Elementos de Cálculo Numérico/Cálculo Numérico

Clase 7

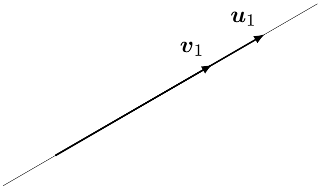
Primer Cuatrimestre 2021

Proceso de ortonormalización

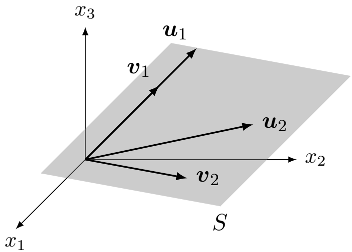
$\{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_d\}$ base del subespacio S

$\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_d\}$ base ortonormal

$\{\boldsymbol{u}_1, \ldots, \boldsymbol{u}_k\}$ y $\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k\}$ generan el mismo subespacio



(a) Paso 1



(b) Paso 2

Fig.: Proceso de ortonormalización.

Método de Gram-Schmidt

Paso 1

$$\boldsymbol{v}_1 = \boldsymbol{u}_1/\|\boldsymbol{u}_1\|$$

Paso 2

$$\tilde{\boldsymbol{v}}_2 = \boldsymbol{u}_2 - (\boldsymbol{v}_1.\boldsymbol{u}_2)\boldsymbol{v}_1 \quad \Longrightarrow \tilde{\boldsymbol{v}}_2 \perp \boldsymbol{v}_1$$

$$\boldsymbol{v}_2 = \tilde{\boldsymbol{v}}_2/\|\tilde{\boldsymbol{v}}_2\|$$

Paso 3

$$\tilde{\boldsymbol{v}}_3 = \boldsymbol{u}_3 - (\boldsymbol{v}_1.\boldsymbol{u}_3)\boldsymbol{v}_1 - (\boldsymbol{v}_2.\boldsymbol{u}_3)\boldsymbol{v}_2 \quad \Longrightarrow \tilde{\boldsymbol{v}}_3 \perp \boldsymbol{v}_1, \tilde{\boldsymbol{v}}_3 \perp \boldsymbol{v}_2$$

$$\boldsymbol{v}_3 = \tilde{\boldsymbol{v}}_3/\|\tilde{\boldsymbol{v}}_3\|$$

Paso k

$$\tilde{\boldsymbol{v}}_k = \boldsymbol{u}_k - \textstyle\sum_{j=1}^{k-1}(\boldsymbol{v}_j.\boldsymbol{u}_3)\boldsymbol{v}_j \quad \Longrightarrow \tilde{\boldsymbol{v}}_k \perp \boldsymbol{v}_j, \quad j = 1, \ldots, k-1$$

$$\boldsymbol{v}_k = \tilde{\boldsymbol{v}}_k/\|\tilde{\boldsymbol{v}}_k\|$$

Método de Gram-Schmidt modificado

Definimos $\boldsymbol{u}_j^{(0)} = \boldsymbol{u}_j$, $j = 1, \ldots, d$

Paso 1: para $j = 2, \ldots, d$

- $\boldsymbol{u}_1^{(1)} = \boldsymbol{u}_1^{(0)} / \|\boldsymbol{u}_1^{(0)}\|$
- $\boldsymbol{u}_j^{(1)} = \boldsymbol{u}_j^{(0)} - \left(\boldsymbol{u}_j^{(0)} . \boldsymbol{u}_1^{(1)}\right) \boldsymbol{u}_1^{(1)}$

$\boldsymbol{u}_j^{(1)} \perp \boldsymbol{u}_1^{(1)} = 0$ para $j = 2, \ldots, d$

Paso 2: para $j = 3, \ldots, d$

- $\boldsymbol{u}_2^{(2)} = \boldsymbol{u}_2^{(1)} / \|\boldsymbol{u}_2^{(1)}\|$
- $\boldsymbol{u}_j^{(2)} = \boldsymbol{u}_j^{(1)} - \left(\boldsymbol{u}_j^{(1)} . \boldsymbol{u}_2^{(2)}\right) \boldsymbol{u}_2^{(2)}$

$\boldsymbol{u}_j^{(2)} \perp \boldsymbol{u}_2^{(2)} = 0$ para $j = 3, \ldots, d$

