Note Title 3/15/2012

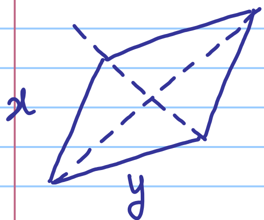
A : $n \times n$ invertible matrix

Aim : To find an orthogonal matrix Q ($Q^t Q = I$) and an upper triangular matrix R such that

$$A = QR$$

Let $x, y \in \mathbb{R}^n$ be such that

$x \neq y$ and $\|x\|_2 = \|y\|_2$



$$u = \frac{x-y}{\|x-y\|_2}, \quad v = \frac{x+y}{\|x+y\|_2}$$

$$\langle u, v \rangle = 0$$

$x \neq y$, $\|x\|_2 = \|y\|_2$

$u = \dfrac{x-y}{\|x-y\|_2}$, $v = \dfrac{x+y}{\|x+y\|_2}$

$Q = I - 2uu^t$

$Qu = u - 2u\underbrace{u^t u}_{=1} = -u$

$Qv = v - 2u\underbrace{u^t v}_{=0} = v$

$$x \neq y \ , \ \|x\|_2 = \|y\|_2$$

$$u = \frac{x-y}{\|x-y\|_2} \ , \ v = \frac{x+y}{\|x+y\|_2}$$

$$Q = I - 2uu^t$$

$$Qu = -u \ , \ Qv = v$$

$$Qx = Q\left(\frac{x+y}{2} + \frac{x-y}{2}\right) = \frac{x+y}{2} - \frac{x-y}{2}$$

$$= y$$

$x \neq y \ , \ \|x\|_2 = \|y\|_2$

$u = \dfrac{x-y}{\|x-y\|_2}$ $\quad Q = I - 2uu^t$

$\boxed{Qx = y}$ $\quad Q^t = Q$

$$Q^2 = (I - 2uu^t)(I - 2uu^t)$$

$$= I - 2uu^t - 2uu^t + 4u\underbrace{u^t u}_{=1}u^t$$

$$= I$$

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}$$

Let

$$x = \begin{bmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{n1} \end{bmatrix}, \quad \sigma_1 = \|x\|_2$$

$$= (a_{11}^2 + \cdots + a_{n1}^2)^{1/2}$$

$$y = \begin{bmatrix} \sigma_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \Rightarrow \|y\|_2 = \|x\|_2$$

$$x = \begin{bmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{n1} \end{bmatrix} \longrightarrow y = \begin{bmatrix} \sigma_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$\sigma_1 = \left(\sum_{i=1}^{n} a_{i1}^2 \right)^{1/2}$$

$$u = \frac{x - y}{\| x - y \|_2}$$

$$Q_1 = I - 2uu^t$$

$$\boxed{Q_1 x = y}$$

$$x - y = \begin{bmatrix} a_{11} - \sigma_1 \\ a_{21} \\ \vdots \\ a_{n1} \end{bmatrix}, \quad \sigma_1^2 = \sum_{i=1}^{n} a_{i1}^2$$

$$\|x - y\|_2^2 = \sum_{i=1}^{n} a_{i1}^2 - 2\sigma_1 a_{11} + \sigma_1^2$$

$$= 2\sigma_1(\sigma_1 - a_{11})$$

$$Q_1 = I - 2uu^t$$

$$= I - 2\frac{(x-y)(x-y)^t}{\|x-y\|_2^2}$$

$$\sigma_1 = (a_{11}^2 + \cdots + a_{n1}^2)^{1/2}$$

$$\|x-y\|_2^2 = 2\sigma_1(\sigma_1 - a_{11})$$

$$Q_1 A = Q_1 [C_1 \; C_2 \cdots C_n]$$
$$= [Q_1 C_1 , \; Q_1 C_2 , \; \cdots , \; Q_1 C_n]$$

$$Q_1 = I - 2 u u^t$$

$$Q_1 C_2 = C_2 - 2 u u^t C_2$$
$$= C_2 - 2 \langle C_2 , u \rangle u$$

$$
\begin{aligned}
Q_1 A &= Q_1 \left[c_1 \; c_2 \; \cdots \; c_n \right] \\
&= \left[Q_1 c_1 , \; Q_1 c_2 , \; \cdots , \; Q_1 c_n \right] \\
&= \left[\begin{array}{c|ccc}
\sigma_1 & a_{12}^{(1)} & \cdots & a_{1n}^{(1)} \\
\hline
0 & a_{22}^{(1)} & \cdots & a_{2n}^{(1)} \\
\vdots & \vdots & & \\
0 & a_{n2}^{(1)} & \cdots & a_{nn}^{(1)}
\end{array} \right]
\end{aligned}
$$

