Chapter 3. Direct Methods for Linear Systems.

Section 1. Gauss Elimination Method.

$$\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 3 \\ 3 \end{pmatrix} \to (2) - (1)\times \tfrac{1}{2}$$

$$\begin{pmatrix} 2 & 1 \\ 0 & 3/2 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 3 \\ 3/2 \end{pmatrix} \to \begin{array}{l} \tfrac{3}{2}y = \tfrac{3}{2} \Rightarrow y = 1 \\ 2x + y = 3 \\ \Rightarrow 2x = 3 - y = 2 \Rightarrow x = 1 \end{array}$$

$$A = (a_{ij})_{n\times n} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \cdots & & \cdots & \cdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \in \mathbb{R}^n$$

Linear System: $Ax = b$ (1). $\quad x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \in \mathbb{R}^n \quad b = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} \in \mathbb{R}^n$

Assume A is invertible

Idea: eliminate the entries in the lower part of the matrix.

For $k = 1, 2, \cdots n-1$ do (as follows)

For $i = k+1, k+2, \cdots n$ do $\Big\langle$ let $l_{ik} = a_{ik}/a_{kk}$

For $j = k, k+1, \cdots n$ do $\quad b_i^{(k+1)} \leftarrow b_i^{(k)} - l_{ik} b_k^{(k)}$

$$a_{ij}^{(k+1)} \leftarrow a_{ij}^{(k)} - l_{ik} a_{kj}^{(k)}$$

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ & a_{22}^{(2)} & \cdots & a_{2n}^{(2)} \\ & & a_{33}^{(3)} \cdots & a_{3n}^{(3)} \\ & & \ddots & \\ & & & a_{nn}^{(n)} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2^{(2)} \\ b_3^{(3)} \\ \vdots \\ b_n^{(n)} \end{pmatrix} \qquad (2)$$

Assumption: The diagonal entries are always non-zero in the elimination process.

$$a_{kk}^{(k)} \neq 0.$$

$$\begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \end{pmatrix} \quad (\times)$$

The upper/right triangular system can be solved by the backward substitution method.

For $k = n, n-1, \cdots, 1$. do

$$a_{kk}^{(k)} x_k = b_k^{(k)} - \sum_{j=k+1}^{n} a_{kj}^{(k)} x_j$$

$$x_k = \left(b_k^{(k)} - \sum_{j=k+1}^{n} a_{kj}^{(k)} x_j \right) / a_{kk}^{(k)} \qquad (*).$$

algorithm complexity.

$$O(n^3) + O(n^2).$$

section 2. LU-decomposition Method.

Decompose A into the product of a lower triangular and an upper triangular matrix.

Denote the lower and upper triangular matrix by L and U, respectively.

$$A = LU \quad \text{with} \quad L = \begin{pmatrix} 1 & & & & \\ l_{21} & 1 & & & \\ l_{31} & l_{32} & 1 & & \\ \cdots & \cdots & \cdots & \ddots & \\ l_{n1} & l_{n2} & \cdots & \cdots & 1 \end{pmatrix}$$

$$U = \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ & u_{22} & \cdots & u_{2n} \\ & & \ddots & \vdots \\ & & & u_{nn} \end{pmatrix}$$

l_{ik}

$$Ax = b \Rightarrow LUx = b.$$

Let $Ux = y$. $\Rightarrow Ly = b$.

step 1. solve $Ly = b$. by forward substitution.

$$\begin{pmatrix} 1 & & & \\ l_{21} & 1 & & \\ l_{31} & l_{32} & 1 & \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} \quad ✓$$

$O(n^2)$

step 2, solve $Ux = y$ by backward substitution.

$$\begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ & u_{22} & \cdots & u_{2n} \\ & & \ddots & \vdots \\ & & & u_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}.$$

$O(n^2)$

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \cdots & & & \cdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} = \begin{pmatrix} 1 & & & \\ l_{21} & 1 & & \\ l_{31} & l_{32} & 1 & \\ & & & \\ l_{n1} & l_{n2} & \cdots & 1 \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ & u_{22} & \cdots & u_{2n} \\ & & \ddots & \\ & & & u_{nn} \end{pmatrix}$$

$a_{11} = u_{11} \qquad a_{12} = u_{12}. \qquad a_{1j} = u_{1j} \qquad j = 1, 2 \cdots n$

$l_{i1} u_{11} = a_{i1} \qquad i = 2, 3 \cdots n \Rightarrow u_{i1} = a_{i1}/u_{11}$

For $K = 1, 2, \cdots n$.

