Krylov subspace methods for symmetric systems

Conjugate gradient, SYMMLQ and MINRES

Anthony J. Rasmussen

Derived by hand, 1996

transcribed, corrected and verified, September 2026

Abstract

In 1996, during the first year of doctoral study, thirty handwritten pages derived three Krylov subspace methods for symmetric linear systems from first principles, working from Paige and Saunders' 1975 paper. This document sets out the spine of those derivations in modern notation, records the four errors the manuscript contains, closes the two results it states without proof, and reports a numerical verification of every recurrence.

The derivations are sound. Every error is one of justification rather than destination: in each case the conclusion reached is correct and the argument offered for it is not. One — an initialisation convention — would break an implementation coded directly from the page, and is corrected here. The manuscript's two acknowledged gaps, both flagged by the author at the time, are proved and hold.

Contents

1 What this document is

This document has two parts.

Part one sets out the spine of the derivations in modern notation: the minimisation framework, the Lanczos process, and each of the three algorithms in turn, followed by a numerical verification and a collected errata.

Part two (§9) reproduces the original thirty handwritten pages in facsimile, exactly as written. Nothing there has been transcribed, corrected or reordered.

The two are complementary and deliberately so. The facsimile is the record; the transcription is the reading copy, with the errors marked where they occur rather than silently repaired. Three conventions are used:

- A small grey note flushed right beneath a heading, *notebook p. n*, gives the corresponding pages of the facsimile.
- A **red box** marks an error in the manuscript. The surrounding text always states the correct result; the box says what the notebook says and why it fails.
- A **blue box** marks a result the notebook states without proving — in both cases explicitly, in the author's own hand — together with the proof.

The bookkeeping is deliberately visible. A document that quietly corrected a thirty-year-old notebook would be less useful than one that shows where a young mathematician's instinct outran his patience, because that is the interesting part of the record.

Problem and standing assumptions

Throughout, $A \in \mathbb{R}^{n\times n}$ is real, symmetric and nonsingular, $b \in \mathbb{R}^n$, and we seek x with

$$Ax = b.$$

A is not assumed positive definite — the indefinite case is the whole point of SYMMLQ and MINRES. We take $x_0 = 0$ throughout, so that $r_0 = b$; the general case follows by shifting.

2 The minimisation framework

notebook p. 1–2

Let $V_k = [v_1, \ldots, v_k]$ have orthonormal columns and seek an iterate in the subspace they span, $x_k = V_k y_k$. Paige and Saunders characterise a family of methods by the quadratic

$$f_k(y) \;=\; (AV_k y - b)^{\mathsf T} B\,(AV_k y - b), \tag{1}$$

with B symmetric and at our disposal. Expanding and differentiating,

$$\frac{\mathrm{d}f_k}{\mathrm{d}y} = 2\,y^{\mathsf T} V_k^{\mathsf T} ABAV_k - 2\,b^{\mathsf T} BAV_k,$$

and setting this to zero, then transposing and using $A^{\mathsf T} = A$, $B^{\mathsf T} = B$:

$$\boxed{V_k^{\mathsf T} ABAV_k\, y_k \;=\; V_k^{\mathsf T} AB\, b} \tag{2}$$

Equivalently $V_k^{\mathsf T} AB\, r_k = 0$ with $r_k = b - Ax_k$: the residual is constrained to be B-orthogonal, through A, to the subspace.

Restricting to $B = A^m$ for integer m, two choices are computationally viable.

Case (a): $m = -1$**,** $B = A^{-1}$**.** *notebook p. 2*

Equation (2) collapses to

$$V_k^\top A V_k\, y_k = V_k^\top b, \qquad V_k^\top r_k = 0. \tag{3}$$

This is the Galerkin condition, and yields conjugate gradient (§4) and SYMMLQ (§5).

Case (b): $m = 0$**,** $B = I$**.** *notebook p. 3*

Equation (2) becomes

$$V_k^\top A^2 V_k\, y_k = V_k^\top A b, \tag{4}$$

which minimises $\|r_k\|_2$ and yields MINRES (§6).

A caveat the notebook does not raise. The objective (1) is a genuine minimisation only when B is positive definite. For $B = A^{-1}$ this requires $A \succ 0$; when A is indefinite, (3) determines a stationary point rather than a minimum. This is not a defect in the derivation — it is exactly why case (a) is the unstable one and case (b) is not, a contrast the manuscript goes on to quantify precisely (§6.4).

3 The Lanczos process

notebook p. 3–4

The basis is generated by the symmetric Lanczos recurrence. With $\beta_1 = \|b\|$, $v_1 = b/\beta_1$ and $v_0 = 0$,

$$\beta_{j+1} v_{j+1} = A v_j - \alpha_j v_j - \beta_j v_{j-1}, \qquad \alpha_j = v_j^\top A v_j, \tag{5}$$

β_{j+1} being chosen non-negative so that $\|v_{j+1}\| = 1$. Collecting k steps,

$$\boxed{A V_k = V_k T_k + \beta_{k+1} v_{k+1} e_k^\top} \tag{6}$$

with T_k symmetric tridiagonal carrying $\alpha_1, \ldots, \alpha_k$ on the diagonal and $\beta_2, \ldots, \beta_k$ off it. Orthonormality gives $V_k^\top V_k = I_k$ and $V_k^\top v_{k+1} = 0$, hence

$$V_k^\top A V_k = T_k. \tag{7}$$

Substituting into (3) and using $V_k^\top b = \beta_1 V_k^\top v_1 = \beta_1 e_1$,

$$T_k y_k = \beta_1 e_1, \qquad x_k = V_k y_k. \tag{8}$$

V_k **is** $n \times k$**, not square.** The notebook flags this in a margin note, and the point is load-bearing: $V_k^\top V_k = I_k$ but $V_k V_k^\top \neq I_n$, so the cancellation in (7) runs one way only. Two of the errors recorded below (§5.4, §6.3) are precisely failures to respect it.

It is convenient to name the $(k{+}1) \times k$ rectangular form

$$\bar{T}_{k+1} = \begin{pmatrix} T_k \\ \beta_{k+1} e_k^\top \end{pmatrix}, \qquad \text{so that} \qquad A V_k = V_{k+1} \bar{T}_{k+1}. \tag{9}$$

It does not appear in the notebook, but it is what §6.3 needs.

4 Conjugate gradient

notebook p. 5–6

Take $A \succ 0$, so $T_k = V_k^\mathsf{T} A V_k \succ 0$ and admits a Cholesky-type factorisation $T_k = L_k D_k L_k^\mathsf{T}$ with L_k unit lower bidiagonal (subdiagonal μ_j) and $D_k = \mathrm{diag}(d_1, \dots, d_k)$.

The difficulty is that y_k changes in every component as k grows, so $x_k = V_k y_k$ cannot be accumulated. Setting

$$p_k \triangleq L_k^\mathsf{T} y_k, \qquad C_k \triangleq V_k L_k^{-\mathsf{T}} = [c_1, \dots, c_k], \tag{10}$$

equation (8) becomes $L_k D_k p_k = \beta_1 e_1$, and $x_k = V_k y_k = C_k p_k$. Both factors are now triangular, which freezes earlier components: reading $C_k L_k^\mathsf{T} = V_k$ column-wise and row j of $L_k D_k p_k = \beta_1 e_1$,

$$c_j = v_j - \mu_{j-1} c_{j-1}, \qquad \mu_0 \equiv 0, \tag{11}$$

$$p_j = \big(v_j^\mathsf{T} b - \mu_{j-1} d_{j-1} p_{j-1}\big)/d_j, \tag{12}$$

$$x_j^c = x_{j-1}^c + p_j c_j. \tag{13}$$

The numerator of (12) is written $v_j^\mathsf{T} b$ rather than $\beta_1 (e_1)_j$. The two agree exactly: $v_1^\mathsf{T} b = \beta_1$, and $v_j^\mathsf{T} b = \beta_1 v_j^\mathsf{T} v_1 = 0$ for $j \geq 2$.

Here c_j is the search direction and p_j the step length; (11)–(13) are conjugate gradient.

5 SYMMLQ

notebook p. 7–21

Cholesky requires definiteness. Replacing it by an orthogonal factorisation removes that requirement, and this is the content of SYMMLQ.

5.1 The LQ factorisation

notebook p. 7–8

Write $T_k = \bar{L}_k Q_k$ with $Q_k Q_k^\mathsf{T} = I$ and $\bar{L}_k$ lower triangular, Q_k^T being a product of plane transformations $Q_{1,2} \cdots Q_{k-1,k}$, so that $T_k Q_k^\mathsf{T} = \bar{L}_k$. Define

$$\bar{W}_k \triangleq V_k Q_k^\mathsf{T} = [w_1, \dots, w_{k-1}, \bar{w}_k], \qquad \bar{z}_k \triangleq Q_k y_k. \tag{14}$$

Then (8) becomes $\bar{L}_k \bar{z}_k = \beta_1 e_1$ with $x_k^c = \bar{W}_k \bar{z}_k$. The matrix $\bar{L}_k$ has the banded form

$$\bar{L}_k = \begin{pmatrix} \gamma_1 & & & & \\ \delta_2 & \gamma_2 & & & \\ \varepsilon_3 & \delta_3 & \gamma_3 & & \\ & \ddots & \ddots & \ddots & \\ & & \varepsilon_k & \delta_k & \bar{\gamma}_k \end{pmatrix}, \tag{15}$$

the final diagonal entry being barred because the next transformation has not yet fixed it. L_k denotes $\bar{L}_k$ with $\bar{\gamma}_k$ replaced by γ_k.

The transformation is a reflection, not a rotation. The notebook uses

$$Q_{i,i+1} \text{ acting through } \begin{pmatrix} c & s \\ s & -c \end{pmatrix}, \qquad c^2 + s^2 = 1,$$

whose determinant is $-(c^2+s^2) = -1$. Paige and Saunders call it a rotation; the notebook observes, correctly, that it is not one — a proper Givens rotation is $\left(\begin{smallmatrix} c & s \\ -s & c \end{smallmatrix}\right)$. The distinction is not cosmetic. This matrix is *symmetric and involutary*, and §5.6 and §6.5 both rely on inverting a relation by re-applying it, which a genuine rotation would not permit.

5.2 The recurrences

notebook p. 9–12

Applying the transformations and matching entries gives, for $k \geq 2$,

$$\boxed{\begin{aligned} \varepsilon_k &= \beta_k s_{k-2}, \\ \delta_k &= -\beta_k c_{k-2} c_{k-1} + \alpha_k s_{k-1}, \\ \bar{\gamma}_k &= -\beta_k c_{k-2} s_{k-1} - \alpha_k c_{k-1}, \end{aligned}} \tag{16}$$

with $\bar{\gamma}_1 = \alpha_1$, and then

$$\gamma_k = \left(\bar{\gamma}_k^2 + \beta_{k+1}^2\right)^{1/2}, \qquad c_k = \frac{\bar{\gamma}_k}{\gamma_k}, \qquad s_k = \frac{\beta_{k+1}}{\gamma_k}. \tag{17}$$

Erratum (notebook p. 12)

The manuscript initialises (16) with $c_0 = s_0 = 1$. **This is wrong**, and contradicts the $k = 2$ entries derived four pages earlier:

	with $c_0 = s_0 = 1$	required (p. 9)
ε_2	β_2	absent
δ_2	$-\beta_2 c_1 + \alpha_2 s_1$	$+\beta_2 c_1 + \alpha_2 s_1$
$\bar{\gamma}_2$	$-\beta_2 s_1 - \alpha_2 c_1$	$+\beta_2 s_1 - \alpha_2 c_1$

The correct convention is $c_0 = -1,\ s_0 = 0$, which reproduces all three and satisfies $c_0^2 + s_0^2 = 1$. It is consistent with the reflection form, which at $c = -1$, $s = 0$ is $\operatorname{diag}(-1, 1)$.

This is the one error in the manuscript that would break an implementation coded from the page. Verified numerically in §7: the recurrences reproduce $T_k Q_k^{\mathsf{T}}$ to 7×10^{-15} with $c_0 = -1$, $s_0 = 0$, and to a relative error of order 10^1 as written. Only the initialisation is affected — every $k \geq 3$ avoids the index-zero terms.

