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Lecture Notes 4: Matrix decompositions

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2. Matrix decomposition

2.1 LU decomposition

- Example: when solving $A\vec{x} = \vec{b}$:

$$\begin{cases} 2x - y + 3z = 2 \\ 4x + 2y + z = 8 \\ -6x - y + 2z = 0 \end{cases}, \quad A = \begin{bmatrix} 2 & -1 & 3 \\ 4 & 2 & 1 \\ -6 & -1 & 2 \end{bmatrix}, \quad \vec{x} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}, \quad \vec{b} = \begin{bmatrix} 2 \\ 8 \\ 0 \end{bmatrix}.$$

$$\begin{aligned} A \quad &\xrightarrow{-2R1+R2} \quad A^{(1)} = \begin{bmatrix} 2 & -1 & 3 \\ 0 & 4 & -5 \\ -6 & -1 & 2 \end{bmatrix} \\ &\xrightarrow{3R1+R3} \quad A^{(2)} = \begin{bmatrix} 2 & -1 & 3 \\ 0 & 4 & -5 \\ 0 & -4 & 11 \end{bmatrix} \\ &\xrightarrow{R2+R3} \quad A^{(3)} = \begin{bmatrix} 2 & -1 & 3 \\ 0 & 4 & -5 \\ 0 & 0 & 6 \end{bmatrix} \end{aligned}$$

- Express the progess as matrix multiplication:

$$A^{(1)} = E^{(1)}A = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \overrightarrow{a_1}^T \\ \overrightarrow{a_2}^T \\ \overrightarrow{a_3}^T \end{bmatrix} = \begin{bmatrix} \overrightarrow{a_1}^T \\ -2\,\overrightarrow{a_1}^T + \overrightarrow{a_2}^T \\ \overrightarrow{a_3}^T \end{bmatrix}$$

$$A^{(2)} = E^{(2)}A^{(1)}, \quad E^{(2)} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 3 & 0 & 1 \end{bmatrix}$$

$$A^{(3)} = E^{(3)}A^{(2)}, \quad E^{(3)} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}$$

- Combine the $E^{(*)}$ matrices:

$$A^{(3)} = E^{(3)}E^{(2)}E^{(1)}A = L^{-1}A = U, \quad A = LU = E^{(1)^{-1}}E^{(2)^{-1}}E^{(3)^{-1}}U$$

$$E^{(3)^{-1}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix}, \quad E^{(2)^{-1}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -3 & 0 & 1 \end{bmatrix}, \quad E^{(1)^{-1}} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

$$L = E^{(1)^{-1}}E^{(2)^{-1}}E^{(3)^{-1}} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -3 & -1 & 1 \end{bmatrix}.$$

- Time complexity:

$$\begin{aligned} T(n) &= 2n(n-1) + T(n-1) \\ &= \sum_{k=1}^{n} 2k(k-1) \\ &= \sum_{k=1}^{n} 2k^2 - \sum_{k=1}^{n} 2k \\ &= 2 \times \frac{n(n+1)(2n+1)}{6} - 2 \times \frac{n(n+1)}{2} \\ &\approx \frac{2}{3}n^3 \end{aligned}$$

- Prove the inverse of a nonsingular lower triangular matrix L is also a lower triangular matrix:

base case: $L = \alpha, L^{-1} = \dfrac{1}{\alpha}$

assume: ${L_k}^{-1}$ is a $k \times k$ lower triangular matrix

induction: $L_{k+1} = \begin{bmatrix} L_k & \vec{0} \\ \overrightarrow{l_k}^T & \lambda \end{bmatrix}$

Let $L_{k+1}M = I, \quad M = \begin{bmatrix} A & \vec{b} \\ \vec{c}^T & d \end{bmatrix}$,

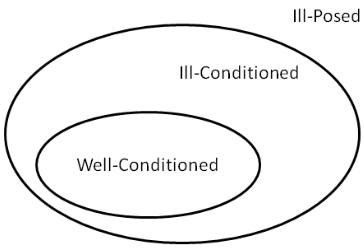
$$L_{k+1}M = \begin{bmatrix} L_kA & L_k\vec{b} \\ \overrightarrow{l_k}^T A + \lambda\vec{c}^T & \overrightarrow{l_k}^T \vec{b} + d\lambda \end{bmatrix},$$

which is equal to I if $A = {L_k}^{-1}, \quad \vec{b} = \vec{0}, \quad d = \dfrac{1}{\lambda}$.

(Thm: For an n×n nonsingular matrix A, $A\vec{b} = 0$ iff $\vec{b} = \vec{0}$.)

$\Rightarrow M = {L_{k+1}}^{-1} = \begin{bmatrix} {L_k}^{-1} & \vec{0} \\ \vec{c}^T & \frac{1}{\lambda} \end{bmatrix}$ is lower triangular.

