Section 5.5. Gram-Schmidt orthogonalization

Take two vectors in $\mathbb{R}^3$ $\cancel{x_1}$ $\cancel{x_2}$

(e.g. $x_1 = \begin{vmatrix} 1 \\ 1 \\ 0 \end{vmatrix}$ $x_2 = \begin{vmatrix} 1 \\ 1 \\ 2 \end{vmatrix}$)

they span a plane in $\mathbb{R}^3$ (dim 2)

Goal find an orthonormal basis $\{u_1, u_2\}$ of the same plane so that

$$\text{span}\{u_1\} = \text{span}\{x_1\}$$

$$\text{span}\{u_1, u_2\} = \text{Span}\{x_1, x_2\}$$

First take $u_1 = \dfrac{x_1}{\|x_1\|}$ since $\|u_1\| = \dfrac{1}{\|x_1\|} \|x_1\| = 1$

i.e. normalize x_1.

then take

$w_2 = x_2 - \langle x_2, u_1 \rangle u_1$ (and then normalize w_2)

Since $\langle w_2, u_1 \rangle = \langle x_2, u_1 \rangle - \langle x_2, u_1 \rangle \underbrace{\langle u_1, u_1 \rangle}_{=1} = 0$

$\langle u_1, u_1 \rangle = \|u_1\|^2$

$$u_2 = \frac{w_2}{\|w_2\|}$$

For the example $\quad \|x_1\| = \sqrt{1^2+1^2} = \sqrt{2}$

$$u_1 = \frac{1}{\sqrt{2}}\begin{vmatrix}1\\1\\0\end{vmatrix} \qquad \langle x_2, u_1\rangle = \frac{1}{\sqrt{2}}(1+1+0) = \frac{2}{\sqrt{2}}$$

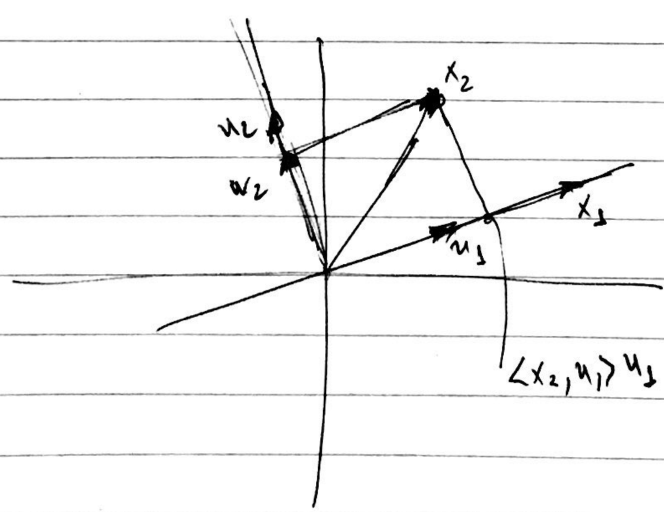
$$w_2 = x_2 - \langle x_2, u_1\rangle u_1$$

$$= \begin{vmatrix}1\\1\\2\end{vmatrix} - \frac{2}{\sqrt{2}}\cdot\frac{1}{\sqrt{2}}\begin{vmatrix}1\\1\\0\end{vmatrix} = \begin{vmatrix}0\\0\\2\end{vmatrix}$$

check. $\langle w_2, u_1\rangle = 0$

$$\|w_2\| = \sqrt{0+0+2^2} = 2 \qquad u_2 = \frac{1}{2}\begin{vmatrix}0\\0\\2\end{vmatrix} = \begin{vmatrix}0\\0\\1\end{vmatrix}$$

$$\text{span}\left\{\begin{vmatrix}1\\1\\0\end{vmatrix}, \begin{vmatrix}1\\1\\2\end{vmatrix}\right\} = \text{span}\left\{\frac{1}{\sqrt{2}}\begin{vmatrix}1\\1\\0\end{vmatrix}, \begin{vmatrix}0\\0\\1\end{vmatrix}\right\}$$



More generally,

Let $\{x_1, x_2, \ldots x_n\}$ be a basis of an n-dimensional subspace S of V (with an inner product)

then, we can obtain an orthonormal basis $\{u_1, u_2, \ldots u_n\}$ of S

such that $\operatorname{span}\{u_1, u_2, \ldots, u_k\} = \operatorname{span}\{x_1, x_2, \ldots, x_k\}$

$k = 0, \ldots, n$

with the Gram-Schmidt process:

$$u_1 = \frac{x_1}{\|x_1}$$

For $k = 1, \ldots, n-1$

$$w_{k+1} = x_{k+1} - \sum_{i=1}^{k} \langle x_{k+1}, u_i \rangle u_i$$

$$u_{k+1} = \frac{w_{k+1}}{\|x_{k+1}\|}$$

Clearly $\|u_i\| = 1 \quad i = 1, \ldots, n$

Clearly $\operatorname{span}\{u_1, \ldots, u_k\} = \operatorname{span}\{x_1, \ldots, x_k\}$

What about orthogonality.

