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Technical Report TR/PA/16/240

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SPECTRAL COUPLING FOR HERMITIAN MATRICES

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Cerfacs Tech. Rep. TR/PA/16/240

Abstract. The report presents the information processing that can be performed by a general hermitian matrix when two of its distinct eigenvalues are coupled, such as $\lambda < \lambda'$, instead of considering only one eigenvalue as traditional spectral theory does. Setting $a = \frac{\lambda+\lambda'}{2} \neq 0$ and $e = \frac{\lambda'-\lambda}{2} > 0$, the information is delivered in geometric form, both metric and trigonometric, associated with various right-angled triangles exhibiting optimality properties quantified as ratios or product of $|a|$ and e. The potential optimisation has a triple nature which offers two possibilities: in the case $\lambda\lambda' > 0$ they are characterised by $\frac{e}{|a|}$ and $|a|e$ and in the case $\lambda\lambda' < 0$ by $\frac{|a|}{e}$ and $|a|e$. This nature is revealed by a key generalisation to indefinite matrices over $\mathbb{R}$ or $\mathbb{C}$ of Gustafson's operator trigonometry.

Keywords: Spectral coupling, indefinite symmetric or hermitian matrix, spectral plane, invariant plane, catchvector, antieigenvector, midvector, local optimisation, Euler equation, balance equation, torus in 3D, angle between complex lines.

1. Spectral coupling

1.1. **Introduction.**

In the work we present below, we focus our attention on the coupling of any two distinct real eigenvalues $\lambda < \lambda'$ of a general hermitian or symmetric matrix A, a coupling called *spectral coupling*. This coupling produces new information about A, of trigonometric and geometric nature based on *triangles*.

Such a coupling can be seen as a self-interference for A, that is an interference of A with itself by means of two of its eigenvalues. The effects of this self-interference for A are generated by vectors in the invariant subspace spanned by the corresponding eigenvectors. Although this seems like a natural line of research, no systematic study of the spectral coupling has been undertaken when the matrix is *indefinite* over $\mathbb{R}$ or $\mathbb{C}$.

On the one hand one finds many scattered results about pairs of eigenvalues for A positive definite in the classic literature [Parlett, 1998, Horn and Johnson, 1985, (chap. 4 and 7)]. In most cases the pair consists of the largest and smallest positive eigenvalues and vectors are usually ignored.

On the other hand, a first attempt to a more systematic approach started in 1968 with the work [Gustafson, 1968] about operator trigonometry vastly expanded in [Gustafson, 2012]. But when applied to matrices this insightful theory leaves room for further development. In the paper we address three issues 1) the matrix is not assumed to be *definite*, 2) Gustafson's *turning* angle $\measuredangle(x, Ax)$, $x \in \mathbb{R}^n$ is interpreted as one instance of *three* relevant angles in a *triangle* based on the data $\lambda < \lambda'$, x and Ax, 3) the question of the geometric definition of an angle between two complex vectors (i.e. two real planes) is considered.

The report serves the following goals: (i) It shows how theory can alleviate the three issues cited above. (ii) It indicates that familiar inequalities about pairs of eigenvalues found in Numerical Analysis and Statistics which seem unrelated are in fact the signature of the existence of deeper *variational principles* applied to functionals defined by A and vectors in $\mathbb{R}^n$ or $\mathbb{C}^n$.

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(iii) It presents a mechanism by which a geometric 2D-image emerges from the complex nD-dynamics of a hermitian matrix when *two* eigenvalues are considered simultaneously rather than *one* only, as this is classically done.

As we fulfil each of these three goals, we uncover new ways by which a hermitian matrix discloses information about the dynamics of its inner potential [Chatelin, 2012, chap. 8].

1.2. **Spectral coupling in the past.** At the bottom of spectral coupling lies the resolution of a quadratic polynomial which is assumed to have two distinct real roots. When the roots are positive, the problem goes back to Sumer four millennia ago.

Let the eigenvalues λ and λ', $\lambda < \lambda'$ be the distinct real roots of the quadratic equation

$$\mu^2 - 2a\mu + g^2 = 0, \quad a = \frac{\lambda + \lambda'}{2}, \;\; g^2 = \lambda\lambda' \tag{1.1}$$

where a is the arithmetic mean and we set $e = \frac{\lambda'-\lambda}{2} > 0$. By assumption $a^2 - g^2 = \frac{1}{4}(\lambda - \lambda')^2 > 0$. Observe that $a^2 = g^2 + e^2 \Leftrightarrow -e^2 \le g^2 \le a^2$ and $g^2 \ge 0 \Leftrightarrow |a| \ge e \ge 0$, $g^2 \le 0 \Leftrightarrow |a| \le e$.

