Is there a Small Skew Cayley Transform with Zero Diagonal?

§0: Abstract

The eigenvectors of an Hermitian matrix H are the columns of some complex unitary matrix Q. For any diagonal unitary matrix Ω the columns of Q· Ω are eigenvectors too. Among all such Q· Ω at least one has a skew-Hermitian Cayley transform S := $(I+Q\cdot\Omega)^{-1} \cdot (I-Q\cdot\Omega)$ with just zeros on its diagonal. Why? The proof is unobvious, as is the further observation that Ω may also be so chosen that no element of this S need exceed 1 in magnitude. Thus, plausible constraints, easy to satisfy by perturbations of complex eigenvectors when Hermitian matrix H is perturbed infinitesimally, can be satisfied for discrete perturbations too. And if H is real symmetric, Q real orthogonal and Ω restricted to diagonals of ±1's, then that at least one real skew-symmetric S has every element between ±1 has been proved by Evan O'Dorney [2014].

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§1: Introduction

After Cayley transforms $(B) := (I+B)^{-1} \cdot (I-B)$ have been described in 2, a transform with only zeros on its diagonal will be shown to exist because it solves this minimization problem:

Among unitary matrices $Q \cdot \Omega$ with a fixed unitary Q and variable unitary diagonal Ω , those matrices $Q \cdot \Omega$ "nearest" the identity I in a sense defined in §3 have skew-Hermitian Cayley transforms $S := \$(Q \cdot \Omega) = -S^H$ with zero diagonals and with no element s_{ik} bigger than 1 in magnitude.

Now, why might this interest us? It's a long story

Let H be an Hermitian matrix (so $H^{H} = H$) whose eigenvalues are ordered monotonically (this is crucial) and put into a real column vector v, and whose corresponding eigenvectors can then be chosen to constitute the columns of some unitary matrix Q satisfying the equations

$$H \cdot Q = Q \cdot Diag(v)$$
 and $Q^H = Q^{-1}$. (†)

(Notational note: We distinguish diagonal matrices Diag(A) and V = Diag(v) from column vectors diag(A) and v = diag(V), unlike MATLAB whose diag(diag(A)) is our Diag(A).

We also distinguish scalar 0 from zero vectors o and zero matrices O. And $Q^{H} = \overline{Q}^{T}$ is the complex conjugate transpose of Q; and $\iota = \sqrt{-1}$; and all identity matrices are called "I". The word "skew" serves to abbreviate either "skew-Hermitian" or "real skew-symmetric".)

If Q and v are not known yet but H is very near an Hermitian H_o with known eigenvaluecolumn v_o (also ordered monotonically) and eigenvector matrix Q_o then, as is well known, v must lie very near v_o . This helps us find v during perturbation analyses or curve tracing or iterative refinement. However, two complications can push Q far from Q_o . First, (†) above does not determine Q uniquely: Replacing Q by $Q \cdot \Omega$ for any unitary diagonal Ω leaves the equations still satisfied. To attenuate this first complication we shall seek a $Q \cdot \Omega$ "nearest" Q_o . Still, no $Q \cdot \Omega$ need be very near Q_o unless gaps between adjacent eigenvalues in v and also in v_o are all rather bigger than $||H-H_o||$; this second complication is unavoidable for

reasons exposed by examples so simple as $H = \begin{bmatrix} 1 + \theta & 0 \\ 0 & 1 - \theta \end{bmatrix}$ and $H_o = \begin{bmatrix} 1 & \phi \\ \phi & 1 \end{bmatrix}$ with tiny θ and ϕ .

To simplify our exposition we assume $Q_o = I$ with no loss of generality; doing so amounts to choosing the columns of Q_o as a new orthonormal basis turning H_o into $Diag(v_o)$. Now we can seek solutions Q and v of (†) above with v ordered and Q "nearest" I in some sense.

§2: The Cayley Transform $(B) := (I+B)^{-1} \cdot (I-B) = (I-B) \cdot (I+B)^{-1}$

On its domain it is an *Involution*: ((B)) = B. However $(-(B)) = B^{-1}$ if it exists. maps certain unitary matrices Q to skew matrices S (real if Q is real orthogonal) and back thus:

If I+Q is nonsingular the Cayley transform of unitary $Q = Q^{-1 \text{ H}}$ is skew $S := \$(Q) = -S^{\text{H}}$; and then the Cayley transform of skew $S = -S^{\text{H}}$ recovers unitary $Q = \$(S) = Q^{-1 \text{ H}}$.