5.3 Accumulating the iterate

notebook p. 13–16

Because L_k and $\bar{L}_k$ differ only in the (k, k) entry, $L_k z_k = \bar{L}_k \bar{z}_k$ forces $\bar{\gamma}_k \bar{\zeta}_k = \gamma_k \zeta_k$, so

$$\zeta_k = c_k \bar{\zeta}_k. \tag{18}$$

The basis vectors satisfy, with $\bar{w}_1 = v_1$,

$$\begin{bmatrix} \bar{w}_k & v_{k+1} \end{bmatrix} \begin{pmatrix} c_k & s_k \\ s_k & -c_k \end{pmatrix} = \begin{bmatrix} w_k & \bar{w}_{k+1} \end{bmatrix}, \tag{19}$$

that is $w_k = c_k \bar{w}_k + s_k v_{k+1}$ and $\bar{w}_{k+1} = s_k \bar{w}_k - c_k v_{k+1}$. Row k of $L_k z_k = \beta_1 e_1$ gives ζ_k, and the iterate accumulates:

$$\varepsilon_k \zeta_{k-2} + \delta_k \zeta_{k-1} + \gamma_k \zeta_k = \beta_1 (e_1)_k, \qquad x_k^L = x_{k-1}^L + \zeta_k w_k. \tag{20}$$

Since $\bar{W}_{k+1} = [W_k \ \ \bar{w}_{k+1}]$ and $\bar{z}_{k+1} = (z_k^{\mathsf{T}}, \bar{\zeta}_{k+1})^{\mathsf{T}}$, the conjugate gradient iterate is recoverable at no extra cost:

$$x_k^c = x_{k-1}^L + \bar{\zeta}_k \bar{w}_k. \tag{21}$$

5.4 L_k is nonsingular

notebook p. 17

Proposition 1. *L_k is nonsingular at every step.*

Proof. L_k is lower triangular with diagonal $\gamma_1, \dots, \gamma_k$, so it is singular only if some $\gamma_k = 0$. By (17), $\gamma_k^2 = \bar{\gamma}_k^2 + \beta_{k+1}^2$.

If $\beta_{k+1} \neq 0$ then $\gamma_k \geq |\beta_{k+1}| > 0$ immediately — *regardless of $\bar{\gamma}_k$*.

If $\beta_{k+1} = 0$ the Lanczos process has terminated, $AV_k = V_k T_k$, and range(V_k) is A-invariant. Suppose $T_k z = 0$ for some $z \neq 0$. Then $AV_k z = V_k T_k z = 0$, while $V_k z \neq 0$ because V_k has orthonormal columns; so A is singular, contrary to assumption. Hence T_k is nonsingular, and $L_k = T_k Q_k^{\mathsf{T}}$ is a product of nonsingular matrices. □

The first branch deserves emphasis, because the manuscript compresses it to the point of invisibility and it is the strongest statement on the page:

> *For $\beta_{k+1} \neq 0$, L_k is nonsingular* even when $\bar{\gamma}_k = 0$ *— that is, even when $\bar{L}_k$ is singular and T_k may be. This is precisely why SYMMLQ survives indefinite systems on which conjugate gradient breaks down.*

Erratum (notebook p. 17)

The manuscript reaches Proposition 1 by two invalid arguments.

(i) "A, V_k and V_k^{T} all have non-zero diagonal elements $\Rightarrow T_k$ has non-zero diagonal elements, i.e. it is nonsingular." Non-zero diagonal entries do not imply nonsingularity — $\left(\begin{smallmatrix}1&1\\1&1\end{smallmatrix}\right)$ — and an indefinite symmetric A need not have a non-zero diagonal at all ($\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right)$). The premise is worse than false: V_k is $n \times k$, so it has neither a diagonal nor a notion of singularity, as the notebook's own margin note insists.

(ii) "Q_k^{T} is nonsingular because it is built from matrices $Q_{i,i+1}$ which have no zero diagonal elements." The premise is false: the diagonal entries of $Q_{i,i+1}$ are c_i and $-c_i$, both zero when $c_i = 0$ — the near-breakdown case of interest. The correct reason is that Q_k^{T} is a product of orthogonal matrices, so $\det Q_k^{\mathsf{T}} = \pm 1$.

(iii) The manuscript writes $L_k = \bar{L}_k = Q_k T_k$; page 8 established $\bar{L}_k = T_k Q_k^{\mathsf{T}}$. Factors reversed and Q untransposed.

> The closing observation of the page is correct and worth keeping. At termination $\beta_{k+1} = 0$ gives $s_k = 0$ and $c_k = 1$, so (18) and (19) yield $\zeta_k = \bar{\zeta}_k$ and $w_k = \bar{w}_k$: the barred and unbarred quantities coincide and $x_k^L = x_k^c$. SYMMLQ and conjugate gradient agree exactly when the Krylov space closes.

5.5 Residuals

notebook p. 18–20

Using (6), (8) and $V_k e_1 = v_1$, the conjugate gradient residual telescopes to $r_k^c = -\beta_{k+1} v_{k+1} \eta_{kk}$, where η_{kk} is the last component of y_k. Comparing the k-th entries of $\bar{L}_k^{\mathsf{T}} y_k = \beta_1 Q_k e_1$ gives $\bar{\gamma}_k \eta_{kk} = \beta_1 s_1 \cdots s_{k-1}$, and since $s_k / c_k = \beta_{k+1} / \bar{\gamma}_k$,

$$\boxed{r_k^c = -\Big(\beta_1 s_1 s_2 \cdots s_k / c_k\Big) v_{k+1}} \tag{22}$$

so that $\|r_k^c\| = \beta_1 |s_1 \cdots s_k| / |c_k|$. *The factor $1/c_k$ is the conjugate gradient breakdown*: it diverges as $c_k \to 0$, i.e. as $\bar{\gamma}_k \to 0$.

Gap closed (notebook p. 20)

The manuscript states, without proof — "*I presume this could be sought by a little induction*" — that

$$r_k^L = \gamma_{k+1}\zeta_{k+1}v_{k+1} - \varepsilon_{k+2}\zeta_k v_{k+2}. \tag{23}$$

It is correct. Write $W_k = V_{k+1}Q_{k+1}^\mathsf{T}E$ with E the first k columns of I_{k+1}. From (9),

$$AW_k = V_kL_k + v_{k+1}\big(\varepsilon_{k+1}e_{k-1}^\mathsf{T} + \delta_{k+1}e_k^\mathsf{T}\big) + \beta_{k+2}v_{k+2}\,e_{k+1}^\mathsf{T}Q_{k+1}^\mathsf{T}E.$$

Then: $L_kz_k = \beta_1e_1$ cancels $\beta_1v_1 - V_kL_kz_k$; row $k+1$ of $L_{k+1}z_{k+1} = \beta_1e_1$ reads $\varepsilon_{k+1}\zeta_{k-1} + \delta_{k+1}\zeta_k + \gamma_{k+1}\zeta_{k+1} = 0$, giving the coefficient $+\gamma_{k+1}\zeta_{k+1}$ on v_{k+1}; and the last row of $Q_{k+1}^\mathsf{T} = Q_{1,2}\cdots Q_{k,k+1}$ is $[0,\ldots,0,s_k,-c_k]$, so E leaves only $s_k\zeta_k$, with $\varepsilon_{k+2} = \beta_{k+2}s_k$ by (16). Orthonormality then gives $\|r_k^L\|^2 = \gamma_{k+1}^2\zeta_{k+1}^2 + \varepsilon_{k+2}^2\zeta_k^2$.

The author's remark that the generalised ε_i gave "a head start" is exactly right: it is the step that closes the argument.

5.6 SYMMLQ against conjugate gradient

notebook p. 21

Subtracting (20) from (21) and using $\bar\zeta_k = \zeta_k/c_k$,

$$x_k^c = x_k^L + \zeta_k\Big(\bar w_k/c_k - w_k\Big).$$

Because the reflection in (19) is involutary, that relation inverts without modification to give $\bar w_k = c_kw_k + s_k\bar w_{k+1}$, whence

$$\boxed{x_k^c = x_k^L + \Big(\frac{\zeta_ks_k}{c_k}\Big)\bar w_{k+1}} \tag{24}$$

Proposition 2. *$\|x_k^c\| \geq \|x_k^L\|$ at every step.*

Proof. The columns of $\bar W_{k+1} = V_{k+1}Q_{k+1}^\mathsf{T} = [W_k\ \ \bar w_{k+1}]$ are orthonormal, being an orthogonal transformation of orthonormal columns. Hence $\bar w_{k+1} \perp w_j$ for all $j \leq k$, and $x_k^L = W_kz_k$ lies in $\operatorname{span}\{w_1,\ldots,w_k\}$, so $\bar w_{k+1} \perp x_k^L$. By Pythagoras and $\|\bar w_{k+1}\| = 1$,

$$\|x_k^c\|^2 = \|x_k^L\|^2 + \Big(\frac{\zeta_ks_k}{c_k}\Big)^2 \ \geq\ \|x_k^L\|^2. \qquad \square$$

Erratum (notebook p. 21)

The manuscript deduces the proposition from the assertion that the coefficient in (24) "*is never negative*". This fails twice.

(i) The coefficient can be negative. $s_k = \beta_{k+1}/\gamma_k \geq 0$, but $c_k = \bar\gamma_k/\gamma_k$ and $\bar\gamma_k$ is sign-indefinite by (16) — as it must be when A is indefinite — and ζ_k likewise.

(ii) Non-negativity would not suffice in any case: $x = y + \lambda w$ with $\lambda \geq 0$ does not imply $\|x\| \geq \|y\|$. Take $y = (1,0)$, $w = (-1,0)$, $\lambda = 1$.

The orthogonality argument above repairs this, and is shorter. Note that it turns on the *square* of the coefficient, which is why the sign question is irrelevant — and that it uses $\|\bar w_{k+1}\| = 1$, which the manuscript itself invokes on its final page.

6 MINRES

notebook p. 22–30

6.1 The normal equations

notebook p. 22–24

Take $B = I$. Transposing (6) and using $A^{\mathsf{T}} = A$, $T_k^{\mathsf{T}} = T_k$,

$$V_k^{\mathsf{T}} A = T_k V_k^{\mathsf{T}} + \beta_{k+1} e_k v_{k+1}^{\mathsf{T}},$$

and multiplying out, all cross terms vanishing by orthonormality,

$$V_k^{\mathsf{T}} A^2 V_k = T_k^2 + \beta_{k+1}^2 e_k e_k^{\mathsf{T}} \quad (= \bar{T}_{k+1}^{\mathsf{T}} \bar{T}_{k+1}). \tag{25}$$

Similarly $V_k^{\mathsf{T}} Ab = \beta_1 T_k e_1$. Now $T_k^2 = T_k T_k^{\mathsf{T}} = \bar{L}_k Q_k Q_k^{\mathsf{T}} \bar{L}_k^{\mathsf{T}} = \bar{L}_k \bar{L}_k^{\mathsf{T}}$, and $\beta_{k+1}^2 = \gamma_k^2 - \bar{\gamma}_k^2$. Since $\bar{L}_k$ and L_k differ only in the (k,k) entry — and, $\bar{L}_k$ being lower triangular, that entry occurs only in row k — the rank-one correction converts one into the other:

$$\boxed{V_k^{\mathsf{T}} A^2 V_k = L_k L_k^{\mathsf{T}}} \tag{26}$$

So (4) reads $L_k L_k^{\mathsf{T}} u_k = \beta_1 T_k e_1 = \beta_1 \bar{L}_k Q_k e_1$. Writing $\bar{L}_k = L_k D_k$ with $D_k = \operatorname{diag}(1, \ldots, 1, c_k)$ — valid because column k of the triangular L_k contains only γ_k — this becomes

$$L_k^{\mathsf{T}} u_k = \beta_1 D_k Q_k e_1 \;\triangleq\; t_k = (\tau_1, \ldots, \tau_k)^{\mathsf{T}}. \tag{27}$$

6.2 The recurrences

notebook p. 25–26

Evaluating (27),

$$\tau_1 = \beta_1 c_1, \qquad \tau_i = \beta_1 s_1 s_2 \cdots s_{i-1} c_i \quad (i \geq 2), \tag{28}$$

which depends only on i — so t_k extends by one entry per step without disturbing its predecessors. Setting $M_k \triangleq V_k L_k^{-\mathsf{T}} = [m_1, \ldots, m_k]$ gives $x_k^M = V_k u_k = M_k t_k$, and reading $M_k L_k^{\mathsf{T}} = V_k$ column-wise,

$$\boxed{\begin{aligned} &m_k = (v_k - \delta_k m_{k-1} - \varepsilon_k m_{k-2})/\gamma_k, \qquad m_0 = m_{-1} = 0, && (29)\\ &x_k^M = x_{k-1}^M + \tau_k m_k. && (30) \end{aligned}}$$

M_k likewise extends without disturbance, the leading block of an upper-triangular inverse being the inverse of the leading block.