If we have $0 < \lambda < \lambda'$, we associate three types of mean: arithmetic $a = \frac{\lambda+\lambda'}{2}$, geometric $g = \sqrt{\lambda\lambda'}$, harmonic $h = \frac{g^2}{a} = \frac{2\lambda\lambda'}{\lambda+\lambda'}$. The three means which satisfy $0 < \lambda < h < g < a < \lambda'$ are known since Antiquity as the *pythagorean means*.

If A is definite then $g^2 = \lambda\lambda'$ is always positive, i.e. $|a| > e$. By contrast, when A is indefinite, $\lambda\lambda'$ may be nonpositive ($|a| \le e$) leading to $g = 0$ ($|a| = e$) or $|g| = \sqrt{-\lambda\lambda'} > 0$ ($|a| < e$).

Let q and q' be orthonormal eigenvectors associated respectively with λ and λ'. The subspace $\mathbf{M}$ spanned by q and q' is *invariant* under A: any $x \in \mathbf{M}$ is such that $Ax \in \mathbf{M}$. The invariant subspace $\mathbf{M}$ has 2 (resp. 4) real dimensions when A is symmetric (resp. hermitian). The orthonormal projection of A onto $\mathbf{M}$ defines a 2×2 symmetric matrix $A_{\restriction \mathbf{M}}$ whose eigenvalues λ and λ' lie on $\mathbb{R}$ called the spectral line: $A_{\restriction \mathbf{M}}$ is similar to the symmetric matrix $\begin{pmatrix} a & e \\ e & a \end{pmatrix} = P$, $\det P = g^2$.

Let us draw in $\mathbb{R}^2$ the circle Γ centered at $(a, 0)$ with radius e: it passes through $(\lambda, 0)$ and $(\lambda', 0)$ and realises the link between λ and λ' in the plane $\mathbb{R}^2$ called the spectral plane. Such a circle Γ is well-known in continuum mechanics as Mohr's circle. C.O. Mohr proposed in 1882 this circle as a graphical tool to analyse, from the perspective of linear elasticity, the dynamics of the Cauchy stress tensor in 2 and 3D which is symmetric positive definite [Timoshenko, 1983]. The 3D-analysis leads to the tricircle, a figure related to that known to Archimedes and other greek geometers as an *arbelos* [Boas, 2006].

The use of Γ that we propose goes in a different direction, trigonometric rather than mechanical. It is valid whether A is definite or not, real or complex. Its main asset is that it provides a way to build a simple 2D-image of the evolution of Ax as the nD-vector x describes the invariant subspace $\mathbf{M}$. The result is fully original when A is hermitian and x is a *complex* vector in $\mathbb{C}^n$.

In modern times, coupled phenomena are ubiquitous in Science and often they are analysed through spectral theory. It seems therefore worthwhile to study the new information provided by structural coupling inside a hermitian matrix. The value of the paper is primarily in the insight it brings about spectral information processing through eigenvector coupling in nD, in particular about data representation and management.

1.3. **Organisation of the paper.** Section 2 sets the scene for the two aspects of spectral coupling expressed in triangles, related to pairs of eigen*values* (λ, λ') in $\mathbb{R}^2$ and of eigen*vectors* (q, q') in $\mathbb{R}^n$ generating an invariant plane $\mathbf{M}$. With the ground field $K = \mathbb{R}$, Section 3 establishes the link between right-angled triangles and local optimisation in $\mathbf{M} \subset \mathbb{R}^n$ of 3 distinct functionals over $\mathbb{R}^n$. In Section 4 with $K = \mathbb{R}$ or $\mathbb{C}$, 3 variational principles are derived from a unique generic functional $K^n \to \mathbb{R}$. Section 5 develops further one of the classes of optimisers found in Section 4. We show how spectral coupling enriches the geometric understanding of inequalities due to Wielandt, Kantorovich and Greub-Rheinboldt in Numerical Analysis, as well as of the Bloomfield-Watson inequality in Statistics. Section 6 presents for $K = \mathbb{C}$ a geometric interpretation in $\mathbb{R}^3$ of the optimality results taking place in the complex invariant subspace $\mathbf{M}$ isomorphic to $\mathbb{R}^4$. The paper closes in Section 7 by summarising the salient features of spectral coupling that have been demonstrated.

