## 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 $\Omega$ the columns of $\mathrm{Q} \cdot \Omega$ are eigenvectors too. Among all such $\mathrm{Q} \cdot \Omega$ at least one has a skew-Hermitian Cayley transform $\mathrm{S}:=(\mathrm{I}+\mathrm{Q} \cdot \Omega)^{-1} \cdot(\mathrm{I}-\mathrm{Q} \cdot \Omega)$ with just zeros on its diagonal. Why? The proof is unobvious, as is the further observation that $\Omega$ 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 $\Omega$ restricted to diagonals of $\pm 1$ 's, then that at least one real skew-symmetric $S$ has every element between $\pm 1$ has been proved by Evan O'Dorney [2014].
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## §1: Introduction

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

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

Now, why might this interest us? It's a long story ... .
Let H be an Hermitian matrix ( so $\mathrm{H}^{\mathrm{H}}=\mathrm{H}$ ) 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

$$
\mathrm{H} \cdot \mathrm{Q}=\mathrm{Q} \cdot \operatorname{Diag}(\mathrm{v}) \text { and } \mathrm{Q}^{\mathrm{H}}=\mathrm{Q}^{-1}
$$

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

We also distinguish scalar 0 from zero vectors o and zero matrices O . And $\mathrm{Q}^{\mathrm{H}}=\overline{\mathrm{Q}}^{\mathrm{T}}$ is the complex conjugate transpose of Q ; and $\boldsymbol{\imath}=\sqrt{-1}$; 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 $\mathrm{H}_{\mathrm{o}}$ with known eigenvaluecolumn $\mathrm{v}_{\mathrm{o}}$ (also ordered monotonically) and eigenvector matrix $\mathrm{Q}_{\mathrm{o}}$ then, as is well known, v must lie very near $\mathrm{v}_{\mathrm{o}}$. This helps us find v during perturbation analyses or curve tracing or iterative refinement. However, two complications can push $Q$ far from $Q_{0}$. First, ( $\dagger$ ) above does not determine Q uniquely: Replacing Q by $\mathrm{Q} \cdot \Omega$ for any unitary diagonal $\Omega$ leaves the equations still satisfied. To attenuate this first complication we shall seek a $\mathrm{Q} \cdot \Omega$ "nearest" $\mathrm{Q}_{0}$. Still, no $\mathrm{Q} \cdot \Omega$ need be very near $\mathrm{Q}_{\mathrm{o}}$ unless gaps between adjacent eigenvalues in v and also in $\mathrm{v}_{\mathrm{o}}$ are all rather bigger than $\left\|\mathrm{H}-\mathrm{H}_{\mathrm{o}}\right\|$; this second complication is unavoidable for reasons exposed by examples so simple as $H=\left[\begin{array}{cc}1+\theta & 0 \\ 0 & 1\end{array}-\theta\right]$ and $H_{o}=\left[\begin{array}{cc}1 & \phi \\ \phi & 1\end{array}\right]$ with tiny $\theta$ and $\phi$.

To simplify our exposition we assume $\mathrm{Q}_{0}=\mathrm{I}$ with no loss of generality; doing so amounts to choosing the columns of $Q_{0}$ as a new orthonormal basis turning $H_{o}$ into $\operatorname{Diag}\left(v_{o}\right)$. Now we can seek solutions Q and v of $(\dagger)$ above with v ordered and Q "nearest" I in some sense.

## §2: The Cayley Transform \$(B):=(I+B)-1.(I-B)=(I-B)•(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 $Q=Q^{-1 H}$ is skew $S:=\$(Q)=-S^{H}$; and then the Cayley transform of skew $S=-S^{H}$ recovers unitary $Q=\$(S)=Q^{-1 H}$.

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 $\mathrm{S}=-\mathrm{S}^{\mathrm{H}}$, though doing so risks losing some solution(s) Q for which $\mathrm{I}+\mathrm{Q}$ 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 $\mathrm{I}+\mathrm{Q}$ is singular, then reversing signs of aptly chosen columns of Q will make $\mathrm{I}+\mathrm{Q}$ nonsingular and provide a finite Cayley transform $\mathrm{S}=\$(\mathrm{Q})$.

