Gram-Schmidt procedure

Thm (Fourier Expansion)

If $\mathcal{B} = \{u_1, u_2, \dots, u_n\}$ is an orthonormal bases for an inner-product space V, then for each $x \in V$ can be expressed as:

$$x = \langle x, u_1 \rangle u_1 + \langle x, u_2 \rangle u_2 + \dots + \langle x, u_n \rangle u_n.$$

The scalars $\langle x | u_i \rangle$ are the coordinates of x with respect to $\mathcal{B}$, and they are called the Fourier coefficients.

Example: Determine the Fourier expansion of $x = \begin{pmatrix} -1 \\ 2 \\ 1 \end{pmatrix}$ with respect to the standard inner product and the orthonormal basis:

$$\mathcal{B} = \left\{ u_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, u_2 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, u_3 = \frac{1}{\sqrt{6}} \begin{pmatrix} -1 \\ -1 \\ 2 \end{pmatrix} \right\}$$

Solution The Fourier coefficients are

$$\xi_1 = \langle x, u_1 \rangle = \frac{-3}{\sqrt{2}}, \quad \xi_2 = \langle x, u_2 \rangle = \frac{2}{\sqrt{3}}, \quad \xi_3 = \langle x, u_3 \rangle = \frac{1}{\sqrt{6}}$$

$$\Rightarrow x = \xi_1 u_1 + \xi_2 u_2 + \xi_3 u_3. *$$

Does every finite dimensional inner-product space V has an orthonormal basis? and if so how can we find them? The answer is in the following Gram-Schmidt procedure.

Let $\mathcal{B} = \{x_1, x_2, \dots, x_n\}$ be an arbitrary basis (not necessarily orthonormal) for n-dim inner product space S and remember $\|\star\| = \langle \star, \star \rangle^{1/2}$.

They use $\mathcal{B}$ to construct an orthonormal basis $\mathcal{O} = \{u_1, u_2, \dots, u_n\}$ for S

In fact they construct O sequentially so that
$O_k = \{u_1, u_2, \ldots, u_k\}$ is orthonormal basis for
$S_k = \text{span}\{x_1, x_2, \ldots, x_k\}$ for $k = 1, \ldots, n$.
for $k=1$ take $u_1 = \frac{x_1}{\|x_1\|}$ so that $O_1 = \{u_1\}$ is an orthonormal set whose span agree with $S_1 = \{x_1\}$.
Suppose that $O_k = \{u_1, u_2, \ldots, u_k\}$ is an orthonormal basis for $S_k = \text{span}\{x_1, \ldots, x_k\}$. Now find u_{k+1} s.th.
$O_{k+1} = \{u_1, u_2, \ldots, u_{k+1}\}$ is an orthonormal basis for $S_k = \{x_1, \ldots, x_{k+1}\}$.
The Fourier expansion w.r.t. O_{k+1} is

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

$$\Rightarrow \qquad u_{k+1} = \frac{x_{k+1} - \sum_{i=1}^{k} \langle x_{k+1}, u_i \rangle u_i}{\langle x_{k+1}, u_{k+1} \rangle}$$

since $\|u_{k+1}\| = 1$, it follows that

$$\left| \langle x_{k+1}, u_{k+1} \rangle \right| = \left\| x_{k+1} - \sum_{i=1}^{k} \langle x_{k+1}, u_i \rangle u_i \right\|$$

so that $\langle x_{k+1}, u_{k+1} \rangle = e^{i\theta} \left\| x_{k+1} - \sum_{i=1}^{k} \langle x_{k+1}, u_i \rangle u_i \right\|$, for some $0 \leq \theta < 2\pi$, and

$$u_{k+1} = \frac{x_{k+1} - \sum_{i=1}^{k} \langle x_{k+1}, u_i \rangle u_i}{e^{i\theta} \left\| x_{k+1} - \sum_{i=1}^{k} \langle x_{k+1}, u_i \rangle u_i \right\|}$$

since $e^{i\theta}$ neither affect $\text{span}\{u_1, u_2, \ldots, u_{k+1}\}$ nor $\|u_{k+1}\| = 1$ and $\langle u_i, u_{k+1} \rangle = 0$ for all $i \leq k$, we can arbitrarily define u_{k+1} by letting $\theta = 0$. Let

$$\nu_{k+1} = \left\| x_{k+1} - \sum_{i=1}^{k} \langle x_{k+1}, u_i \rangle u_i \right\|$$

