{\sqrt{2}}{2})\}$.

Properties of orthonormal sets

Lemma

If $\{v_1, v_2, \ldots, v_n\}$ *is an orthonormal set, then*

$$(a_1 v_1 + \cdots + a_n v_n)^\top (b_1 v_1 + \cdots + b_n v_n) = \sum_{i=1}^{n} a_i b_i.$$

Properties of orthonormal sets

Lemma

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Proof.

Let $v_i = [v_{i1}, \ldots, v_{im}]^\top$.

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Proof.

Let $v_i = [v_{i1}, \ldots, v_{im}]^\top$.

$$(a_1 v_1 + \cdots + a_n v_n)^\top (b_1 v_1 + \cdots + b_n v_n)$$

$$= \begin{bmatrix} \sum_{i=1}^{n} a_i v_{i1} & \ldots & \sum_{i=1}^{n} a_i v_{im} \end{bmatrix} \begin{bmatrix} \sum_{j=1}^{n} b_j v_{j1} \\ \vdots \\ \sum_{j=1}^{n} b_j v_{jm} \end{bmatrix}$$

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$$(a_1 v_1 + \cdots + a_n v_n)^\top (b_1 v_1 + \cdots + b_n v_n) = \sum_{i=1}^{n} a_i b_i.$$

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Let $v_i = [v_{i1}, \ldots, v_{im}]^\top$.

$$(a_1 v_1 + \cdots + a_n v_n)^\top (b_1 v_1 + \cdots + b_n v_n)$$

$$= \begin{bmatrix} \sum_{i=1}^{n} a_i v_{i1} & \ldots & \sum_{i=1}^{n} a_i v_{im} \end{bmatrix} \begin{bmatrix} \sum_{j=1}^{n} b_j v_{j1} \\ \vdots \\ \sum_{j=1}^{n} b_j v_{jm} \end{bmatrix}$$

$$= \sum_{k=1}^{m} (\sum_{i=1}^{n} a_i v_{ik}) \cdot (\sum_{j=1}^{n} b_j v_{jk})$$

Properties of orthonormal sets

Proof.

$$= \sum_{k=1}^{m} \sum_{i=1}^{n} \sum_{j=1}^{n} (a_i b_j v_{ik} v_{jk})$$

Properties of orthonormal sets

Proof.

$$= \sum_{k=1}^{m} \sum_{i=1}^{n} \sum_{j=1}^{n} (a_i b_j v_{ik} v_{jk})$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} [(a_i b_j) \cdot \sum_{k=1}^{m} (v_{ik} v_{jk})]$$

Properties of orthonormal sets

Proof.

$$= \sum_{k=1}^{m} \sum_{i=1}^{n} \sum_{j=1}^{n} (a_i b_j v_{ik} v_{jk})$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} [(a_i b_j) \cdot \sum_{k=1}^{m} (v_{ik} v_{jk})]$$

If $i \neq j$, then $\sum_{k=1}^{m} v_{ik} v_{jk} = v_i^\top v_j = 0$.

Ow, $\sum_{k=1}^{m} v_{ik} v_{jk} = v_i^\top v_j = 1$.

Properties of orthonormal sets

Proof.

$$= \sum_{k=1}^{m} \sum_{i=1}^{n} \sum_{j=1}^{n} (a_i b_j v_{ik} v_{jk})$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} [(a_i b_j) \cdot \sum_{k=1}^{m} (v_{ik} v_{jk})]$$

If $i \neq j$, then $\sum_{k=1}^{m} v_{ik} v_{jk} = v_i^\top v_j = 0$.

Ow, $\sum_{k=1}^{m} v_{ik} v_{jk} = v_i^\top v_j = 1$.

We get $\sum_{i=1}^{n} a_i b_i$

Outline

Jacobi Method

Example

A linear equation is as follows:

$$\begin{aligned} 3u + v &= 5 \\ u + 2v &= 5. \end{aligned}$$

We have:

$$\begin{aligned} u &= \frac{5-v}{3} \\ v &= \frac{5-u}{2}. \end{aligned}$$

Jacobi Method

Example (Iteration process)

1. $$\begin{bmatrix} u_0 \\ v_0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$
2. $$\begin{bmatrix} u_1 \\ v_1 \end{bmatrix} = \begin{bmatrix} \frac{5-v_0}{3} \\ \frac{5-u_0}{2} \end{bmatrix} = \begin{bmatrix} \frac{5-0}{3} \\ \frac{5-0}{2} \end{bmatrix} = \begin{bmatrix} \frac{5}{3} \\ \frac{5}{2} \end{bmatrix}$$
3. $$\begin{bmatrix} u_2 \\ v_2 \end{bmatrix} = \begin{bmatrix} \frac{5-v_1}{3} \\ \frac{5-u_1}{2} \end{bmatrix} = \begin{bmatrix} \frac{5-5/2}{3} \\ \frac{5-5/3}{2} \end{bmatrix} = \begin{bmatrix} \frac{5}{6} \\ \frac{5}{3} \end{bmatrix}$$
4. $$\begin{bmatrix} u_3 \\ v_3 \end{bmatrix} = \begin{bmatrix} \frac{5-v_2}{3} \\ \frac{5-u_2}{2} \end{bmatrix} = \begin{bmatrix} \frac{5-5/3}{3} \\ \frac{5-5/6}{2} \end{bmatrix} = \begin{bmatrix} \frac{10}{9} \\ \frac{25}{12} \end{bmatrix}$$
5. The process converges to the solution, which is $[1, 2]$.

Jacobi Method

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A linear equation is as follows:

$$\begin{aligned} u + 2v &= 5 \\ 3u + v &= 5. \end{aligned}$$

We have:

$$\begin{aligned} u &= 5 - 2v \\ v &= 5 - 3u. \end{aligned}$$

Jacobi method

Example (Iteration process)

1. $\begin{bmatrix} u_0 \\ v_0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$
2. $\begin{bmatrix} u_1 \\ v_1 \end{bmatrix} = \begin{bmatrix} 5 - 2v_0 \\ 5 - 3u_0 \end{bmatrix} = \begin{bmatrix} 5 - 2 \times 0 \\ 5 - 3 \times 0 \end{bmatrix} = \begin{bmatrix} 5 \\ 5 \end{bmatrix}$
3. $\begin{bmatrix} u_2 \\ v_2 \end{bmatrix} = \begin{bmatrix} 5 - 2v_1 \\ 5 - 3u_1 \end{bmatrix} = \begin{bmatrix} 5 - 2 \times 5 \\ 5 - 3 \times 5 \end{bmatrix} = \begin{bmatrix} -5 \\ -10 \end{bmatrix}$
4. $\begin{bmatrix} u_3 \\ v_3 \end{bmatrix} = \begin{bmatrix} 5 - 2v_2 \\ 5 - 3u_2 \end{bmatrix} = \begin{bmatrix} 5 - 2 \times (-10) \\ 5 - 3 \times (-5) \end{bmatrix} = \begin{bmatrix} 25 \\ 20 \end{bmatrix}$
5. The process tends to diverge.

Strictly diagonally dominance

Question: What is the condition under which Jabobi method does work?

Strictly diagonally dominance

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Definition

The $n \times n$ matrix $A = (a_{ij})$ is **strictly diagonally dominant**, if for each $1 \leq i \leq n$, $|a_{ii}| > \sum_{j \neq i} |a_{ij}|$.

Example

$\begin{bmatrix} 3 & 1 & -1 \\ 2 & -5 & 2 \\ 1 & 6 & 8 \end{bmatrix}$ is strictly diagonally dominant.

1. $|3| > |1| + |-1|$;
2. $|-5| > |2| + |2|$;
3. $|8| > |1| + |6|$.

Strictly diagonally dominance

Example

$$\begin{bmatrix} 3 & 2 & 6 \\ 1 & 8 & 1 \\ 9 & 2 & -2 \end{bmatrix}$$ is not strictly diagonally dominant.

1. $|3| < |2| + |6|$;
2. $|-2| < |9| + |2|$.

Strictly diagonally dominance

Example

$$\begin{bmatrix} 3 & 2 & 6 \\ 1 & 8 & 1 \\ 9 & 2 & -2 \end{bmatrix}$$ is not strictly diagonally dominant.

1. $|3| < |2| + |6|$;
2. $|-2| < |9| + |2|$.

But $$\begin{bmatrix} 9 & 2 & -2 \\ 1 & 8 & 1 \\ 3 & 2 & 6 \end{bmatrix}$$ is strictly diagonally dominant.

1. $|9| > |2| + |-2|$;
2. $|8| > |1| + |1|$;
3. $|6| > |3| + |2|$.

Strictly diagonally dominance

Theorem

If the $n \times n$ matrix A is strictly diagonally dominant, then

1. *A is a nonsingular matrix;*
2. *for every vector b and every starting guess, the Jacobi Method applied to $Ax = b$ converges to the unique solution.*

The matrix form of Jacobi Method

Definition

Suppose that A is a matrix.

- D: the main diagonal of A;
- L: the lower triangle of A;
- U: the upper triangle of A.