Find a $(n-1)\times(n-1)$ matrix $\tilde{Q}_2$

such that

$$\tilde{Q}_2 \begin{bmatrix} a_{22}^{(1)} \\ \vdots \\ a_{n2}^{(1)} \end{bmatrix} = \begin{bmatrix} \sigma_2 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$\sigma_2 = \left\{ \sum_{i=2}^{n} \left(a_{i2}^{(1)} \right)^2 \right\}^{1/2}$$

Define $Q_2 = \begin{bmatrix} 1 & \bar{0} \\ \bar{0} & \tilde{Q}_2 \end{bmatrix}_{n \times n}$

$$Q_2 Q_1 A = \begin{bmatrix} \sigma_1 & a_{12}^{(1)} & a_{13}^{(2)} & \cdots & a_{1n}^{(2)} \\ 0 & \sigma_2 & a_{23}^{(2)} & \cdots & a_{2n}^{(2)} \\ \vdots & 0 & \vdots & & \\ \vdots & \vdots & \vdots & & \\ 0 & 0 & a_{n3}^{(2)} & \cdots & a_{nn}^{(2)} \end{bmatrix}$$

$$Q_{n-1} Q_{n-2} \cdots Q_1 A = R$$

$$Q_i^t = Q_i , \quad Q_i^2 = I .$$

$$A = Q_1 Q_2 \cdots Q_{n-1} R$$
$$= Q R .$$

$$Q^t Q = (Q_{n-1} \cdots Q_1)(Q_1 Q_2 \cdots Q_{n-1})$$
$$= I \quad , \quad Q^t \neq Q .$$

Example

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

$$x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \|x\|_2 = \sqrt{2}, \quad y = \begin{bmatrix} \sqrt{2} \\ 0 \end{bmatrix}.$$

$$u = \frac{x - y}{\|x - y\|_2}, \quad Q = I - 2uu^t$$

$$x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad y = \begin{bmatrix} \sqrt{2} \\ 0 \end{bmatrix}$$

$$(x-y)(x-y)^t = \begin{bmatrix} 1-\sqrt{2} \\ 1 \end{bmatrix} \begin{bmatrix} 1-\sqrt{2} & 1 \end{bmatrix}$$

$$= \begin{bmatrix} (1-\sqrt{2})^2 & 1-\sqrt{2} \\ 1-\sqrt{2} & 1 \end{bmatrix}$$

$$\|x-y\|_2^2 = 4 - 2\sqrt{2}$$

$$Q = I - \frac{2(x-y)(x-y)^t}{\|x-y\|_2^2}$$

$$= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{2}{4-2\sqrt{2}} \begin{bmatrix} (1-\sqrt{2})^2 & 1-\sqrt{2} \\ 1-\sqrt{2} & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \frac{1}{\sqrt{2}} \begin{bmatrix} 1-\sqrt{2} & 1 \\ 1 & \frac{1}{1-\sqrt{2}} \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$A = \begin{bmatrix} 1 & 2 \\ 1 & 3 \end{bmatrix}, \quad Q = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$QA = \begin{bmatrix} \sqrt{2} & \frac{5}{\sqrt{2}} \\ 0 & -\frac{1}{\sqrt{2}} \end{bmatrix} = \underbrace{\frac{1}{\sqrt{2}} \begin{bmatrix} 2 & 5 \\ 0 & -1 \end{bmatrix}}_{= R}$$

$$Q^t = Q^{-1}$$

$$A = QR$$

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

$$= QR = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad \frac{1}{\sqrt{2}} \begin{bmatrix} 2 & 5 \\ 0 & -1 \end{bmatrix}$$

$$A = \hat{Q}\,\hat{R} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 2 & 5 \\ 0 & 1 \end{bmatrix}$$

QR method

Write $A = Q_0 R_0$

Define $A_1 = R_0 Q_0$

Write $A_1 = Q_1 R_1$,

Define $A_2 = R_1 Q_1$, ...