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 $\mathrm{m}:=2^{\mathrm{n}}-1$, and for each $\mathrm{k}=0,1,2, \ldots, \mathrm{~m}$ obtain n -by-n unitary $\mathrm{Q}_{\mathrm{k}}$ 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 $\mathrm{Q}_{0}=\mathrm{Q}, \mathrm{Q}_{\mathrm{m}}=-\mathrm{Q}$, and $\mathrm{Q}_{1}$ is obtained by reversing the sign of just the last column of Q . Were the lemma false we would find every $\operatorname{det}\left(\mathrm{I}+\mathrm{Q}_{\mathrm{k}}\right)=0$. For argument's sake let us suppose all $2^{\mathrm{n}}$ of these equations to be satisfied.

Recall that $\operatorname{det}(\ldots)$ is a linear function of each column separately; whenever $n$-by-n $B$ and $C$ differ in only one column, $\operatorname{det}(B+C)=2^{\mathrm{n}-1} \cdot(\operatorname{det}(\mathrm{~B})+\operatorname{det}(\mathrm{C}))$. Therefore our supposition would imply $\operatorname{det}\left(\mathrm{I}+\mathrm{Q}_{2 \mathrm{i}}+\mathrm{I}+\mathrm{Q}_{2 \mathrm{i}+1}\right)=2^{\mathrm{n}-1} \cdot\left(\operatorname{det}\left(\mathrm{I}+\mathrm{Q}_{2 \mathrm{i}}\right)+\operatorname{det}\left(\mathrm{I}+\mathrm{Q}_{2 \mathrm{i}+1}\right)\right)=0$ whenever $0 \leq \mathrm{i} \leq(\mathrm{m}-1) / 2$. Similarly $\operatorname{det}\left(\left(I+Q_{4 j}+I+Q_{4 j+1}\right)+\left(I+Q_{4 j+2}+I+Q_{4 j+3}\right)\right)=0$ whenever $0 \leq j \leq(m-3) / 4$. And so on. Ultimately $\operatorname{det}\left(\mathrm{I}+\mathrm{Q}_{0}+\mathrm{I}+\mathrm{Q}_{1}+\mathrm{I}+\mathrm{Q}_{2}+\ldots+\mathrm{I}+\mathrm{Q}_{\mathrm{m}}\right)=0$ would be inferred though the sum amounts to $2^{\mathrm{n}} \cdot \mathrm{I}$, 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 $\mathrm{Q}:=(\mathrm{I}+\mathrm{S})^{-1} \cdot(\mathrm{I}-\mathrm{S})$. Constraining the search to skew-Hermitian S with $\operatorname{diag}(S)=0$ is justified in §3. A further constraint keeping every $\left|s_{j k}\right| \leq 1$ to render $Q$ easy to compute accurately is justified in $\S 5$ for complex S . Real Q and S require something else.

Substituting Cayley transform $\mathrm{Q}=\$(\mathrm{~S})$ into $(\dagger)$ turns them into equations more nearly linear:

$$
(\mathrm{I}+\mathrm{S}) \cdot \mathrm{H} \cdot(\mathrm{I}-\mathrm{S})=(\mathrm{I}-\mathrm{S}) \cdot \operatorname{Diag}(\mathrm{v}) \cdot(\mathrm{I}+\mathrm{S}) \quad \text { and } \quad \mathrm{S}^{\mathrm{H}}=-\mathrm{S} .
$$

If all off-diagonal elements $\mathrm{h}_{\mathrm{jk}}$ of H are so tiny compared with differences $\mathrm{h}_{\mathrm{jj}}-\mathrm{h}_{\mathrm{kk}}$ between diagonal elements that 3rd-order terms $S \cdot(\mathrm{H}-\operatorname{Diag}(\mathrm{H})) \cdot \mathrm{S}$ can be neglected, equations ( $\ddagger$ ) have approximate solutions $\mathrm{v} \approx \operatorname{diag}(\mathrm{H})$ and $\mathrm{s}_{\mathrm{jk}} \approx \frac{1}{2} \mathrm{~h}_{\mathrm{jk}} /\left(\mathrm{h}_{\mathrm{jj}}-\mathrm{h}_{\mathrm{kk}}\right)$ for $\mathrm{j} \neq \mathrm{k}$. Diagonal elements $\mathrm{s}_{\mathrm{jj}}$ can be arbitrary imaginaries but small lest 3rd-order terms be not negligible. Forcing $\mathrm{s}_{\mathrm{jj}}:=0$ 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 $(\ddagger)$ must still have at least one solution v and S with $\operatorname{diag}(\mathrm{S})=\mathrm{o}$ 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 $\mathrm{Q}:=\mathrm{G} \cdot \Omega$ of $(\dagger)$ whose skew-Hermitian Cayley transforms $\mathrm{S}:=\$(\mathrm{G} \cdot \Omega)$ satisfying ( $\ddagger$ ) sweep out a continuum as $\Omega$ runs through all complex unitary diagonal matrices for which $\mathrm{I}+\mathrm{G} \cdot \Omega$ is nonsingular. This continuum happens to include at least one skew $S$ with $\operatorname{diag}(S)=0$ and no huge elements, as we'll see in $\S 3$ and $\S 5$.