- Well/ill-condictioned (in problem domain)
  - Relationship between well-condictioned, ill-condictioned, and ill-posed



  - Example: solve quartic equation. The problem is ill-condition when a is small.

$$ax^2 + bx + c = 0, \quad x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$
$$\text{when } \frac{|a - \tilde{a}|}{|a|} = 10^{-5}, \quad \frac{|x - \tilde{x}|}{|x|} = 10^{-1}$$

- stability (in algorithm domain)
  - Example: $10000 + 0.0001 - 10000$. The result is zero if we calculate $10000 + 0.0001$ first while the precision is not enough.
  - Example: solving $A\vec{x} = \vec{b}$ (unstable).

$$\begin{cases} 0.001x_1 + x_2 = 3 \\ x_1 + 2x_2 = 5 \end{cases}, \quad A = \begin{bmatrix} 0.001 & 1 \\ 1 & 2 \end{bmatrix}, \quad A^{(1)} = \begin{bmatrix} 0.001 & 1 \\ 0 & -998 \end{bmatrix}.$$

$$\text{with } \begin{bmatrix} 0.001 & 1 \\ 0 & -998 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3 \\ -2995 \end{bmatrix}, \quad \begin{cases} x_2 = \frac{2995}{998} \approx 3.001 \\ x_1 \approx -1.002 \end{cases}, \quad \begin{cases} \tilde{x_2} = 3 \\ \tilde{x_1} = 0 \end{cases}.$$

$$\frac{|x_1 - \tilde{x_1}|}{|x_1|} = \frac{1.002}{1.002} = 1, \quad \frac{|x_2 - \tilde{x_2}|}{|x_2|} = \frac{0.001}{3} \approx 3 \times 10^{-4}.$$

  - Example: solving $A\vec{x} = \vec{b}$ (stable, with pivoting).

$$\begin{cases} 0.001x_1 + x_2 = 3 \\ x_1 + 2x_2 = 5 \end{cases}, \quad A' = \begin{bmatrix} 1 & 2 \\ 0.001 & 1 \end{bmatrix}, \quad A^{(1)'} = \begin{bmatrix} 1 & 2 \\ 0 & 0.998 \end{bmatrix}.$$

$$\text{with } \begin{bmatrix} 1 & 2 \\ 0 & 0.998 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 5 \\ 2.995 \end{bmatrix}, \quad x_2 = \frac{2.995}{0.998} \approx 3, \quad x_1 \approx -1,$$
$$\frac{|x_1 - \tilde{x_1}|}{|x_1|} = \frac{0.002}{1.002} \approx 0.002$$

– Example: solving $ax^2 + bx + c = 0$.

when $a = c = 10^{-4}$, $b = 10^4$, $d = b^2 - 4ac = 10^8 - 4 \times 10^{-8} \approx 10^8$,

$$x^{(+)} = \frac{-b + \sqrt{d}}{2a} = \frac{-10^4 + 10^4}{2 \times 10^{-4}} = 0,$$

$$x^{(-)} = \frac{-b - \sqrt{d}}{2a} = \frac{-10^4 - 10^4}{2 \times 10^{-4}} = -10^8.$$

However, by calcuating $x^{(+)}$ from $\dfrac{(\sqrt{d} + b)(\sqrt{d} - b)}{(\sqrt{d} + b)2a}$,

$$x^{(+)} = \frac{d - b^2}{(\sqrt{d} + b)2a} = \frac{-4ac}{(\sqrt{d} + b)2a} = \frac{-2c}{\sqrt{d} + b} = \frac{-2 \times 10^{-4}}{\sqrt{10^8} + 10^4} = -10^{-8}.$$

- Definition of condition number:
  The relative error of input × condition number = The relative error of output
- The condition number of $A\vec{x} = \vec{b}$: (assume all errors are in A)

$$\tilde{A} = A + E, \quad \tilde{\vec{x}} = \vec{x} + \Delta\vec{x}, \quad \text{input error: } \frac{\|E\|}{\|A\|}, \quad \text{output error: } \frac{\|\Delta\vec{x}\|}{\|\vec{x}\|}.$$

$$A\vec{x} = \vec{b} = (A + E)(\vec{x} + \Delta\vec{x}), \quad A\vec{x} = A\vec{x} + E\vec{x} + A\Delta\vec{x} + E\Delta\vec{x}$$

$$A\Delta\vec{x} = -E(\vec{x} + \Delta\vec{x})$$

$$\Delta\vec{x} = -A^{-1}E(\vec{x} + \Delta\vec{x})$$

$$\begin{aligned} \|\Delta\vec{x}\| &= \left\|A^{-1}E(\vec{x} + \Delta\vec{x})\right\| \\ &\le \left\|A^{-1}\right\| \|E\| \|(\vec{x} + \Delta\vec{x})\| \end{aligned}$$

$$\begin{aligned} \frac{\|\Delta\vec{x}\|}{\|\vec{x}\|} &\approx \frac{\|\Delta\vec{x}\|}{\|(\vec{x} + \Delta\vec{x})\|} \ (\text{ approximation holds if } \Delta\vec{x} \ll \vec{x}) \\ &\le \left\|A^{-1}\right\| \|E\| \\ &= \left\|A^{-1}\right\| \|A\| \frac{\|E\|}{\|A\|} \end{aligned}$$

where $\dfrac{\|E\|}{\|A\|}$ is the input error, and $\left\|A^{-1}\right\| \|A\|$ is the condition number.