The matrix form of Jacobi Method

Example

- $A = \begin{bmatrix} 3 & 1 \\ 1 & 2 \end{bmatrix}$
- $D = \begin{bmatrix} 3 & 0 \\ 0 & 2 \end{bmatrix}$
- $L = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$
- $U = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$

The matrix form of Jacobi Method

$$
\begin{aligned}
Ax &= b \\
(D+L+U)x &= b \\
Dx &= b-(L+U)x \\
Dx_{k+1} &= b-(L+U)x_k \\
x_{k+1} &= D^{-1}(b-(L+U)x_k).
\end{aligned}
$$

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\end{aligned}
$$

Jacobi Method is as follows:

$$
\begin{aligned}
x_0 &= \text{initial vector} \\
x_{k+1} &= D^{-1}(b-(L+U)x_k) \\
x_{k+1,i} &= \frac{1}{a_{ii}}(b_i - \sum_{j\neq i} a_{ij}x_{k,j}) \textbf{ for } 1 \leq i \leq n.
\end{aligned}
$$

The matrix form of Jacobi Method

Example

- $\begin{bmatrix} 3 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 5 \\ 5 \end{bmatrix}$,
- $$\begin{aligned} x_{k+1} = \begin{bmatrix} u_{k+1} \\ v_{k+1} \end{bmatrix} &= D^{-1}(b - (L+U)x_k) \\ &= \begin{bmatrix} \frac{1}{3} & 0 \\ 0 & \frac{1}{2} \end{bmatrix} \left(\begin{bmatrix} 5 \\ 5 \end{bmatrix} - \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} u_k \\ v_k \end{bmatrix} \right) \\ &= \begin{bmatrix} \frac{5-v_k}{3} \\ \frac{5-u_k}{2} \end{bmatrix}. \end{aligned}$$

Outline

Gauss-Seidel Method

Question: Are there some methods converging faster than the Jacobi Method?

Gauss-Seidel Method

Question: Are there some methods converging faster than the Jacobi Method?

Answer: Yes! The Gauss-Seidel Method.

Gauss-Seidel Method

Example

- The definition of v_{k+1} uses u_{k+1} instead of u_k;
- $\begin{bmatrix} u_{k+1} \\ v_{k+1} \end{bmatrix} = \begin{bmatrix} \frac{5-v_k}{3} \\ \frac{5-u_{k+1}}{2} \end{bmatrix}$.

1. $\begin{bmatrix} u_0 \\ v_0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$
2. $\begin{bmatrix} u_1 \\ v_1 \end{bmatrix} = \begin{bmatrix} \frac{5-v_0}{3} \\ \frac{5-u_1}{2} \end{bmatrix} = \begin{bmatrix} \frac{5-0}{3} \\ \frac{5-5/3}{2} \end{bmatrix} = \begin{bmatrix} \frac{5}{3} \\ \frac{5}{3} \end{bmatrix}$
3. $\begin{bmatrix} u_2 \\ v_2 \end{bmatrix} = \begin{bmatrix} \frac{5-v_1}{3} \\ \frac{5-u_2}{2} \end{bmatrix} = \begin{bmatrix} \frac{5-5/3}{3} \\ \frac{5-10/9}{2} \end{bmatrix} = \begin{bmatrix} \frac{10}{9} \\ \frac{35}{18} \end{bmatrix}$
4. $\begin{bmatrix} u_3 \\ v_3 \end{bmatrix} = \begin{bmatrix} \frac{5-v_2}{3} \\ \frac{5-u_3}{2} \end{bmatrix} = \begin{bmatrix} \frac{5-35/18}{3} \\ \frac{5-55/54}{2} \end{bmatrix} = \begin{bmatrix} \frac{55}{54} \\ \frac{215}{108} \end{bmatrix}$.

Gauss-Seidel Method

Times	Jacobi	Gauss-Seidel
1	0.8333	0.7454
2	0.3727	0.1242
3	0.1389	0.0207

After 3 iterations, Gauss-Seidel converges faster than Jacobi.

The matrix form of Gauss-Seidel Method

$$
\begin{aligned}
Ax &= b \\
(D+L+U)x &= b \\
(D+L)x &= b - Ux \\
(D+L)x_{k+1} &= b - Ux_k
\end{aligned}
$$

For computation:

$$x_{k+1} = D^{-1}(b - Ux_k - Lx_{k+1})$$

For the proof of convergence:

$$x_{k+1} = (D+L)^{-1}(b - Ux_k).$$

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Gauss-Seidel Method is as follows:

$$
\begin{aligned}
x_0 &= \text{initial vector} \\
x_{k+1} &= D^{-1}(b - Ux_k - Lx_{k+1}) \\
x_{k+1,i} &= \frac{1}{a_{ii}}(b_i - \sum_{j>i} a_{ij}x_{k,j} - \sum_{j<i} a_{ij}x_{k+1,j}) \text{ for } 1 \le i \le n
\end{aligned}
$$

The matrix form of Gauss-Seidel Method

Example

- $\begin{bmatrix} 3 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 5 \\ 5 \end{bmatrix}$,
- $$\begin{aligned} x_{k+1} = \begin{bmatrix} u_{k+1} \\ v_{k+1} \end{bmatrix} &= D^{-1}(b - Ux_k - Lx_{k+1}) \\ &= \begin{bmatrix} \frac{1}{3} & 0 \\ 0 & \frac{1}{2} \end{bmatrix} \left(\begin{bmatrix} 5 \\ 5 \end{bmatrix} - \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} u_k \\ v_k \end{bmatrix} - \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} u_{k+1} \\ v_{k+1} \end{bmatrix} \right) \\ &= \begin{bmatrix} \frac{5 - v_k}{3} \\ \frac{5 - u_{k+1}}{2} \end{bmatrix}. \end{aligned}$$

Convergence of Gauss-Seidel Method

Theorem

If the $n \times n$ matrix A is strictly diagonally dominant, then

1. *A is a nonsingular matrix;*
2. *for every vector b and every starting guess, the Gauss-Seidel Method applied to $Ax = b$ converges to the unique solution.*

Outline

Successive Over-Relaxation

Question: Are there some methods converging faster than the Gauss-Seidel Method?

Successive Over-Relaxation

Question: Are there some methods converging faster than the Gauss-Seidel Method?

Answer: Yes! Successive Over-Relaxation, a variant of the Gauss-Seidel Method.

Relaxation parameter

Example

- Relaxation parameter ω: used to define each component of the new guess x_{k+1} as ω times, and $1-\omega$ times the current guess x_k;
- $\begin{bmatrix} u_{k+1} \\ v_{k+1} \end{bmatrix} = \begin{bmatrix} (1-\omega)u_k + \omega\frac{5-v_k}{3} \\ (1-\omega)v_k + \omega\frac{5-u_{k+1}}{2} \end{bmatrix}$.

1. Let $\omega = \frac{11}{10}$, so $1-\omega = -\frac{1}{10}$;
2. $\begin{bmatrix} u_1 \\ v_1 \end{bmatrix} = \begin{bmatrix} -\frac{u_0}{10} + \frac{11}{10}\cdot\frac{5-v_0}{3} \\ -\frac{v_0}{10} + \frac{11}{10}\cdot\frac{5-u_1}{2} \end{bmatrix} = \begin{bmatrix} \frac{11}{10}\cdot\frac{5-0}{3} \\ \frac{11}{10}\cdot\frac{5-11/6}{2} \end{bmatrix} \approx \begin{bmatrix} 1.8333 \\ 1.7416 \end{bmatrix}$
3. $\begin{bmatrix} u_2 \\ v_2 \end{bmatrix} = \begin{bmatrix} -\frac{u_1}{10} + \frac{11}{10}\cdot\frac{5-v_1}{3} \\ -\frac{v_1}{10} + \frac{11}{10}\cdot\frac{5-u_2}{2} \end{bmatrix} = \begin{bmatrix} -\frac{1.8333}{10} + \frac{11}{10}\cdot\frac{5-1.7416}{3} \\ -\frac{1.7416}{10} + \frac{11}{10}\cdot\frac{5-1.0114}{2} \end{bmatrix} \approx \begin{bmatrix} 1.0114 \\ 2.0196 \end{bmatrix}$

Relaxation parameter

Example

1. $$\begin{bmatrix} u_3 \\ v_3 \end{bmatrix} = \begin{bmatrix} -\frac{u_2}{10} + \frac{11}{10} \cdot \frac{5-v_2}{3} \\ -\frac{v_2}{10} + \frac{11}{10} \cdot \frac{5-u_3}{2} \end{bmatrix} = \begin{bmatrix} -\frac{1.0114}{10} + \frac{11}{10} \cdot \frac{5-2.0196}{3} \\ -\frac{2.0196}{10} + \frac{11}{10} \cdot \frac{5-0.9917}{2} \end{bmatrix} \approx \begin{bmatrix} 0.9917 \\ 2.0026 \end{bmatrix}$$

Successive Over-Relaxation

Times	Jacobi	Gauss-Seidel	SOR($\omega = \frac{11}{10}$)
1	0.8333	0.7454	0.8724
2	0.3727	0.1242	0.0227
3	0.1389	0.0207	0.0087

After 3 iterations, SOR converges faster than Jacobi and Gauss-Seidel.

Relaxation parameter

- Over-relaxation: $\omega > 1$;
- The Gauss-Seidel Method: $\omega = 1$;
- Under-relaxation: $\omega < 1$.