Thus, given an algebraic equation like (\dagger) to solve for Q subject to a nonlinear side-condition like $Q^{H} = Q^{-1}$, we can solve instead an equivalent algebraic equation for S subject to a nearlinear and thus simpler side-condition $S = -S^{H}$, though doing so risks losing some solution(s) Q for which I+Q is singular and the Cayley transform S is infinite. But no eigenvectors need be lost that way. Instead their unitary matrix Q can appear post–multiplied harmlessly by a diagonal matrix whose diagonal elements are each either +1 or -1. Here is why: ...

Lemma: If Q is unitary and if I+Q is singular, then reversing signs of aptly chosen columns of Q will make I+Q nonsingular and provide a finite Cayley transform S = \$(Q).

Proof: I am grateful to Prof. Jean Gallier for pointing out that Richard Bellman published this lemma in 1960 as an exercise; see Exs. 7 - 11, pp. 92-3 in §4 of Ch. 6 of his book *Introduction to Matrix Analysis* (2d ed. 1970 McGraw-Hill, New York). The non-constructive proof hereunder is utterly different. Let n be the dimension of Q, let $m := 2^n - 1$, and for each k = 0, 1, 2, ..., m obtain n-by-n unitary Q_k by reversing the signs of whichever columns of Q have the same positions as have the nonzero bits in the binary representation of k. For example $Q_0 = Q$, $Q_m = -Q$, and Q_1 is obtained by reversing the sign of just the last column of Q. Were the lemma false we would find every det(I+Q_k) = 0. For argument's sake let us suppose all 2^n of these equations to be satisfied.

Recall that det(...) is a linear function of each column separately; whenever n-by-n B and C differ in only one column, det(B+C) = $2^{n-1} \cdot (det(B) + det(C))$. Therefore our supposition would imply det(I+Q_{2i} + I+Q_{2i+1}) = $2^{n-1} \cdot (det(I+Q_{2i}) + det(I+Q_{2i+1})) = 0$ whenever $0 \le i \le (m-1)/2$. Similarly det((I+Q_{4j} + I+Q_{4j+1}) + (I+Q_{4j+2} + I+Q_{4j+3})) = 0 whenever $0 \le j \le (m-3)/4$. And so on. Ultimately det(I+Q₀ + I+Q₁ + I+Q₂ + ... + I+Q_m) = 0 would be inferred though the sum amounts to $2^n \cdot I$, whose determinant cannot vanish! This contradiction ends the lemma's proof.

The lemma lets us replace any search for a unitary or real orthogonal matrix Q of eigenvectors by a search for a skew matrix S from which a Cayley transform will recover one of the sought eigenvector matrices $Q := (I+S)^{-1} \cdot (I-S)$. Constraining the search to skew-Hermitian S with diag(S) = o is justified in §3. A further constraint keeping every $|s_{jk}| \le 1$ to render Q easy to compute accurately is justified in §5 for complex S. Real Q and S require something else.

Substituting Cayley transform Q = (I-S) into (\dagger) turns them into equations more nearly linear: $(I+S)\cdot H \cdot (I-S) = (I-S) \cdot Diag(v) \cdot (I+S)$ and $S^H = -S$. (\ddagger)

If all off-diagonal elements h_{jk} of H are so tiny compared with differences $h_{jj} - h_{kk}$ between diagonal elements that 3rd-order terms $S \cdot (H-Diag(H)) \cdot S$ can be neglected, equations (‡) have approximate solutions $v \approx diag(H)$ and $s_{jk} \approx \frac{1}{2} h_{jk}/(h_{jj} - h_{kk})$ for $j \neq k$. Diagonal elements s_{jj} can be arbitrary imaginaries but small lest 3rd-order terms be not negligible. Forcing $s_{jj} := 0$ seems plausible. But if done when, as happens more often, off-diagonal elements are too big for the foregoing approximations for v and S to be acceptable, how do we know equations (‡) must still have at least one solution v and S with diag(S) = o and no huge elements in S ?