Cambio de base

$\{\boldsymbol{u}_1, \dots, \boldsymbol{u}_k\}$ y $\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_k\}$ generan el mismo subespacio $1 \leq k \leq d$

Existen coeficientes $\{r_{i,j} : j = 1, \dots, d \quad i = 1, \dots, j\}$

$$\begin{aligned} \boldsymbol{u}_1 &= r_{1,1}\,\boldsymbol{v}_1 \\ &\vdots \\ \boldsymbol{u}_d &= r_{1,d}\,\boldsymbol{v}_1 + \dots + r_{d,d}\,\boldsymbol{v}_d \end{aligned}$$

$$[\boldsymbol{u}_1 \ \boldsymbol{u}_2 \ \cdots \ \boldsymbol{u}_d] = [\boldsymbol{v}_1 \ \boldsymbol{v}_2 \ \cdots \ \boldsymbol{v}_d] \begin{bmatrix} r_{1,1} & r_{1,2} & \dots & r_{1,d} \\ 0 & r_{2,2} & \dots & r_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & r_{d,d} \end{bmatrix}$$

Descomposición QR

$\mathrm{A} = [\boldsymbol{a}_1 \ \cdots \ \boldsymbol{a}_n]$ inversible,

$\{\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n\}$ columnas de A forman una base

$\{\boldsymbol{q}_1, \ldots, \boldsymbol{q}_n\}$ base ortonormal obtenida por G-S

$\mathrm{A} = \mathrm{Q.R}$

$\mathrm{Q} = [\boldsymbol{q}_1 \ \cdots \ \boldsymbol{q}_n]$ (matriz ortogonal)

$$\mathrm{R} = \begin{bmatrix} r_{1,1} & r_{1,2} & \ldots & r_{1,n} \\ 0 & r_{2,2} & \ldots & r_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & r_{n,n} \end{bmatrix}$$ (matriz triangular superior)

Resolución de sistema usando descomposición QR

$\mathrm{A} \in \mathbb{R}^{n\times n}$ inversible

Sistema: $\mathrm{A}.\boldsymbol{x} = \boldsymbol{b}$

$\mathrm{Q}.\mathrm{R}.\boldsymbol{x} = \boldsymbol{b}$

$\mathrm{Q}.\boldsymbol{y} = \boldsymbol{b}, \quad \mathrm{R}.\boldsymbol{x} = \boldsymbol{y}$

Q ortogonal $\Longrightarrow y = \mathrm{Q}^{\mathrm{T}}.\boldsymbol{b}$

R triangular: $\mathrm{R}.\boldsymbol{x} = \boldsymbol{y}$ (eliminación recursiva)

Matrices ortogonales

$\mathrm{Q} \in \mathbb{R}^{n \times n}$, son equivalentes:

- Las columnas de Q forman una base ortonormal
- Las filas de Q forman una base ortonormal
- $\mathrm{Q}^{\mathrm{T}} = \mathrm{Q}^{-1}$
- $\|\mathrm{Q}.\boldsymbol{x}\|_2 = \|\boldsymbol{x}\|_2$
- $(\mathrm{Q}.\boldsymbol{x}).(\mathrm{Q}.\boldsymbol{y}) = \boldsymbol{x}.\boldsymbol{y}$

En este caso $\mathrm{Q} \in \mathbb{R}^{n \times n}$ es ortogonal

Matrices ortogonales

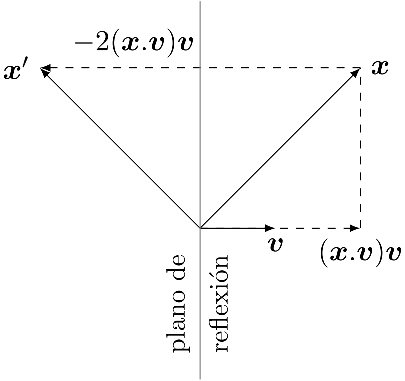
$Q \in \mathbb{R}^{n \times n}$ ortogonal

- $\det(Q) = \pm 1$
- $\|Q\|_2 = 1$
- $\kappa_2(Q) = 1$
- λ autovalor $\Longrightarrow |\lambda| = 1$
- Ejemplo: Q rotación $\Longrightarrow \det(Q) = 1$
- Ejemplo: Q reflexión $\Longrightarrow \det(Q) = -1$