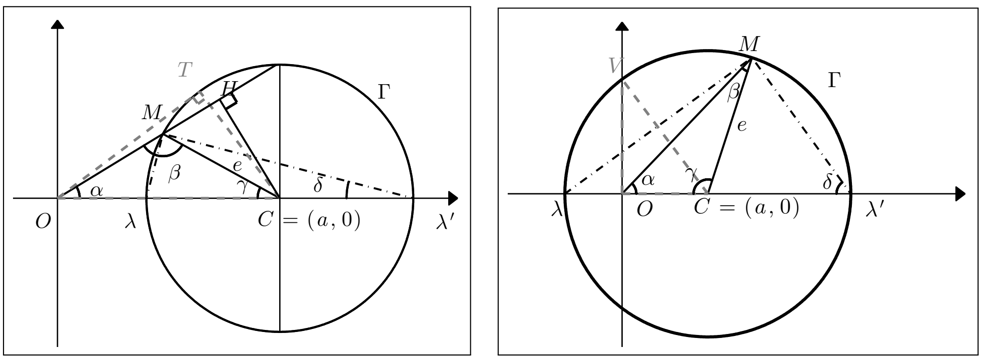
2. Spectral information processing

Let $A \in K^{n\times n}$, $K = \mathbb{R}$ or $\mathbb{C}$, be a symmetric ($K = \mathbb{R}$, $A = A^T$) or hermitian ($K = \mathbb{C}$, $A = A^H$) matrix . The spectrum of A consists of n real eigenvalues $\lambda_1 \leq \ldots \leq \lambda_n$ lying on the spectral line $\mathbb{R}$. If $A \neq \lambda I$, the spectrum contains at least two distinct eigenvalues. The matrix A is diagonalisable in the eigenbasis $Q = [q_1, \ldots, q_n]$, with $Q^{-1} = Q^H$ if $K = \mathbb{C}$ and $Q^{-1} = Q^T \in \mathbb{R}^{n\times n}$ if $K = \mathbb{R}$. We denote $\langle x, y\rangle = x^H y$ or $x^T y$ and $\|x\|^2 = x^H x$ or $x^T x$. For the sake of simplicity we consider in Sections 2.2 and 3 only the case $K = \mathbb{R}$. The treatment of $K = \mathbb{C}$ (A hermitian) is deferred to Sections 4, 5 and 6.

The information processing takes place in the Spectral plane $\cong \mathbb{R}^2$ (Section 2.1) and the Invariant plane $\subset \mathbb{R}^n$ (Section 2.2).

2.1. **Spectral plane,** $K = \mathbb{R}$ **or** $\mathbb{C}$**.** Let be given the pair $\{\lambda, \lambda'\}$, $\lambda < \lambda'$ lying on the spectral line. We consider the circle Γ centered at C, $\overline{OC} = a$ with radius e, which passes through the points $(\lambda, 0)$ and $(\lambda', 0)$ and lies in the spectral plane, see Figure 1. Depending on the sign of $g^2 = \lambda\lambda'$, the origin O is outside Γ ($g^2 > 0$), Figure 1 (a), on Γ ($g = 0$) or inside Γ ($g^2 < 0$), Figure 1 (b). g^2 is the *power* of O with respect to Γ. The circle Γ can be thought of as a *linking curve* between the isolated eigenvalues λ and λ', a curve specifying a plane where elementary geometric constructions and trigonometric calculations can be performed.

Assuming that $ae \neq 0$ ($\lambda' \neq \pm\lambda$), we consider M a point lying on Γ and the corresponding triangle OMC. Two of the side lengths are fixed: $OC = |a|$ and $MC = e$, while the third length OM varies with M. We denote the three *ordinary* angles of OMC as follows: $\alpha = \angle(OC, OM)$, $\beta = \angle(MC, MO)$ and $\gamma = \angle(CO, CM)$. For future reference, we also introduce $\delta = \frac{\gamma}{2} = \angle(\Lambda'\Lambda, \Lambda'M)$, $0 < \delta < \frac{\pi}{2}$ ($\Lambda = (\lambda, 0)$, $\Lambda' = (\lambda', 0)$). See Figure 1. We recall that $\alpha + \beta + \gamma = \pi$ and $\frac{\sin\alpha}{e} = \frac{\sin\beta}{|a|} = \frac{\sin\gamma}{OM}$, hence the ratio $\frac{\sin\alpha}{\sin\beta} = \frac{e}{|a|}$ is fixed.