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 $\Omega$ is a real diagonal of -1 's and/or +1 's for which the Cayley transform $\$(\mathrm{G} \cdot \Omega)$ exists, it is a real skew matrix with zeros on its diagonal. The Lemma above ensures that some such $\$(\mathrm{G} \cdot \Omega)$ exists. O'Dorney [2014] has proved that at least one such $\$(\mathrm{G} \cdot \Omega)$ has every element between $\pm 1$. Examples in $\S 4$ are on the brink; these are n-by-n real orthogonal matrices $G$ for which every off-diagonal element of every (there are $2^{\mathrm{n}-1}$ of them) such $\$(\mathrm{G} \cdot \Omega)$ is $\pm 1$.

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

## §3: $£(Q)$ Gauges How "Near" a Unitary $\mathbf{Q}$ is to $I$

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

When ( $\mathrm{I}+\mathrm{Q}$ ) is nonsingular, every eigenvalue of unitary Q has magnitude 1 but none is -1 , so matrix $\left(2 \mathrm{I}+\mathrm{Q}+\mathrm{Q}^{-1}\right) / 4=(\mathrm{I}+\mathrm{Q})^{\mathrm{H}} \cdot(\mathrm{I}+\mathrm{Q}) / 4$ 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 $£(\mathrm{Q}) \geq 0$. Only $£(\mathrm{I})=0$. Another way to confirm this is to observe that $f(\mathrm{Q})=\log \left(\operatorname{det}\left(\mathrm{I}-\$(\mathrm{Q})^{2}\right)\right)=\log \left(\operatorname{det}\left(\mathrm{I}+\$(\mathrm{Q})^{\mathrm{H}} . \$(\mathrm{Q})\right)\right)>0($ or $+\infty)$ for every unitary $\mathrm{Q} \neq \mathrm{I}$.
$£(\mathrm{Q})$ and $\$(\mathrm{Q})$ are differentiable functions of Q except at their poles, where $\$(\mathrm{Q})$ is infinite and $£(\mathrm{Q})=+\infty$ because $\operatorname{det}(\mathrm{I}+\mathrm{Q})=0$. The differential of $£(\mathrm{Q})$ is simpler to derive than its derivative is because of Jacobi's formula $d \log (\operatorname{det}(B))=\operatorname{trace}\left(B^{-1} \cdot d B\right)$ and another formula $d\left(B^{-1}\right)=-B^{-1} \cdot d B \cdot B^{-1}$, and because $\operatorname{trace}(B \cdot C)=\operatorname{trace}(C \cdot B)$ whenever both matrix products $B \cdot C$ and $C \cdot B$ are square. By applying these formulas we find that

$$
\begin{aligned}
\mathrm{d} £(\mathrm{~B}) & =-\operatorname{trace}\left(\left(2 \mathrm{I}+\mathrm{B}+\mathrm{B}^{-1}\right)^{-1} \cdot\left(\mathrm{~dB}-\mathrm{B}^{-1} \cdot \mathrm{~dB} \cdot \mathrm{~B}^{-1}\right)\right) \\
& =\operatorname{trace}\left((\mathrm{I}+\mathrm{B})^{-1} \cdot(\mathrm{I}-\mathrm{B}) \cdot \mathrm{B}^{-1} \cdot \mathrm{~dB}\right)=\operatorname{trace}\left(\$(\mathrm{~B}) \cdot \mathrm{B}^{-1} \cdot \mathrm{~dB}\right) .
\end{aligned}
$$

