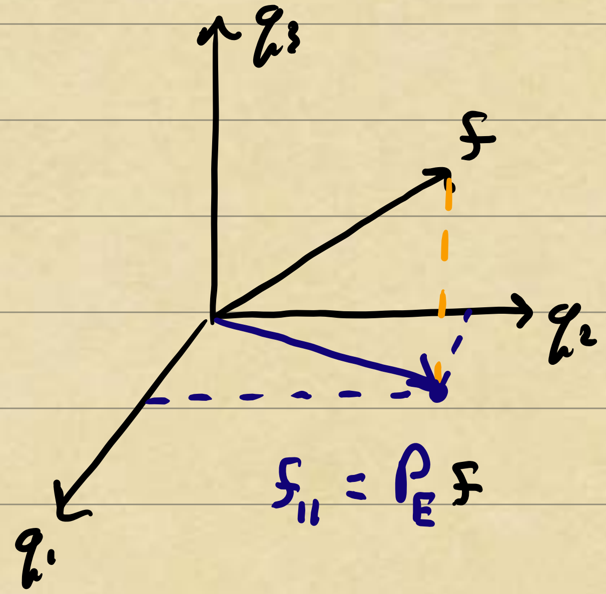
Gram-Schmidt & QR

Goal: Minimize $\|f - Ec\|$ in Hilbert norm.

$\uparrow$ $E : \mathbb{R}^N \to H$ (quasimatrix)



Two step procedure:

$\Rightarrow$ Project $\quad f_\parallel = P_E f$

$\Rightarrow$ Solve $\quad Ec = f_\parallel$

Here, $P_E : H \to \mathrm{col}(E)$ is the orthogonal projection of H onto $\mathrm{col}(E)$. If the columns of E are orthonormal, then

$\Rightarrow$ Project $\to$ $f_\parallel = E E^* f$

$\Rightarrow$ Solve $\to$ $\overbrace{\cancel{E^* E}}^{=I} c = \overbrace{\cancel{E^* E}}^{=I} E^* f \quad \to \quad c = E^* f$

Question: What if columns of E are not ONB?

E.g. $\quad E = [1 \;\; x \;\; x^2 \; \cdots \; x^n]$

Gram-Schmidt Orthogonalization

Given linearly independent vectors $\{v_k\}_{k=1}^N$ in a Hilbert Space, w/inner product $\langle \cdot, \cdot \rangle$, Gram-Schmidt systematically constructs ONB.

Input: $v_1, v_2, \ldots, v_N$

normalize so $\|q_1\| = 1$ $\Rightarrow$ $q_1 = v_1 / \|v_1\|$

orthogonalize $v_2 \perp q_1$ $\Rightarrow$ $\tilde{q}_2 = v_2 - \langle v_2, q_1 \rangle q_1$

normalize $q_2 = \tilde{q}_2 / \|\tilde{q}_2\|$

$\vdots$

orthogonalize $v_k \perp q_1, \ldots, q_{k-1}$ $\Rightarrow$ $\tilde{q}_k = v_k - \langle v_k, q_{k-1} \rangle q_{k-1} \cdots - \langle v_k, q_1 \rangle q_1$

normalize $q_k = \tilde{q}_k / \|q_k\|$

Output: $q_1, q_2, \ldots, q_N$

$\{q_1, \ldots, q_N\}$ is an ONB for span$\{v_1, \ldots, v_N\}$

Example: Construct ONB for span$\{1, x, x^2\}$ using the $L^2([-1,1])$ inner product $\langle f,g\rangle = \int_{-1}^{+1} f g \, dx$.

$\underline{v_1 = 1}$ $\Rightarrow$ $\|v_1\|^2 = \int_{-1}^{+1} 1^2 \, dx = 2$

$$q_1 = v_1/\|v_1\| = 1/\sqrt{2}$$

$\underline{v_2 = x}$ $\Rightarrow$ $\langle v_2, q_1\rangle = \frac{1}{\sqrt{2}} \int_{-1}^{+1} 1 \cdot x \, dx = 0$

$$\tilde{q}_2 = x$$

$$\|\tilde{q}_2\|^2 = \int_{-1}^{+1} x^2 \, dx = \frac{x^3}{3}\Big|_{-1}^{+1} = \frac{2}{3}$$

$$q_2 = \tilde{q}_2/\|\tilde{q}_2\| = \sqrt{\tfrac{3}{2}}\, x$$

$\underline{v_3 = x^2}$ $\Rightarrow$ $\langle v_3, q_1\rangle = \frac{1}{\sqrt{2}} \int_{-1}^{+1} 1 \cdot x^2 \, dx = \frac{1}{\sqrt{2}} \frac{2}{3} = \frac{\sqrt{2}}{3}$