Gap closed (notebook p. 26)

Against (29) the manuscript records: "*I recommend verifying this progression formulation before implementing it!*" It is correct, as a column-by-column expansion of $M_k L_k^{\mathsf{T}} = V_k$ confirms, and as §7 confirms numerically. The recommendation is nonetheless sound practice; the three-term form of (29), against the two-term (11) of conjugate gradient, is exactly the extra superdiagonal that the orthogonal factorisation fills in where Cholesky did not.

6.3 $AM_k = W_k$

notebook p. 29

Lemma 3. *$AM_k = W_k$ for every k.*

Proof. By (9), $AM_k = AV_kL_k^{-\mathsf{T}} = V_{k+1}\bar{T}_{k+1}L_k^{-\mathsf{T}}$. The transformations that lower-triangularise T_k also furnish a QR factorisation of the rectangular $\bar{T}_{k+1}$, with L_k^{T} as triangular factor:

$$\bar{T}_{k+1} = Q_{k+1}^{\mathsf{T}} E\, L_k^{\mathsf{T}}, \tag{31}$$

E being the first k columns of I_{k+1}. Hence $AM_k = V_{k+1}Q_{k+1}^{\mathsf{T}}E = W_k$. □

Identity (31) at $k = 2$ makes the mechanism visible; the off-diagonal entries recover $\bar{T}_3$ only through $c_1^2 + s_1^2 = 1$:

$$c_1\delta_2 + s_1c_2\gamma_2 = c_1(\beta_2c_1 + \alpha_2s_1) + s_1(\beta_2s_1 - \alpha_2c_1) = \beta_2,$$

$$s_1\delta_2 - c_1c_2\gamma_2 = s_1(\beta_2c_1 + \alpha_2s_1) - c_1(\beta_2s_1 - \alpha_2c_1) = \alpha_2.$$

Erratum (notebook p. 29)

This is the most serious gap in the manuscript, and it has two parts.

(i) The page writes $AV_mV_m^{-1} = A = V_mT_mV_m^{-1}$. V_m **has no inverse**: it is $n \times m$, invertible only if $m = n$, and Lanczos terminating at $m < n$ is the ordinary case, not a pathology. The step is also unnecessary — $AV_m = V_mT_m$ gives $AM_m = V_mT_mL_m^{-\mathsf{T}} = V_mQ_m^{\mathsf{T}} = W_m$ directly.

(ii) More seriously, the page establishes $AM = W$ *only at termination* — the whole argument assumes $\beta_{m+1} = 0$, which is what licenses $\bar{L}_m = L_m$ — and then applies $Am_k = w_k$ at arbitrary k two lines later. For $k < m$ the derivation given does not hold, since $T_k = \bar{L}_kQ_k$ with $\bar{L}_k \neq L_k$, so $T_kL_k^{-\mathsf{T}} \neq Q_k^{\mathsf{T}}$. Lemma 3 supplies the general statement, by routing through the rectangular $\bar{T}_{k+1}$ rather than the square T_m. With it in place the conclusion of the page stands unaltered.

6.4 MINRES against conjugate gradient

notebook p. 27–28

Manipulating (27) through $\bar{L}_k = L_kD_k$ gives $x_k^c = M_kD_k^{-2}t_k$, which differs from $x_k^M = M_kt_k$ in its last coefficient alone. Since $c_k^{-2} - 1 = s_k^2/c_k^2$,

$$x_k^c = x_k^M + \tau_km_k\left(\frac{s_k}{c_k}\right)^2, \tag{32}$$

and therefore, by Lemma 3,

$$r_k^M = r_k^c + \tau_k\left(\frac{s_k}{c_k}\right)^2 w_k. \tag{33}$$

Compare (24) with (32). Each expresses the conjugate gradient iterate as the stable method's iterate plus a correction carrying a power of $1/c_k$ — the same story told twice, once for SYMMLQ and once for MINRES.

6.5 Monotonicity of the residual

notebook p. 30

Proposition 4. $r_k^M = \beta_1 s_1 s_2 \cdots s_k \, \bar{w}_{k+1}$, *and consequently* $\|r_k^M\|$ *is non-increasing in* k.

Proof. By (28), $\tau_k s_k^2/c_k^2 = (\beta_1 s_1 \cdots s_k)(s_k/c_k)$, so combining (33) with (22),

$$r_k^M = \frac{\beta_1 s_1 \cdots s_k}{c_k}\big(s_k w_k - v_{k+1}\big).$$

The reflection (19) is involutary, so it inverts to give $v_{k+1} = s_k w_k - c_k \bar{w}_{k+1}$, whence $s_k w_k - v_{k+1} = c_k \bar{w}_{k+1}$ and

$$r_k^M = \beta_1 s_1 s_2 \cdots s_k \, \bar{w}_{k+1}.$$

With $\|\bar{w}_{k+1}\| = 1$ and $0 \le s_i \le 1$, the norm $\beta_1 \prod_{i \le k} s_i$ is non-increasing. □

The c_k cancels. The factor that made $\|r_k^c\|$ diverge in (22) is absent here, and that cancellation is what the thirty pages are built toward.

An immediate corollary the manuscript does not state. Comparing norms in (22) and the proposition,

$$\|r_k^M\| = |c_k| \cdot \|r_k^c\| \;\le\; \|r_k^c\|.$$

The MINRES residual is never larger than the conjugate gradient residual — as it must not be, MINRES being *defined* by minimising it. That the derivation closes on a statement it was obliged to produce is good evidence that it hangs together.

7 Numerical verification

The recurrences above — (5), (16), (17), (11)–(13), (18)–(20), (28)–(30) — were implemented exactly as the notebook gives them, with no textbook forms substituted, and run on a symmetric positive definite and a symmetric *indefinite* system, each 60×60, the latter with eigenvalues straddling zero. Script: `verify/verify_1996.py`; the full working notes are in `ALGEBRA_CHECK.md`.

Check	**Source**	**SPD**	**Indefinite**
LQ recurrences vs. $T_k Q_k^\top$, $c_0 = -1$, $s_0 = 0$	(16)	7e−15	2e−15
same, with the manuscript's $c_0 = s_0 = 1$		*2e+01*	*2e+01*
Conjugate gradient, final relative error	(13)	2.6e−15	1.1e−14
SYMMLQ, final relative error	(20)	2.0e−15	2.0e−15
MINRES, final relative error	(30)	2.1e−15	2.1e−15
$r_k^M = \beta_1 s_1 \cdots s_k \bar{w}_{k+1}$	§6.5	1.4e−14	8.6e−15
$\|r_k^M\| = \|c_k\|\|r_k^c\|$	§6.5	2.3e−15	8.8e−14
r_k^L closed form	(23)	1.3e−14	8.6e−15
$\|x_k^c\| \ge \|x_k^L\|$	§5.6	holds	holds
$\|r_k^M\|$ non-increasing	§6.5	†	holds

† Two apparent violations in the definite case, both at $\|r\| \approx 1.1 \times 10^{-14}$ against a floor of $\varepsilon\|A\|\|x\| \approx 9.7 \times 10^{-15}$, with ratios 1.03 and 1.004. This is round-off, not a failure of the proposition.

The Lanczos step in the verification uses full reorthogonalisation. This is *not* a correction to the notebook and is not part of any derivation above: it isolates the algebra from the well-known loss of orthogonality of the Lanczos process in finite precision. Without it, conjugate gradient drifts to a relative error of 2.7×10^{-2} on a matrix of condition number 40 — a property of the basis generation, not of (11)–(13).

8 Errata, collected

p.	Locus	Issue	Status
11	(**), line 2	$\bar{\gamma}_2 s_2 - \beta_3 c_3 = 0$ should read $\beta_3 c_2$	typo; self-corrected lower on the same page
12	initialisation of (16)	"$c_0 = s_0 = 1$" should read $c_0 = -1$, $s_0 = 0$	**would break an implementation**
17	nonsingularity of L_k	non-zero diagonal $\Rightarrow$ nonsingular; Q nonsingular "because no zero diagonal"; $Q_k T_k$ for $T_k Q_k^\top$	conclusion correct, arguments invalid
18	below $(*)$	"multiplying both sides by y_k" describes a substitution followed by premultiplication	wording only
21	$\|x^c\| \geq \|x^L\|$	"this term is never negative" is false, and would not suffice	conclusion correct, proof replaced
28	$c_k^{-2} - 1$	five lines for $\sec^2\theta - 1 = \tan^2\theta$	valid, merely long
29	$AM = W$	V_m^{-1} does not exist; result proved at termination but used at general k	**conclusion correct, proof replaced**

Every error is one of justification, never of destination. In each case the result asserted is correct and the argument offered for it is not — a consistently better failure mode than its converse, and the one that formal training exists to remedy.

9 The original pages

The thirty pages that follow are reproduced exactly as written — worked by hand, with reference texts, over several months of evenings during the first year of doctoral study, from the source paper:

> C. C. Paige and M. A. Saunders, *Solution of Sparse Indefinite Systems of Linear Equations*, SIAM Journal on Numerical Analysis **12**(4), 617–629, 1975.

No internet. Nothing has been transcribed, corrected or reordered, and the errors recorded in §8 are left standing where they fall.

Notebook pages	Content	Above at
1–2	The minimisation framework	§2
3–4	Lanczos vectors	§3
5–6	Conjugate gradient	§4
7–21	SYMMLQ	§5
22–30	MINRES	§6

Conjugate gradient predates the source paper — Hestenes and Stiefel, 1952 — and is derived here as the foundation the other two are built on. Two loose sheets tucked between pages 2–3 and 25–26 carry supplementary notes; they are reproduced in sequence at those points.

Photographed and assembled 2026. The mathematics is the author's.

The following pages contain derivations of the algorithms developed in a paper, "SOLUTION of SPARSE INDEFINITE SYSTEMS of LINEAR EQUATIONS" by C.C. Paige & M.A. Saunders (SIAM J. Numer. Anal. Vol 12 No.4, 1975)

Introduction / Background mathematics

We seek to solve $Ax = b$ (ideally)

$A =$ real, symmetric, large, sparse, & square

Realistically it's difficult to solve the above equation exactly. Usually,

$$r + Ax = b, \qquad Ar = 0$$

Finding solutions $x_k \triangleq V_k y_k$ (where $V_k = [v_1, v_2, \cdots v_k]$) that will minimise r_k is achieved by acquiring x_k that give stationary values to the B-norm of vector r_k given by

$$f_k(y) \equiv (AV_k y - b)^T B (AV_k y - b) \qquad B \text{ is +ve, definite}$$

That is, we want x_k that satisfy $\frac{d f(y)}{dy} = 0$.

$\frac{df(y)}{dy}$ is found firstly by expanding $f_k(y)$

$$f_k(y) = \cancel{AV_k^T y B}\ (AV_k y - b)^T B (AV_k y - b)$$

$$= (y^T V_k^T AB - b^T B)(AV_k y - b) \qquad A \text{ symmetric ie } A \equiv A^T$$

$$= y^T V_k^T A B A V_k y - y^T V_k^T A B b - b^T B A V_k y - b^T B b$$

$$\frac{df}{dy} = \left(u \frac{dv}{dy} + \frac{du}{dy} v\right) - \left(\bar{u} \frac{d\bar{v}}{dy} + \frac{d\bar{u}}{dy} \bar{v}\right) - b^T B A V_k$$

$$= \left(u \frac{dv}{dy} + v^T \frac{du^T}{dy}\right) - \left(\bar{u} \frac{d\bar{v}}{dy} + \bar{v}^T \frac{d\bar{u}^T}{dy}\right) - b^T B A V_k$$

(recall that dot products are conserved under transpose, $b^T a = a^T b$)

$$\therefore \frac{df}{dy} = \left(u\frac{dv}{dy} + v^T\frac{du^T}{dy}\right) - \left(\bar{u}\frac{d\bar{v}}{dy} + \bar{v}^T\frac{d\bar{u}^T}{dy}\right) - b^TBAV_k$$

$$= y^TV_k^TABAV_k + y^TV_k^TABAV_k - \left(y^T.0 + b^TBAV_k\right) - b^TBAV_k$$

$$= 2y^TV_k^TABAV_k - \cancel{2y^T}\, 2b^TBAV_k$$

but we want the conditions for when $\frac{df}{dy} = 0$

ie $\quad \cancel{2}y^TV_k^TABAV_k = \cancel{2}b^TBAV_k$

$$(y^TV_k^TABAV_k)^T = (b^TBAV_k)^T$$

$$\boxed{V_k^TABAV_ky_k = V_k^TAB\,b}$$

$$\Rightarrow \quad V_k^TAB\left(b - AV_ky_k\right) = 0 \qquad V_ky_k \triangleq x_k$$

or $\quad V_k^TABr_k = 0 \qquad$ where $r_k = b - AV_ky_k = b - Ax_k$

The positive definite matrix B isn't explicitly required; we are free to choose its form.