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

Abbreviate $\operatorname{Diag}(\mathrm{x})=\mathrm{X}$ and $\operatorname{Diag}(\mathrm{dx})=\mathrm{dX}$; and note that X and dX commute, so that $\mathrm{d} \Omega=\mathrm{d} e^{\boldsymbol{\imath} \mathrm{X}}=\boldsymbol{t} e^{\boldsymbol{\lambda} \mathrm{X}} \cdot \mathrm{d} \mathrm{X}=\boldsymbol{\imath} \Omega \cdot \mathrm{dX}$, and therefore

$$
\mathrm{d} \mathfrak{f}(\mathrm{Q} \cdot \Omega)=\operatorname{trace}\left(\$(\mathrm{Q} \cdot \Omega) \cdot e^{-\boldsymbol{l} \mathrm{X}} \mathrm{Q}^{-1} \cdot \mathrm{Q} \cdot \boldsymbol{l} e^{\boldsymbol{} \mathrm{X}} \cdot \mathrm{dX}\right)=\boldsymbol{t} \operatorname{diag}(\$(\mathrm{Q} \cdot \Omega))^{\mathrm{T}} \mathrm{dx}
$$

Since this $d £$ must vanish at a minimum of $£$ for every real $d x$, so $\operatorname{diag}(\$(Q \cdot \Omega))=0$ 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 $\Omega$ for which the skewHermitian Cayley transform $\mathrm{S}:=(\mathrm{I}+\mathrm{Q} \cdot \Omega)^{-1} \cdot(\mathrm{I}-\mathrm{Q} \cdot \Omega)=-\mathrm{S}^{\mathrm{H}}$ has $\operatorname{diag}(\mathrm{S})=\mathrm{o}$.

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

$$
\begin{equation*}
\operatorname{det}(\cos (\operatorname{Diag}(\mathrm{x} / 2))-\boldsymbol{\imath} \mathrm{Z} \cdot \sin (\operatorname{Diag}(\mathrm{x} / 2)))=0 \tag{*}
\end{equation*}
$$

Despite first appearances, the left-hand side of this equation is a real function of the real vector x because matrix $\cot (\operatorname{Diag}(\mathrm{x} / 2))-\boldsymbol{\imath} \mathrm{Z}$ 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 $2 \pi$. 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 $\partial £ / \partial \mathrm{x}=\mathrm{o}^{\mathrm{T}}$ ) of $£$ provides another of the theorem's diagonals $\Omega:=e^{\imath \operatorname{Diag}(\mathrm{x})}$. 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 $\Omega$ is infinite in the general complex case, $2^{\mathrm{n}-1}$ in the restricted-to-real case. All these diagonals $\Omega$ minimize $£$; all of them provide skew Cayley transforms $S$ whose $\operatorname{diag}(S)=0$ and whose every off-diagonal element has magnitude 1 . Here is such an example:
Define n-by-n real orthogonal $\mathrm{G}:=\left[\begin{array}{cccccccc}0 & 1 & & & & & & \\ & 0 & 1 & & & & \\ & & \ldots & \ldots & & & \\ & & & \cdots & \ldots & & \\ & & & & 0 & 1 & \\ (-1)^{\mathrm{n}-1} & & & & & 0 & 1 \\ & & & & & & 0\end{array}\right]$, and
let $\Omega$ run through unitary diagonal matrices with $\operatorname{det}(\Omega) \neq-1$. Then unitary $\mathrm{Q}:=\mathrm{G} \cdot \Omega$ has a skew-Hermitian Cayley transform $\mathrm{S}=\$(\mathrm{Q}):=(\mathrm{I}+\mathrm{Q})^{-1} \cdot(\mathrm{I}-\mathrm{Q})=-\mathrm{S}^{\mathrm{T}}$ which, as we shall show, has off-diagonal elements all of the same magnitude $2 /|1+\operatorname{det}(\Omega)|$. Moreover this magnitude is minimized just when $\operatorname{det}(\Omega)=+1$, the minimized magnitude is 1 , and $\operatorname{diag}(S)=0$. In particular, for every real orthogonal diagonal $\Omega$ of $\pm 1$ 's with an even number of -1 's, S is a real skew matrix all of whose off-diagonal elements are $\pm 1$ 's. We'll prove these claims next.