Different relaxation parameters lead to different convergence speeds

Times	Jacobi	Gauss-Seidel	SOR($\omega = \frac{11}{10}$)	SOR($\omega = \frac{6}{5}$)
1	0.8333	0.7454	0.8724	1.0198
2	0.3727	0.1242	0.0227	0.1641
3	0.1389	0.0207	0.0087	0.0230

SOR with parameter $\frac{6}{5}$ converges faster than Jacobi, but slower than Gauss-Seidel.

The matrix form of Successive Over-Relaxation

$$
\begin{aligned}
Ax &= b \\
\omega Ax &= \omega b \\
(\omega D + \omega L + \omega U)x &= \omega b \\
(D + \omega L)x &= \omega b - \omega Ux + (1-\omega)Dx \\
(D + \omega L)x_{k+1} &= \omega b - \omega Ux_k + (1-\omega)Dx_k \\
Dx_{k+1} &= \omega b + (1-\omega)Dx_k - \omega Ux_k - \omega Lx_{k+1}) \\
x_{k+1} &= (1-\omega)x_k + D^{-1}(\omega b - \omega Ux_k - \omega Lx_{k+1})
\end{aligned}
$$

The matrix form of Successive Over-Relaxation

$$
\begin{aligned}
Ax &= b \\
\omega Ax &= \omega b \\
(\omega D + \omega L + \omega U)x &= \omega b \\
(D + \omega L)x &= \omega b - \omega Ux + (1-\omega)Dx \\
(D + \omega L)x_{k+1} &= \omega b - \omega Ux_k + (1-\omega)Dx_k \\
Dx_{k+1} &= \omega b + (1-\omega)Dx_k - \omega Ux_k - \omega Lx_{k+1}) \\
x_{k+1} &= (1-\omega)x_k + D^{-1}(\omega b - \omega Ux_k - \omega Lx_{k+1})
\end{aligned}
$$

Successive Over-Relaxation is as follows:

$$
\begin{aligned}
x_0 &= \text{initial vector} \\
x_{k+1} &= (1-\omega)x_k + D^{-1}(\omega b - \omega Ux_k - \omega Lx_{k+1}) \\
x_{k+1,i} &= (1-\omega)x_{k,i} + \frac{\omega}{a_{ii}}(b_i - \sum_{j>i} a_{ij}x_{k,j} - \sum_{j<i} a_{ij}x_{k+1,j}) \text{ for } 1 \le i \le n.
\end{aligned}
$$

Outline

Eigenvalues and eigenvectors

Definition (Eigenvalues and eigenvectors)

- A: an $n \times n$ matrix;
- λ: a real number;
- v: a nonzero n-dimensional real vector.

If $Av = \lambda v$, then λ is called an **eigenvalue** of A, and v is its corresponding **eigenvector**.

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Eigenvalues are the roots of the ***characteristic polynomial*** $\det(A - \lambda I) = 0$.

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Proposition

Eigenvalues are the roots of the ***characteristic polynomial*** $\det(A - \lambda I) = 0$.

Proposition

Suppose that A is an $n \times n$ matrix, λ is an eigenvalue of A, v is the eigenvector of A w.r.t. λ.
Then, $A^m v = \lambda^m v$.

Eigenvalues and eigenvectors

Example

- $A = \begin{bmatrix} 1 & 3 \\ 2 & 2 \end{bmatrix}$;

Eigenvalues and eigenvectors

Example

- $A = \begin{bmatrix} 1 & 3 \\ 2 & 2 \end{bmatrix}$;
- $\det(A-\lambda I) = \begin{vmatrix} 1-\lambda & 3 \\ 2 & 2-\lambda \end{vmatrix} = (1-\lambda)(2-\lambda)-6 = (\lambda-4)(\lambda+1)$;
- The eigenvalues: 4 and -1;

Eigenvalues and eigenvectors

Example

- $A = \begin{bmatrix} 1 & 3 \\ 2 & 2 \end{bmatrix}$;
- $\det(A-\lambda I) = \begin{vmatrix} 1-\lambda & 3 \\ 2 & 2-\lambda \end{vmatrix} = (1-\lambda)(2-\lambda)-6 = (\lambda-4)(\lambda+1)$;
- The eigenvalues: 4 and -1;
- $(A-4I)x = 0 \Rightarrow \begin{bmatrix} -3 & 3 \\ 2 & -2 \end{bmatrix} x = 0 \Rightarrow -3x_1 + 3x_2 = 0 \Rightarrow x_1 = x_2$;
- The eigenvectors wrt $\lambda = 4$: all nonzero multiples of $\begin{bmatrix} 1 & 1 \end{bmatrix}^\top$;

Eigenvalues and eigenvectors

Example

- $A = \begin{bmatrix} 1 & 3 \\ 2 & 2 \end{bmatrix}$;
- $\det(A-\lambda I) = \begin{vmatrix} 1-\lambda & 3 \\ 2 & 2-\lambda \end{vmatrix} = (1-\lambda)(2-\lambda)-6 = (\lambda-4)(\lambda+1)$;
- The eigenvalues: 4 and -1;
- $(A-4I)x = 0 \Rightarrow \begin{bmatrix} -3 & 3 \\ 2 & -2 \end{bmatrix} x = 0 \Rightarrow -3x_1 + 3x_2 = 0 \Rightarrow x_1 = x_2$;
- The eigenvectors wrt $\lambda = 4$: all nonzero multiples of $\begin{bmatrix} 1 & 1 \end{bmatrix}^\top$;
- $(A+I)x = 0 \Rightarrow \begin{bmatrix} 2 & 3 \\ 2 & 3 \end{bmatrix} x = 0 \Rightarrow 2x_1 + 3x_2 = 0 \Rightarrow x_1 = -\frac{3}{2}x_2$;
- The eigenvectors wrt $\lambda = -1$: all nonzero multiples of $\begin{bmatrix} 3 & -2 \end{bmatrix}^\top$;

Diagonalizable

Definition (Similarity)

Two $n \times n$ matrices A_1 and A_2 are **similar**, denoted by $A_1 \sim A_2$, if there exists a nonsingular $n \times n$ matrix S s.t. $A_1 = SA_2S^{-1}$.

Definition (Diagonal matrix)

The $n \times n$ diagonal matrix D_n is the matrix with $I_{ii} \neq 0$ for $1 \leq i \leq n$.

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & -2 \end{bmatrix}$$

Definition (Diagonalizable matrix)

An $n \times n$ matrix A is **diagonalizable**, if it is similar to a diagonal matrix B.

Diagonalizable

Proposition

- A: *an* $n \times n$ *matrix;*
- $\lambda_1, \lambda_2, \ldots, \lambda_n$: *the eigenvalues of* A*;*
- v_i: *the eigenvector of* A *wrt* λ_i*;*
- $S = \begin{bmatrix} v_1 & v_2 & \ldots & v_n \end{bmatrix}$;
- $B = \begin{bmatrix} \lambda_1 & 0 & \ldots & 0 \\ 0 & \lambda_2 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \lambda_n \end{bmatrix}$.

Then, $A = SBS^{-1}$.

Diagonalizable

Example

- $A = \begin{bmatrix} 1 & 3 \\ 2 & 2 \end{bmatrix}$;
- The eigenvalues: 4 and -1;

Diagonalizable

Example

- $A = \begin{bmatrix} 1 & 3 \\ 2 & 2 \end{bmatrix}$;
- The eigenvalues: 4 and -1;
- $B = \begin{bmatrix} 4 & 0 \\ 0 & -1 \end{bmatrix}$;

Diagonalizable

Example

- $A = \begin{bmatrix} 1 & 3 \\ 2 & 2 \end{bmatrix}$;
- The eigenvalues: 4 and -1;
- $B = \begin{bmatrix} 4 & 0 \\ 0 & -1 \end{bmatrix}$;
- An eigenvector wrt $\lambda_1 = 4$: $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$;
- An eigenvector wrt $\lambda_2 = -1$: $\begin{bmatrix} 3 \\ -2 \end{bmatrix}$;

Diagonalizable

Example

- $A = \begin{bmatrix} 1 & 3 \\ 2 & 2 \end{bmatrix}$;
- The eigenvalues: 4 and -1;
- $B = \begin{bmatrix} 4 & 0 \\ 0 & -1 \end{bmatrix}$;
- An eigenvector wrt $\lambda_1 = 4$: $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$;
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- $A = \begin{bmatrix} 1 & 3 \\ 2 & 2 \end{bmatrix}$;
- The eigenvalues: 4 and -1;
- $B = \begin{bmatrix} 4 & 0 \\ 0 & -1 \end{bmatrix}$;
- An eigenvector wrt $\lambda_1 = 4$: $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$;
- An eigenvector wrt $\lambda_2 = -1$: $\begin{bmatrix} 3 \\ -2 \end{bmatrix}$;
- $S = \begin{bmatrix} 1 & 3 \\ 1 & -2 \end{bmatrix}$;
- $\begin{bmatrix} 1 & 3 \\ 2 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 3 \\ 1 & -2 \end{bmatrix} \begin{bmatrix} 4 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 3 \\ 1 & -2 \end{bmatrix}^{-1}.$

Spectral radius

Definition

Let A be an $n \times n$ matrix and $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of A. The **spectral radius** $\rho(A)$ is defined as $\max\{|\lambda_1|, \ldots, |\lambda_n|\}$.