Now the question that is this work's title has been motivated: Every unitary matrix G of H's eigenvectors spawns an infinitude of solutions $Q := G \cdot \Omega$ of (†) whose skew-Hermitian Cayley transforms $S := \$(G \cdot \Omega)$ satisfying (‡) sweep out a continuum as Ω runs through all complex unitary diagonal matrices for which $I+G \cdot \Omega$ is nonsingular. This continuum happens to include at least one skew S with diag(S) = 0 and no huge elements, as we'll see in \$3 and \$5.

Lacking this continuum, an ostensibly simpler special case turns out not so simple: When H is real symmetric and G is real orthogonal then, whenever Ω is a real diagonal of -1's and/or +1's for which the Cayley transform $(G \cdot \Omega)$ exists, it is a real skew matrix with zeros on its diagonal. The Lemma above ensures that some such $(G \cdot \Omega)$ exists. O'Dorney [2014] has proved that at least one such $(G \cdot \Omega)$ has every element between ± 1 . Examples in 4 are on the brink; these are n-by-n real orthogonal matrices G for which *every* off-diagonal element of *every* (there are 2^{n-1} of them) such $(G \cdot \Omega)$ is ± 1 .

The continuum swept out in the complex case helps us answer our questions. For any given real or complex unitary G, as Ω ranges through all complex unitary diagonal matrices for which I+G· Ω is nonsingular, the unitary G· Ω that comes nearest the identity matrix I in a peculiar sense to be explained forthwith has a Cayley transform $(G \cdot \Omega)$ with only zeros on its diagonal and no element bigger than 1 in magnitude.

§3: £(Q) Gauges How "Near" a Unitary Q is to I

The function $\pounds(B) := -\log(\det((2I + B + B^{-1})/4)) = -\log(\det((I+B^{-1})\cdot(I+B)/4)))$ will be used to gauge how "near" any unitary matrix $Q = Q^{-1 \text{ H}}$ is to I. The closer is $\pounds(Q)$ to 0, the "nearer" shall Q be deemed to I. The following digression explores properties of $\pounds(Q)$:

When (I+Q) is nonsingular, every eigenvalue of unitary Q has magnitude 1 but none is -1, so matrix $(2I+Q+Q^{-1})/4 = (I+Q)^{H} \cdot (I+Q)/4$ is Hermitian with real eigenvalues all positive and no bigger than 1. Therefore its determinant, their product, is also positive and no bigger than 1; therefore $\pounds(Q) \ge 0$. Only $\pounds(I) = 0$. Another way to confirm this is to observe that $\pounds(Q) = log(det(I - \$(Q)^2)) = log(det(I + \$(Q)^{H} \cdot \$(Q))) > 0 \text{ (or } +\infty) for every unitary } Q \neq I$.

 $\pounds(Q)$ and \$(Q) are differentiable functions of Q except at their poles, where \$(Q) is infinite and $\pounds(Q) = +\infty$ because det(I+Q) = 0. The differential of $\pounds(Q)$ is simpler to derive than its derivative is because of Jacobi's formula $d \log(det(B)) = trace(B^{-1} \cdot dB)$ and another formula $d(B^{-1}) = -B^{-1} \cdot dB \cdot B^{-1}$, and because trace(B \cdot C) = trace(C \cdot B) whenever both matrix products B \cdot C and C \cdot B are square. By applying these formulas we find that

$$d \pounds(B) = -\operatorname{trace}((2I + B + B^{-1})^{-1} \cdot (dB - B^{-1} \cdot dB \cdot B^{-1}))$$

= trace((I+B)^{-1} \cdot (I-B) \cdot B^{-1} \cdot dB) = trace(\\$(B) \cdot B^{-1} \cdot dB).