Paige & Saunders restrict their analysis to cases where $B = A^m$ where m is some integer. They consider $m = 0, -1$ to be the most computationally viable.

case 1a) $m = -1 \Rightarrow B = A^{-1}$

$$\therefore V_k^TAV_ky_k = V_k^Tb \qquad x_k = V_ky_k\,, \quad V_k^Tr = 0$$

this formulation will be used for: the (standard) conjugate gradient method, CGM, that is the method utilising the Cholesky factorisation; Paige & Saunders variation of the CGM using an orthogonal LQ factorisation; & the SYMMLQ procedure, again requiring an LQ factorisation.

A note on Lanczos:

For A n rows × n columns

V_k is $n \times k$ (k is iteration #) V_k aint necessarily square !!

a vector $\underset{(n\times 1)}{v_k}$ is produced for every iteration

case (b) $m = 0 \Rightarrow B = A^0 = I$

$$V_k^T A^2 V_k u_k = V_k^T A b$$

This formulation will lead u[...]
the residual norm $\|r_k\|$, MINRE[...]

LANCZOS VECTORS

Vectors $v_1 \cdots v_k$ are obtai[...]
best choice of the initial [...]
is

$$v_1 = b/\beta_1 \qquad \beta_1 \triangleq \|$$

Adopting the notation of Saad's
(6.19 on p 184)

$$v_{j+1} = w_j/\beta_{j+1}$$

$$\beta_{j+1} v_{j+1} = w_j = \bar{w}_j$$

$$\text{but } \bar{w}_j = Av_j - \beta_j$$

So, $\beta_{j+1} v_{j+1} = Av_j - \beta$

The best way to place [...]
induction (a tool f.M u[...]
algorithms. Define $v_0 \equiv$ [...]

$$A v_1 = \underbrace{\cancel{\beta v_0}}_{=0} + \alpha_1 v_1 + \beta$$
$$A v_2 = \beta_2 v_1 + \alpha$$
$$A v_3 = \beta$$
$$A v_4 =$$

case (b) $m = 0 \Rightarrow B = A^0 = I$

$$V_k^T A^2 V_k u_k = V_k^T A b \qquad x_k = V_k u_k$$

This formulation will lead us to a method that progressively minimises the residual norm $\|r_k\|$, MINRES.

LANCZOS VECTORS

Vectors $v_1 \cdots v_k$ are obtained by the Lanczos algorithm. The best choice of the initial vector according to Paige & Saunders is

$$v_1 = b/\beta_1 \qquad \beta_1 \triangleq \|b\|$$

Adopting the notation of Saad's formulation of the Lanczos algorithm (6.19 on p 184)

$$v_{j+1} = w_j/\beta_{j+1}$$

$$\beta_{j+1} v_{j+1} = w_j = \bar{w}_j - \alpha_j v_j$$

but $\bar{w}_j = A v_j - \beta_j v_{j-1}$

So, $\beta_{j+1} v_{j+1} = A v_j - \beta_j v_{j-1} - \alpha_j v_j$ where $\alpha_j = v_j^T A v_j$

The best way to place this into matrix notation is to use induction (a tool I'll use frequently during the derivation of these algorithms. Define $v_0 \equiv 0$ & consider the $k=4$ example

$$\begin{aligned}
A v_1 &= \overset{=0}{\cancel{\beta_1 v_0}} + \alpha_1 v_1 + \beta_2 v_2 \\
A v_2 &= \beta_2 v_1 + \alpha_2 v_2 + \beta_3 v_3 \\
A v_3 &= \beta_3 v_2 + \alpha_3 v_3 + \beta_4 v_4 \\
A v_4 &= \beta_4 v_3 + \alpha_4 v_4 + \beta_5 v_5
\end{aligned}$$

ie $A[v_1\ v_2\ v_3\ v_4] = [v_1\ v_2\ v_3\ v_4]\begin{bmatrix}\alpha_1 & \beta_2 & 0 & 0\\ \beta_2 & \alpha_2 & \beta_3 & 0\\ 0 & \beta_3 & \alpha_3 & \beta_4\\ 0 & 0 & \beta_4 & \alpha_4\end{bmatrix} + v_5\begin{pmatrix}0\\0\\0\\\beta_5\end{pmatrix}^T$

since $[Av_1, Av_2, Av_3, Av_4] = [\alpha_1 v_1 + \beta_2 v_2,\ \beta_2 v_1 + \alpha_2 v_2 + \beta_3 v_3,\ \beta_3 v_2 + \alpha_3 v_3 + \beta_4 v_4,\ \beta_4 v_3 + \alpha_4 v_4 + \beta_5 v_5]$

corresponding 'elements' give the 4 explicit equations from last page

$\Rightarrow \quad AV_4 = V_4 T_4 + \beta_5 v_5 e_4^T$

In general, $\boxed{AV_k = V_k T_k + \beta_{k+1} v_{k+1} e_k^T}$

tridiagonal $T_k = \begin{bmatrix}\alpha_1 & \beta_2 & & \\ \beta_2 & \alpha_2 & \beta_3 & \\ & \ddots & \ddots & \ddots \\ & & \beta_k & \alpha_k\end{bmatrix}$

Since vectors v_k are built from an orthonormal Krylov sequence

$$V_k^T V_k = I = [e_1 \cdots e_k] \quad \& \quad V_k^T v_{k+1} = 0$$

With these two equalities in mind, multiplying both sides of the above boxed eq. yields

$$V_k^T A V_k = \overbrace{\cancel{V_k^T V_k}}^{I} T_k + \beta_{k+1} \cancel{V_k^T v_{k+1}} e_k^T$$

$$\boxed{V_k^T A V_k = T_k}$$

then case (a), $V_k^T A V_k \underline{y_k} = V_k^T b$ becomes $T_k y_k = \beta_1 V_k^T v_1$
(recall $v_1 \equiv b/\beta_1$),

$$\therefore \quad \boxed{T_k y_k = \beta_1 e_1 \quad x_k^c = V_k y_k}$$

x_k^c is the solution obtainable with the (standard) CGM.

CONJUGATE GRADIENT METHOD

see Golub / van Loan pp 494 → 497

If A is +ve definite, so too is $T_k = V_k^T A V_k$, which means $\exists$ a Cholesky factorisation,

$$T_k = L_k D_k L_k^T \qquad \text{(see B\&F pp 376} \to \text{379)}$$

$$L_k = \begin{bmatrix} 1 & \cdots & 0 \\ \mu_1 & 1 & \vdots \\ \vdots & \ddots & \ddots \\ 0 & \cdots \ \mu_{k-1} & 1 \end{bmatrix} \qquad D_k = \begin{bmatrix} d_1 & & \cdots & 0 \\ & d_2 & & \vdots \\ \vdots & & \ddots & \\ 0 & \cdots & & d_k \end{bmatrix}$$

lower bidiagonal
diagonal is unit

As k increases, y_k changes its form fully, hence $V_k y_k$ cannot be acquired as k increases. To overcome this, define

$$\underset{(k\times 1)}{p_k} \triangleq L_k^T y_k \quad \& \quad \underset{\cancel{(k\times k)}}{C_k} \triangleq \underset{n\times k \otimes k\times k}{V_k L_k^{-T}} \quad \left\{ = [c_1 \cdots c_k] \right\}$$

→ C_k is $(n\times k)$!!

so, the eq. $\underset{k\times k \otimes k\times 1}{T_k y_k} = \underset{(1\times k)}{\beta_1 e_1}$ becomes

$$L_k D_k L_k^T y_k = \beta_1 e_1$$

or $\boxed{L_k D_k p_k = \beta_1 e_1}$

Similarly $x_k^c = V_k y_k$ becomes

$$x_k^c = V_k L_k^{-T} L_k^T y_k$$

or $\boxed{x_k^c = C_k p_k}$ $\quad (n\times k)\times(k\times 1) = n\times 1$ ✓

By induction I found the columns that compose matrix C_k to be

$$c_j = v_j - \mu_{j-1} c_{j-1} \qquad (\mu_0 \equiv 0)$$

this means matrix C_k can be accumulated with increasing iterations

For efficiency we wish to be able to discard the columns of V_k & C_k after each iteration. This constraint means that we can't explicitly obtain p_k from $L_k D_k p_k = \beta_1 e_1$ & then use $x_k^c = C_k p_k$ (since we've only got the k^{th} column of C_k).

Exploit the fact that vector $p_j = \begin{bmatrix} p_{j-1} \\ P_j \end{bmatrix} = \begin{pmatrix} P_1 \\ P_2 \\ \vdots \\ P_j \end{pmatrix}$

& use $L_k D_k p_k = \beta_1 e_1$ (& induction) to see

$$P_j = \left(v_j^T b - \mu_{j-1} d_{j-1} P_{j-1} \right) / d_j$$

$$x_k = C_k p_k = C_{k-1} p_{k-1} + P_k c_k$$

$$\Rightarrow \quad \boxed{x_k^c = x_{k-1}^c + P_k c_k}$$

where P_j & c_j have been shown

Algorithm :

- Input A, b
- Use Lanczos, tridiagonalise. (T_k, v_k)
- Factorise $T_k = L_k D_k L_k^T$ $(\mu_{k-1}, d_{k-1}, d_k)$
- Calculate P_k, c_k
- find x_k^c & store it
- step
- next

Indefinite symmetric systems - SYMMLQ

For a stable method that won't have the problems that CGM might face when handling indefinite symmetric systems, try an orthogonal factorisation of T_k:

$$T_k = \bar{L}_k Q_k \qquad Q_k^T Q_k = I$$

lower triangular

Define $[w_1, \cdots w_{k-1}, \bar{w}_k] \equiv \bar{W}_k \equiv V_k Q_k^T$

also $\bar{z}_k \equiv (\zeta_1, \cdots, \zeta_{k-1}, \bar{\zeta}_k)^T \equiv Q_k y_k$

The expression $T_k y_k = \beta_1 e_1$ may be written:

$$\bar{L}_k Q_k y_k = \beta_1 e_1$$

$$\Rightarrow \bar{L}_k \bar{z}_k = \beta_1 e_1$$

Similarly, the expression $x_k^c = V_k y_k$ may be written:

$$x_k^c = V_k Q_k^T Q_k y_k = \bar{W}_k \bar{z}_k$$

We then have

$$\boxed{\begin{array}{c} \bar{L}_k \bar{z}_k = \beta_1 e_1 \\ \text{with } x_k^c = \bar{W}_k \bar{z}_k \end{array}}$$

This formulation is not unlike the standard CGM derived earlier. Obviously, the main difference between the two is the factorisation. The method being considered now relies on orthogonal factorisations, which are considerably more stable for dealing with an indefinite T_k. The factorisation being employed can be summarised:

$$T_k Q_{1,2} \cdots Q_{k-1,k} \triangleq T_k Q_k^T = \bar{L}_k = \begin{bmatrix} \gamma_1 & & & & \\ \delta_2 & \gamma_2 & & & \\ \varepsilon_3 & \delta_3 & \gamma_3 & & \\ & \cdot & \cdot & \cdot & \\ & & \varepsilon_k & \delta_k & \bar{\gamma}_k \end{bmatrix}$$

$Q_{i,i+1}$ is an orthonormal matrix differing from the unit matrix only in the elements $q_{i,i}$ & $q_{i,i+1} = q_{i+1,i}$, $q_{i+1,i+1}$

↑ easy to see by induction

This variation on the (standard) CGM is not without its weaknesses. If $\bar{L}_k$ is singular (see note below) then $\bar{z}_k$ is undefined, so a solution x_k^c depending ~~of~~ on $\bar{z}_k$ is impossible to find. All is not lost though - a few modifications can be made to ensure the algorithm is dealing with nonsingular matrices (L_k) ALL the time

Let L_k be $\bar{L}_k$ with $\bar{\gamma}_k$ replaced by γ_k. (We'll now spend considerable time examining the $\bar{L}Q$ factorisation). Noting that the orthogonal matrix Q has the form of a reflection (Paige & Saunders call it a rotation).

$$Q = \begin{bmatrix} 1 & \ddots & & & \cdots & 0 \\ & & q_{ii} & q_{i,i+1} & & \vdots \\ & & q_{i+1,i} & q_{i+1,i+1} & & \\ \vdots & & & & \ddots & \\ 0 & \cdots & & & & 1 \end{bmatrix} = \begin{bmatrix} 1 & \ddots & & & \cdots & 0 \\ & & \cos\theta & \sin\theta & & \vdots \\ & & \sin\theta & -\cos\theta & & \\ \vdots & & & & \ddots & \\ 0 & \cdots & & & & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & \ddots & & & \cdots & 0 \\ & & c & s & & \vdots \\ & & s & -c & & \\ \vdots & & & & \ddots & \\ 0 & \cdots & & & & 1 \end{bmatrix}$$

An $n \times n$ matrix A is nonsingular if $\exists$ an $n \times n$ matrix B s.t. $AB = BA = I_n$. If this is the case, B is said to be the inverse of A. If not, A is singular.