$\Rightarrow$ $\langle v_3, q_2\rangle = \sqrt{\tfrac{3}{2}} \int_{-1}^{+1} x \cdot x^2 \, dx = 0$

$$\tilde{q}_3 = x^2 - \frac{\sqrt{2}}{3} \frac{1}{\sqrt{2}} = x^2 - 1/3$$

$$\|\tilde{q}_3\|^2 = \int_{-1}^{+1} (x^2 - 1/3)^2 dx = \int_{-1}^{+1} x^4 - \frac{2}{3}x^2 + \frac{1}{9}\, dx$$

$$= \frac{x^5}{5}\Big|_{-1}^{+1} - \frac{2}{3}\frac{x^3}{3}\Big|_{-1}^{+1} + \frac{1}{9}x\Big|_{-1}^{+1}$$

$$= \frac{2}{5} - \frac{4}{9} + \frac{2}{9} = \frac{18}{45} - \frac{10}{45} = \frac{8}{45}$$

$$q_3 = \sqrt{\frac{45}{8}}\,(x^2 - 1/3)$$

In general, applying the Gram-Schmidt algorithm to monomials $\{1, x, \ldots, x^N\}$ leads to the Legendre polynomials, normalized to have $L^2([-1,1])$ norm equal to one.

Classically, the Legendre polynomials are normalized to have $\hat{q}_k(1) = 1$ and they form an orthogonal basis for $L^2([-1,1])$.

<u>Question:</u> How can we use Gram-Schmidt to solve the best approximation problem?

The QR decomposition

Given a quasimatrix w/lin. indep. columns:

$$E = \begin{bmatrix} | & | & & | \\ e_1 & e_2 & \cdots & e_N \\ | & | & & | \end{bmatrix},$$

Gram Schmidt finds an ONB for col(E) by taking linear combinations of $e_1, \ldots, e_N$.

$$\underbrace{\begin{bmatrix} | & | & & | \\ e_1 & e_2 & \cdots & e_N \\ | & | & & | \end{bmatrix}}_{E} \underbrace{\begin{bmatrix} t_{11} & t_{12} & \cdots & t_{1N} \\ & t_{22} & \cdots & t_{2N} \\ & & \ddots & \vdots \\ & & & t_{NN} \end{bmatrix}}_{T} = \underbrace{\begin{bmatrix} | & | & & | \\ q_1 & q_2 & \cdots & q_N \\ | & | & & | \end{bmatrix}}_{Q}$$

The combinations are upper triangular, and we can reverse the process!

$$E = QT^{-1} = QR \qquad (R = T^{-1})$$

The inverse of a triangular matrix is triangular so E is factored into ONB Q × Tri R.

QR solution to Best Approximation

We can now use the QR decomposition of E to solve $\underline{c}_* = \operatorname{argmin}_{c \in \mathbb{R}} \| f - E\underline{c} \|$:

$$\text{Project} \Rightarrow \quad f_{\parallel} = P_V f = QQ^* f$$

$$\text{Solve} \Rightarrow \quad E\underline{c} = f_{\parallel}$$

$$(QR)\underline{c} = QQ^* f \rightarrow \underbrace{Q^* Q}_{=1} R\underline{c} = \underbrace{Q^* Q}_{=1} Q^* f$$

$$\rightarrow R\underline{c} = Q^* f \rightarrow \underline{c} = R^{-1} Q^* f$$

Change-of-Basis

R is the change-of-basis matrix $E \rightarrow Q$

$$E\underline{c} = QR\underline{c} = Q\underline{b}, \qquad \underline{b} = R\underline{c}$$

$\underline{b}$ = coords in Q basis, $\underline{c}$ = coords in E basis.

Question: What about changing between other non-orthogonal bases?