How does $\pounds(Q \cdot \Omega)$ behave for any fixed unitary Q as Ω runs through the set of all diagonal unitary matrices? This set is swept out by $\Omega := e^{i \text{Diag}(x)}$ as real vector x runs throughout any hypercube with side-lengths bigger than 2π ; and $\pounds(Q \cdot e^{i \text{Diag}(x)})$ must assume its minimum value at some real vector(s) x strictly inside such a hypercube. Such a minimizing $Q \cdot e^{i \text{Diag}(x)}$ is a unitary $Q \cdot \Omega$ "nearest" I. Let's investigate the Cayley transform of a "nearest" $Q \cdot \Omega$.

Abbreviate Diag(x) = X and Diag(dx) = dX; and note that X and dX commute, so that $d\Omega = de^{iX} = ie^{iX} \cdot dX = i\Omega \cdot dX$, and therefore

 $d \pounds (\mathbf{Q} \cdot \mathbf{\Omega}) = \operatorname{trace}(\$ (\mathbf{Q} \cdot \mathbf{\Omega}) \cdot e^{-\iota \mathbf{X}} \mathbf{Q}^{-1} \cdot \mathbf{Q} \cdot \iota e^{\iota \mathbf{X}} \cdot d \mathbf{X}) = \iota \operatorname{diag}(\$ (\mathbf{Q} \cdot \mathbf{\Omega}))^{\mathrm{T}} d \mathbf{x}.$

Since this $d \pounds$ must vanish at a minimum of \pounds for every real dx, so $diag(\$(Q \cdot \Omega)) = o$ there. Thus the question that is this work's title must have an affirmative answer, namely ...

Theorem: For each unitary Q there exists at least one unitary diagonal Ω for which the skew-Hermitian Cayley transform $S := (I + Q \cdot \Omega)^{-1} \cdot (I - Q \cdot \Omega) = -S^H$ has diag(S) = 0.

The theorem's "at least one" tends to understate how many such diagonals Ω exist. To see why, set $\Omega := e^{i \text{Diag}(x)}$ again and consider the locus of poles of the function $\pounds(Q \cdot e^{i \text{Diag}(x)})$ of the real column x. These poles are the zeros x of $\det(I + Q \cdot e^{i \text{Diag}(x)})$. Substitution of the Cayley transform $Z := \$(Q) = -Z^H$, perhaps after shifting x's origin by applying \$2's Lemma, transforms the determinantal equation for the locus of poles into an equivalent equation

 $det(\cos(\operatorname{Diag}(x/2)) - \iota Z \cdot \sin(\operatorname{Diag}(x/2))) = 0.$ (*)

Despite first appearances, the left-hand side of this equation is a real function of the real vector x because matrix $\cot(\text{Diag}(x/2)) - \iota Z$ is Hermitian wherever it is finite. Moreover that left-

hand side reverses sign somewhere because it takes both positive and negative values at vectors x whose elements are various integer multiples of 2π . Therefore the space of real vectors x is partitioned into cells by the locus of poles of £; inside each cell £ is finite and nonnegative, and the left-hand side of (*) takes on a constant nonzero sign probably opposite to the sign in adjacent cells. Inside every cell each local minimum (or any other *critical point* x where $\partial \pounds/\partial x = o^T$) of £ provides another of the theorem's diagonals $\Omega := e^{i\text{Diag}(x)}$. These are likely to be numerous, as we shall see next.

§4: Examples

For every integer n > 1 examples exist for which the number of the theorem's diagonals Ω is infinite in the general complex case, 2^{n-1} in the restricted-to-real case. All these diagonals Ω minimize £; all of them provide skew Cayley transforms S whose diag(S) = 0 and whose every off-diagonal element has magnitude 1. Here is such an example:

let Ω run through unitary diagonal matrices with $\det(\Omega) \neq -1$. Then unitary $Q := G \cdot \Omega$ has a skew-Hermitian Cayley transform $S = \$(Q) := (I+Q)^{-1} \cdot (I-Q) = -S^T$ which, as we shall show, has off-diagonal elements all of the same magnitude $2/|1 + \det(\Omega)|$. Moreover this magnitude is minimized just when $\det(\Omega) = +1$, the minimized magnitude is 1, and $\operatorname{diag}(S) = o$. In particular, for every real orthogonal diagonal Ω of ± 1 's with an even number of -1's, S is a real skew matrix all of whose off-diagonal elements are ± 1 's. We'll prove these claims next.