By induction.

~~When~~ We saw $\langle w_2, u_1 \rangle = 0$

$\Rightarrow \langle u_2, u_1 \rangle = 0$

Assume $\langle u_j, u_i \rangle = 0 \quad j \neq i, \ j = 1, \dots, k$

We want to show $\langle u_{k+1}, u_j \rangle = 0 \quad j = 1 \dots k$

It suffices to show $\langle w_{k+1}, u_j \rangle = 0$

Compute

$$\langle w_{k+1}, u_j \rangle = \langle x_{k+1}, u_j \rangle - \sum_{i=1}^{k} \langle x_{k+1}, u_i \rangle \langle u_i, u_j \rangle$$

since $\langle u_i, u_j \rangle = 0 \quad j \neq i$

we are left with

$$\langle w_{k+1}, u_j \rangle = \langle x_{k+1}, u_j \rangle - \langle x_{k+1}, u_j \rangle \langle u_j, u_j \rangle$$

again $\langle u_j, u_j \rangle = \|u_j\|^2 = 1$

so $\langle w_{k+1}, u_j \rangle = 0$ i.e. $w_{k+1} \perp u_j \quad j = 1, \dots, k$

q.e.d

Example $x_1 = \begin{vmatrix} 1 \\ 1 \\ 0 \end{vmatrix}$ $x_2 = \begin{vmatrix} 1 \\ 1 \\ 2 \end{vmatrix}$ $x_3 = \begin{vmatrix} 1 \\ 0 \\ 1 \end{vmatrix}$

We obtained already $u_1 = \frac{1}{\sqrt{2}}\begin{vmatrix} 1 \\ 1 \\ 0 \end{vmatrix}$ $u_2 = \begin{vmatrix} 0 \\ 0 \\ 1 \end{vmatrix}$

$$\langle x_3, u_1 \rangle = \frac{1}{\sqrt{2}} \qquad \langle x_3, u_2 \rangle = 1$$

$$w_3 = x_3 - \langle x_3, u_1 \rangle u_1 - \langle x_3, u_2 \rangle u_2$$

$$= \begin{vmatrix} 1 \\ 0 \\ 1 \end{vmatrix} - \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} \begin{vmatrix} 1 \\ 1 \\ 0 \end{vmatrix} - 1 \begin{vmatrix} 0 \\ 0 \\ 1 \end{vmatrix} = \begin{vmatrix} 1/2 \\ -1/2 \\ 0 \end{vmatrix}$$

$$\| w_3 \| = \sqrt{\frac{1}{4} + \frac{1}{4}} = \sqrt{\frac{1}{2}} \qquad u_3 = \sqrt{2} \cdot \begin{vmatrix} 1/2 \\ -1/2 \\ 0 \end{vmatrix} = \sqrt{2} \cdot \frac{1}{2} \begin{vmatrix} 1 \\ -1 \\ 0 \end{vmatrix} = \frac{1}{\sqrt{2}} \begin{vmatrix} 1 \\ -1 \\ 0 \end{vmatrix}$$

$\frac{1}{\sqrt{2}}$ $u_3 = \frac{1}{\sqrt{2}} \begin{vmatrix} 1 \\ -1 \\ 0 \end{vmatrix}$ check. $\langle u_3, u_1 \rangle = 0$

$\langle u_3, u_2 \rangle = 0$

Let us rephrase the question: Given an $n \times n$ matrix A, find Q $n \times n$ such that its columns are orthonormal (ie. $Q^T Q = I$, ie. Q orthogonal matrix) such that $\text{span}\{q_1\, q_2 \cdots q_k\} = \text{span}\{a_1\, a_2 \cdots a_k\}$ where $Q = [q_1\, q_2 \cdots q_n]$, $A = [a_1\, a_2 \cdots a_n]$

Same answer: Gram-Schmidt.
But now observe that

$$A = Q \cdot R \quad \text{, where } R \text{ is upper triangular.}$$

with positive diagonals

$$a_1 = q_1 \cdot \|a_1\| \qquad \left(q_1 = a_1 / \|a_1\| \right)$$

$$a_2 = \langle a_2, q_1 \rangle q_1 + \|w_2\| q_2$$

$$w_2 = \|w_2\| q_2 = a_2 - \langle a_2, q_1 \rangle q_1$$

$$R_{ij} = \langle a_j, q_i \rangle \qquad i < j$$

$$R_{ii} = \|w_i\|$$

In example $R_{11} = \|x_1\| = \sqrt{2}$

$R_{12} = \langle x_2, u_1 \rangle = \frac{2}{\sqrt{2}}$

$R_{22} = \|w_2\| = 2$

$R_{13} = \langle x_3, u_1 \rangle = 1/\sqrt{2}$

$R_{23} = \langle x_3, u_2 \rangle = 1$

$R_{33} = \|w_3\| = 1/\sqrt{2}$

$$R = \begin{bmatrix} \sqrt{2} & 2/\sqrt{2} & 1/\sqrt{2} \\ 0 & 2 & 1 \\ 0 & 0 & 1/\sqrt{2} \end{bmatrix}$$

check $A = Q.R$

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 0 & 2 & 1 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 0 & 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} \sqrt{2} & 2/\sqrt{2} & 1/\sqrt{2} \\ 0 & 2 & 1 \\ 0 & 0 & 1/\sqrt{2} \end{bmatrix}$$

$$A \qquad\qquad Q \qquad\qquad R$$

<u>lemma</u>. A $n \times n$. $A = QR$

$Q^T Q = I$. R ∇ upper triang with positive diagonals.

