

→ Once the optimal coefficients $\gamma^* = [\alpha_1^*, \dots, \alpha_m^*]^T$ have been determined, we can finally assemble our approximation

$$X^{(m)} = X^{(0)} + \sum_{k=1}^m \alpha_k^* V_k = X^{(0)} + V_m \gamma^*$$

→ This is what we call the Generalised Minimal Residual (GMRES) method. The key algorithmic feature of the GMRES method, however, is that the entire process can be done "on the fly", as we build each column of V_m, \bar{H}_m , etc, and every factor of $G = G_m G_{m-1} \dots G_1$ for increasing m . An efficient, classical implementation is:

Algorithm: GMRES($A, X^{(0)}, b, m, \text{tol}$)

1. $r^{(0)} = b - AX^{(0)}$, $v_1 = r^{(0)} / \|r^{(0)}\|$, $\beta = \|r^{(0)}\|$
2. for $j = 1, \dots, m$
3. $[v_{j+1}, h_j] = \text{get Krylov}(A, v_j)$ (from the previous lecture)
 ↳ j -th column of \bar{H}_m

4. for $k=2, \dots, j$
5.
$$\begin{bmatrix} h_{k-1,j} \\ h_{k,j} \end{bmatrix} \leftarrow \begin{bmatrix} C_{k-1} & S_{k-1} \\ -S_{k-1} & C_{k-1} \end{bmatrix} \begin{bmatrix} h_{k-1,j} \\ h_{k,j} \end{bmatrix}$$
6. end
7. $d = \sqrt{h_{j,j}^2 + h_{j+1,j}^2}$, $C_j = \overbrace{h_{j,j}/d}^{\cos\theta}$, $S_j = \overbrace{h_{j+1,j}/d}^{\sin\theta}$
8. $h_{j,j} \leftarrow d$
9.
$$\begin{bmatrix} g_j \\ g_{j+1} \end{bmatrix} \leftarrow \begin{bmatrix} C_j & S_j \\ -S_j & C_j \end{bmatrix} \begin{bmatrix} g_j \\ 0 \end{bmatrix}$$
10. if $|g_{j+1}| < \text{tol}$, exit loop! (because $\|r^{(j)}\| = |g_{j+1}|$)
11. end

12. Solve the upper triangular system $R Y^* = g$, where overwritten values

$$r_{ij} = \begin{cases} h_{ij}, & \text{if } i \leq j \\ 0, & \text{otherwise} \end{cases}$$

13. $X^{(j)} = X^{(0)} + \sqrt{J_j} Y^*$

→ Notice how we only solve the triangular system (and compute the actual iterate $x^{(j)}$) at the end, but we still know how large the residual is after each iteration ($\|r^{(j)}\| = |g_{j+1}|$)!