So that we can write

$$(1)\quad u_1 = \frac{x_1}{\|x_1\|} \quad \text{and} \quad u_{k+1} = \frac{x_{k+1} - \sum_{i=1}^{k} \langle x_{k+1}, u_i \rangle u_i}{v_{k+1}} \qquad k>0$$

This sequence is called Gram-Schmidt sequence.

Exc: Prove that $O_k = \{u_1, u_2, \ldots, u_k\}$ is an orthonormal basis for $\text{span}\{x_1, \ldots, x_k\}$ for each $k = 1, 2, \ldots, n$.

Now let us consider $\mathbb{R}^m$ or $\mathbb{C}^m$ with the standard inner product and euclidean norm we can formulate (1) in term of matrices. Suppose $B = \{x_1, \ldots, x_n\}$ is a basis for an n-dim subspace S of $\mathbb{C}^{m\times 1}$, so that the Gram-Schmidt $\Rightarrow$

$$u_1 = \frac{x_1}{\|x_1\|} \quad \text{and} \quad u_k = \frac{x_k - \sum_{i=1}^{k-1} (u_i^* x_k) u_i}{\|x_k - \sum_{i=1}^{k-1} (u_i^* x_k) u_i\|} \qquad k = 2, 3, \ldots, n.$$

in matrix notations set

$$U_1 = O_{m\times 1} \quad \& \quad U_k = \begin{pmatrix} u_1 & u_2 & \ldots & u_{k-1} \end{pmatrix}_{m\times k-1} \qquad k>1$$

and notice that

$$U_k^* x_k = \begin{pmatrix} u_1^* x_k \\ u_2^* x_k \\ \vdots \\ u_{k-1}^* x_k \end{pmatrix} \quad \text{and} \quad U_k U_k^* x_k = \sum_{i=1}^{k-1} u_i (u_i^* x_k) = \sum_{i=1}^{k-1} (u_i^* x_k) u_i$$

Since $x_k - \sum_{i=1}^{k-1} (u_i^* x_k) u_i = x_k - U_k U_k^* x_k = (I - U_k U_k^*) x_k$.

$$\Rightarrow u_k = \frac{(I - U_k U_k^*) x_k}{\|(I - U_k U_k^*) x_k\|} \qquad \text{for } k = 1, 2, \ldots, n.$$

Summary (Gram-Schmidt orthogonalization proced.)

If $\mathcal{B}=\{x_1, \dots, x_n\}$ is a basis for a general inner-product space S, then the Gram-Schmidt sequence defined by:

$$u_1 = \frac{x_1}{\|x_1\|} \quad \text{and} \quad u_k = \frac{x_k - \sum_{i=1}^{k-1} \langle x_k, u_i \rangle u_i}{\left\| x_k - \sum_{i=1}^{k-1} \langle x_k, u_i \rangle u_i \right\|} \qquad k=2, \dots, n$$

is an orthonormal basis for S. When S is an n-dim subspace of $\mathbb{C}^{m\times 1}$, the Gram-Schmidt sequence:

$$u_k = \frac{(I - U_k U_k^*) x_k}{\|(I - U_k U_k^*) x_k\|} \qquad \text{for } k=1, 2, \dots, n$$

in which $U_1 = 0$ and $U_k = (u_1 \ u_2 \cdots u_{k-1})_{m\times k-1}$ $k>1$.