The spectral radius: the upper bound of $\frac{\|Ax\|_2}{\|x\|_2}$.

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The spectral radius: the upper bound of $\frac{\|Ax\|_2}{\|x\|_2}$.

Example

- $A = \begin{bmatrix} 1 & 3 \\ 2 & 2 \end{bmatrix}$;
- The eigenvalues: 4 and -1;
- $\rho(A) = \max\{|4|, |-1|\} = 4$.

Convergence

Theorem

- *A: an $n \times n$ matrix with spectral radius $\rho(A) < 1$;*
- *b: an vector.*

For any initial vector x_0, the iteration $x_{k+1} = Ax_k + b$ converges, i.e., there exists a unique x_* s.t. $\lim_{k\to\infty} x_k = x_*$ and $x_* = Ax_* + b$.

Proof of the convergence of Jacobi Method

Proof.

- Matrix form: $x_{k+1} = -D^{-1}(L+U)x_k + D^{-1}b$;
- Reduce the proof of convergence to that of $\rho(D^{-1}(L+U)) < 1$;
- Let λ be any eigenvalue of $D^{-1}(L+U)$ with corresponding eigenvector v;
- m: the index such that $|v_m| \geq |v_i|$ for $1 \leq i \neq m \leq n$;
- $D^{-1}(L+U)v = \lambda v \Rightarrow (L+U)v = \lambda Dv$.

Proof of the convergence of Jacobi Method

Proof.

- Take absolute values of the mth component of this vector equation:

$$\begin{aligned} |\lambda||v_m||a_{mm}| &= |\lambda a_{mm} v_m| \\ &= |\sum_{i \neq m} a_{mi} v_i| \\ &\leq |v_m| \sum_{i \neq m} |a_{mi}| \\ &< |v_m||a_{mm}|. \end{aligned}$$

- Hence, $|\lambda| < 1$.
- Since λ is an arbitrary eigenvalue, we have that $\rho(D^{-1}(L+U)) < 1$.

Proof of the convergence of Gauss-Seidel Method

Proof.

- Matrix form: $x_{k+1} = -(L+D)^{-1}Ux_k + (L+D)^{-1}b$
- Reduce the proof of convergence to that of $\rho((L+D)^{-1}U) < 1$;
- Let λ be any eigenvalue of $(L+D)^{-1}U$ with corresponding eigenvector v;
- m: the index such that $|v_m| \geq |v_i|$ for $1 \leq i \neq m \leq n$;
- $(L+D)^{-1}Uv = \lambda v \Rightarrow Uv = \lambda(D+L)v$.

Proof of the convergence of Gauss-Seidel Method

Proof.

- $$\begin{aligned} |\lambda||v_m| \cdot \sum_{i>m} |a_{mi}| &< |\lambda||v_m| \cdot (|a_{mm}| - \sum_{i<m} |a_{mi}|) \\ &\leq |\lambda| \cdot (|a_{mm}v_m| - \sum_{i<m} |a_{mi}v_i|) \\ &\leq |\lambda| \cdot |a_{mm}v_m + \sum_{i<m} a_{mi}v_i| \\ &= |\sum_{i>m} a_{mi}v_i| \\ &\leq |v_m| \sum_{i>m} |a_{mi}| \end{aligned}$$
- Hence, $|\lambda| < 1$.
- Since λ is arbitrary, we have that $\rho((L+D)^{-1}U) < 1$.

Outline

Methods for symmetric positive-definite matrices

Sometimes, we handle some special matrices, *e.g.*, symmetric and positive-definite.

Question: For this type of matrices, are there some methods converging faster?

Methods for symmetric positive-definite matrices

Sometimes, we handle some special matrices, *e.g.*, symmetric and positive-definite.

Question: For this type of matrices, are there some methods converging faster?

Answer: Yes! Conjugate Gradient Method.

Symmetric positive-definite matrices

Definition

The $n \times n$ matrix A is

- **symmetric**: $A^\top = A$;
- **positive-definite**: $x^\top A x > 0$ for all vectors $x \neq 0$.

Example

$A = \begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix}$ is symmetric positive-definite.

- symmetric: $A^\top = \begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix} = A$;
- positive-definite:
$$\begin{aligned} x^\top A x &= \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\ &= 2x_1^2 + 4x_1 x_2 + 5x_2^2 \\ &= 2(x_1 + x_2)^2 + 3x_2^2 \\ &> 0 \text{ if } x_1, x_2 > 0 \end{aligned}$$

Symmetric positive-definite matrices

Example

$A = \begin{bmatrix} 2 & 4 \\ 4 & 5 \end{bmatrix}$ is not positive-definite.

$$
\begin{aligned}
x^\top A x &= \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 2 & 4 \\ 4 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\
&= 2x_1^2 + 8x_1x_2 + 5x_2^2 \\
&= 2(x_1 + 2x_2)^2 - 3x_2^2 \\
&= 2(-2 + 2 \cdot 1)^2 - 3 \cdot 1^2 \quad (x_1 = -2, x_2 = 1) \\
&= -3 \\
&< 0
\end{aligned}
$$

Properties of positive-definite matrices

Lemma

A matrix is nonsingular iff $Ax = 0$ implies that $x = 0$.

Proposition

A positive-definite matrix is nonsingular.

Proof.

We want to prove that $x = 0$ when A is positive-definite and $Ax = 0$.
Since $y^\top Ay > 0$ for every nonzero vector y, we have $Ay \neq 0$.
Hence, x must be zero vector.
So A is nonsingular.

Properties of symmetric matrices

Theorem (The finite-dimensional spectral theorem)

Let A be a symmetric $n \times n$ matrix. Then the set of unit eigenvectors of A is an orthonormal set $\{v_1, \ldots, v_n\}$ forming a basis of R^n.

Properties of symmetric matrices

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Let A be a symmetric $n \times n$ matrix. Then the set of unit eigenvectors of A is an orthonormal set $\{v_1, \ldots, v_n\}$ forming a basis of R^n.

Example

- $A = \begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix}$;

Properties of symmetric matrices

Theorem (The finite-dimensional spectral theorem)

Let A be a symmetric $n \times n$ matrix. Then the set of unit eigenvectors of A is an orthonormal set $\{v_1, \ldots, v_n\}$ forming a basis of R^n.

Example

- $A = \begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix}$;
- $\det(A - \lambda I) = \begin{vmatrix} 2-\lambda & 2 \\ 2 & 5-\lambda \end{vmatrix} = (2-\lambda)(5-\lambda) - 4 = (\lambda-6)(\lambda-1)$;
- The eigenvalues: 6 and 1.

Properties of symmetric matrices

Example

- $(A-6I)x=0 \Rightarrow \begin{bmatrix} -4 & 2 \\ 2 & -1 \end{bmatrix} x = 0 \Rightarrow 2x_1 - x_2 = 0 \Rightarrow x_1 = \frac{1}{2}x_2$;
- An eigenvector wrt $\lambda = 6$: $\begin{bmatrix} 1 & 2 \end{bmatrix}^\top$;
- The unit eigenvector wrt $\lambda = 6$ via normalization: $\begin{bmatrix} \frac{v_1}{\|v\|_2} & \frac{v_2}{\|v\|_2} \end{bmatrix}^\top = \begin{bmatrix} \frac{1}{\sqrt{2^2+1^2}} & \frac{2}{\sqrt{2^2+1^2}} \end{bmatrix}^\top = \begin{bmatrix} \frac{\sqrt{5}}{5} & \frac{2\sqrt{5}}{5} \end{bmatrix}^\top$;

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- $(A-I)x=0 \Rightarrow \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} x = 0 \Rightarrow x_1 + 2x_2 = 0 \Rightarrow x_1 = -2x_2$;
- An eigenvector wrt $\lambda = 1$: $\begin{bmatrix} 2 & -1 \end{bmatrix}^\top$;
- The unit eigenvector wrt $\lambda = 1$ via normalization: $\begin{bmatrix} \frac{v_1}{\|v\|_2} & \frac{v_2}{\|v\|_2} \end{bmatrix}^\top = \begin{bmatrix} \frac{2}{\sqrt{2^2+(-1)^2}} & -\frac{1}{\sqrt{2^2+(-1)^2}} \end{bmatrix}^\top = \begin{bmatrix} \frac{2\sqrt{5}}{5} & -\frac{\sqrt{5}}{5} \end{bmatrix}^\top$;