First we must confirm that $\$(\mathrm{Q})$ exists; it will follow from $\Omega^{-1}=\bar{\Omega}$ (the complex conjugate):

$$
\operatorname{det}(\mathrm{I}+\mathrm{Q})=\operatorname{det}(\mathrm{I}+\mathrm{G} \cdot \Omega)=\operatorname{det}(\bar{\Omega}+\mathrm{G}) \cdot \operatorname{det}(\Omega)=(\operatorname{det}(\bar{\Omega})+1) \cdot \operatorname{det}(\Omega)=1+\operatorname{det}(\Omega) \neq 0 .
$$

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

Start by defining the n -vector $\mathrm{u}:=\operatorname{diag}(\Omega)$ so that $\Omega=\operatorname{Diag}(\mathrm{u})$ and the elements of u all have magnitude 1 and product $\operatorname{det}(\Omega)$. Next observe that $G \cdot \operatorname{Diag}(v)=\operatorname{Diag}(G \cdot v) \cdot G$ for any n -vector v . Use this to confirm by induction that
$(\mathrm{G} \cdot \Omega)^{\mathrm{k}}=\operatorname{Diag}(\mathrm{G} \cdot \mathrm{u}) \cdot \operatorname{Diag}\left(\mathrm{G}^{2} \cdot \mathrm{u}\right) \cdot \operatorname{Diag}\left(\mathrm{G}^{3} \cdot \mathrm{u}\right) \cdot \ldots \cdot \operatorname{Diag}\left(\mathrm{G}^{\mathrm{k}} \cdot \mathrm{u}\right) \cdot \mathrm{G}^{\mathrm{k}}$ for each $\mathrm{k}=1,2,3, \ldots$ in turn.
In particular, when $\mathrm{k}=\mathrm{n}$ we find that $\mathrm{Q}^{\mathrm{n}}=(\mathrm{G} \cdot \Omega)^{\mathrm{n}}=(-1)^{\mathrm{n}-1} \cdot \prod_{1 \leq \mathrm{k} \leq \mathrm{n}} \operatorname{Diag}\left(\mathrm{G}^{\mathrm{k}} \cdot \mathrm{u}\right)$. Each
diagonal element of this product includes the product of all the elements of $u$ each once, and their product is $\operatorname{det}(\Omega)$. Factor it out to obtain $Q^{n}=\operatorname{det}(\Omega) \cdot(G \cdot I)^{n}=\operatorname{det}(\Omega) \cdot(-1)^{\mathrm{n}-1} \cdot I$.

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

$$
\$(\mathrm{Q})=(\mathrm{I}+\mathrm{Q})^{-1} \cdot(\mathrm{I}-\mathrm{Q})=\left((1-\operatorname{det}(\Omega)) \cdot \mathrm{I}+2 \sum_{1 \leq \mathrm{k} \leq \mathrm{n}-1}(-1)^{\mathrm{k}} \mathrm{Q}^{\mathrm{k}}\right) /(1+\operatorname{det}(\Omega))
$$

To confirm it multiply by $\mathrm{I}+\mathrm{Q}$ and collect terms. This formula validates every claim uttered above for $\$(\mathrm{Q})$ because every unitary diagonal $\Omega$ has $|\operatorname{det}(\Omega)|=1$.
$\mathfrak{f}(\mathrm{Q})$, the gauge of "nearness" to I , is minimized when $\operatorname{det}(\Omega)=1$ and $\operatorname{diag}(\mathrm{S})=0$ since $\mathfrak{f}(\mathrm{Q})=\mathrm{n} \cdot \log (4)-2 \cdot \log |1+\operatorname{det}(\Omega)| \geq(\mathrm{n}-1) \cdot \log (4)$ with equality just when $\operatorname{det}(\Omega)=1$.

Here is a different example $\left.Q:=\$\left(\begin{array}{ccc}0 & 2 & -2 \\ -2 & 0 & 2 \\ 2 & -2 & 0\end{array}\right]\right)=\left[\begin{array}{ccc}-3 & 4 & 1 \\ 12 & -3 & 4 \\ 4 & 12 & -3\end{array}\right] / 13$. Six unitary diagonals $\Omega$ satisfy the theorem. Four are real: $\Omega=\mathrm{I}, \operatorname{Diag}([-1 ;-1 ; 1]), \operatorname{Diag}([1 ;-1 ;-1])$ and $\operatorname{Diag}([-1 ; 1 ;-1])$.
Typical of the last three is $\$(\mathrm{Q} \cdot \operatorname{Diag}([-1 ; 1 ;-1]))=\left[\begin{array}{ccc}0 & -1 & \frac{1}{2} \\ 1 & 0 & 1 \\ -\frac{1}{2} & -1 & 0\end{array}\right]$; none of them minimizes $£(\mathrm{Q} \cdot \Omega)$.
It is minimized by two complex scalar diagonals $\Omega:=(-5 \pm 12 \imath) \mathrm{I} / 13$ for which respectively $\$(\mathrm{Q} \cdot \Omega)=\left[\begin{array}{cccc}0 & -1-3 \imath & 1-3 l \\ 1-3 \imath & 0 & -3 & -3 l \\ -1-3 l & 1-3 l & 0\end{array}\right] / 4$ 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 $£(\mathbb{Q} \cdot \Omega)$ Makes $\$(Q \cdot \Omega)$ Small.