$u_{kj} = ? \qquad a_{kj} = \sum_{m=1}^{K} l_{km} u_{mj} \qquad j = k, k+1 \cdots n$

$= u_{kj} + \sum_{m=1}^{k-1} l_{km} u_{mj}$

$u_{kj} = a_{kj} - \sum_{m=1}^{k-1} l_{km} u_{mj} \leftarrow j = k, k+1 \cdots n$

$l_{ik} = ? \qquad a_{ik} = \sum_{m=1}^{K} l_{im} u_{mk}, \qquad i = k+1, \cdots n$

$$l_{ik} \cdot u_{kk} = a_{ik} - \sum_{m=1}^{k-1} l_{im} u_{mk}$$

$$i = k+1, k+2, \cdots n$$

$$\Rightarrow \quad l_{ik} = \left(a_{ik} - \sum_{m=1}^{k-1} l_{im} u_{mk} \right) / u_{kk}$$

Doolittle decomposition.

section 3. QR decomposition

$$A = QR.$$

First, decompose a matrix A into the product of an orthogonal matrix Q and a right triangular matrix R.

$$Ax = b \Rightarrow QRx = b.$$

Let $Rx = y$. $\quad Qy = b.$

$$\Downarrow$$

$$y = Q^T b.$$

$$\Rightarrow Rx = Q^T b.$$

$$R = \begin{pmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \cdots & r_{2n} \\ & & \ddots & \vdots \\ & & & r_{nn} \end{pmatrix}. \qquad Q = (q_1, q_2 \cdots q_n)$$

q_j : j^{th} column vector of Q.

$q_j \in \mathbb{R}^n$.

$$(q_1,\ q_2\ \cdots\ q_n)\begin{pmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \cdots & r_{2n} \\ & & \ddots & \vdots \\ & & & r_{nn} \end{pmatrix} = (a_1, a_2, \cdots a_n)$$

$$q_i^T q_j = \begin{cases} 1. & j=i \\ 0 & j \neq i \end{cases}$$

$\|q_j\|_2 = 1.$

a_j : j^{th} column vector of A.

$a_j \in \mathbb{R}^n$

$$\begin{cases} q_1 r_{11} = a_1 & (1) \\ q_1 r_{12} + q_2 r_{22} = a_2 & (2). \\ q_1 r_{13} + q_2 r_{23} + q_3 r_{33} = a_3 \\ q_1 r_{14} + q_2 r_{24} + q_3 r_{34} + q_4 r_{44} = a_4 \end{cases}$$

$|r_{11}| = \|a_1\|_2 \Rightarrow r_{11} = \|a_1\|_2$

$q_1 = \dfrac{a_1}{r_{11}}$

$\cdots \quad \cdots$

$$\sum_{i=1}^{j} q_i r_{ij} = a_j \qquad (3)$$

Take inner product of (2) with q_1

$$(q_1, q_1) r_{12} + \cancelto{0}{(q_1, q_2)} r_{22} = (q_1, a_2) \Rightarrow r_{12} = (q_1, a_2).$$

inner product of (2) with q_2.

$$(q_2, q_1) r_{12} + (q_2, q_2) r_{22} = (q_2, a_2) \Rightarrow r_{22} = (\underline{q_2}, a_2)\ ?$$

$q_2 r_{22} = \underline{a_2 - q_1 r_{12}}$

$r_{22} = \|a_2 - q_1 r_{12}\|_2$ ✓

$q_2 = (a_2 - q_1 r_{12}) / r_{22}$

Take inner product of (3) with q_m, $m=1,2,\cdots j-1$.

$$\left(q_m, \sum_{i=1}^{j} q_i r_{ij}\right) = (q_m, a_j).$$

$$(q_m, q_m) r_{mj} = (q_m, a_j) \Rightarrow r_{mj} = (q_m, a_j).$$

$m=1,2\cdots j-1$.

$$q_j r_{jj} = a_j - \sum_{i=1}^{j-1} q_i r_{ij}$$

$$r_{jj} = \|a_j - \sum_{i=1}^{j-1} q_i r_{ij}\|_2. \Rightarrow q_j = \left(a_j - \sum_{i=1}^{j-1} q_i r_{ij}\right)/r_{jj}$$

Gram-Schmidt orthogonalization

$(a_1, a_2, \cdots a_n)$

normalize a_1: $q_1 \Leftarrow a_1$, $\|q_1\|_2 = 1$.

$a_1 = r_{11} q_1$ $r_{11} = \|a_1\|_2$

$q_1 = a_1/r_{11}$

$$a_2 - (a_2, q_1) q_1 = p_2.$$

$$r_{22} = \|p_2\|_2. \quad r_{22} q_2 = p_2. \Rightarrow q_2 = p_2/r_{22}$$

$$a_j - \sum_{i=1}^{j-1} (a_j, q_i) q_i = p_j \qquad j=1,2\cdots n.$$

$$r_{jj} = \|p_j\|_2 \quad r_{jj} q_j = p_j \Rightarrow q_j = p_j/r_{jj}.$$

QR method to solve linear system:

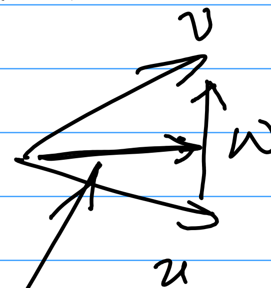
$$Ax = b$$

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ a_{31} & a_{32} & \cdots & a_{3n} \\ \vdots & \vdots & \ddots & \\ a_{n1} & a_{n2} & & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

Householder matrix. (reflection matrix.)