Let's examine the consequences of the relationship $T_k Q_k^T = \bar{L}_k$. Perhaps the best way to do this is to examine the progression of relationships as the dimension of the system increases (ie use induction). We'll use $k = 2, 3, \& 4$ & then generalise for any k

2×2 : $k=2$, $i+1 = k \Rightarrow i=1$

$$\underset{T_{k=2}}{\begin{bmatrix} \alpha_1 & \beta_2 \\ \beta_2 & \alpha_2 \end{bmatrix}} \underset{Q_{12}}{\begin{bmatrix} c_1 & s_1 \\ s_1 & -c_1 \end{bmatrix}} = \begin{bmatrix} \alpha_1 c_1 + \beta_2 s_1 & \alpha_1 s_1 - \beta_2 c_1 \\ \beta_2 c_1 + \alpha_2 s_1 & \beta_2 s_1 - \alpha_2 c_1 \end{bmatrix} \triangleq \underset{\bar{L}_{k=2}}{\begin{bmatrix} \gamma_1 & 0 \\ \delta_2 & \bar{\gamma}_2 \end{bmatrix}}$$

So, we have

$$\begin{aligned} \alpha_1 c_1 + \beta_2 s_1 &= \gamma_1 \\ \alpha_1 s_1 - \beta_2 c_1 &= 0 \\ \beta_2 c_1 + \alpha_2 s_1 &= \delta_2 \\ \beta_2 s_1 - \alpha_2 c_1 &= \bar{\gamma}_2 \end{aligned}$$

We can use these relationships for higher-k systems

3×3 $k=3$

$$\begin{bmatrix} \alpha_1 & \beta_2 & 0 \\ \beta_2 & \alpha_2 & \beta_3 \\ 0 & \beta_3 & \alpha_3 \end{bmatrix} \begin{bmatrix} c_1 & s_1 & 0 \\ s_1 & -c_1 & 0 \\ 0 & 0 & 1 \end{bmatrix} Q_{23} = \bar{L}_{k=3}$$

$$\begin{bmatrix} \cancel{\alpha_1 c_1 + \beta_2 s_1}^{\,\gamma_1} & \cancel{\alpha_1 s_1 - \beta_2 c_1}^{\,0} & 0 \\ \cancel{\beta_2 c_1 + \alpha_2 s_1}^{\,\delta_2} & \cancel{\beta_2 s_1 - \alpha_2 c_1}^{\,\bar{\gamma}_2} & \beta_3 \\ \beta_3 s_1 & -c_1 \beta_3 & \alpha_3 \end{bmatrix} Q_{23} = \bar{L}_{k=3}$$

$$\begin{bmatrix} \gamma_1 & 0 & 0 \\ \delta_2 & \bar{\gamma}_2 & \beta_3 \\ \beta_3 s_1 & -\beta_3 c_1 & \alpha_3 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & c_2 & s_2 \\ 0 & s_2 & -c_2 \end{bmatrix} = \bar{L}_{k=3}$$

$$\begin{bmatrix} \gamma_1 & 0 & 0 \\ \delta_2 & \bar{\gamma}_2 c_2 + \beta_3 s_2 & \bar{\gamma}_2 s_2 - \beta_3 c_2 \\ \beta_3 s_1 & -\beta_3 c_1 c_2 + \alpha_3 s_2 & -\beta_3 c_1 s_2 - \alpha_3 c_2 \end{bmatrix} \triangleq \begin{bmatrix} \gamma_1 & 0 & 0 \\ \delta_2 & \gamma_2 & 0 \\ \varepsilon_3 & \delta_3 & \bar{\gamma}_3 \end{bmatrix}$$

$$T_k Q_{12} Q_{23} = T_k Q_k^T \qquad \bar{L}_{k=3}$$

From the above:

$$\bar{\gamma}_2 c_2 + \beta_3 s_2 = \gamma_2$$
$$\bar{\gamma}_2 s_2 - \beta_3 c_2 = 0$$
$$\beta_3 s_1 = \varepsilon_3$$
$$-\beta_3 c_1 c_2 + \alpha_3 s_2 = \delta_3$$
$$-\beta_3 c_1 s_2 - \alpha_3 c_2 = \bar{\gamma}_3$$

These, in turn, can be used to simplify the 4×4 formulation.

4×4

$$\begin{bmatrix} \alpha_1 & \beta_2 & 0 & 0 \\ \beta_2 & \alpha_2 & \beta_3 & 0 \\ 0 & \beta_3 & \alpha_3 & \beta_4 \\ 0 & 0 & \beta_4 & \alpha_4 \end{bmatrix} \begin{bmatrix} c_1 & s_1 & 0 & 0 \\ s_1 & -c_1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} Q_{23} Q_{34} = \bar{L}_{k=4}$$

$$\begin{bmatrix} \alpha_1 c_1 + \beta_2 s_1 = \gamma_1 & \alpha_1 s_1 - \beta_2 c_1 = 0 & 0 & 0 \\ \beta_2 c_1 + \alpha_2 s_1 = \delta_2 & \beta_2 s_1 - \alpha_2 c_1 = \bar{\gamma}_2 & \beta_3 & 0 \\ s_1 \beta_3 = \varepsilon_3 & -c_1 \beta_3 & \alpha_3 & \beta_4 \\ 0 & 0 & \beta_4 & \alpha_4 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & c_2 & s_2 & 0 \\ 0 & s_2 & -c_2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} Q_{34} = \bar{L}_{k=4}$$

$$\begin{bmatrix} \gamma_1 & 0 & 0 & 0 \\ \delta_2 & c_2 \bar{\gamma}_2 + \beta_3 s_2 = \gamma_2 & s_2 \bar{\gamma}_2 - c_2 \beta_3 = 0 & 0 \\ \varepsilon_3 & -\beta_3 c_1 c_2 + \alpha_3 s_2 = \delta_3 & -s_2 c_1 \beta_3 - \alpha_3 c_2 = \bar{\gamma}_3 & \beta_4 \\ 0 & s_2 \beta_4 & -c_2 \beta_4 & \alpha_4 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & c_3 & s_3 \\ 0 & 0 & s_3 & -c_3 \end{bmatrix} = \bar{L}_{k=4}$$

$$\begin{bmatrix} \gamma_1 & 0 & 0 & 0 \\ \delta_2 & \gamma_2 & 0 & 0 \\ \varepsilon_3 & \delta_3 & c_3 \bar{\gamma}_3 + s_3 \beta_4 & s_3 \bar{\gamma}_3 - c_3 \beta_4 \\ 0 & s_2 \beta_4 & -c_2 c_3 \beta_4 + s_3 \alpha_4 & -c_2 s_3 \beta_4 - c_3 \alpha_4 \end{bmatrix} = \begin{bmatrix} \gamma_1 & 0 & 0 & 0 \\ \delta_2 & \gamma_2 & 0 & 0 \\ \varepsilon_3 & \delta_3 & \gamma_3 & 0 \\ 0 & \varepsilon_4 & \delta_4 & \bar{\gamma}_4 \end{bmatrix}$$

Can clearly obtain another set of relationships!

Now see if we can see any trends from the three systems were investigated:

$$(*)\quad \left.\begin{array}{l} \alpha_1 c_1 + \beta_2 s_1 = \gamma_1 \\ \alpha_1 s_1 - \beta_2 c_1 = 0 \\ \beta_2 c_1 + \alpha_2 s_1 = \delta_2 \\ \beta_2 s_1 - \alpha_2 c_1 = \bar{\gamma}_2 \end{array}\right\} \; 2\times 2$$

$$(**)\quad \left.\begin{array}{l} \bar{\gamma}_2 c_2 + \beta_3 s_2 = \gamma_2 \\ \bar{\gamma}_2 s_2 - \beta_3 c_3 = 0 \\ \beta_3 s_1 = \varepsilon_3 \\ -\beta_3 c_1 c_2 + \alpha_3 s_2 = \delta_3 \\ -\beta_3 c_1 s_2 - \alpha_3 c_2 = \bar{\gamma}_3 \end{array}\right\} \; 3\times 3$$

$$(***)\quad \left.\begin{array}{l} \bar{\gamma}_3 c_3 + \beta_4 s_3 = \gamma_3 \\ \bar{\gamma}_3 s_3 - \beta_4 c_3 = 0 \\ \beta_4 s_2 = \varepsilon_4 \\ -\beta_4 c_2 c_3 + \alpha_4 s_3 = \delta_4 \\ -\beta_4 c_2 s_3 - \alpha_4 c_3 = \bar{\gamma}_4 \end{array}\right\} \; 4\times 4$$

Look at the sets of eq.s marked (*), (**) & (***):

$$\alpha_1 c_1 + \beta_2 s_1 = \gamma_1$$
$$\bar{\gamma}_2 c_2 + \beta_3 s_2 = \gamma_2$$
$$\bar{\gamma}_3 c_3 + \beta_4 s_3 = \gamma_3$$

In general $\bar{\gamma}_k c_k + \beta_{k+1} s_k = \gamma_k$ with $\bar{\gamma}_1 \equiv \alpha_1$

Likewise
$$\left.\begin{array}{l} \alpha_1 s_1 - \beta_2 c_1 = 0 \\ \bar{\gamma}_2 s_2 - \beta_3 c_2 = 0 \\ \bar{\gamma}_3 s_3 - \beta_4 c_3 = 0 \end{array}\right\} \quad \boxed{\bar{\gamma}_k s_k = \beta_{k+1} c_k}$$

Upon first glance one is tempted to set $s_k = \beta_{k+1}$ & $c_k = \bar{\gamma}_k$ in order to satisfy the boxed eq. This would $s_k^2 + c_k^2 = 1 \overset{?}{=} \beta_{k+1}^2 + \bar{\gamma}_k^2$

which may not hold in all cases. A more satisfactory & consistent solution may be of the form

$$\boxed{s_k = \frac{\beta_{k+1}}{(\beta_{k+1}^2 + \bar{\gamma}_k^2)^{1/2}} \quad , \quad c_k = \frac{\bar{\gamma}_k}{(\beta_{k+1}^2 + \bar{\gamma}_k^2)^{1/2}}}$$

This too clearly satisfy the identity $\sin^2\theta + \cos^2\theta = 1$.

Substituting these two into $\bar{\gamma}_k c_k + \beta_{k+1} s_k = \gamma_k$ gives

$$\gamma_k = \frac{(\bar{\gamma}_k^2 + \beta_{k+1}^2)^1}{(\bar{\gamma}_k^2 + \beta_{k+1}^2)^{1/2}} = (\beta_{k+1}^2 + \bar{\gamma}_k^2)^{1/2}$$

thus,

$$\boxed{\begin{gathered} s_k = \frac{\beta_{k+1}}{\gamma_k} \quad , \quad c_k = \frac{\bar{\gamma}_k}{\gamma_k} \\ \text{where} \quad \gamma_k = (\beta_{k+1}^2 + \bar{\gamma}_k^2)^{1/2} \end{gathered}}$$

Also using the trends summarised on the last page,

$$\varepsilon_k = \beta_k s_{k-2}$$
$$\delta_k = -\beta_k c_{k-2} c_{k-1} + \alpha_k s_{k-1} \qquad (\text{assume } c_0 = s_0 = 1)$$
$$\bar{\gamma}_k = -\beta_k c_{k-2} s_{k-1} - \alpha_k c_{k-1}$$

So now we've seen how the $\bar{L}Q$ factorisation works. Recall that algorithms utilising the $\bar{L}Q$ factorisation are numerically equivalent to the CGM, only more stable. As mentioned before, the $\bar{L}Q$ method may encounter singularities & crash. SYMMLQ is similar to the algorithm employing the orthogonal $\bar{L}Q$ factorisation.