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

$$
\mathfrak{f}\left(\mathrm{Q} \cdot \Omega \cdot e^{i \Delta \mathrm{X}}\right)=\mathfrak{f}(\mathrm{Q} \cdot \Omega)+(\partial £(\mathrm{Q} \cdot \Omega) / \partial \mathrm{x}) \cdot \Delta \mathrm{x}+\left(\partial^{2} £(\mathrm{Q} \cdot \Omega) / \partial \mathrm{x}^{2}\right) \cdot \Delta \mathrm{x} \cdot \Delta \mathrm{x} / 2+O(\Delta \mathrm{x})^{3}
$$

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

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 $f^{\prime}(x)=\partial f(x) / \partial x$. It must be a row vector since scalar $d f(x)=f^{\prime}(x) \cdot d x$. 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 $\mu$, the chain rule yields a derivative $\mathrm{d} f(\mathrm{x}(\mu)) / \mathrm{d} \mu=f^{\prime}(\mathrm{x}(\mu)) \cdot \mathrm{x}^{\prime}(\mu)$. For any fixed x this $f^{\prime}(\mathrm{x})$ 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 $\partial £\left(\mathrm{Q} \cdot e^{\boldsymbol{l} \operatorname{Diag}(\mathrm{x})}\right) / \partial \mathrm{x}=\boldsymbol{t} \operatorname{diag}(\mathrm{S})^{\mathrm{T}}$.

If $f(x)$ is continuously twice differentiable its second derivative, denoted by $f^{\prime \prime}(x)=\partial^{2} f(x) / \partial x^{2}$, is a symmetric bilinear operator acting upon pairs of vectors in the same space as x . "Symmetric" means $f$ " $(\mathrm{x}) \cdot \mathrm{y} \cdot \mathrm{z}=f$ " $(\mathrm{x}) \cdot \mathrm{z} \cdot \mathrm{y}$ 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 $f^{\prime \prime}(x) \cdot y \cdot z=z^{T} \cdot H(x) \cdot y$. Sometimes we can derive the differential $d f^{\prime}(x) \cdot y=f^{\prime \prime}(x) \cdot y \cdot d x=d x^{T} \cdot H(x) \cdot y$ more easily than the derivative. Such will be the case for the second derivative $\partial^{2} £\left(\mathrm{Q} \cdot e^{\iota \operatorname{Diag}(\mathrm{x})}\right) / \partial \mathrm{x}^{2}$ derived hereunder.

Recall that the differential of the unitary diagonal $\Omega:=e^{\boldsymbol{t}}$ is $\mathrm{d} \Omega=\boldsymbol{\iota} \Omega \cdot \mathrm{dX}$. Then rewrite

$$
\mathrm{S}=\$(\mathrm{Q} \cdot \Omega)=(\mathrm{I}+\mathrm{Q} \cdot \Omega)^{-1}(\mathrm{I}-\mathrm{Q} \cdot \Omega)=2(\mathrm{I}+\mathrm{Q} \cdot \Omega)^{-1}-\mathrm{I}
$$

to see easily why

$$
\begin{aligned}
\mathrm{d} \mathrm{~S} & =-2(\mathrm{I}+\mathrm{Q} \cdot \Omega)^{-1} \cdot \mathrm{Q} \cdot \mathrm{~d} \Omega \cdot(\mathrm{I}+\mathrm{Q} \cdot \Omega)^{-1}=-2 \boldsymbol{\imath}(\mathrm{I}+\mathrm{Q} \cdot \Omega)^{-1} \cdot \mathrm{Q} \cdot \Omega \cdot \mathrm{dX} \cdot(\mathrm{I}+\mathrm{Q} \cdot \Omega)^{-1} \\
& =-\boldsymbol{\imath}(\mathrm{I}+\mathrm{S}) \cdot(\mathrm{I}+\mathrm{S})^{-1} \cdot(\mathrm{I}-\mathrm{S}) \cdot \mathrm{dX} \cdot(\mathrm{I}+\mathrm{S}) / 2=-\boldsymbol{l}(\mathrm{I}-\mathrm{S}) \cdot \mathrm{dX} \cdot(\mathrm{I}+\mathrm{S}) / 2 .
\end{aligned}
$$