First we must confirm that (Q) exists; it will follow from $\Omega^{-1} = \overline{\Omega}$ (the complex conjugate): $\det(I+Q) = \det(I + G \cdot \Omega) = \det(\overline{\Omega} + G) \cdot \det(\Omega) = (\det(\overline{\Omega}) + 1) \cdot \det(\Omega) = 1 + \det(\Omega) \neq 0$.

Next confirm that the powers $Q^0 = I$, $Q, Q^2, Q^3, ..., Q^{n-1}$ are linearly independent because their nonzero elements occupy non-overlapping positions in the matrix. Just as $G^n = (-1)^{n-1} \cdot I$, so does Q^n turns out to be a scalar multiple of I. Our next task is to determine this scalar.

Start by defining the n-vector $u := diag(\Omega)$ so that $\Omega = Diag(u)$ and the elements of u all have magnitude 1 and product $det(\Omega)$. Next observe that $G \cdot Diag(v) = Diag(G \cdot v) \cdot G$ for any n-vector v. Use this to confirm by induction that

 $(G \cdot \Omega)^k = Diag(G \cdot u) \cdot Diag(G^2 \cdot u) \cdot Diag(G^3 \cdot u) \cdot ... \cdot Diag(G^k \cdot u) \cdot G^k$ for each k = 1, 2, 3, ... in turn. In particular, when k = n we find that $Q^n = (G \cdot \Omega)^n = (-1)^{n-1} \cdot \prod_{1 \le k \le n} Diag(G^k \cdot u)$. Each diagonal element of this product includes the product of all the elements of u each once, and their product is $det(\Omega)$. Factor it out to obtain $Q^n = det(\Omega) \cdot (G \cdot I)^n = det(\Omega) \cdot (-1)^{n-1} \cdot I$.

The last equation figures in the confirmation of an explicit formula for the Cayley transform:

 $(Q) = (I+Q)^{-1} \cdot (I-Q) = ((1 - \det(\Omega)) \cdot I + 2\sum_{1 \le k \le n-1} (-1)^k Q^k) / (1 + \det(\Omega)).$

To confirm it multiply by I+Q and collect terms. This formula validates every claim uttered above for (Q) because every unitary diagonal Ω has $|\det(\Omega)| = 1$.

 $\pounds(Q)$, the gauge of "nearness" to I, is minimized when $\det(\Omega) = 1$ and $\operatorname{diag}(S) = 0$ since $\pounds(Q) = n \cdot \log(4) - 2 \cdot \log|1 + \det(\Omega)| \ge (n-1) \cdot \log(4)$ with equality just when $\det(\Omega) = 1$.

Here is a different example $Q := \$(\begin{bmatrix} 0 & 2 & -2 \\ -2 & 0 & 2 \\ 2 & -2 & 0 \end{bmatrix}) = \begin{bmatrix} -3 & 4 & 12 \\ 12 & -3 & 4 \\ 4 & 12 & -3 \end{bmatrix}/13$. Six unitary diagonals Ω satisfy the theorem. Four are real: $\Omega = I$, Diag([-1; -1; 1]), Diag([1; -1; -1]) and Diag([-1; 1; -1]). Typical of the last three is $\$(Q \cdot Diag([-1; 1; -1])) = \begin{bmatrix} 0 & -1 & \frac{1}{2} \\ 1 & 0 & 1 \\ -\frac{1}{2} & -1 & 0 \end{bmatrix}$; none of them minimizes $\pounds(Q \cdot \Omega)$.

It is minimized by two complex scalar diagonals $\Omega := (-5 \pm 12i)I/13$ for which respectively

 $\$(\mathbf{Q}\cdot\mathbf{\Omega}) = \begin{bmatrix} 0 & -1-3\iota & 1-3\iota \\ 1-3\iota & 0 & -1-3\iota \\ -1-3\iota & 1-3\iota & 0 \end{bmatrix} / 4 \text{ and its complex conjugate. Note that its every element is strictly}$

smaller than 1 in magnitude, unlike the theorem's four real instances.

§5: Why Minimizing $\pounds(\mathbf{Q}\cdot\Omega)$ Makes $\$(\mathbf{Q}\cdot\Omega)$ Small.