(a) $\lambda'\lambda > 0$ (b) $\lambda'\lambda < 0$

Figure 1. Spectral plane, $|\lambda| = 0.2$, $\lambda' = 0.8$

2.2. **Invariant plane,** $K = \mathbb{R}$**.** Let q and q' be an orthonormal pair of eigenvectors associated with λ and λ': $\|q\| = \|q'\| = 1$ and $\langle q, q'\rangle = q^T q' = 0$. The subspace of real linear combinations of q and q' is a real plane invariant under the action of A when $K = \mathbb{R}$. It is worth to keep in mind that we work with matrices of dimension $n \times n$ so that the corresponding invariant plane in $\mathbb{R}^n$ is isomorphic to $\mathbb{R}^2$.

We consider the real combination $u = (\cos\theta)q + (\sin\theta)q'$, with unit norm $\|u\| = 1$, $\theta \in [0, 2\pi[$. When θ varies in $[0, 2\pi[$, the vector u describes the unit circle $(\mathcal{C})$ centered at O and passing through the eigenvectors $\pm q$, $\pm q'$, see Figure 2 (a).

A key matrix for spectral coupling is the locally centered matrix $B = A - aI$ (see Figure 2 (a)), a matrix which commutes with A: $F = AB = BA = A^2 - aA$ and which has the following property.

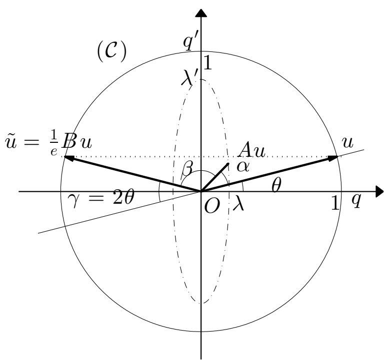
Lemma 2.1. $\|Bu\| = e$ *and* $\|Fu - e^2 u\| = |a|e$ *for any* $u \in (C)$.

Proof. $Bu = \cos\theta(\lambda - a)q + \sin\theta(\lambda' - a)q = e\tilde{u}$ with $\tilde{u} = -q\cos\theta + q'\sin\theta$, $\|\tilde{u}\| = 1$, $\langle u, \tilde{u}\rangle = -\cos 2\theta$. Hence $\|Bu\| = e$ for any θ. Next $Fu - e^2 u = ea\tilde{u}$. □

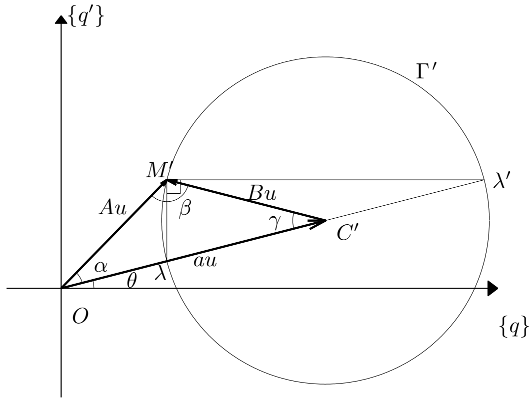
When u is not an eigenvector ($\theta \notin \{0, \frac{\pi}{2}, \frac{3\pi}{2}, \pi\}$) and $a \neq 0$, the 3 vectors au, Au and Bu are linearly independent. Since $Bu = Au - au$ they form a non degenerate triangle $OM'C'$, see Figure 2 (b) when $a > e$ and (c) when $a < e$. In order that $OM'C'$ be non degenerate ($C' \neq O$), we assume below that $a \neq 0$ when $g^2 < 0$. As θ varies in $[0, 2\pi]$, M' describes the ellipse given in

Lemma 2.2. *The point* $M' = (r, r')$ *describes the ellipse of equation* $\left(\frac{r}{\lambda}\right)^2 + \left(\frac{r'}{\lambda'}\right)^2 = 1$ *iff* $g^2 \neq 0$. *The ellipse is reduced to a segment, if* $g^2 = 0$ *and to a circle if* $a = 0$.