Reflexiones

Si $\|\boldsymbol{v}\| = 1$, la transformación $\boldsymbol{x} \mapsto \boldsymbol{x} - 2(\boldsymbol{v}.\boldsymbol{x})\boldsymbol{v}$ es ortogonal:

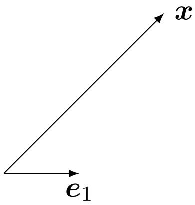
$$\|\boldsymbol{x} - 2(\boldsymbol{v}.\boldsymbol{x})\boldsymbol{v}\|_2^2 = \|\boldsymbol{x}\|_2^2 - 4(\boldsymbol{v}.\boldsymbol{x})^2 + 4(\boldsymbol{v}.\boldsymbol{x})^2 = \|\boldsymbol{x}\|_2^2$$



Matrices de Householder

$$\boldsymbol{e}_1 = (1\ 0 \ldots 0) \in \mathbb{R}^n$$

$$\tilde{\boldsymbol{v}} = \boldsymbol{x} + \|\boldsymbol{x}\|\boldsymbol{e}_1 \ \ \text{si } x_1 \geq 0 \quad \tilde{\boldsymbol{v}} = \boldsymbol{x} - \|\boldsymbol{x}\|\boldsymbol{e}_1 \ \ \text{si } x_1 < 0$$
$$\boldsymbol{v} = \tilde{\boldsymbol{v}}/\|\tilde{\boldsymbol{v}}\|$$
$$\boldsymbol{x}' = \boldsymbol{x} - 2\,(\boldsymbol{v}.\boldsymbol{x})\,\boldsymbol{v} = \pm\|\boldsymbol{x}\|\,\boldsymbol{e}_1$$



Matrices de Householder

Si $\mathrm{A} \in \mathbb{R}^{n \times n}$, $\mathrm{A} = [\boldsymbol{a}_1 \boldsymbol{a}_2 \ldots \boldsymbol{a}_n]$

Definimos: $\boldsymbol{v} \in \mathbb{R}^n$, $\tilde{\boldsymbol{v}} = \boldsymbol{a}_1 \pm \|\boldsymbol{a}_1\| \boldsymbol{e}_1$, $\boldsymbol{v} = \tilde{\boldsymbol{v}} / \|\tilde{\boldsymbol{v}}\|$

$\mathrm{Q}_1 . \boldsymbol{a}_1 = \boldsymbol{a}_1 - 2(\boldsymbol{a}_1 . \boldsymbol{v}) \boldsymbol{v} = \alpha_1 \, \boldsymbol{e}_1$

$$\mathrm{Q}_1 . \mathrm{A} = [\alpha_1 \boldsymbol{e}_1 \ \boldsymbol{a}'_2 \ldots \boldsymbol{a}'_{\mathrm{n}}] = \begin{bmatrix} \alpha_1 & a'_{1,2} & a'_{1,3} & \ldots & a'_{1,n} \\ 0 & a'_{2,2} & a'_{3,3} & \ldots & a'_{3,n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & a'_{n,2} & a'_{n,3} & \ldots & a'_{n,n} \end{bmatrix} \left[\begin{array}{c|} \alpha_1 \\ \hline 0 \\ \vdots \\ 0 \end{array} \right.$$

Matrices de Householder

Existe $\mathrm{Q}' \in \mathbb{R}^{(n-1)\times(n-1)}$

$$\mathrm{Q}'.\begin{bmatrix} a'_{2,2} & a'_{2,3} & \dots & a'_{2,n} \\ a'_{3,2} & a'_{3,3} & \dots & a'_{3,n} \\ \vdots & \vdots & \ddots & \vdots \\ a'_{n,2} & a'_{n,3} & \dots & a'_{n,n} \end{bmatrix} = \begin{bmatrix} \alpha_2 & a''_{2,3} & \dots & a''_{2,n} \\ 0 & a''_{3,3} & \dots & a''_{3,n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a''_{n,3} & \dots & a''_{n,n} \end{bmatrix}$$

Existe $\mathrm{Q}_2 \in \mathbb{R}^{n\times n}$ ortogonal

$$\mathrm{Q}_2.\mathrm{Q}_1.\mathrm{A} = \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & \mathrm{Q}' \end{array}\right].\mathrm{Q}_1.\mathrm{A} = \begin{bmatrix} \alpha_1 & a'_{1,2} & a'_{1,3} & \dots & a'_{1,n} \\ 0 & \alpha_2 & a''_{2,3} & \dots & a''_{2,n} \\ 0 & 0 & a''_{3,3} & \dots & a''_{3,n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & a''_{n,3} & \dots & a''_{n,n} \end{bmatrix}$$

