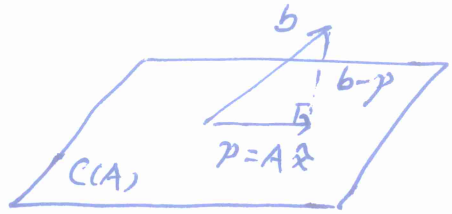
Recall:

1. Least Squares Approximation:

   Given a $m\times n$ matrix A, $b \in \mathbb{R}^m$, find $\hat{x} \in \mathbb{R}^n$ such that
   $\|b - A\hat{x}\|^2$ is minimal

2. By geometry, $A^T(b - A\hat{x}) = 0$

   $A^TA\hat{x} = A^Tb$



3. By calculus,

   $E = \|Ax - b\|^2$ is minimal

   $\Rightarrow \frac{\partial E}{\partial x_i} = 0, \ i = 1, \cdots, n$

   $\Leftrightarrow A^TA\hat{x} = A^Tb$

4. Application: Line Fitting.

§4.4 Orthonormal Bases and Gram-Schmidt

Motivation: Consider

$$A^TA\hat{x} = A^Tb$$

if $A^TA = I$, $\Rightarrow \hat{x} = A^Tb$

$A \xrightarrow{\text{Gram-Schmidt}} A = QR$, where $Q^TQ = I$, R is upper trangular

Def Vectors $q_1, \cdots, q_n$ are orthonormal if

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

Set $Q = [q_1, \cdots, q_n]$ (to be a matrix with orthonormal columns).

Then $Q^TQ = I$

②

$$Q^TQ = \begin{bmatrix} q_1^T \\ q_2^T \\ \vdots \\ q_n^T \end{bmatrix} \begin{bmatrix} q_1 & q_2 & \cdots & q_n \end{bmatrix} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix} = I$$

If Q is square, $Q^TQ = I \Rightarrow Q^T = Q^{-1}$

~~In this case, we~~

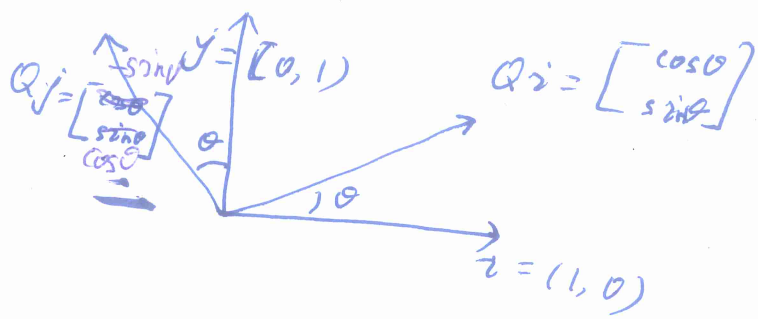
In square case, we call Q an orthogonal matrix.

(Let us look at three important ~~exa~~ examples of orthogonal matrices)

Ex 1 (Rotation)

$$Q = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}, \quad Q^T = Q^{-1} = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$$

$QQ^T = I$



Ex 2 (Permutation)

$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} y \\ z \\ x \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} y \\ x \end{bmatrix}$$

inverse
‖
transpose

$$\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} y \\ z \\ x \end{bmatrix} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} = \begin{bmatrix} y \\ x \end{bmatrix}$$

every permutation matrix is an orthogonal matrix.

Ex 3 (Reflection)

If u is a unit vector, set $Q = I - 2uu^T$.

Then $Q^T = I - 2uu^T = Q$ and $Q^TQ = I - 4uu^T + 4u(u^Tu)u^T = I$.

Q is called a reflection matrix.

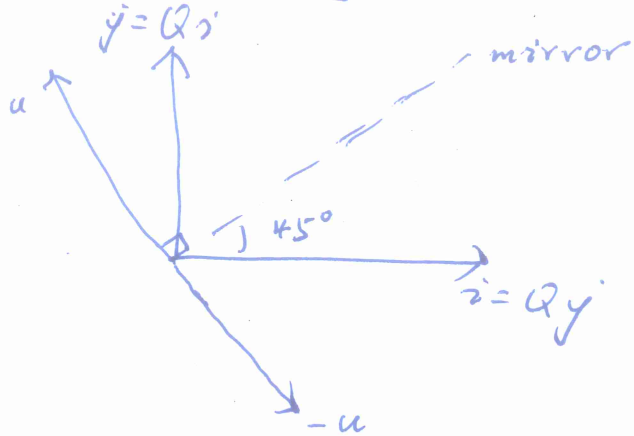
③

$Q^2 = Q^TQ = I.$

(Refleting twice through a mirror will get the original one)

Let $u = \left(-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right)$

Then $Q = I - 2uu^T = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $Q\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} y \\ x \end{bmatrix}$



Note: Orthogonal matrices preserve lengths and angles

If Q has ~~is a~~ ~~orthogonal~~ orthonomal columns ($Q^TQ = I$), then

$\|Qx\| = \|x\|$ for each x

Q preserves dot (Π) product. $(Qx)^T(Qy) = x^TQ^TQy = x^Ty.$

Projections Using Orthonormal Bases: Q Replaces A.

Assume $A = Q$, where Q has orthonormal columns

Then the least squares solution of $Qx = b$ $(Q^TQ\hat{x} = Q^Tb)$

is $\hat{x} = Q^Tb$ $(Q^TQ = I)$

The projection matrix is

$$P = Q(Q^TQ)^{-1}Q^T$$
$$= QQ^T$$

The projection

$$p = Q\hat{x} = QQ^Tb$$

$$p = [q_1 \cdots q_n] \begin{bmatrix} q_1^T b \\ \vdots \\ q_n^T b \end{bmatrix}$$

$$= q_1(q_1^T b) + \cdots + q_n(q_n^T b)$$

p is a sum of projections of b onto the lines in direction of q's.