SYMMLQ uses L_k instead of $\bar{L}_k$. L_k is the same as $\bar{L}_k$ except $\bar{\gamma}_k$ is replaced by γ_k (easily accomplished by $c_k = \bar{\gamma}_k / \gamma_k$).

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We can now define z_k & W_k

$$z_k \triangleq (\zeta_1, \cdots, \zeta_k)^T$$
$$W_k \triangleq [w_1, \cdots, w_k]$$

Set $L_k z_k = \beta_1 e_1$

Now $\because$ $\beta_1 e_1 = \bar{L}_k \bar{z}_k \Rightarrow L_k z_k = \bar{L}_k \bar{z}_k$

In a 2×2 system

$$\begin{bmatrix} \gamma_1 & 0 \\ \delta_2 & \bar{\gamma}_2 \end{bmatrix} \begin{pmatrix} \zeta_1 \\ \bar{\zeta}_2 \end{pmatrix} = \begin{bmatrix} \gamma_1 & 0 \\ \delta_2 & \gamma_2 \end{bmatrix} \begin{pmatrix} \zeta_1 \\ \zeta_2 \end{pmatrix}$$

Plainly, $\cancel{\delta_2 \zeta_1} + \bar{\gamma}_2 \bar{\zeta}_2 = \cancel{\delta_2 \zeta_1} + \gamma_2 \zeta_2$

or $\zeta_2 = \dfrac{\bar{\gamma}_2 \bar{\zeta}_2}{\gamma_2} = c_2 \bar{\zeta}_2$

&, in general $\boxed{\zeta_k = c_k \bar{\zeta}_k}$

So far we've taken care of L_k & z_k. We need now turn our attention to finding vector $\bar{w}_k$ & its relationship to w_k by induction again.

2×2 $\quad V_k Q_k^T \triangleq \bar{W}_k$

$$[w_1, w_2] \begin{bmatrix} c_1 & s_1 \\ s_1 & -c_1 \end{bmatrix} = [w_1 c_1 + w_2 s_1, \; w_1 s_1 - w_2 c_1] \triangleq [w_1, \bar{w}_2]$$

$$\left.\begin{aligned} w_1 c_1 + w_2 s_1 &= w_1 \\ w_1 s_1 - w_2 c_1 &= \bar{w}_2 \end{aligned}\right\} \text{use for } 3\times 3 \text{ case}$$

3x3 $\begin{bmatrix} v_1 & v_2 & v_3 \end{bmatrix} \begin{bmatrix} c_1 & s_1 & 0 \\ s_1 & -c_1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & c_2 & s_2 \\ 0 & s_2 & -c_2 \end{bmatrix} \triangleq \begin{bmatrix} w_1 & w_2 & \bar{w}_3 \end{bmatrix}$

$\Rightarrow \begin{bmatrix} w_1 & \bar{w}_2 & v_3 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & c_2 & s_2 \\ 0 & s_2 & -c_2 \end{bmatrix} = \begin{bmatrix} w_1, & \bar{w}_2 c_2 + v_3 s_2, & \bar{w}_2 s_2 - v_3 c_2 \end{bmatrix}$

$\triangleq \begin{bmatrix} w_1, & w_2, & \bar{w}_3 \end{bmatrix}$

$\therefore \left.\begin{aligned} \bar{w}_2 c_2 + v_3 s_2 &= w_2 \\ \bar{w}_2 s_2 - v_3 c_2 &= \bar{w}_3 \end{aligned}\right\}$ use for 4x4

4x4: $\begin{bmatrix} w_1, & v_2, & v_3, & v_4 \end{bmatrix} \begin{bmatrix} c_1 & s_1 & 0 & 0 \\ s_1 & -c_1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & c_2 & s_2 & 0 \\ 0 & s_2 & -c_2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & c_3 & s_3 \\ 0 & 0 & s_3 & -c_3 \end{bmatrix} \triangleq \begin{bmatrix} w_1, & w_2, & w_3, & \bar{w}_4 \end{bmatrix}$

$\Rightarrow \begin{bmatrix} w_1, & \bar{w}_2, & v_3, & v_4 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & c_2 & s_2 & 0 \\ 0 & s_2 & -c_2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & c_3 & s_3 \\ 0 & 0 & s_3 & -c_3 \end{bmatrix} \triangleq \begin{bmatrix} w_1, & w_2, & w_3, & \bar{w}_4 \end{bmatrix}$

$\Rightarrow \begin{bmatrix} w_1, & w_2, & \bar{w}_3, & v_4 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \boxed{\begin{matrix} c_3 & s_3 \\ s_3 & -c_3 \end{matrix}} \end{bmatrix} \triangleq \begin{bmatrix} w_1, & w_2, & \boxed{w_3, \ \bar{w}_4} \end{bmatrix}$

$\begin{bmatrix} w_1, & w_2, & \bar{w}_3 c_3 + v_4 s_3, & \bar{w}_3 s_3 - v_4 c_3 \end{bmatrix} \triangleq \begin{bmatrix} w_1, & w_2, & w_3, & \bar{w}_4 \end{bmatrix}$

$$\Rightarrow \quad \left.\begin{aligned} \bar{w}_3 c_3 + v_4 s_3 &= w_3 \\ \bar{w}_3 s_3 - v_4 c_3 &= \bar{w}_4 \end{aligned}\right\} \text{ use for } 5\times 4 \text{ etc...}$$

Now, provided v_1 is set to $\bar{w}_1$, then the relationships ($\square$, $\bigcirc$, $\square$) can clearly be generalised for any k

$$\boxed{\begin{bmatrix} \bar{w}_k & v_{k+1} \end{bmatrix} \begin{bmatrix} c_k & s_k \\ s_k & -c_k \end{bmatrix} = \begin{bmatrix} w_k , & \bar{w}_{k+1} \end{bmatrix}}$$

We now have a recursion allowing us to obtain w_k from $\bar{w}_k$ whilst also producing the next vector, $\bar{w}_{k+1}$, to be plugged back into the recursion!

What's involved with the SYMMLQ algorithm (after k iterations

- Obtain Tridiagonal T_k $\left\{ \begin{array}{l} \beta_k \\ \alpha_k \\ v_k \end{array} \right.$ * also know β_{k+1} (see Cullum / Willoughby 2-3-4 on p. 46)

- Factorise $T_k = \bar{L}_k Q_k$, get $\bar{\gamma}_k$

- Use $\bar{\gamma}_k$ & β_{k+1} to find γ_k (ie acquire L_k)
  Use all three to find c_k & s_k (which aren't available explicitly from the factorisation

- Use Q_k^T & V_k to obtain $\bar{W}_k$ (by def. $\bar{W}_k = V_k Q_k^T$)
  Use $\bar{w}_k$ (from $\bar{W}_k$) to find w_k by $[\bar{w}_k, v_{k+1}]\begin{bmatrix} c_k & s_k \\ s_k & -c_k\end{bmatrix} = [w_k, \bar{w}_{k+1}]$
  & hence W_k

- Similarly, use $\bar{L}_k$ to get $\bar{z}_k$ ($\because \bar{L}_k \bar{z}_k = \beta_1 e_1$)
  Can find z_k from $L_k z_k = \beta_1 e_1$ too!! However
  we seek $\zeta_k = c_k \bar{\zeta}_k$ for an efficient algorithm p.t.o.

- Update $\boxed{x_k^L = W_k z_k = x_{k-1}^L + \zeta_k w_k}$
- Store x_k^L, step, repeat.

Aside: $x_k^C = \bar{W}_k \bar{z}_k$

$$\therefore x_{k+1}^C = \bar{W}_{k+1} \bar{z}_{k+1}$$

$$= W_k z_k + \bar{\zeta}_{k+1} \bar{w}_{k+1}$$

$$\Rightarrow \boxed{x_{k+1}^C = x_k^L + \bar{\zeta}_{k+1} \bar{w}_{k+1}}$$

It's possible to obtain the CG solution x_{k+1}^C from the SYMMLQ solution x_k^L. After the $k+1$ th step we know x_k^L (stored) as well as $\bar{\zeta}_{k+1}$ & $\bar{w}_{k+1}$. ✓

Here I find Paige & Saunders' choice of notation poor - it breeds confusion about the question 'How can one get information about the $k+1$ th iteration if only k iterations have been performed?' They should have stated a proviso (ie possible to compute iff $k+1$ iterations had been completed) or changed their notation:

$$\boxed{x_k^C = x_{k-1}^L + \bar{\zeta}_k \bar{w}_k}$$

* More about this relationship to come later!

Proof that L_k is always non-singular

Assume $\bar{L}_k$ is singular. The only chance we have of forcing L_k to be singular is to set (or attempt to) $\bar{L}_k = L_k$. This would imply $\beta_{k+1} = 0 \;\because\; \gamma_k = (\bar{\gamma}_k^2 + \beta_{k+1}^2)^{1/2} = \bar{\gamma}_k$. But if $\beta_{k+1} = 0$, then:

$$AV_k = V_k T_k + \beta_{k+1} v_{k+1} e_k^T = V_k T_k$$

Since A, V_k, & V_k^T all have non-zero diagonal elements $\Rightarrow$ T_k will have non-zero diagonal elements, ie it'll be non-singular

We know that Q_k^T is non-singular because it's built from multiplications of rotation matrices, $Q_{i,i+1}$, which have no zero diagonal elements.

Now $L_k = \bar{L}_k = Q_k T_k$ which is a product of two non-singular matrices, ie its nonsingular

QED

In attempting to make L_k singular, the form of the problem was altered, the effect of which was to resist that attempt

So, z_k, found from $L_k z_k = \beta_1 e_1$ is well defined allowing x_k^L to always be found

non singular (for L_k); both well-defined (for $\beta_1 e_1$)

$(\beta_1 = \|b\|)$

(It's damn cool too since $\bar{\gamma}_k = \gamma_k$, $c_k = 1$ $\therefore$ $\zeta_k = \bar{\zeta}_k$, $\beta_{k+1} = 0$ means $s_k = \beta_{k+1}/\gamma_k = 0$, so $[\bar{w}_k, w_{k+1}]\begin{bmatrix} c_k & s_k \\ s_k & -c_k \end{bmatrix} = [w_k, \bar{w}_{k+1}]$

means $c_k \bar{w}_k + s_k w_{k+1} = w_k$

ie $\bar{w}_k = w_k$ Beautiful!

Turn attention to finding residuals. They are, afterall, a measure of a method's success.

We know $r_k^c = b - Ax_k^c$

but $b = \beta_1 v_1$ (from def. of initial vector)

& $x_k^c = V_k y_k$

So, $r_k^c = \beta_1 v_1 - AV_k y_k$

but $AV_k = V_k T_k + \beta_{k+1} v_{k+1} e_k^T$

$\therefore \quad r_k^c = \beta_1 v_1 - V_k T_k y_k - \beta_{k+1} v_{k+1} e_k^T y_k$

$= \beta_1 v_1 - V_k \beta_1 e_1 - \beta_{k+1} v_{k+1} e_k^T y_k \qquad (\because T_k y_k = \beta_1 e_1)$

$= \beta_1 v_1 - \beta_1 v_1 - \beta_{k+1} v_{k+1} e_k^T y_k \qquad (\because V_k e_1 = v_1)$

Thus, $r_k^c = -\beta_{k+1} v_{k+1} \eta_{kk}$ where η_{kk} is the k^{th} element of y_k

We don't know what y_k is ... it's inaccessible. All's not lost however.

$T_k = T_k^T = Q_k^T \bar{L}_k^T$ (*)

but $T_k y_k = \beta_1 e_1$

$\Rightarrow \quad Q_k^T \bar{L}_k^T y_k = \beta_1 e_1$ (by multiplying both sides of (*) by y_k)

$\bar{L}_k^T y_k = \beta_1 Q_k e_1$ (**)

p.t.o. Look at the LH & RH sides of (**) ...