Properties of symmetric matrices

Example

- $(A-6I)x=0 \Rightarrow \begin{bmatrix} -4 & 2 \\ 2 & -1 \end{bmatrix} x = 0 \Rightarrow 2x_1 - x_2 = 0 \Rightarrow x_1 = \frac{1}{2}x_2;$
- An eigenvector wrt $\lambda = 6$: $\begin{bmatrix} 1 & 2 \end{bmatrix}^\top;$
- The unit eigenvector wrt $\lambda = 6$ via normalization: $\begin{bmatrix} \frac{v_1}{\|v\|_2} & \frac{v_2}{\|v\|_2} \end{bmatrix}^\top = \begin{bmatrix} \frac{1}{\sqrt{2^2+1^2}} & \frac{2}{\sqrt{2^2+1^2}} \end{bmatrix}^\top = \begin{bmatrix} \frac{\sqrt{5}}{5} & \frac{2\sqrt{5}}{5} \end{bmatrix}^\top;$
- $(A-I)x=0 \Rightarrow \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix} x = 0 \Rightarrow x_1 + 2x_2 = 0 \Rightarrow x_1 = -2x_2;$
- An eigenvector wrt $\lambda = 1$: $\begin{bmatrix} 2 & -1 \end{bmatrix}^\top;$
- The unit eigenvector wrt $\lambda = 1$ via normalization: $\begin{bmatrix} \frac{v_1}{\|v\|_2} & \frac{v_2}{\|v\|_2} \end{bmatrix}^\top = \begin{bmatrix} \frac{2}{\sqrt{2^2+(-1)^2}} & -\frac{1}{\sqrt{2^2+(-1)^2}} \end{bmatrix}^\top = \begin{bmatrix} \frac{2\sqrt{5}}{5} & -\frac{\sqrt{5}}{5} \end{bmatrix}^\top;$
- $\left\{ \begin{bmatrix} \frac{\sqrt{5}}{5} & \frac{2\sqrt{5}}{5} \end{bmatrix}^\top, \begin{bmatrix} \frac{2\sqrt{5}}{5} & -\frac{\sqrt{5}}{5} \end{bmatrix}^\top \right\}$ are an orthonormal set of R^2.

Properties of symmetric positive-definite matrices

Proposition

Suppose that the $n \times n$ matrix A is symmetric.
Then, A is positive-definite iff all of its eigenvalues are positve.

Proof.

($\Longrightarrow$) A is positive-definite and $Av = \lambda v$ for any nonzero vector v.
$0 < v^\top A v = v^\top \lambda v = \lambda \|v\|_2^2$.
Since $\|v\|_2^2 > 0$, $\lambda > 0$.

Properties of symmetric positive-definite matrices

Proof.

($\Longleftarrow$) By the finite-dimensional spectral theorem, any nonzero vector x can be represented by

$$x = c_1 v_1 + \ldots + c_n v_n$$

where $v_1, \ldots, v_n$ are the eigenvectors of A and not all c_i are zero.

$$\begin{aligned} x^\top A x &= (c_1 v_1 + \ldots + c_n v_n)^\top A (c_1 v_1 + \ldots + c_n v_n) \\ &= (c_1 v_1 + \ldots + c_n v_n)^\top (\lambda_1 c_1 v_1 + \ldots + \lambda_n c_n v_n) \\ &= \lambda_1 c_1^2 + \ldots + \lambda_n c_n^2 \\ &> 0 \end{aligned}$$

Properties of symmetric positive-definite matrices

Definition

A principal submatrix of a square matrix A is a square submatrix whose diagonal entries are diagonal entries of A.

Proposition

Any principal submatrix of a symmetric positive-definite matrix is symmetric positive-definite.

Example

If $\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}$ is symmetric positive-definite,

then so is $\begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix}$.

Outline

A-Conjugate

Assume we have a symmetric positive-definite $n \times n$ matrix A.

Definition

For two n-vectors v and w, define the A-**inner product** as

$$(v, w)_A = v^\top A w.$$

The vectors v and w are A-**conjugate** if $(v, w)_A = 0$.

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For two n-vectors v and w, define the A-**inner product** as

$$(v, w)_A = v^\top A w.$$

The vectors v and w are A-**conjugate** if $(v, w)_A = 0$.

Proposition

- *Symmetry:* $(v, w)_A = (w, v)_A$;
- *Linearity:* $(\alpha v, w)_A = \alpha(v, w)_A$ *and* $(v, \alpha w)_A = \alpha(v, w)_A$;
- *Positive-definiteness:* $(v, v)_A > 0$ *if* $v \neq 0$;
- *Classical inner-product:* $(v, w) = (v, w)_I$.

Conjugate Gradient Method

Lemma

Let $D = \{d_1, \cdots, d_n\}$ a set of n mutually conjugate vectors wrt to A. Then D forms a basis for R^n.

Conjugate Gradient Method

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Let $D = \{d_1, \cdots, d_n\}$ a set of n mutually conjugate vectors wrt to A. Then D forms a basis for R^n.

Proposition

The solution x^* of $Ax = b$ can be represented by

$$x^* = \sum_{k=1}^{n} \alpha_k d_k.$$

Question: How to compute the mutually conjugate vectors D and their corresponding coefficients α_k's?

Some notations of Conjugate Gradient Method

1. d_k: the k-th mutually conjugate vector;
2. α_k: the coefficient of d_k for x^* ensuring $(d_k, r_{k+1}) = 0$;
3. x_k: the approximate solution at step k;
   - the projection of x^* onto $\{d_1, \ldots, d_{k-1}\}$, *i.e.*, $\sum_{i=1}^{k-1} \alpha_i d_i$;

Some notations of Conjugate Gradient Method

1. d_k: the k-th mutually conjugate vector;
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3. x_k: the approximate solution at step k;
   - the projection of x^* onto $\{d_1, \ldots, d_{k-1}\}$, *i.e.*, $\sum_{i=1}^{k-1} \alpha_i d_i$;
4. r_k: the residual of x_k at step k, *i.e.*, $b - Ax_k$;
   - $(r_i, r_k) = 0$ for $0 \leq i < k$;
5. β_k: the coefficient ensuring $(d_k, d_{k+1})_A = 0$.

An iterative framework for Conjugate Gradient Method

Algorithm 1: Conjugate Gradient Method

$x_0 =$ initial guess
$d_0 = r_0 = b - Ax_0$
for $k = 0, 1, 2, \ldots, n-1$ **do**
    if r_k *is sufficiently small* **then**
        return x_k
    Compute the parameters $\alpha_k, x_{k+1}, r_{k+1}, \beta_k$ and d_{k+1}.

An iterative framework for Conjugate Gradient Method

Algorithm 2: Conjugate Gradient Method

$x_0 =$ initial guess
$d_0 = r_0 = b - Ax_0$
for $k = 0, 1, 2, \ldots, n-1$ **do**
  if r_k *is sufficiently small* **then**
    return x_k
  Compute the parameters $\alpha_k, x_{k+1}, r_{k+1}, \beta_k$ and d_{k+1}.

- $(r_i, r_k) = 0$ for $0 \leq i < k$ implies the method ends in n iterations.
- To achieve this, we need $(r_{k+1}, d_k) = 0$ for each iteration.
- In addition, $(d_k, d_{k+1})_A = 0$ is guaranteed for each iteration.

Computation of x_{k+1}, r_{k+1} and d_{k+1}

By definition:

$$
\begin{aligned}
x_{k+1} &= x_k + \alpha_k d_k \\
b - Ax_{k+1} &= b - Ax_k - \alpha_k A d_k \\
r_{k+1} &= r_k - \alpha_k A d_k
\end{aligned}
$$

Update d_{k+1} by r_{k+1} and d_k:

$$d_{k+1} = r_{k+1} + \beta_k d_k.$$

Computation of α_k

Choose α_k s.t. $r_{k+1}^\top d_k = 0$:

Computation of α_k

Choose α_k s.t. $r_{k+1}^\top d_k = 0$:

$$\begin{aligned} r_{k+1} &= r_k - \alpha_k A d_k \\ 0 = d_k^\top r_{k+1} &= d_k^\top r_k - \alpha_k d_k^\top A d_k \\ \alpha_k &= \frac{d_k^\top r_k}{d_k^\top A d_k} \end{aligned}$$

Computation of α_k

Choose α_k s.t. $r_{k+1}^\top d_k = 0$:

$$
\begin{aligned}
r_{k+1} &= r_k - \alpha_k A d_k \\
0 = d_k^\top r_{k+1} &= d_k^\top r_k - \alpha_k d_k^\top A d_k \\
\alpha_k &= \frac{d_k^\top r_k}{d_k^\top A d_k}
\end{aligned}
$$

α_k can be transformed as $\frac{r_k^\top r_k}{d_k^\top A d_k}$ because the following

$$
\begin{aligned}
d_k - r_k &= \beta_{k-1} d_{k-1} \\
r_k^\top d_k - r_k^\top r_k &= 0 \qquad\qquad (r_k^\top d_{k-1} = 0)
\end{aligned}
$$

Computation of β_k

Choose β_k s.t. $d_k^\top A d_{k+1} = 0$:

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d_{k+1} &= r_{k+1} + \beta_k d_k \\
0 = d_k^\top A d_{k+1} &= d_k^\top A r_{k+1} + \beta_k d_k^\top A d_k \\
\beta_k &= -\frac{d_k^\top A r_{k+1}}{d_k^\top A d_k}.
\end{aligned}
$$

Computation of β_k

Choose β_k s.t. $d_k^\top A d_{k+1} = 0$:

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β_k can be simplified as $\frac{r_{k+1}^\top r_{k+1}}{r_k^\top r_k}$ because the following

- $d_k^\top A r_{k+1} = \frac{1}{\alpha_k}(r_k - r_{k+1})^\top r_{k+1} = -\frac{1}{\alpha_k} r_{k+1}^\top r_{k+1}$;
- $d_k^\top A d_k = (r_k + \beta_{k-1} d_{k-1})^\top A d_k = \frac{1}{\alpha_k} r_k^\top (r_k - r_{k+1}) = \frac{1}{\alpha_k} r_k^\top r_k$.