$A_m = Q_m R_m$, Define

$A_{m+1} = R_m Q_m$

Theorem: Let A be a real $n \times n$ matrix with eigenvalues $\lambda_1, \cdots, \lambda_n$ such that $|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n| > 0$.
Then A_m converge to an upper triangular matrix that contains λ_i in the diagonal position.
If A is symmetric, then A_m converge to a diagonal matrix.

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \det(A - zI) = z^2 - 1 = 0$$

$\Rightarrow$ evs of A: $\lambda_1 = -1$, $\lambda_2 = 1$

$|\lambda_1| = |\lambda_2|$

$A^T = A$, $A^2 = I$: A orthogonal

$A = Q_0 R_0$ with $Q_0 = A$, $R_0 = I$

$A_1 = R_0 Q = A \Rightarrow A_m = A$ for all m

A_m does not converge to a diagonal matrix

Solution of a system of linear equations

$Ax = b$, A invertible

$A = QR$: $Q^tQ = I$, R: upper triangular

$QRx = b \iff Qy = b$ and $Rx = y$.

$y = Q^t b$

$Rx = y$: back substitution

Number of Computations

$A = QR$

$\frac{2n^3}{3}$ multiplications and

$\frac{2n^3}{3}$ additions

Twice expensive as compared to LU decomposition

Polynomial Approximation

Bernstein Polynomials :

$f \in C[0,1]$

$$(B_n f)(x) = \sum_{k=0}^{n} \frac{n!}{k!(n-k)!} x^k (1-x)^{n-k}$$

Slow Convergence, does not reproduce polynomials

Best Approximation

$\mathcal{P}_n$: polynomials of degree $\leq n$

Aim: To find $p_n^* \in \mathcal{P}_n$ such that

$$\| f - p_n^* \|_\infty = \min_{p \in \mathcal{P}_n} \| f - p \|_\infty .$$

$$\| $$

$$\mathrm{dist}_\infty (f , \mathcal{P}_n)$$

Second Algorithm of Remes

$f, g \in C[a, b]$

<u>Inner Product</u>

$$\langle f, g \rangle = \int_a^b f(x)\, g(x)\, dx$$

<u>Induced norm</u>

$$\| f \|_2 = \left(\int_a^b f(x)^2\, dx \right)^{1/2}$$

Least-Squares Approximation

$\mathcal{P}_n$: space of polynomials of degree $\leq n$.

Let $f \in C[a,b]$

Aim: To find $p_n^* \in \mathcal{P}_n$ such that

$$\| f - p_n^* \|_2 = \min_{p_n \in \mathcal{P}_n} \| f - p_n \|_2$$

$\{1, x, x^2, \cdots\}$ linearly independent

Use Gram-Schmidt orthonormalization to obtain Legendre polynomials

$q_0, q_1, q_2, \cdots$

q_i : polynomial of degree i

$$\langle q_i, q_j \rangle = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

Legendre Polynomials

q_i : polynomial of degree i

$$i = 0, 1, 2, \cdots$$

$$\text{span}\{q_0, q_1, \cdots, q_n\} = \mathcal{P}_n$$

$$\langle q_i, q_j \rangle = 0, \quad i \neq j, \quad \langle q_i, q_i \rangle = 1$$

$$p_n \in \mathcal{P}_n : \ p_n = \alpha_0 q_0 + \cdots + \alpha_n q_n$$

To find $p_n^* \in \mathcal{P}_n$ such that

$$\|f - p_n^*\|_2 \le \|f - p_n\|_2, \quad p_n \in \mathcal{P}_n.$$

<u>Claim:</u> $p_n^* = \sum_{j=0}^{n} \langle f, q_j \rangle q_j$

Note that $\langle p_n^*, q_i \rangle = \sum_{j=0}^{n} \langle f, q_j \rangle \langle q_j, q_i \rangle$

$$= \langle f, q_i \rangle, \quad i = 0, 1, \cdots, n$$

$$\langle f - p_n^*, q_i \rangle = 0, \quad i = 0, 1, \cdots, n$$

Let $p_n = \alpha_0 q_0 + \cdots + \alpha_n q_n \in \mathcal{P}_n$

and $p_n^* = \sum_{j=0}^{n} \langle f, q_j \rangle q_j$

Since $\langle f - p_n^*, q_i \rangle = 0$, $i = 0, 1, \cdots, n$,

it follows that

$$\langle f - p_n^*, p_n \rangle = 0 \quad \forall\, p_n \in \mathcal{P}_n$$

$f \in C[a,b]$, $p_n^* = \sum_{j=0}^{n} \langle f, q_j \rangle q_j$,

$\langle f - p_n^*, p_n \rangle = 0$ for $p_n \in \mathcal{P}_n$.