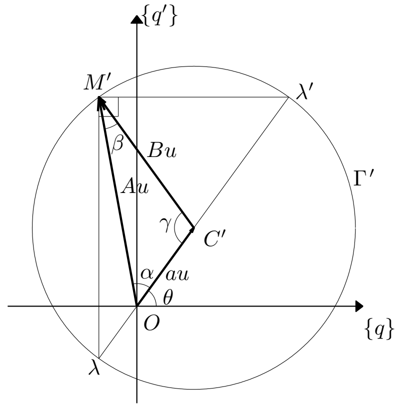
Proof. $Au = \lambda\cos\theta q + \lambda'\sin\theta q' = rq + r'q'$, hence $\cos^2\theta + \sin^2\theta = 1 = \left(\frac{r}{\lambda}\right)^2 + \left(\frac{r'}{\lambda'}\right)^2$ when $\lambda\lambda' \neq 0$. See Figure 2 (a). If $g^2 = 0$, $\lambda = 0 < \lambda'$, $r = 0$ and $r' \in [-\lambda', \lambda']$ (say). The ellipse is the cercle centered at $O = C'$ with radius e if $a = 0 \Leftrightarrow \lambda' = -\lambda = e$. □



(a)



(b) $\lambda'\lambda > 0$



(c) $\lambda'\lambda < 0$

FIGURE 2. Invariant plane, $|\lambda| = 0.2$, $\lambda' = 0.8$, $K = \mathbb{R}$

A remarkable consequence is that the spectral information processing in the spectral plane is mirrored in the invariant plane. Indeed if we compare the triangle OMC parameterised by δ and the triangle $OM'C'$ parameterised by θ we obtain the following result.

Corollary 2.3. *The equality $\delta = \theta$ in $]0, \frac{\pi}{2}[$ yields the congruence $OMC = OM'C'$.*

Proof. The triangles have two fixed side lengths $OC = OC' = |a|$ and $CM = C'M' = e$. Each pair of sides envelops the same (ordinary) angle γ if $\delta = \theta$ in $]0, \frac{\pi}{2}[$: $\gamma = 2\theta = 2\delta \in]0, \pi[$.

□

Therefore we denote the angles of the triangle $OM'C'$ by $\alpha = \angle(u, Au)$, $\beta = \angle(Au, Bu)$, $\gamma = \angle(-au, Bu)$. When M' describes its ellipse once in the invariant plane, θ varies in $[0, 2\pi[$. This entails that the corresponding point M describes its circle Γ *twice* in the spectral plane. The reference triangle OMC in the spectral plane has only one moving vertex M. By comparison, in the invariant plane both vertices M' and C' evolve for $OM'C'$.
Let Γ' be the circle (C', e) which intersects its diameter line OC' at the points λ and λ' (Fig.2 (b), (c)). The evolution of M on Γ is equivalent to that of M' on Γ'. Observe that the sides $M'\lambda$ and $M'\lambda'$ of the right-angled triangle $\lambda M'\lambda'$ inscribed in Γ' are parallel to the eigenvectors q' and q respectively.

Remark 2.1. The Figures presented in Sections 2 and 3 are computed with the numerical data $\lambda = 0.2$ and $\lambda' = 0.8$ when $\lambda'\lambda > 0$ and $\lambda = -0.2$ and $\lambda' = 0.8$ when $\lambda'\lambda < 0$. Thus we can observe the congruence between the triangles OMC in the spectral plane and the triangles $OM'C'$ in the invariant plane, Figure 1 (a) and Figure 2 (b) when $\lambda\lambda' > 0$ and Figure 1 (b) and Figure 2 (c) when $\lambda\lambda' < 0$. The only difference lies in the graphical scaling which was found necessary to get a clear enough figure.

3. Right-angled triangles for optimality, $K = \mathbb{R}$

In the previous section we introduced how the spectral information processing can be observed in the spectral plane and in the invariant plane. In this section we show that the possibility for one of the three angles α, β and γ to equal $\frac{\pi}{2}$ expresses one of three kinds of optimal property.