QR Factorization <u>is unique</u>.

<u>Proof</u>. Let $A = Q_1 R_1 = Q_2 R_2$

$Q_1^{-1} = Q_1^T \qquad R_1 = Q_1^T Q_2 R_2$

$R_1 R_2^{-1} = Q_1^T Q_2$

Note first. product of orthogonal matrix is orthogonal. $U^T U = I \quad V^T V = I$

$$(UV)^T UV = V^T U^T U V = V^T I V = I.$$

so. left hand side ∇, r.h.s. orthonormal columns

$\Rightarrow \nabla = \diagdown = I. \Rightarrow Q_1 = Q_2 \quad R_1 = R_2$

(triangular, orthonormal $\Rightarrow I$)

qed

Example $A = \begin{vmatrix} 1 & 1 \\ 2 & 1 \end{vmatrix}$

$$q_1 = a_1 / \|a_1\| = \frac{1}{\sqrt{5}} \begin{vmatrix} 1 \\ 2 \end{vmatrix}$$

since $\|a_1\| = \sqrt{1+2^2} = \sqrt{5}$

$$\langle a_2, q_1 \rangle = \frac{1}{\sqrt{5}}(1+2) = \frac{3}{\sqrt{5}}$$

$$w_2 = a_2 - \langle a_2, q_1 \rangle q_1$$

$$= \begin{vmatrix} 1 \\ 1 \end{vmatrix} - \frac{3}{\sqrt{5}} \frac{1}{\sqrt{5}} \begin{vmatrix} 1 \\ 2 \end{vmatrix} = \begin{vmatrix} 1 \\ 1 \end{vmatrix} - \frac{3}{5} \begin{vmatrix} 1 \\ 2 \end{vmatrix} = \frac{1}{5} \begin{vmatrix} 2 \\ -1 \end{vmatrix}$$

$$\|w_2\| = \frac{1}{5} \cdot \sqrt{4+1} = \frac{\sqrt{5}}{5} = \frac{1}{\sqrt{5}}$$

$$q_2 = \frac{1}{\sqrt{5}} \begin{vmatrix} 2 \\ -1 \end{vmatrix}$$

$$A = QR = \begin{vmatrix} 1 & 1 \\ 2 & 1 \end{vmatrix} = \underbrace{\frac{1}{\sqrt{5}} \begin{vmatrix} 1 & 2 \\ 2 & -1 \end{vmatrix}}_{Q} \cdot \underbrace{\begin{vmatrix} \sqrt{5} & 3/\sqrt{5} \\ 0 & 1/\sqrt{5} \end{vmatrix}}_{R}$$

$$= \underbrace{\frac{1}{\sqrt{5}} \cdot \left(\frac{1}{\sqrt{5}}\right.}_{=\frac{1}{5}} \underbrace{\left.\begin{vmatrix} 1 & 2 \\ 2 & -1 \end{vmatrix}\right)}_{Q} \cdot \begin{vmatrix} 5 & 3 \\ 0 & 1 \end{vmatrix}$$

We have now two factorizations

$$A = LU \qquad \text{(assuming no pivoting)}$$
$$A = QR$$

Can use the latter also to solve $Ax = b$

Indeed $\quad QRx = b$

$$Rx = Q^T b$$

back substitution

$Rx = Q^T b$ same cost as $Ux = y$

but computationally more stable.

Solve $\begin{vmatrix} 1 & 1 \\ 2 & 1 \end{vmatrix} \begin{vmatrix} x_1 \\ x_2 \end{vmatrix} = \begin{vmatrix} -1 \\ 0 \end{vmatrix}$

$$A \quad x \quad = \quad b$$

$$Q^T b = \frac{1}{\sqrt{5}} \begin{vmatrix} 1 & 2 \\ 2 & -1 \end{vmatrix} \begin{vmatrix} -1 \\ 0 \end{vmatrix} = \frac{1}{\sqrt{5}} \begin{vmatrix} -1 \\ -2 \end{vmatrix}$$

$$Ux = \frac{1}{\sqrt{5}} \begin{vmatrix} 5 & 3 \\ 0 & 1 \end{vmatrix} = \frac{1}{\sqrt{5}} \begin{vmatrix} -1 \\ -2 \end{vmatrix}$$

$$x_2 = -2$$
$$x_1 = \left(-1 - 3(-2)\right)/5 = (-1+6)/5 = 1$$

$x = \begin{vmatrix} 1 \\ -2 \end{vmatrix}$ check ✓