Next, $(\partial £(\mathrm{Q} \cdot \Omega) / \partial \mathrm{x}) \cdot \Delta \mathrm{x}=\boldsymbol{\imath} \operatorname{diag}(\mathrm{S})^{\mathrm{T}} \cdot \Delta \mathrm{x}=\boldsymbol{t}$ trace $(\mathrm{S} \cdot \Delta \mathrm{X})$ for any fixed column $\Delta \mathrm{x}$ and therefore

$$
\begin{aligned}
& \left(\partial^{2} £(\mathrm{Q} \cdot \Omega) / \partial \mathrm{x}^{2}\right) \cdot \mathrm{dx} \cdot \Delta \mathrm{x}=\mathrm{d}(\partial £(\mathrm{Q} \cdot \Omega) / \partial \mathrm{x}) \cdot \Delta \mathrm{x}=\boldsymbol{\imath} \mathrm{d} \operatorname{trace}(\mathrm{~S} \cdot \Delta \mathrm{X})=\boldsymbol{\imath} \text { trace }(\mathrm{d} \mathrm{~S} \cdot \Delta \mathrm{X}) \\
& \quad=\boldsymbol{\imath} \operatorname{trace}(-\boldsymbol{\imath}(\mathrm{I}-\mathrm{S}) \cdot \mathrm{dX} \cdot(\mathrm{I}+\mathrm{S}) \cdot \Delta \mathrm{X}) / 2=\operatorname{trace}(\mathrm{dX} \cdot \Delta \mathrm{X}-\mathrm{S} \cdot \mathrm{dX} \cdot \Delta \mathrm{X}+\mathrm{dX} \cdot \mathrm{~S} \cdot \Delta \mathrm{X}-\mathrm{S} \cdot \mathrm{dX} \cdot \mathrm{~S} \cdot \Delta \mathrm{X}) / 2 \\
& \quad=\operatorname{trace}\left(\mathrm{dX} \cdot \Delta \mathrm{X}+\left(\mathrm{S}^{\mathrm{H}} \cdot \mathrm{dX}\right) \cdot(\mathrm{S} \cdot \Delta \mathrm{X})\right) / 2=\mathrm{dx}^{\mathrm{T}} \cdot\left(\mathrm{I}+|\mathrm{S}|^{2}\right) \cdot \Delta \mathrm{x} / 2
\end{aligned}
$$

wherein $|S|^{2}$ is obtained elementwise by substituting $\left|s_{i j}\right|^{2}$ for each element $s_{i j}$ in $S$.
Thus we have derived the first three terms of the Taylor Series expansion

$$
\mathfrak{£}\left(\mathrm{Q} \cdot \Omega \cdot e^{\iota \Delta \mathrm{X}}\right)=£(\mathrm{Q} \cdot \Omega)+\boldsymbol{\imath} \operatorname{diag}(\mathrm{S})^{\mathrm{T}} \cdot \Delta \mathrm{x}+\Delta \mathrm{x}^{\mathrm{T}} \cdot\left(\mathrm{I}+|\mathrm{S}|^{2}\right) \cdot \Delta \mathrm{x} / 4+O(\Delta \mathrm{x})^{3} .
$$

Since $\operatorname{diag}(S)=0$ and $I+|S|^{2}$ must be a positive (semi)definite matrix at a minimum of $£$, every $\left|\mathrm{s}_{\mathrm{ij}}\right| \leq 1$ there. Consequently $\ldots$

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

## §6: Conclusion:

Perturbing a complex Hermitian matrix $H$ changes its unitary matrix $Q$ of eigenvectors to a perturbed unitary $\mathrm{Q} \cdot(\mathrm{I}+\mathrm{S})^{-1} \cdot(\mathrm{I}-\mathrm{S})$ in which the skew-Hermitian $\mathrm{S}=-\mathrm{S}^{\mathrm{H}}$ 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 skewsymmetric, Evan O'Dorney [2014] has proved S can always be chosen to have every element between $\pm 1$. 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<br>Mathematics Dept. \#3840<br>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.