Matrices de Householder

Existen $\mathrm{Q}_1, \ldots \mathrm{Q}_{n-1}$ ortogonales y R triangular superior:

$$\mathrm{Q}_{n-1}.\mathrm{Q}_{\mathrm{n}-2}.\ldots.\mathrm{Q}_2.\mathrm{Q}_1.\mathrm{A} = \mathrm{R}$$

El sistema $\mathrm{A}.\boldsymbol{x} = \boldsymbol{b}$ es equivalente a:

$$\mathrm{Q}_{n-1}.\mathrm{Q}_{\mathrm{n}-2}.\ldots.\mathrm{Q}_2.\mathrm{Q}_1.\mathrm{A}.\boldsymbol{x} = \mathrm{R}.\boldsymbol{x}$$

Se obtiene: $\mathrm{R}.\boldsymbol{x} = \mathrm{Q}_{n-1}.\mathrm{Q}_{\mathrm{n}-2}.\ldots.\mathrm{Q}_2.\mathrm{Q}_1.\boldsymbol{b}$

Descomposición QR por matrices de Householder

Ejemplo: $\mathrm{A} \in \mathbb{R}^{3\times 3}$, $\boldsymbol{b} \in \mathbb{R}^3$, $\mathrm{A}.\boldsymbol{x} = \boldsymbol{b}$

$$\mathrm{A} = \left[\begin{array}{rrr} 2.31378 & -0.80272 & -2.53906 \\ 1.12035 & -5.84402 & -1.16536 \\ 5.46919 & 4.91904 & -3.19922 \end{array}\right], \ \boldsymbol{b} = \left[\begin{array}{r} 3.83421 \\ 3.99835 \\ -5.24273 \end{array}\right]$$

Paso 1:

$\boldsymbol{a}_1 = (2.31378, 1.12035, 5.46919)$, $\|\boldsymbol{a}_1\| = 6.04324$

$\tilde{\boldsymbol{v}}_1 = (8.35702, 1.12035, 5.46919)$, $\boldsymbol{v}_1 = (0.83153, 0.11148, 0.54419)$

$$\mathrm{Q}_1 = \left[\begin{array}{rrr} -0.38287 & -0.18539 & -0.90501 \\ -0.18539 & 0.97515 & -0.12133 \\ -0.90501 & -0.12133 & 0.40772 \end{array}\right]$$

Descomposición QR por matrices de Householder

Paso 1:

$$Q_1.A = \begin{bmatrix} -6.04324 & -3.06102 & 4.08350 \\ 0.0 & -6.14677 & -0.27754 \\ 0.0 & 3.44111 & 1.13487 \end{bmatrix}$$

Paso 2:

$\boldsymbol{a}_2 = (-6.14677, 3.44111)$, $\|\boldsymbol{a}_2\| = 7.04443$

$\tilde{\boldsymbol{v}}_2 = (0., 0.89766, 3.44111)$, $\boldsymbol{v}_2 = (0., 0.25242, 0.96762)$

$$Q_2 = \begin{bmatrix} 1.0 & 0.0 & 0.0 \\ 0.0 & 0.87257 & -0.48849 \\ 0.0 & -0.48849 & -0.87257 \end{bmatrix}$$

Descomposición QR por matrices de Householder

Paso 2:

$$\mathrm{R} = \mathrm{Q}_2.\mathrm{Q}_1.\mathrm{A} = \begin{bmatrix} -6.04324 & -3.06102 & 4.08350 \\ 0.0 & -7.04443 & -0.79654 \\ 0.0 & 0.0 & -0.85468 \end{bmatrix}$$

Resolución: $\mathrm{R}.\boldsymbol{x} = \mathrm{Q}_2.\mathrm{Q}_1.\boldsymbol{b}$

$$\begin{bmatrix} -6.04324 & -3.06102 & 4.08350 \\ 0.0 & -7.04443 & -0.79654 \\ 0.0 & 0.0 & -0.85468 \end{bmatrix} . \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2.53546 \\ 6.31312 \\ 3.44821 \end{bmatrix}$$

$$\boldsymbol{x} = (-2.92287, -0.43999, -4.03452)$$