In general, can the theorem's $S := \$(Q \cdot \Omega)$ be huge for a $Q \cdot \Omega$ "nearest" I? No; here is why: Once again abbreviate $Diag(x+\Delta x) = X+\Delta X$ for real columns $x+\Delta x$, and set unitary diagonal $\Omega := e^{tX}$, and abbreviate $\$(Q \cdot \Omega) = S$. The second term of the Taylor series expansion

 $\mathbf{\pounds}(\mathbf{Q}\cdot\mathbf{\Omega}\cdot e^{t\Delta X}) = \mathbf{\pounds}(\mathbf{Q}\cdot\mathbf{\Omega}) + (\partial\mathbf{\pounds}(\mathbf{Q}\cdot\mathbf{\Omega})/\partial\mathbf{x})\cdot\Delta\mathbf{x} + (\partial^{2}\mathbf{\pounds}(\mathbf{Q}\cdot\mathbf{\Omega})/\partial\mathbf{x}^{2})\cdot\Delta\mathbf{x}\cdot\Delta\mathbf{x}/2 + O(\Delta\mathbf{x})^{3}$ must vanish and the third must be nonnegative for all $\Delta\mathbf{x}$ at a local minimum \mathbf{x} of $\mathbf{\pounds}$. We already have $\partial\mathbf{\pounds}(\mathbf{Q}\cdot\mathbf{\Omega})/\partial\mathbf{x} = \iota \operatorname{diag}(\mathbf{S})^{T}$, and next we shall compute $\partial^{2}\mathbf{\pounds}(\mathbf{Q}\cdot\mathbf{\Omega})/\partial\mathbf{x}^{2}$.

The next two paragraphs serve only to introduce my notation to readers unacquainted with it. Others may skip them.

A continuously differentiable scalar function f(x) of a column-vector argument x has a first *derivative* denoted by $f'(x) = \partial f(x)/\partial x$. It must be a row vector since scalar $df(x) = f'(x) \cdot dx$. Sometimes this *differential* is easier to derive than the derivative; it means that, for every differentiable vector-valued function $x(\mu)$ of any scalar variable μ , the chain rule yields a derivative $df(x(\mu))/d\mu = f'(x(\mu)) \cdot x'(\mu)$. For any fixed x this f'(x) is a *linear functional* acting linearly upon vectors in the same space as x and represented by a row often called "The Jacobian Array of First partial Derivatives". Such is $\partial \pounds(Q \cdot e^{t \operatorname{Diag}(x)})/\partial x = t \operatorname{diag}(S)^{T}$.

If f(x) is continuously twice differentiable its second derivative, denoted by $f''(x) = \partial^2 f(x)/\partial x^2$, is a *symmetric* bilinear operator acting upon pairs of vectors in the same space as x. "Symmetric" means $f''(x) \cdot y \cdot z = f''(x) \cdot z \cdot y$ because of H.A. Schwarz's lemma that tells when the order of differentiation does not matter. The "Hessian Array of Second partial Derivatives" is a symmetric matrix H(x) that yields $f''(x) \cdot y \cdot z = z^T \cdot H(x) \cdot y$. Sometimes we can derive the differential $df'(x) \cdot y = f''(x) \cdot y \cdot dx = dx^T \cdot H(x) \cdot y$ more easily than the derivative. Such will be the case for the second derivative $\partial^2 \pounds(Q \cdot e^t \operatorname{Diag}(x))/\partial x^2$ derived hereunder.

Recall that the differential of the unitary diagonal $\Omega := e^{iX}$ is $d\Omega = i \Omega \cdot dX$. Then rewrite

$$dS = -2(I+Q\cdot\Omega)^{-1} \cdot Q \cdot d\Omega \cdot (I+Q\cdot\Omega)^{-1} = -2\iota (I+Q\cdot\Omega)^{-1} \cdot Q \cdot \Omega \cdot dX \cdot (I+Q\cdot\Omega)^{-1}$$
$$= -\iota (I+S) \cdot (I+S)^{-1} \cdot (I-S) \cdot dX \cdot (I+S)/2 = -\iota (I-S) \cdot dX \cdot (I+S)/2 .$$