To see where this is leading to, look at the k^{th} element of $\bar{L}_k^T y_k$

$$\begin{bmatrix} \gamma_1 & \delta_2 & \varepsilon_3 & & \vdots \\ & \gamma_2 & \delta_3 & & \vdots \\ & & \gamma_3 & & \varepsilon_k \\ \vdots & & & \ddots & \delta_k \\ 0 & \cdots & & & \bar{\gamma}_k \end{bmatrix} \begin{pmatrix} y_k^{(1)} \\ y_k^{(2)} \\ \vdots \\ \vdots \\ y_k^{(k)} = \eta_{kk} \end{pmatrix} = \begin{pmatrix} \\ \\ \\ \\ 0 \cdot y_k^{(1)} + 0 \cdot y_k^{(2)} + \cdots + \eta_{kk} \bar{\gamma}_k \end{pmatrix} = \begin{pmatrix} \\ \\ \\ \\ \eta_{kk} \bar{\gamma}_k \end{pmatrix}$$

On our LHS we $\eta_{kk} \bar{\gamma}_k$. To see what it's equal to, we must look at the k^{th} element of $\beta_1 Q_k e_1$. Do this by induction

$k=3$

$$Q_{k=3} = \left(Q_{k=3}^T\right)^T = \left(Q_{12} Q_{23}\right)^T$$

$$= \left[\begin{bmatrix} c_1 & s_1 & 0 \\ s_1 & -c_1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & c_2 & s_2 \\ 0 & s_2 & -c_2 \end{bmatrix}\right]^T$$

$$= \begin{bmatrix} c_1 & s_1 c_2 & s_1 s_2 \\ s_1 & -c_1 c_2 & -c_1 s_2 \\ 0 & s_2 & -c_2 \end{bmatrix}^T = \begin{bmatrix} c_1 & s_1 & 0 \\ s_1 c_2 & -c_1 c_2 & s_2 \\ s_1 s_2 & -c_1 s_2 & -c_2 \end{bmatrix}$$

So, $\beta_1 Q_k e_1 = \beta_1 \begin{bmatrix} c_1 & s_1 & 0 \\ s_1 c_2 & -c_1 c_2 & s_2 \\ s_1 s_2 & -c_1 s_2 & -c_2 \end{bmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$

$$= \beta_1 \begin{pmatrix} c_1 \\ s_1 c_2 \\ s_1 s_2 \end{pmatrix}$$

$\therefore$ $k=3^{th}$ element of $\beta_1 Q_{\underset{(=3)}{k}} e_1 = \beta_1 s_1 s_2$

Generalising this for any k: the k^{th} element of $\beta_1 Q_k e_1$ is:

$$\beta_1 s_1 s_2 \cdots s_{k-1}$$

Looking ~~at~~ at the k^{th} elements of both sides of $\bar{L}_k^T y_k = \beta_1 Q_k e_1$

$$\Rightarrow \quad y_{kk} \bar{\gamma}_k = \beta_1 s_1 s_2 \cdots s_{k-1}$$

$$\therefore \quad y_{kk} = \beta_1 s_1 s_2 \cdots s_{k-1} / \bar{\gamma}_k$$

The expression for the residual is therefore:

$$r_k^c = -\beta_{k+1} v_{k+1} y_{kk}$$

$$= -\beta_{k+1} v_{k+1} \beta_1 s_1 s_2 \cdots s_{k-1} / \bar{\gamma}_k$$

tidy up by noting $\frac{s_k}{c_k} = \frac{\beta_{k+1}}{\gamma_k} \frac{\gamma_k}{\bar{\gamma}_k}$, we're left with:

$$\boxed{r_k^c = -(\beta_1 s_1 s_2 \cdots s_k / c_k) v_{k+1}}$$

One can likewise show

$$\boxed{r_k^L = b - A x_k^L = \gamma_{k+1} \zeta_{k+1} v_{k+1} - \varepsilon_{k+2} \zeta_k v_{k+2}}$$

I presume this could be sought by a little induction. Recall that I already generalised the element ε_i - there's a head-start already.

Also, $\| r_k^L \|^2 = \gamma_{k+1}^2 \zeta_{k+1}^2 + \varepsilon_{k+2}^2 \zeta_k^2$

Before I mentioned my preferred notation for x_k^C, that is,

$$x_k^C = x_{k-1}^L + \bar{\zeta}_k \bar{w}_k$$

This is the same as $x_k^C = x_k^L - \zeta_k w_k + \bar{\zeta}_k \bar{w}_k$

$$= x_k^L - \zeta_k w_k + \frac{\zeta_k}{c_k}\bar{w}_k$$

$$\Rightarrow \quad \boxed{x_k^C = x_k^L + \zeta_k\left(\frac{\bar{w}_k}{c_k} - w_k\right)}$$

But, $[\bar{w}_k, w_{k+1}]\begin{bmatrix} c_k & s_k \\ s_k & -c_k \end{bmatrix} = [w_k, \bar{w}_{k+1}]$ showed that:

$$\bar{w}_k = c_k w_k + s_k \bar{w}_{k+1}$$

then $x_k^C = x_k^L + \zeta_k\left(\frac{\cancel{c_k} w_k}{\cancel{c_k}} + \frac{s_k \bar{w}_{k+1}}{c_k} - \cancel{w_k}\right)$

$$\Rightarrow \quad \boxed{x_k^C = x_k^L + \underbrace{\left(\frac{\zeta_k s_k}{c_k}\right)\bar{w}_{k+1}}_{\text{this term is never negative}}}$$

$$\therefore \quad \|x_k^C\| \geq \|x_k^L\|$$

The minimum residual method - MINRES

case (b) $m=0 \quad \therefore \quad B = A^0 = I$

Previously we found $V_k^T A^2 V_k u_k = V_k^T A b$, $x_k = V_k u_k$

Also, $AV_k = V_k T_k + \beta_{k+1} v_{k+1} e_k^T$

Recall matrix identities $(AB)^T = B^T A^T$ & $(A+B)^T = A^T + B^T$

$$
\begin{aligned}
(AV_k)^T &= V_k^T A^T \\
&= V_k^T A \qquad \because A \text{ symmetric } (A^T \equiv A) \\
&= \left(V_k T_k + \beta_{k+1} v_{k+1} e_k^T\right)^T \\
&= (V_k T_k)^T + (\beta_{k+1} v_{k+1} e_k^T)^T \\
&= T_k^T V_k^T + \beta_{k+1} e_k v_{k+1}^T \\
&= T_k V_k^T + \beta_{k+1} e_k v_{k+1}^T
\end{aligned}
$$

So,

$$
\begin{aligned}
V_k^T A A V_k = V_k^T A^2 V_k &= \left(T_k V_k^T + \beta_{k+1} e_k v_{k+1}^T\right)\left(V_k T_k + \beta_{k+1} v_{k+1} e_k^T\right) \\
&= T_k \underbrace{\cancel{V_k^T V_k}}_{=I} T_k + T_k V_k^T \beta_{k+1} v_{k+1} e_k^T + \beta_{k+1} e_k \underbrace{v_{k+1}^T V_k}_{= V_k^T v_{k+1} = 0} T_k + \dots \\
&\qquad \dots + \beta_{k+1} e_k v_{k+1}^T \beta_{k+1} v_{k+1} e_k^T \\
&= T_k^2 + \beta_{k+1} T_k \overbrace{V_k^T v_{k+1}}^{=0} e_k^T + \beta_{k+1}^2 e_k \underbrace{v_{k+1}^T v_{k+1}}_{=1} e_k^T
\end{aligned}
$$

thus $V_k^T A^2 V_k = T_k^2 + \beta_{k+1}^2 e_k e_k^T$ ✓

Now, before we found $V_k^T A = T_k V_k^T + \beta_{k+1} e_k v_{k+1}^T$

$$\Rightarrow \quad V_k^T A b = V_k^T A \beta_1 v_1 \qquad \text{(from initial vector definition)}$$

$$= T_k V_k^T \beta_1 v_1 + \beta_{k+1} e_k v_{k+1} \beta_1 v_1$$

$$= \beta_1 T_k V_k^T v_1 + \beta_1 \beta_{k+1} e_k \underbrace{v_{k+1} v_1}_{=0}$$

$$= \beta_1 T_k e_1$$

At present we have
$$\boxed{\begin{aligned} V_k^T A^2 V_k &= T_k^2 + \beta_{k+1}^2 e_k e_k^T \\ V_k^T A b &= \beta_1 T_k e_1 \end{aligned}}$$

We can relate the two by $V_k^T A^2 V_k u_k = V_k^T A b$. But first perform orthogonal factorisation: $T_k = \bar{L}_k Q_k$

$$T_k^2 = T_k T_k^T \qquad \because T_k \text{ symmetric}$$

$$= \bar{L}_k Q_k (\bar{L}_k Q_k)^T$$

$$= \bar{L}_k \underbrace{Q_k Q_k^T}_{I} \bar{L}_k^T = \bar{L}_k \bar{L}_k^T$$

Also, since $\gamma_k = (\bar{\gamma}_k^2 + \beta_{k+1}^2)^{1/2} \Rightarrow \beta_{k+1}^2 = \gamma_k^2 - \bar{\gamma}_k^2$

So, $$\beta_{k+1}^2 e_k e_k^T = \begin{bmatrix} 0 & \cdots & \cdots & 0 \\ \vdots & \ddots & & \vdots \\ \vdots & & 0 & 0 \\ 0 & \cdots & 0 & \gamma_k^2 - \bar{\gamma}_k^2 \end{bmatrix}$$

then $V_k^T A^2 V_k = T_k^2 + \beta_{k+1}^2 e_k e_k^T$

$$= \bar{L}_k \bar{L}_k^T + \beta_{k+1}^2 e_k e_k^T$$

$$= \begin{bmatrix} \ddots & & \vdots \\ & \ddots & \vdots \\ \cdots & \cdots & \bar{\gamma}_k^2 \end{bmatrix} + \begin{bmatrix} 0 & \cdots & \cdots & 0 \\ \vdots & \ddots & & \vdots \\ \vdots & & 0 & 0 \\ 0 & \cdots & 0 & \gamma_k^2 - \bar{\gamma}_k^2 \end{bmatrix}$$

$$= \begin{bmatrix} \ddots & & \vdots \\ & \ddots & \vdots \\ \cdots & \cdots & \gamma_k^2 \end{bmatrix} = L_k L_k^T$$

$$\boxed{V_k^T A^2 V_k = L_k L_k^T}$$

Our relationship $V_k^T A^2 V_k u_k = V_k^T A b$ becomes

$$L_k L_k^T u_k = \beta_1 T_k e_1$$

ie $$\boxed{L_k L_k^T u_k = \beta_1 \bar{L}_k Q_k e_1}$$

$\bar{L}_k$ & L_k differ only in the (k, k) element $\bar{\gamma}_k = c_k \gamma_k$, hence

$\bar{L}_k = L_k D_k$ where $D_k = \text{diag}(1, 1 \cdots c_k)$

So $L_k^T u_k = \beta_1 L_k^{-1} \bar{L}_k Q_k e_1$

ie $L_k^T u_k = \beta_1 D_k Q_k e_1$ = a vector t_k say $= (\tau_1, \cdots \tau_k)^T$

How does one acquire the elements of t_k? Again, use induction to infer a generalised expression

