

Gram-Schmidt Orthogonalization II [nl91]

First three iterations in step #1 of [nl90].

Initial condition:

$$|f_0\rangle = A|\phi_0\rangle.$$

First iteration:

$$\begin{aligned} |f_1\rangle &= \bar{\mathcal{H}}|f_0\rangle - a_0|f_0\rangle \\ \Rightarrow \langle f_0|f_1\rangle &= \langle f_0|\bar{\mathcal{H}}|f_0\rangle - a_0\langle f_0|f_0\rangle = 0 \\ &\text{if } a_0 = \frac{\langle f_0|\bar{\mathcal{H}}|f_0\rangle}{\langle f_0|f_0\rangle}. \end{aligned}$$

Second iteration:

$$\begin{aligned} |f_2\rangle &= \bar{\mathcal{H}}|f_1\rangle - a_1|f_1\rangle - b_1^2|f_0\rangle \\ \Rightarrow \langle f_0|f_2\rangle &= \underbrace{\langle f_0|\bar{\mathcal{H}}|f_1\rangle}_{\langle f_1|f_1\rangle} - a_1 \underbrace{\langle f_0|f_1\rangle}_0 - b_1^2\langle f_0|f_0\rangle = 0 \\ &\text{if } b_1^2 = \frac{\langle f_1|f_1\rangle}{\langle f_0|f_0\rangle}, \\ \Rightarrow \langle f_1|f_2\rangle &= \langle f_1|\bar{\mathcal{H}}|f_1\rangle - a_1 \underbrace{\langle f_1|f_1\rangle}_0 - b_1^2 \underbrace{\langle f_1|f_0\rangle}_0 = 0 \\ &\text{if } a_1 = \frac{\langle f_1|\bar{\mathcal{H}}|f_1\rangle}{\langle f_1|f_1\rangle}. \end{aligned}$$

Third iteration:

$$\begin{aligned} |f_3\rangle &= \bar{\mathcal{H}}|f_2\rangle - a_2|f_1\rangle - b_2^2|f_0\rangle - c_2|f_0\rangle \\ \Rightarrow \langle f_0|f_3\rangle &= \dots = 0 \quad \text{if } c_2 = 0, \\ \Rightarrow \langle f_1|f_3\rangle &= \dots = 0 \quad \text{if } b_2^2 = \frac{\langle f_2|f_2\rangle}{\langle f_1|f_1\rangle}, \\ \Rightarrow \langle f_2|f_3\rangle &= \dots = 0 \quad \text{if } a_2 = \frac{\langle f_2|\bar{\mathcal{H}}|f_2\rangle}{\langle f_2|f_2\rangle}. \end{aligned}$$