$H = I - 2ww^T$ $\quad \|w\|_2 = 1.$

$u, v \in \mathbb{R}^n$ $\quad \|u\|_2 = \|v\|_2$

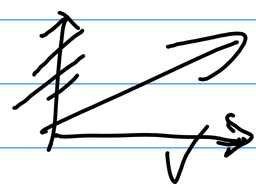


$$w = \frac{u-v}{\|u-v\|_2}$$

$Hu = v$ $\quad Hv = u.$

$(I - q_1 q_1^T) a_1$

$= a_1 - (q_1, a_1) q_1$



$(I - ww^T)v \Rightarrow$

$$Hv = (I - 2ww^T)v = v - 2\frac{(u-v)(u-v)^T}{\|u-v\|_2^2} v = u$$

H: orthogonal matrix

$\downarrow$

symmetric

$H^T H$

$= (I - 2ww^T)(I - 2ww^T)$

$= I - 2ww^T - 2ww^T + 4w\underline{w^T w}w^T = I$

$$u = \begin{pmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{n1} \end{pmatrix} \to v = \begin{pmatrix} r_{11} \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$\|v\|_2 = |r_{11}| = \|u\|_2 = \|a_1\|_2.$

$r_{11} = \pm \|a_1\|_2$

$$\tilde{w}_1 = u - v. = \begin{pmatrix} a_{11} - r_{11} \\ a_{21} \\ a_{31} \\ \vdots \\ a_{n1} \end{pmatrix}$$

$$w_1 = \frac{\hat{w}_1}{\|\hat{w}\|_2} = \frac{u-v}{\|u-v\|_2}$$

$a_{11} - r_{11} = ?$

$H_1 = I - 2 w_1 w_1^T.$

Next,

$H_1 A x = H_1 b$

$$\hat{a}_2 = \begin{pmatrix} a_{22} \\ a_{23} \\ \vdots \\ a_{2n} \end{pmatrix} \in \mathbb{R}^{n-1} \to \begin{pmatrix} r_2 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$= u_2 \qquad = v_2$

$|r_2| = \pm \|\hat{a}_2\|_2$

$$w_2 = \frac{u_2 - v_2}{\|u_2 - v_2\|_2} \in \mathbb{R}^{n-1}. \qquad H_2 = I - 2 w_2 w_2^T \in \mathbb{R}^{(n-1)\times(n-1)}$$

$$H_2 H_1 A x = H_2 H_1 b.$$

$$\begin{pmatrix} a_{33} \\ a_{43} \\ \vdots \\ a_{n3} \end{pmatrix} \in \mathbb{R}^{n-2} \to \begin{pmatrix} r_{33} \\ 0 \\ \vdots \\ 0 \end{pmatrix} \in \mathbb{R}^{n-2}.$$

$$\underline{H_{n-1} \cdots H_2 H_1 A}\, x = \underline{H_{n-1} \cdots H_2 H_1}\, b$$

$$R x = H_{n-1} \cdots H_2 H_1 b.$$

algorithm complexity $O(n^3)$.

Section 4. Stability Analysis

$$Ax = b. \qquad \text{(original)}$$

$$\tilde{A}\tilde{x} = \hat{b} \qquad \text{(practical)}$$

Step 1. Only b is perturbed.

$$A\hat{x} = \hat{b}$$

Let $\hat{b} = b + \delta b$ $\qquad$ $\delta b \in \mathbb{R}^n$. perturbation

$\tilde{x} = x + \delta x.$ $\qquad$ δx : error.

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

$$\Rightarrow \quad A\delta x = \delta b \quad \Rightarrow \quad \delta x = \underline{A^{-1}\delta b}.$$

$\|\delta x\|$: absolute error.

relative error : $\dfrac{\|\delta x\|}{\|x\|}$

$$\|\delta x\| = \|A^{-1}\delta b\| \le \|A^{-1}\| \cdot \|\delta b\|.$$

$$\frac{\|\delta x\|}{\|x\|} \le \frac{\|A^{-1}\| \cdot \|\delta b\|}{\|x\|} \qquad Ax = b.$$

$$\|b\| = \|Ax\| \le \|A\| \cdot \|x\| \quad \Rightarrow \quad \|x\| \ge \|b\| / \|A\|.$$

$$\Rightarrow \quad \frac{\|\delta x\|}{\|x\|} \le \frac{\|A^{-1}\| \cdot \|\delta b\|}{\|b\| / \|A\|} = \|A\| \cdot \|A^{-1}\| \cdot \frac{\|\delta b\|}{\|b\|}$$