Next, $(\partial \pounds (Q \cdot \Omega) / \partial x) \cdot \Delta x = \iota \operatorname{diag}(S)^{\mathrm{T}} \cdot \Delta x = \iota \operatorname{trace}(S \cdot \Delta X)$ for any fixed column Δx and therefore $(\partial^2 \pounds (Q \cdot \Omega) / \partial x^2) \cdot dx \cdot \Delta x = d (\partial \pounds (Q \cdot \Omega) / \partial x) \cdot \Delta x = \iota \operatorname{dtrace}(S \cdot \Delta X) = \iota \operatorname{trace}(d \cdot S \cdot \Delta X)$

$${}^{2}\mathfrak{t}(Q\cdot\Omega)/\partial x^{2})\cdot dx\cdot\Delta x = d\left(\partial\mathfrak{t}(Q\cdot\Omega)/\partial x\right)\cdot\Delta x = \iota d\operatorname{trace}(S\cdot\Delta X) = \iota \operatorname{trace}(dS\cdot\Delta X)$$

$$= \iota \operatorname{trace}(-\iota (I-S) \cdot dX \cdot (I+S) \cdot \Delta X)/2 = \operatorname{trace}(dX \cdot \Delta X - S \cdot dX \cdot \Delta X + dX \cdot S \cdot \Delta X - S \cdot dX \cdot S \cdot \Delta X)/2$$

= trace(dX \cdot \Delta X + (S^{H} \cdot dX) \cdot (S \cdot \Delta X))/2 = dx^{T} \cdot (I + |S|^{2}) \cdot \Delta x/2

 $= \mbox{trace}(dX \cdot \Delta X + (S^{H} \cdot dX) \cdot (S \cdot \Delta X))/2 = dx^{-1} \cdot (I + |S|^{2}) \cdot \Delta x/2$ wherein $|S|^{2}$ is obtained elementwise by substituting $|s_{ij}|^{2}$ for each element s_{ij} in S.

Thus we have derived the first three terms of the Taylor Series expansion

$$\pounds(\mathbf{Q}\cdot\mathbf{\Omega}\cdot e^{\iota\Delta \mathbf{X}}) = \pounds(\mathbf{Q}\cdot\mathbf{\Omega}) + \iota\operatorname{diag}(\mathbf{S})^{\mathrm{T}}\cdot\Delta\mathbf{x} + \Delta\mathbf{x}^{\mathrm{T}}\cdot(\mathbf{I}+|\mathbf{S}|^{2})\cdot\Delta\mathbf{x}/4 + O(\Delta\mathbf{x})^{3}$$

Since diag(S) = o and $I + |S|^2$ must be a positive (semi)definite matrix at a minimum of £, every $|s_{ij}| \le 1$ there. Consequently ...

Corollary: At least one of the Theorem's complex skew-Hermitian Cayley transforms $S := \$(Q \cdot \Omega)$ with diag(S) = o also has every element $|s_{ij}| \le 1$.

§6: Conclusion:

Perturbing a complex Hermitian matrix H changes its unitary matrix Q of eigenvectors to a perturbed unitary $Q \cdot (I+S)^{-1} \cdot (I-S)$ in which the skew-Hermitian $S = -S^H$ can always be chosen to be small (no element bigger than 1 in magnitude) and to have only zeros on its diagonal. When H is real symmetric, Q is real orthogonal, and S is restricted to be real skew-symmetric, Evan O'Dorney [2014] has proved S can always be chosen to have every element between ± 1 . But how to construct such skews S efficiently and infallibly is not known yet.

Citations:

Evan O'Dorney [2014] "Minimizing the Cayley transform of an orthogonal matrix by multiplying by signature matrices" pp. 97-103 in *Linear Algebra & Appl.* **448**. Evan did this in 2010 while still an undergraduate at U.C. Berkeley.

W. Kahan [2006] "Is there a small skew Cayley transform with zero diagonal?" pp. 335-341 in *Linear Algebra & Appl.* **448**. ... The earlier version of this document.

Prof. W. Kahan Mathematics Dept. #3840 University of California Berkeley CA 94720-3840

As an old acquaintance since 1959, I proffered this work to Prof. Dr. F.L. Bauer of Munich for his 80th birthday.