Conjugate Gradient Method

Algorithm 3: Conjugate Gradient Method

$x_0 =$ initial guess

$d_0 = r_0 = b - Ax_0$

for $k = 0, 1, 2, \ldots, n-1$ **do**

  if r_k *is sufficiently small* **then**

    return x_k

  $\alpha_k = \frac{r_k^\top r_k}{d_k^\top A d_k}$

  $x_{k+1} = x_k + \alpha_k d_k$

  $r_{k+1} = r_k - \alpha_k A d_k$

  $\beta_k = \frac{r_{k+1}^\top r_{k+1}}{r_k^\top r_k}$

  $d_{k+1} = r_{k+1} + \beta_k d_k$

Example

Example (Initialize x_0, d_0 and r_0)

Solve $\begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 6 \\ 3 \end{bmatrix}$ using the Conjugate Gradient Method. .

- $x_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$;
- $r_0 = d_0 = \begin{bmatrix} 6 \\ 3 \end{bmatrix}$.

Example

Example (1st step)

- $\alpha_0 = \dfrac{\begin{bmatrix} 6 & 3 \end{bmatrix}\begin{bmatrix} 6 \\ 3 \end{bmatrix}}{\begin{bmatrix} 6 & 3 \end{bmatrix}\begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix}\begin{bmatrix} 6 \\ 3 \end{bmatrix}} = \frac{45}{6\cdot 18+3\cdot 27} = \frac{5}{21}$;
- $x_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix} + \frac{5}{21}\begin{bmatrix} 6 \\ 3 \end{bmatrix} = \begin{bmatrix} \frac{10}{7} \\ \frac{5}{7} \end{bmatrix}$;
- $r_1 = \begin{bmatrix} 6 \\ 3 \end{bmatrix} - \frac{5}{21}\begin{bmatrix} 18 \\ 27 \end{bmatrix} = 12\begin{bmatrix} \frac{1}{7} \\ -\frac{2}{7} \end{bmatrix}$;
- $\beta_0 = \frac{144\cdot 5/49}{36+9} = \frac{16}{49}$;
- $d_1 = 12\begin{bmatrix} \frac{1}{7} \\ -\frac{2}{7} \end{bmatrix} + \frac{16}{49}\begin{bmatrix} 6 \\ 3 \end{bmatrix} = \begin{bmatrix} \frac{180}{49} \\ -\frac{120}{49} \end{bmatrix}$.

Example

Example (2nd step)

- $$\alpha_1 = \frac{\begin{bmatrix} \frac{12}{7} & -\frac{24}{7} \end{bmatrix} \begin{bmatrix} \frac{12}{7} \\ -\frac{24}{7} \end{bmatrix}}{\begin{bmatrix} \frac{180}{49} & -\frac{120}{49} \end{bmatrix} \begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix} \begin{bmatrix} \frac{180}{49} \\ -\frac{120}{49} \end{bmatrix}} = \frac{7}{10};$$
- $$x_2 = \begin{bmatrix} \frac{10}{7} \\ \frac{5}{7} \end{bmatrix} + \frac{7}{10} \begin{bmatrix} \frac{180}{49} \\ -\frac{120}{49} \end{bmatrix} = \begin{bmatrix} 4 \\ -1 \end{bmatrix};$$
- $$r_2 = 12 \begin{bmatrix} \frac{1}{7} \\ -\frac{2}{7} \end{bmatrix} - \frac{7}{10} \begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix} \begin{bmatrix} \frac{180}{49} \\ -\frac{120}{49} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix};$$
- The solution is $x_2 = \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 4 \\ -1 \end{bmatrix}$ since $r_2 = 0$.

Main theorem

Theorem (Main theorem)

Let $b \neq 0$, $x_0 = 0$, *and* $r_k \neq 0$ *for* $k < n$. *Then for each* $1 \leq k \leq n$,

1. *the following three subspaces of* R^n *are equal:*
$$(x_1, \dots, x_k) = (r_0, \dots, r_{k-1}) = (d_0, \dots, d_{k-1});$$
2. *distinct residuals are pairwise orthogonal:*
$$r_k^\top r_j = 0 \text{ for } j < k;$$
3. *distinct vectors of a subspace span are pairwise* A*-conjugate:*
$$d_k^\top A d_j = 0 \text{ for } j < k.$$

Proof of 1st item

Proof.

- Base case ($k = 1$): $(x_1) = (r_0) = (d_0)$ since
  $x_1 = x_0 + \alpha\, d_0 = \alpha_0\, d_0 = \alpha_0\, r_0$.

Proof of 1st item

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- Base case ($k = 1$): $(x_1) = (r_0) = (d_0)$ since $x_1 = x_0 + \alpha d_0 = \alpha_0 d_0 = \alpha_0 r_0$.
- Inductive step ($k > 1$): Suppose that the $k - 1$ case hold.

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Proof.

- Base case ($k = 1$): $(x_1) = (r_0) = (d_0)$ since $x_1 = x_0 + \alpha d_0 = \alpha_0 d_0 = \alpha_0 r_0$.
- Inductive step ($k > 1$): Suppose that the $k - 1$ case hold.

  1. $(x_1, \dots, x_k) \subseteq (d_0, \dots, d_{k-1})$: $x_k = \sum_{i=0}^{k-1} \alpha_i d_i$;

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- Inductive step ($k > 1$): Suppose that the $k - 1$ case hold.
  1. $(x_1, \ldots, x_k) \subseteq (d_0, \ldots, d_{k-1})$: $x_k = \sum_{i=0}^{k-1} \alpha_i d_i$;
  2. $(x_1, \ldots, x_k) \supseteq (d_0, \ldots, d_{k-1})$: $x_k = x_{k-1} + \alpha_{k-1} d_{k-1} \Rightarrow d_{k-1} = \frac{1}{\alpha_{k-1}} x_k - \frac{1}{\alpha_{k-1}} x_{k-1}$.

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  1. $(r_0, \dots, r_{k-1}) \subseteq (d_0, \dots, d_{k-1})$: $d_{k-1} = r_{k-1} + \beta_{k-2}\, d_{k-2} \Rightarrow r_{k-1} = d_{k-1} - \beta_{k-2}\, d_{k-2}$;

Proof of 1st item

Proof.

- Base case ($k=1$): $(x_1)=(r_0)=(d_0)$ since $x_1 = x_0 + \alpha d_0 = \alpha_0 d_0 = \alpha_0 r_0$.
- Inductive step ($k>1$): Suppose that the $k-1$ case hold.
  1. $(x_1,\ldots,x_k) \subseteq (d_0,\ldots,d_{k-1})$: $x_k = \sum_{i=0}^{k-1} \alpha_i d_i$;
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     $x_k = x_{k-1} + \alpha_{k-1} d_{k-1} \Rightarrow d_{k-1} = \frac{1}{\alpha_{k-1}} x_k - \frac{1}{\alpha_{k-1}} x_{k-1}$.

  1. $(r_0,\ldots,r_{k-1}) \subseteq (d_0,\ldots,d_{k-1})$:
     $d_{k-1} = r_{k-1} + \beta_{k-2} d_{k-2} \Rightarrow r_{k-1} = d_{k-1} - \beta_{k-2} d_{k-2}$;
  2. $(r_0,\ldots,r_{k-1}) \supseteq (d_0,\ldots,d_{k-1})$:
     $$d_{k-2} = \sum_{i=0}^{k-2} \gamma_i r_i \Rightarrow$$
     $$d_{k-1} = r_{k-1} + \beta_{k-2} d_{k-2} = r_{k-1} + \sum_{i=0}^{k-2} (\beta_{k-2}\gamma_i) r_i.$$

Lemmas of the 2nd and 3rd items

Lemma

$(r_j, d_k)_A = 0$ *for* $0 \leq j < k$ *or* $0 \leq k < j+1$.

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Here we only prove the case that $0 \leq j < k$.
If $j = 0$, then $d_k^\top A r_0 = d_k^\top A d_0 = 0$;

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$d_k^\top A r_j = d_k^\top A(d_j - \beta_{j-1} d_{j-1}) = d_k^\top A d_j - \beta_{j-1} d_k^\top A d_{j-1} = 0.$

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$d_k^\top A d_k = r_k^\top A d_k.$

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If $j = 0$, then $d_k^\top A r_0 = d_k^\top A d_0 = 0$;
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Lemma

$d_k^\top A d_k = r_k^\top A d_k$.

Proof.

$d_k^\top A d_k = r_k^\top A d_k + \beta_{k-1} d_{k-1}^\top A d_k = r_k^\top A d_k$.

Proof of the 2nd and 3rd items

Proof.