Note: If Q is square, then

$$P = QQ^T = I$$

$$p = b \iff b = QQ^T b$$

$$= q_1(q_1^T b) + q_2(q_2^T b) + \cdots + q_n(q_n^T b)$$

Ex 4. Consider Q with orthonormal columns

$$Q = \frac{1}{3} \begin{array}{c} \begin{array}{ccc} q_1 & q_2 & q_3 \end{array} \\ \begin{bmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{bmatrix} \end{array}$$

Let $b = (0, 0, 1)$. projections into q's

$q_1(q_1^T b) = \frac{2}{3} q_1$, $q_2(q_2^T b) = \frac{2}{3} q_2$, $q_3(q_3^T b) = -\frac{1}{3} q_3$

$$b = p_1 + p_2 + p_3$$

$$= \frac{2}{3} q_1 + \frac{2}{3} q_2 - \frac{1}{3} q_3$$

The Gram-Schmidt Process.

Let a, b, c be independent vectors.

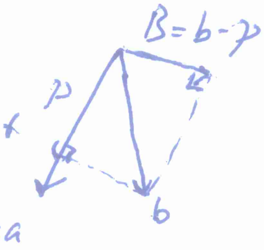
Goal: construct orthogonal vectors A, B, C in the vector space spanned by a, b, c.

Set $q_1 = A/\|A\|$, $q_2 = B/\|B\|$, $q_3 = C/\|C\|$.

Gram-Schmidt: Set $A = a$.

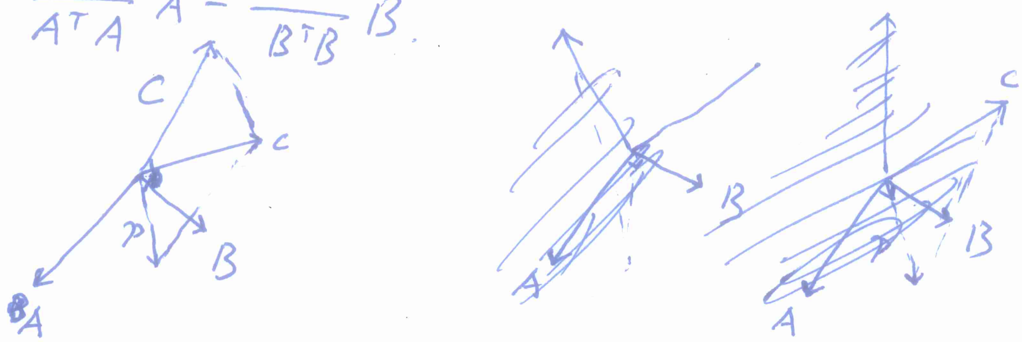
⑤ Step 1. Set $B = b - \frac{A^Tb}{A^TA}A$

Note: $B \neq 0$ because a and b are independent



Step 2:

$$C = c - \overbrace{\frac{A^Tc}{A^TA}A - \frac{B^Tc}{B^TB}}^{p}B.$$



Step 3. Set $q_1 = \frac{A}{\|A\|}$, $q_2 = \frac{B}{\|B\|}$, $q_3 = \frac{C}{\|C\|}$.

Ex Let

$$a = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}, \quad b = \begin{bmatrix} 2 \\ 0 \\ -2 \end{bmatrix}, \quad c = \begin{bmatrix} 3 \\ -3 \\ 3 \end{bmatrix}.$$

$A = a$, $A^TA = 2$, $A^Tb = 2$

$$B = b - \frac{A^Tb}{A^TA}A = \begin{bmatrix} 1 \\ 1 \\ -2 \end{bmatrix}$$

$$C = c - \frac{A^Tc}{A^TA}A - \frac{B^Tc}{B^TB}B = c - \frac{6}{2}A + \frac{6}{6}B = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\Rightarrow q_1 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}, \quad q_2 = \frac{1}{\sqrt{6}}\begin{bmatrix} 1 \\ 1 \\ -2 \end{bmatrix}, \quad q_3 = \frac{1}{\sqrt{3}}\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}.$$

The Factorization $A = QR$. (put Gram-Schmidt process in a nutshell)

Let $A = [a \ b \ c]$

$$a, b, c \xrightarrow{\text{Gram-Schmidt}} q_1, q_2, q_3.$$

⑥

$$a = q_1(q_1^T a)$$

$$b = q_1(q_1^T b) + q_2(q_2^T b)$$

$$c = q_1(q_1^T c) + q_2(q_2^T c) + q_3(q_3^T c)$$

$$A = [a\ b\ c] = [q_1\ q_2\ q_3] \begin{bmatrix} q_1^T a & q_1^T b & q_1^T c \\ & q_2^T b & q_2^T c \\ & & q_3^T c \end{bmatrix}$$

$$= QR$$

Note: it can be generalized to n-dimensional case

~~Ex~~. Least squares:

$$A^T A x = A^T b \iff R^T R \hat{x} = R^T Q^T b$$

(R^T is invertible by independence of columns of A)

$$A^T A = (QR)^T QR = R^T(Q^T Q)R = R^T R$$

$$\Rightarrow R\hat{x} = Q^T b$$

$$\Rightarrow \hat{x} = R^{-1} Q^T b \text{ (back substitution)}$$