3×3

$$L_k^T u_k = \beta_1 D_k Q_k e_1$$

$$Q_{k=3} = (Q_{k=3}^T)^T = \begin{bmatrix} c_1 & s_1 & 0 \\ s_1 c_2 & -c_1 c_2 & s_2 \\ s_1 s_2 & -c_1 s_2 & -c_2 \end{bmatrix}$$

$$\beta_1 D_{k=3} = \beta_1 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & c_3 \end{bmatrix} = \begin{bmatrix} \beta_1 & 0 & 0 \\ 0 & \beta_1 & 0 \\ 0 & 0 & \beta_1 c_3 \end{bmatrix}$$

$$\therefore \beta_1 D_{k=3} Q_{k=3} = \begin{bmatrix} \beta_1 & 0 & 0 \\ 0 & \beta_1 & 0 \\ 0 & 0 & \beta_1 c_3 \end{bmatrix} \begin{bmatrix} c_1 & s_1 & 0 \\ s_1 c_2 & -c_1 c_2 & s_2 \\ s_1 s_2 & -c_1 s_2 & -c_2 \end{bmatrix} = \begin{bmatrix} c_1\beta_1 & s_1\beta_1 & 0 \\ \beta_1 s_1 c_2 & -\beta_1 c_1 c_2 & s_2\beta_1 \\ \beta_1 s_1 s_2 c_3 & -\beta_1 c_3 c_1 s_2 & -\beta_1 c_3 c_2 \end{bmatrix}$$

$$\therefore \beta_1 D_{k=3} Q_{k=3} e_1 = \begin{bmatrix} c_1\beta_1 & s_1\beta_1 & 0 \\ \beta_1 s_1 c_2 & -\beta_1 c_1 c_2 & s_2\beta_1 \\ \beta_1 s_1 s_2 c_3 & -\beta_1 c_3 c_1 s_2 & -\beta_1 c_3 c_2 \end{bmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\therefore L_{k=3}^T u_3 = \beta_1 D_{k=3} Q_{k=3} e_1 = \begin{pmatrix} \beta_1 c_1 \\ \beta_1 s_1 c_2 \\ \beta_1 s_1 s_2 c_3 \end{pmatrix} = t_{k=3} = \begin{pmatrix} \tau_1 \\ \tau_2 \\ \tau_3 \end{pmatrix}$$

In general
$$\boxed{\begin{aligned} \tau_i &= \beta_1 s_1 \cdots s_{i-1} c_i \\ \tau_1 &= \beta_1 c_1 \end{aligned}} \qquad i \geq 2 \cdots k$$

$$M_k = V_k L_k^{-T} \quad \therefore \quad M_k L_k^{T} = V_k$$

$$[m_1, m_2, m_3, m_4] \begin{bmatrix} \gamma_1 & \delta_2 & \varepsilon_3 & 0 \\ 0 & \gamma_2 & \delta_3 & \varepsilon_4 \\ 0 & 0 & \gamma_3 & \delta_4 \\ 0 & 0 & 0 & \gamma_4 \end{bmatrix} = [\nu_1, \nu_2, \nu_3, \nu_4]$$

$$\nu_1 = m_1 \gamma_1 \quad \Rightarrow \quad m_1 = \frac{\nu_1}{\gamma_1}$$
$$\nu_2 = m_1 \delta_2 + m_2 \gamma_2 \quad \Rightarrow \quad m_2 = \frac{1}{\gamma_2}[\nu_2 - \delta_2 m_1]$$
$$\nu_3 = m_1 \varepsilon_3 + m_2 \delta_3 + m_3 \gamma_3 \quad \Rightarrow \quad m_3 = \frac{1}{\gamma_3}[\nu_3 - \delta_3 m_2 - \varepsilon_3 m_1]$$
$$\nu_4 = m_2 \varepsilon_4 + m_3 \delta_4 + m_4 \gamma_4 \quad \Rightarrow \quad m_4 = \frac{1}{\gamma_4}[\nu_4 - \delta_4 m_3 - \varepsilon_4 m_2]$$

In general $m_k = \frac{1}{\gamma_k}[\nu_k - \delta_k m_{k-1} - \varepsilon_k m_{k-2}]$

where $m_0 = m_{-1} = 0$

Define $M_k = [m_1, \dots, m_k] \cdot V_k L_k^{-T}$ in order to tackle the 'I can't find u_k until the very end!!' problem

then $x_k^M \triangleq V_k u_k = \underbrace{V_k L_k^{-T}}_{M_k} \underbrace{L_k^T u_k}_{t_k}$

$$\boxed{x_k^M = M_k t_k}$$

Like the other methods, we can formulate x_k^M progressively

ie $\boxed{x_k^M = x_{k-1}^M + \tau_k m_k}$

We know the general expression for $\tau_i = \beta_1 s_1 \cdots s_{i-1} c_i$ with $\tau_1 = \beta_1 c_1$

By induction I found a general expression for vector m_k:

$$m_k = \frac{1}{\bar{\gamma}_k} \left[v_k - \delta_k m_{k-1} - \epsilon_k m_{k-2} \right] \qquad \left\{ \begin{array}{l} m_0 \\ m_{-1} = 0 \end{array} \right.$$

(this requires knowledge (ie storage) of previous two vectors!
* I recommend verifying this progressive formulation before implementing it! *

Algorithm:

Tridiagonalise T_k get β_k, α_k, v_k (& β_{k+1})
Factorise $T_k = \bar{L}_k Q_k$ get s_k c_k $\bar{\gamma}_k$ etc..
Obtain L_k ∴ now know ϵ_k δ_k γ_k
Form $\tau_k = \beta_1 s_1 \cdots s_{k-1} c_i$
& $m_k = \frac{1}{\gamma_k}[v_k - \delta_k m_{k-1} - \epsilon_k m_{k-2}]$
Update $x_k^M = x_{k-1}^M + \tau_k m_k$
Store, stop & repeat until converged

Turn attention to finding residual r_k^M, a measure of the algorithm's success. We find it by relating x_k^M to x_k^c

We know $x_k^c = V_k y_k$

$$= V_k L_k^{-T} L_k^T y_k = M_k L_k^T y_k$$

Also $Q_k T_k y_k = \bar{L}_k^T y_k$ (*) $\left(\because T_k Q_k^T = \bar{L}_k \rightarrow Q_k T_k^T = \bar{L}_k^T \rightarrow Q_k T_k = \bar{L}_k^T \right)$

But, $T_k^T y_k \equiv T_k y_k = \beta_1 e_1$ $\left(\& \ T_k^T = (\bar{L}_k Q_k)^T = Q_k^T \bar{L}_k^T \right)$

So, $Q_k T_k y_k = \beta_1 Q_k e_1$ too (**)

Considering x_k^c again, $x_k^c = M_k L_k^T y_k$

ie $x_k^c = M_k D_k^{-1} \bar{L}_k^T y_k$ $\left(\because \bar{L}_k = L_k D_k \Rightarrow L_k^T = D_k^{-1} \bar{L}_k^T \ \& \ D_k^T \equiv D_k \right)$

$x_k^c = M_k D_k^{-1} (\beta_1 Q_k e_1)$ from (*) & (**)

$$= M_k D_k^{-1} D_k^{-1} D_k \beta_1 Q_k e_1$$

$$= M_k D_k^{-2} \beta_1 D_k Q_k e_1$$

$x_k^c = M_k D_k^{-2} t_k$ (recall $L_k^T u_k = \beta_1 D_k Q_k e_1 \triangleq t_k$)

Now $M_k D_k^{-2} t_k = (\tau_1 m_1 + \tau_2 m_2 + \cdots + c_k^{-2} \tau_k m_k)$

Can we relate this vector with the form of vector x_k^M? yes.

$$x_k^M = M_k t_k = (\tau_1 m_1 + \tau_2 m_2 + \dots \tau_k m_k)$$

the only difference between $M_k D_k^{-2} t_k$ & x_k^M is that the last term/component to be added in $M_k D_k^{-2} t_k$ is the last component in x_k^M only multiplied by c_k^{-2}

We need $M_k D_k^{-2} t_k = (\tau_1 m_1 + \dots + c_k^{-2} \tau_k m_k)$

$$= \underbrace{(\tau_1 m_1 + \dots + \tau_k m_k)}_{x_k^M} - (\tau_k m_k) + (c_k^{-2} \tau_k m_k)$$

$$\Rightarrow \quad x_k^c = x_k^M + \tau_k m_k (c_k^{-2} - 1)$$

but $c_k^{-2} - 1 = \frac{1}{\cos^2\theta} - 1$

$$= \frac{1}{\cos^2\theta} - (\cos^2\theta + \sin^2\theta)$$

$$= \frac{1}{\cos^2\theta} - \frac{(\cos^2\theta + \sin^2\theta)\cos^2\theta}{\cos^2\theta}$$

$$= \frac{1}{\cos^2\theta} - \left(\frac{\cos^2\theta\cos^2\theta + \cos^2\theta\sin^2\theta}{\cos^2\theta}\right)$$

$$= \frac{(\cos^2\theta + \sin^2\theta)}{\cos^2\theta} - \frac{(\cos^2\theta\cos^2\theta + \cos^2\theta\sin^2\theta)}{\cos^2\theta}$$

$$= \frac{\cos^2\theta + \sin^2\theta - \cos^2\theta\cos^2\theta - \cos^2\theta\sin^2\theta}{\cos^2\theta}$$

$$= \frac{\cos^2\theta\,[1 - \overset{1-1=0}{\cancel{(\cos^2\theta + \sin^2\theta)}}] + \sin^2\theta}{\cos^2\theta}$$

ie $c_k^{-2} - 1 = \frac{\sin^2\theta}{\cos^2\theta} = \frac{s_k^2}{c_k^2}$

$$\boxed{x_k^c = x_k^M + \tau_k m_k \left(\frac{s_k}{c_k}\right)^2}$$

x_k^c can be obtained from MINRES calculation.

The Lanczos procedure should stop at $\beta_{m+1} = 0$

then $AV_m = V_m T_m + 0 \cdot v_{m+1} e_m^T$

$\Rightarrow AV_m = V_m T_m \qquad \left(AV_m V_m^{-1} = A = V_m T_m V_m^{-1} \right)$

when $\beta_{m+1} = 0$, $\gamma_m = \bar{\gamma}_m$ so $\bar{L}_m = L_m$

then $T_m = L_m Q_m \Rightarrow T_m^T = Q_m^T L_m^T \quad \therefore T_m L_m^{-T} = Q_m^T$

& we defined $M_m = V_m L_m^{-T}$

$$\begin{aligned} \Rightarrow AM_m &= V_m T_m V_m^{-1} V_m L_m^{-T} \\ &= V_m T_m L_m^{-T} \\ &= V_m Q_m^T \\ &\triangleq W_m \end{aligned}$$

This means $\boxed{Am_m = w_m}$

Now $r_k^M - r_k^c \equiv A(x_k^c - x_k^M) = A\cancel{x_k^c} - \cancel{Ax_k^c} + A\tau_k m_k \left(\frac{s_k}{c_k}\right)^2$

$$r_k^M - r_k^c = Am_k \left(\frac{s_k}{c_k}\right)^2 \tau_k = \tau_k \left(\frac{s_k}{c_k}\right)^2 w_k$$

$$\therefore \boxed{r_k^M = \tau_k \left(\frac{s_k}{c_k}\right)^2 w_k + r_k^c}$$

recall that we found $r_k^C = -(\beta_1 s_1 s_2 \cdots s_k / c_k)\, v_{k+1}$

$\underline{\text{simplifying}}$ $r_k^M = \tau_k \left(\frac{s_k}{c_k}\right)^2 w_k - (\beta_1 s_1 s_2 \cdots s_k / c_k)\, v_{k+1}$

$\underline{\text{but}}$ $\tau_k = \beta_1 s_1 s_2 \cdots s_{k-1} c_k$

$$r_k^M = (\beta_1 s_1 s_2 \cdots s_{k-1} c_k) \frac{s_k^2}{c_k^2} w_k - (\beta_1 s_1 s_2 \cdots s_k / c_k)\, v_{k+1}$$

$$= (\beta_1 s_1 s_2 \cdots s_k)\, {}^{s_k}/_{c_k}\, w_k - (\beta_1 s_1 s_2 \cdots s_k) \frac{v_{k+1}}{c_k}$$

$$= \beta_1 s_1 s_2 \cdots s_k \,(s_k w_k - v_{k+1}) / c_k$$

remember $[\bar{w}_k, v_{k+1}] \begin{bmatrix} c_k & s_k \\ s_k & -c_k \end{bmatrix} = [w_k, \bar{w}_{k+1}]$

$\Rightarrow$ $[\bar{w}_k, v_{k+1}] = [w_k, \bar{w}_{k+1}] \begin{bmatrix} c_k & s_k \\ s_k & -c_k \end{bmatrix}$ since $Q_{i,i+1} Q_{i,i+1} = I$

then $v_{k+1} = s_k w_k + - c_k \bar{w}_{k+1}$

$$\Rightarrow \quad r_k^M = \beta_1 s_1 s_2 \cdots s_k (\cancel{s_k w_k} - \cancel{s_k w_k} + c_k \bar{w}_{k+1}) / c_k$$

$$r_k^M = \beta_1 s_1 s_2 \cdots s_k \bar{w}_{k+1}$$

$\| r_k^M \|$ never increases $\quad$ β_1 constant

$0 \le |s_i| \le 1$

$\| \bar{w}_{k+1} \| = 1$