Base case ($k = 1$):

1. $r_0^\top r_1 = r_0^\top r_0 - \alpha_0 r_0^\top A d_0 = r_0^\top r_0 - \frac{r_0^\top r_0}{d_0^\top A d_0} d_0^\top A d_0 = 0;$

Proof of the 2nd and 3rd items

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2. $\beta_0 = -\frac{r_1^\top A d_0}{d_0^\top A d_0};$
3. $d_0^\top A d_1 = d_0^\top A r_1 + \beta_0 d_0^\top A d_0 = d_0^\top A r_1 - \frac{r_1^\top A d_0}{d_0^\top A d_0} d_0^\top A d_0 = 0.$

Proof of the 2nd and 3rd items

Proof.

Inductive step ($k > 1$): Suppose that the $k-1$ case hold.

The 2nd item:

1. $r_j^\top r_k = r_j^\top r_{k-1} - \alpha_{k-1} r_j^\top A d_{k-1}$;

Proof of the 2nd and 3rd items

Proof.

Inductive step $(k > 1)$: Suppose that the $k-1$ case hold.

The 2nd item:

1. $r_j^\top r_k = r_j^\top r_{k-1} - \alpha_{k-1} r_j^\top A d_{k-1}$;
2. If $j < k-1$, then $r_j^\top r_k = 0$;

Proof of the 2nd and 3rd items

Proof.

Inductive step $(k > 1)$: Suppose that the $k-1$ case hold.

The 2nd item:

1. $r_j^\top r_k = r_j^\top r_{k-1} - \alpha_{k-1} r_j^\top A d_{k-1}$;
2. If $j < k-1$, then $r_j^\top r_k = 0$;
3. If $j = k-1$, then $\alpha_{k-1} = \frac{r_{k-1}^\top r_{k-1}}{d_{k-1}^\top A d_{k-1}}$;

Proof of the 2nd and 3rd items

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The 2nd item:

1. $r_j^\top r_k = r_j^\top r_{k-1} - \alpha_{k-1} r_j^\top A d_{k-1}$;
2. If $j < k-1$, then $r_j^\top r_k = 0$;
3. If $j = k-1$, then $\alpha_{k-1} = \frac{r_{k-1}^\top r_{k-1}}{d_{k-1}^\top A d_{k-1}}$;
4. $$\begin{aligned} r_{k-1}^\top r_k &= r_{k-1}^\top r_{k-1} - \alpha_{k-1} r_{k-1}^\top A d_{k-1} \\ &= r_{k-1}^\top r_{k-1} - \frac{r_{k-1}^\top r_{k-1}}{d_{k-1}^\top A d_{k-1}} d_{k-1}^\top A d_{k-1} = 0. \end{aligned}$$

Proof of the 2nd and 3rd items

Proof.

Inductive step ($k > 1$): Suppose that the $k-1$ case hold.

The 3rd item:

1. $d_j^\top A d_k = d_j^\top A r_k + \beta_{k-1} d_j^\top A d_{k-1}$;

Proof of the 2nd and 3rd items

Proof.

Inductive step ($k > 1$): Suppose that the $k-1$ case hold.

The 3rd item:

1. $d_j^\top A d_k = d_j^\top A r_k + \beta_{k-1} d_j^\top A d_{k-1}$;
2. If $j < k-1$, then $A d_j = \frac{r_j - r_{j+1}}{\alpha_j}$ is orthogonal to r_k, *i.e.*, $d_j^\top A r_k = 0$;

Proof of the 2nd and 3rd items

Proof.

Inductive step ($k > 1$): Suppose that the $k-1$ case hold.

The 3rd item:

1. $d_j^\top A d_k = d_j^\top A r_k + \beta_{k-1} d_j^\top A d_{k-1}$;
2. If $j < k-1$, then $A d_j = \frac{r_j - r_{j+1}}{\alpha_j}$ is orthogonal to r_k, *i.e.*, $d_j^\top A r_k = 0$;
3. So $d_j^\top A d_k = 0$.

Proof of the 2nd and 3rd items

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Inductive step ($k > 1$): Suppose that the $k-1$ case hold.
The 3rd item:

1. $d_j^\top A d_k = d_j^\top A r_k + \beta_{k-1} d_j^\top A d_{k-1}$;
2. If $j < k-1$, then $A d_j = \frac{r_j - r_{j+1}}{\alpha_j}$ is orthogonal to r_k, *i.e.*, $d_j^\top A r_k = 0$;
3. So $d_j^\top A d_k = 0$.
4. If $j = k-1$, then $\beta_{k-1} = -\frac{r_k^\top A d_{k-1}}{d_{k-1}^\top A d_{k-1}}$.

Proof of the 2nd and 3rd items

Proof.

Inductive step ($k > 1$): Suppose that the $k-1$ case hold.

The 3rd item:

1. $d_j^\top A d_k = d_j^\top A r_k + \beta_{k-1} d_j^\top A d_{k-1}$;
2. If $j < k-1$, then $A d_j = \frac{r_j - r_{j+1}}{\alpha_j}$ is orthogonal to r_k, *i.e.*, $d_j^\top A r_k = 0$;
3. So $d_j^\top A d_k = 0$.
4. If $j = k-1$, then $\beta_{k-1} = -\frac{r_k^\top A d_{k-1}}{d_{k-1}^\top A d_{k-1}}$.
5. So $$\begin{aligned} d_{k-1}^\top A d_k &= d_{k-1}^\top A r_k + \beta_{k-1} d_{k-1}^\top A d_{k-1} \\ &= d_{k-1}^\top A r_k - \frac{r_k^\top A d_{k-1}}{d_{k-1}^\top A d_{k-1}} d_{k-1}^\top A d_{k-1} = 0. \end{aligned}$$

Outline

Motivation of Preconditioning

- Suppose that $Ax = b$ is a linear system.
- Condition number of A: a bound on how inaccurate the solution x will be after approximation.
- A is ill-conditioned: the condition number of A is very large.
- A is ill-conditioned $\Rightarrow$ Conjugate Gradient Method fails.

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- Suppose that $Ax = b$ is a linear system.
- Condition number of A: a bound on how inaccurate the solution x will be after approximation.
- A is ill-conditioned: the condition number of A is very large.
- A is ill-conditioned $\Rightarrow$ Conjugate Gradient Method fails.
- Questions: Is it possible to handle the ill-conditioned matrix?
- Answer: Precondition.

Motivation of Preconditioning

Definition

Suppose $M = M_1 M_2$ is nonsingular and $Ax = b$ is a linear system. Let $\tilde{A}\tilde{x} = \tilde{b}$ be the linear system where

- $\tilde{A} = {M_1}^{-1} A {M_2}^{-1}$;
- $\tilde{x} = M_2 x$;
- $\tilde{b} = {M_1}^{-1} b$.

The matrix M is called a **preconditioner**.

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The matrix M is called a **preconditioner**.

- An effective preconditioner reduces the condition number, *i.e.*, $\mathrm{cond}({M_1}^{-1} A {M_2}^{-1})$ is small.
- Two criterion of choosing M:
  1. M as close to A;
  2. M is simple to invert.

Three preconditioners

Let $A = L + D + L^\top$.

1. **Jacobi preconditioner**: $M = D$;
2. **Gauss-Seidel preconditioner**: $M = (D + L)D^{-1}(D + L)^\top$;
3. **SSOR preconditioner**: $M = (D + \omega L)D^{-1}(D + \omega L)^\top$ where $0 \le \omega \le 2$.

Preconditioner

Lemma

Let M be symmetric positive-definite matrix. Then, there exists a unique symmetric positive-definite matrix C s.t. $M = C^2$.

Preconditioner

Lemma

Let M be symmetric positive-definite matrix. Then, there exists a unique symmetric positive-definite matrix C s.t. $M = C^2$.

Since A is symmetric positive-definite, we choose a symmetric positive-definite preconditioner M.

Definition

Suppose $M = C^2$ is symmetric positive-definite and $Ax = b$ is a linear system. Let $\tilde{A}\tilde{x} = \tilde{b}$ be the linear system where

- $\tilde{A} = C^{-1}AC^{-1}$;
- $\tilde{x} = Cx$;
- $\tilde{b} = C^{-1}b$.

The matrix M is called a **preconditioner**.

Some notations of Conjugate Gradient Method to preconditioned linear system

We use the Conjugate Gradient method to solve

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

1. $\tilde{d}_k$: the k-th mutually conjugate vector wrt $C^{-1}AC^{-1}$;
2. $\tilde{\alpha}_k$: the coefficient of $\tilde{d}_k$ for $\tilde{x}^*$;
3. $\tilde{x}_k$: the approximate solution to $\tilde{x}^*$ at step k;
4. $\tilde{r}_k$: the residual of $\tilde{x}_k$ of preconditioned system at step k, *i.e.*, $\tilde{b} - \tilde{A}\tilde{x}_k = C^{-1}(b - Ax_k) = C^{-1}r_k$;
5. $\tilde{\beta}_k$: the coefficient ensuring $(\tilde{d}_k, \tilde{d}_{k+1})_{\tilde{A}} = 0$.