Consider

$$\|f - p_n\|_2^2 = \|\underbrace{f - p_n^*} + \underbrace{p_n^* - p_n}\|_2^2$$

$$= \|f - p_n^*\|_2^2 + \|p_n^* - p_n\|_2^2$$

$\Rightarrow \|f - p_n^*\|_2 \leq \|f - p_n\|_2$, $p_n \in \mathcal{P}_n$

Interpolating Polynomial

$f \in C[a, b]$

$x_0, x_1, \cdots, x_n$: distinct points in $[a, b]$

$$p_n(x) = f(x_0) + f[x_0, x_1](x - x_0) + \cdots + f[x_0, x_1, \cdots, x_n](x - x_0)\cdots(x - x_{n-1})$$

$$f(x) = p_n(x) + f[x_0, x_1, \cdots, x_n\, x](x - x_0)\cdots(x - x_n)$$

Numerical Integration

$$\int_a^b f(x)\,dx \simeq \int_a^b p_n(x)\,dx$$

$$p_n(x) = \sum_{i=0}^{n} f(x_i)\, l_i(x)$$

$$l_i(x) = \prod_{\substack{j=0 \\ i \neq j}}^{n} \frac{(x - x_j)}{(x_i - x_j)}$$

$$\int_a^b p_n(x)\,dx = \sum_{i=0}^{n} w_i\, f(x_i)$$

Basic Rules

Midpoint Rule, Trapezoidal Rule,
Simpson Rule, Newton-Cotes Rules

Composite Rules

Gaussian Integration

Numerical Differentiation

$f : [a, b] \longrightarrow \mathbb{R}$

$p_n(x)$: interpolating polynomial

$$f'(c) \simeq p_n'(c)$$

Finite Difference Method

System of linear equations

$Ax = b$: $A : n \times n$ invertible

Gauss elimination : $A = LU$,

L : unit lower triangular

U : upper triangular

Gauss elimination with partial pivoting

$PA = LU$: P : Permutation matrix

Cholesky Decomposition

A : positive-definite

$A^t = A$, $x \neq \bar{0} \Rightarrow \langle Ax, x \rangle > 0$

$A = GG^t$: G : lower triangular

Vector and Matrix Norms

$x \in \mathbb{R}^n$, $\|x\|_1 = \sum_{j=1}^{n} |x(j)|$,

$\|x\|_2 = \left(\sum_{j=1}^{n} |x(j)|^2\right)^{1/2}$, $\|x\|_\infty = \max_{1 \le j \le n} |x(j)|$

$\|A\| = \max_{x \neq \bar{0}} \frac{\|Ax\|}{\|x\|}$: Induced Matrix Norm

Perturbed Systems

$$Ax = b \,, \quad (A+\delta A)(x+\delta x) = b+\delta b$$

x : exact solution , $\hat{x} = x+\delta x$: Computed Solution

Relative error : $\dfrac{\|x-\hat{x}\|}{\|x\|}$

Condition Number : $\|A\|\,\|A^{-1}\|$

Iterative Methods

$$Ax = b$$

Jacobi and Gauss-Seidel Methods

Solution of a non-linear equation

$f(x) = 0$

Fixed Point: $g(c) = c$

Picard's fixed point iteration

Newton's and Secant Methods

Initial Value Problem

$y' = f(x, y)$, $y(a) = y_0$

Single Step Methods :

Euler and Rungé-Kutta Methods

Multi-Step Methods

Adams-Bashforth, Adams-Moulton Methods

Stability

Boundary Value Problem

$$y''(x) + f(x)\,y'(x) + g(x)\,y(x) = r(x),$$

$$x \in [a, b]$$

$$y(a) = \alpha, \quad y(b) = \beta$$

$$y' = \frac{dy}{dx}, \quad y'' = \frac{d^2y}{dx^2}$$

f, g, r : continuous.

Finite Difference Method

Eigenvalue Problem

localization results,
Power Method and its extensions
QR method