The input error can be reduced by increasing the precision.

- LU decomposition in MATLAB
  - [L, U] = lu(A)

    $A = LU, \quad \|A - LU\| \approx 0.$
  - [L, U, P] = lu(A)

    $PA = LU, \quad \|PA - LU\| \approx 0.$

2.2 Cholesky decomposition

- For symmetric positive definite (S.P.D.) matrix
  - symmetric: $A = A^T$
  - positive definite: $\forall \vec{x} \neq 0, \vec{x}^T A \vec{x} > 0$
  - A is S.P.D. iff Cholesky decomposition exist
- Considering from LU decomposition
  - in LU decomposition: $A = LU, \quad A^T = U^T L^T$
  - when $A = A^T$: $LU = U^T L^T$
  - $U = L^T$ if A is S.P.D. $\rightarrow \quad A = LL^T$
- Steps of computation
  - base case:

$$A = a_{11}, \quad L = L^T = \sqrt{a_{11}}$$

  - recursion:

$$A_n = \begin{bmatrix} A_{n-1} & \overrightarrow{a_{n-1}} \\ \overrightarrow{a_{n-1}}^T & a_{nn} \end{bmatrix}, \quad L_n = \begin{bmatrix} L_{n-1} & \vec{0} \\ \overrightarrow{l_{n-1}}^T & l_{nn} \end{bmatrix}, \quad L_n^T = \begin{bmatrix} {L_{n-1}}^T & \overrightarrow{l_{n-1}} \\ \vec{0} & l_{nn} \end{bmatrix}.$$

$$A_n = L_n {L_n}^T = \begin{bmatrix} L_{n-1}{L_{n-1}}^T & L_{n-1}\overrightarrow{l_{n-1}} \\ \overrightarrow{l_{n-1}}^T {L_{n-1}}^T & \overrightarrow{l_{n-1}}^T \overrightarrow{l_{n-1}} + {l_{nn}}^2 \end{bmatrix},$$

$$\begin{cases} a_{nn} &= \overrightarrow{l_{n-1}}^T \overrightarrow{l_{n-1}} + {l_{nn}}^2 \\ \overrightarrow{a_{n-1}} &= L_{n-1}\overrightarrow{l_{n-1}} \end{cases} \Rightarrow \begin{cases} l_{nn} &= \sqrt{a_{nn} - \overrightarrow{l_{n-1}}^T \overrightarrow{l_{n-1}}} \\ \overrightarrow{l_{n-1}} &= {L_{n-1}}^{-1} \overrightarrow{a_{n-1}} \end{cases}.$$

  - solving $L_n \vec{x} = \vec{b}$:

$$\begin{cases} l_{11}x_1 & & & & & = b_1 \\ l_{21}x_1 & + l_{22}x_2 & & & & = b_2 \\ l_{31}x_1 & + l_{32}x_2 & + l_{33}x_3 & & & = b_3 \\ \vdots & & & & & \\ l_{n1}x_1 & + l_{n2}x_2 & + l_{n3}x_3 & + \cdots & + l_{nn}x_n & = b_n \end{cases},$$

$$x_1 = \frac{b_1}{l_{11}}. \quad \begin{bmatrix} L_{n-1} & \vec{0} \\ \overrightarrow{l_{n-1}}^T & l_{nn} \end{bmatrix} \begin{bmatrix} \overrightarrow{x_{n-1}} \\ x_n \end{bmatrix} = \begin{bmatrix} \overrightarrow{b_{n-1}} \\ b_n \end{bmatrix} \Rightarrow x_n = \frac{b_n - \overrightarrow{l_{n-1}}^T \overrightarrow{x_{n-1}}}{l_{nn}}$$

- Time complexity
  - for $\overrightarrow{l_{n-1}}$:

$$\begin{cases} l_{11}x_1 & & & & & = b_1 & \rightarrow & 1 \\ l_{21}x_1 & + l_{22}x_2 & & & & = b_2 & \rightarrow & 3 \\ l_{31}x_1 & + l_{32}x_2 & + l_{33}x_3 & & & = b_3 & \rightarrow & 5 \\ \quad\vdots & & & & & & & \\ l_{n1}x_1 & + l_{n2}x_2 & + l_{n3}x_3 & + \cdots & + l_{nn}x_n & = b_n & \rightarrow & 2n-1 \end{cases}$$

$$\Rightarrow (n-1)^2 \text{ in total.}$$

  - for l_{nn}:

$$\begin{cases} \times & : & n-1 \\ + & : & n-2 \\ - & : & 1 \\ \sqrt{\ } & : & 1 \end{cases} \quad \Rightarrow \quad 2n-1 \text{ in total.}$$

  - total:

$$\sum_{k=1}^{n}[(k-1)^2 + 2k - 1] = \sum_{k=1}^{n} k^2 = \frac{n(n+1)(2n+1)}{6} \approx \frac{n^3}{3}$$

  - About 2 times faster than LU decomposition
  - Even faster in practical, since pivoting is not needed.