Computation of the forementioned notations

1. $\tilde{\alpha}_k = \frac{\tilde{r}_k^\top \tilde{r}_k}{\tilde{d}_k^\top \tilde{A} \tilde{d}_k}$;
2. $\tilde{x}_{k+1} = \tilde{x}_k + \tilde{\alpha}_k \tilde{d}_k$;
3. $\tilde{r}_{k+1} = \tilde{r}_k - \tilde{\alpha}_k \tilde{A} \tilde{d}_k$;
4. $\tilde{\beta}_k = \frac{\tilde{r}_{k+1}^\top \tilde{r}_{k+1}}{\tilde{r}_k^\top \tilde{r}_k}$;
5. $\tilde{d}_{k+1} = \tilde{r}_{k+1} + \tilde{\beta}_k \tilde{d}_k$.

The Extra Computation of Direct Usage of CGM

1. Decompose M as $C \cdot C$;
2. Compute C^{-1};
3. Compute $\tilde{A} = C^{-1} A C^{-1}$;
4. Compute $\tilde{b} = C^{-1} b$;
5. Compute $x_k = C^{-1} \tilde{x}_k$.

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5. Compute $x_k = C^{-1}\tilde{x}_k$.

To reduce the extra computations, we incorporate the above computations into CGM.

Simplified Computation

1. Let $z_k = M^{-1} r_k$;
2. $\tilde{r}_k^\top \tilde{r}_k = r_k^\top (C^{-1})^\top C^{-1} r_k = r_k^\top M^{-1} r_k = r_k^\top z_k$;
3. Let $d_k = C^{-1} \tilde{d}_k$;
4. $\tilde{d}_k^\top \tilde{A} \tilde{d}_k = d_k^\top C^\top C^{-1} A C^{-1} C d_k = d_k^\top A d_k$.

Simplified Computation

1. $\tilde{\alpha}_k = \dfrac{\tilde{r}_k^\top \tilde{r}_k}{\tilde{d}_k^\top \tilde{A} \tilde{d}_k} = \dfrac{r_k^\top z_k}{d_k^\top A d_k}$;

Simplified Computation

1. $\tilde{\alpha}_k = \dfrac{\tilde{r}_k^\top \tilde{r}_k}{\tilde{d}_k^\top \tilde{A} \tilde{d}_k} = \dfrac{r_k^\top z_k}{d_k^\top A d_k}$;
2. $\tilde{x}_{k+1} = \tilde{x}_k + \tilde{\alpha}_k \tilde{d}_k \Rightarrow Cx_{k+1} = Cx_k + \tilde{\alpha}_k C d_k \Rightarrow$
   $Cx_{k+1} = C(x_k + \tilde{\alpha}_k d_k) \Rightarrow x_{k+1} = x_k + \tilde{\alpha}_k d_k$;

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1. $\tilde{\alpha}_k = \dfrac{\tilde{r}_k^\top \tilde{r}_k}{\tilde{d}_k^\top \tilde{A} \tilde{d}_k} = \dfrac{r_k^\top z_k}{d_k^\top A d_k}$;

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$C x_{k+1} = C(x_k + \tilde{\alpha}_k d_k) \Rightarrow x_{k+1} = x_k + \tilde{\alpha}_k d_k$;

3. $\tilde{r}_{k+1} = \tilde{r}_k - \tilde{\alpha}_k \tilde{A} \tilde{d}_k \Rightarrow$
$C^{-1} r_{k+1} = C^{-1} r_k - \tilde{\alpha}_k C^{-1} A C^{-1} C d_k \Rightarrow$
$C^{-1} r_{k+1} = C^{-1}(r_k - \tilde{\alpha}_k A d_k) \Rightarrow$
$r_{k+1} = r_k + \tilde{\alpha}_k A d_k$;

Simplified Computation

1. $\tilde{\alpha}_k = \frac{\tilde{r}_k^\top \tilde{r}_k}{\tilde{d}_k^\top \tilde{A} \tilde{d}_k} = \frac{r_k^\top z_k}{d_k^\top A d_k}$;
2. $\tilde{x}_{k+1} = \tilde{x}_k + \tilde{\alpha}_k \tilde{d}_k \Rightarrow Cx_{k+1} = Cx_k + \tilde{\alpha}_k Cd_k \Rightarrow$
   $Cx_{k+1} = C(x_k + \tilde{\alpha}_k d_k) \Rightarrow x_{k+1} = x_k + \tilde{\alpha}_k d_k$;
3. $\tilde{r}_{k+1} = \tilde{r}_k - \tilde{\alpha}_k \tilde{A} \tilde{d}_k \Rightarrow$
   $C^{-1} r_{k+1} = C^{-1} r_k - \tilde{\alpha}_k C^{-1} A C^{-1} C d_k \Rightarrow$
   $C^{-1} r_{k+1} = C^{-1}(r_k - \tilde{\alpha}_k A d_k) \Rightarrow$
   $r_{k+1} = r_k + \tilde{\alpha}_k A d_k$;
4. $z_{k+1} = M^{-1} r_{k+1}$;

Simplified Computation

1. $\tilde{\alpha}_k = \dfrac{\tilde{r}_k^\top \tilde{r}_k}{\tilde{d}_k^\top \tilde{A} \tilde{d}_k} = \dfrac{r_k^\top z_k}{d_k^\top A d_k}$;

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   $Cx_{k+1} = C(x_k + \tilde{\alpha}_k d_k) \Rightarrow x_{k+1} = x_k + \tilde{\alpha}_k d_k$;

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   $C^{-1} r_{k+1} = C^{-1}(r_k - \tilde{\alpha}_k A d_k) \Rightarrow$
   $r_{k+1} = r_k + \tilde{\alpha}_k A d_k$;

4. $z_{k+1} = M^{-1} r_{k+1}$;

5. $\tilde{\beta}_k = \dfrac{\tilde{r}_{k+1}^\top \tilde{r}_{k+1}}{\tilde{r}_k^\top \tilde{r}_k} = \dfrac{r_{k+1}^\top z_{k+1}}{r_k^\top z_k}$;

Simplified Computation

1. $\tilde{\alpha}_k = \frac{\tilde{r}_k^\top \tilde{r}_k}{\tilde{d}_k^\top \tilde{A} \tilde{d}_k} = \frac{r_k^\top z_k}{d_k^\top A d_k}$;
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$Cx_{k+1} = C(x_k + \tilde{\alpha}_k d_k) \Rightarrow x_{k+1} = x_k + \tilde{\alpha}_k d_k$;
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$C^{-1} r_{k+1} = C^{-1} r_k - \tilde{\alpha}_k C^{-1} A C^{-1} C d_k \Rightarrow$
$C^{-1} r_{k+1} = C^{-1}(r_k - \tilde{\alpha}_k A d_k) \Rightarrow$
$r_{k+1} = r_k + \tilde{\alpha}_k A d_k$;
4. $z_{k+1} = M^{-1} r_{k+1}$;
5. $\tilde{\beta}_k = \frac{\tilde{r}_{k+1}^\top \tilde{r}_{k+1}}{\tilde{r}_k^\top \tilde{r}_k} = \frac{r_{k+1}^\top z_{k+1}}{r_k^\top z_k}$;
6. $\tilde{d}_{k+1} = \tilde{r}_{k+1} + \tilde{\beta}_k \tilde{d}_k \Rightarrow Cd_{k+1} = C^{-1} r_{k+1} + \tilde{\beta}_k C d_k \Rightarrow$
$d_{k+1} = M^{-1} r_{k+1} + \tilde{\beta}_k d_k \Rightarrow d_{k+1} = z_{k+1} + \tilde{\beta}_k d_k$.

Some notations of preconditioned Conjugate Gradient Method

1. d_k: the k-th mutually conjugate vector wrt A;
2. z_k: the auxiliary vector instead of $\tilde{r}_k$;
3. $\tilde{\alpha}_k$: the coefficient of $\tilde{d}_k$ for $\tilde{x}^*$;
4. x_k: the approximate solution to x^* at step k;
5. r_k: the residual of x_k of original system at step k;
6. $\tilde{\beta}_k$: the coefficient ensuring $(\tilde{d}_k, \tilde{d}_{k+1})_{\tilde{A}} = 0$.

Preconditioned Conjugate Gradient Method

Algorithm 4: Preconditioned Conjugate Gradient Method

$x_0 =$ initial guess
$r_0 = b - Ax_0$
$d_0 = z_0 = M^{-1} r_0$
for $k = 0, 1, 2, \ldots, n-1$ **do**
    if r_k *is sufficiently small* **then**
        return x_k
    $\tilde{\alpha}_k = \frac{r_k^\top z_k}{d_k^\top A d_k}$
    $x_{k+1} = x_k + \tilde{\alpha}_k d_k$
    $r_{k+1} = r_k - \tilde{\alpha}_k A d_k$
    $z_{k+1} = M^{-1} r_{k+1}$
    $\tilde{\beta}_k = \frac{r_{k+1}^\top z_{k+1}}{r_k^\top z_k}$
    $d_{k+1} = z_{k+1} + \tilde{\beta}_k d_k$

Outline

Conclusions

- Three iterative methods for strictly diagonally dominant matrix
  1. Jacobi Method
  2. Gauss-Seidel Method
  3. Successive Over-Relaxation

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- Three iterative methods for strictly diagonally dominant matrix
  1. Jacobi Method
  2. Gauss-Seidel Method
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- Two iterative methods for symmetric positive-definite matrix
  1. Conjugate Gradient Method
  2. Preconditioned Conjugate Gradient Method

Thank you!