Example: Find an orthonormal basis for the space spanned by the following three linearly independent vectors.

$$x_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}, \quad x_2 = \begin{pmatrix} 1 \\ 2 \\ 0 \\ -1 \end{pmatrix}, \quad x_3 = \begin{pmatrix} 3 \\ 1 \\ 1 \\ -1 \end{pmatrix}$$

Solution

$k=1$: $u_1 = \frac{x_1}{\|x_1\|} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}$

$k=2$: $u_2 = x_2 - (u_1^T x_2)\, u_1 = \begin{pmatrix} 0 \\ 2 \\ 0 \\ 0 \end{pmatrix} \Rightarrow u_2 = \frac{u_2}{\|u_2\|} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$

$k=3$: $u_3 = x_3 - (u_1^T x_3) u_1 - (u_2^T x_3) u_2 = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix} \Rightarrow u_3 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 1 \end{pmatrix}$ #

QR Factorization

Let $\underset{m\times n}{A}=(a_1\ a_2 \dots a_n)$ be a matrix with linearly independent columns. When Gram-Schmidt applied the result is an orthonormal basis $\{q_1, q_2, \dots, q_n\}$ for $R(A)$, where

$$q_1 = \frac{a_1}{r_1} \quad \text{and} \quad q_k = \frac{a_k - \sum_{i=1}^{k-1} \langle a_k, q_i\rangle q_i}{r_k} \qquad k=2,3,\dots,n.$$

where $q_1 = \dfrac{a_1}{r_1}$ and $r_k = \left\| a_k - \sum_{i=1}^{k-1} \langle a_k, q_i\rangle q_i \right\|$ for $k>1$.

So we can write

$a_1 = r_1 q_1$ and $a_k = \langle a_k, q_1\rangle q_1 + \dots + \langle a_k, q_{k-1}\rangle q_{k-1} + r_k q_k$, $k>1$

in matrix form

$$(a_1\ a_2\ \dots a_n) = (q_1\ q_2 \cdots q_n)\begin{pmatrix} r_1 & \langle a_2,q_1\rangle & \langle a_3,q_1\rangle & \cdots & \langle a_n,q_1\rangle \\ 0 & r_2 & \langle a_3,q_2\rangle & \cdots & \langle a_n,q_2\rangle \\ \vdots & 0 & r_3 & & \vdots \\ & \vdots & 0 & \ddots & \vdots \\ 0 & 0 & 0 & \cdots\ 0 & r_n \end{pmatrix}$$

i.e it is possible to factor a matrix with independent columns as $A_{m\times n} = Q_{m\times n} R_{n\times n}$ $\quad Q$: orthonormal basis for $R(A)$

and R is upper-triangular matrix with positive diagonal els

<u>Example:</u> Find the QR factrorization for

$$A = \begin{pmatrix} 0 & -20 & -14 \\ 3 & 27 & -4 \\ 4 & 11 & -2 \end{pmatrix}$$

<u>Solution:</u> $k=1$: $r_{11} = \|a_1\| = 5$ & $q_1 = \dfrac{a_1}{r_{11}} = \begin{pmatrix} 0 \\ 3/5 \\ 4/5 \end{pmatrix}$

$k=2$: $r_{12} = q_1^T a_2 = 25$, $q_2 = a_2 - r_{12} q_1 = \begin{pmatrix} -20 \\ 12 \\ -9 \end{pmatrix}$, $r_{22} = \|q_2\| = 25$

and $q_2 = \dfrac{q_2}{r_{22}} = \dfrac{1}{25}\begin{pmatrix} -20 \\ 12 \\ -9 \end{pmatrix}$

$k=3$, $r_{13} = q_1^T a_3 = -4$ and $r_{23} = q_2^T a_3 = 10$

$$q_3 = a_3 - r_{13} q_1 - r_{23} q_2 = \frac{2}{5}\begin{pmatrix} -15 \\ -16 \\ 12 \end{pmatrix}, \quad r_{33} = \| q_3 \| = 10 \text{ and}$$

$$q_3 = \frac{q_3}{r_{33}} = \frac{1}{25}\begin{pmatrix} -15 \\ -16 \\ 12 \end{pmatrix} \Rightarrow$$

$$Q = \begin{pmatrix} 0 & -20 & -15 \\ 15 & 12 & -16 \\ 20 & -9 & 12 \end{pmatrix} \text{ and } R = \begin{pmatrix} 5 & 25 & -4 \\ 0 & 25 & 10 \\ 0 & 0 & 10 \end{pmatrix}.$$