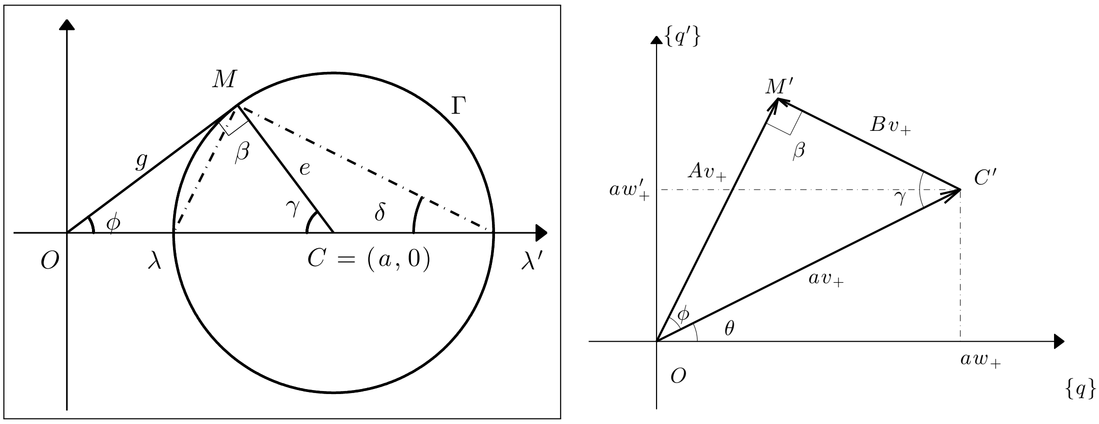
3.1. $g^2 > 0$, $\beta = \frac{\pi}{2}$, α maximum, catchvectors.

When $\beta = \frac{\pi}{2}$, the optimality property corresponds to the maximisation of the angle α when $g^2 = \lambda'\lambda > 0$. In the spectral plane the optimality result illustrated in Figure 3 (a) is given by the

Lemma 3.1. *When $0 < g^2 < a^2$, the angle α is maximum at the value ϕ with $\sin\phi = \frac{e}{|a|}$, $\cos\phi = \frac{|g|}{a}$ and $\alpha = \phi < \frac{\pi}{2} \Leftrightarrow \beta = \psi = \frac{\pi}{2}$, $\gamma = \frac{\pi}{2} - \phi$.*

Proof. Elementary trigonometry. $CH \leq CT = e$, see Figure 1 (a). The angle α is maximum at the value ϕ when the secant line OM is tangent to Γ at T . Then $OT^2 + e^2 = a^2$, $OT = g$, $\cos\phi = \frac{OT}{|a|} = \frac{g}{|a|} = \sin\gamma$.

□



(a) Spectral plane (b) Invariant plane

FIGURE 3. $\lambda'\lambda > 0$, $\alpha = \phi$ maximum, $\beta = \frac{\pi}{2}$, v_+: catchvector

The key Corollary 2.3 allows us to transfer the optimality results of Lemma 3.1 about the triangle OMC in the spectral plane to the triangle $OM'C'$ in the invariant plane, see Figure 3 (b). The optimality property $\alpha \le \phi$ ($g^2 > 0$) is valid for the corresponding ordinary angles $\alpha = \angle(u, Au)$ in $OM'C'$. When $g^2 > 0$, we define w_+ and w'_+ as the positive square roots of $w_+^2 = \frac{\lambda'}{\lambda+\lambda'} > 0$ and $w_+'^2 = \frac{\lambda}{\lambda+\lambda'} > 0$. Indeed $\lambda'(\lambda+\lambda') = \lambda'^2 + g^2$ and $\lambda(\lambda+\lambda') = \lambda^2 + g^2$ are positive quantities.

Then we define the set of four *catchvectors* (see Figure 3 (b))

$$D_+ = \left\{v_+ \ : \ v_+ = \varepsilon w_+ q + \varepsilon' w'_+ q', \ \ \varepsilon = \pm 1, \ \ \varepsilon' = \pm 1\right\}$$

which are the maximisers for α.

Theorem 3.2. *When $g^2 > 0$, the minimum value $\cos\phi = \frac{g}{|a|}$ is achieved by any v_+ in D_+ and $\langle Bv_+, Av_+\rangle = 0$, $\|Av_+\| = \frac{1}{e}\|Fv_+\| = g$.*

Proof. i) When $g^2 > 0$ and $v_+ = w_+q + w'_+q'$, $Av_+ = \lambda w_+ q + \lambda' w'_+ q'$, $Bv_+ = e(-w_+q + w'_+q')$ and $BAv_+ = e(-\lambda w_+ q + \lambda' w'_+ q')$. Therefore $\|Av_+\| = g$, $\langle v_+, Av_+\rangle = \frac{g^2}{a}$, hence $\cos\angle(v_+, Av_+) = \frac{g}{a}$. ($|\cos\alpha| \ge \cos\phi = \frac{g}{|a|}$). Moreover $\langle Bv_+, Av_+\rangle = 0$ as expected. The vector $\frac{1}{|a|}Fv_+$ is orthogonal to v_+ with length $\frac{eg}{|a|}$.

□

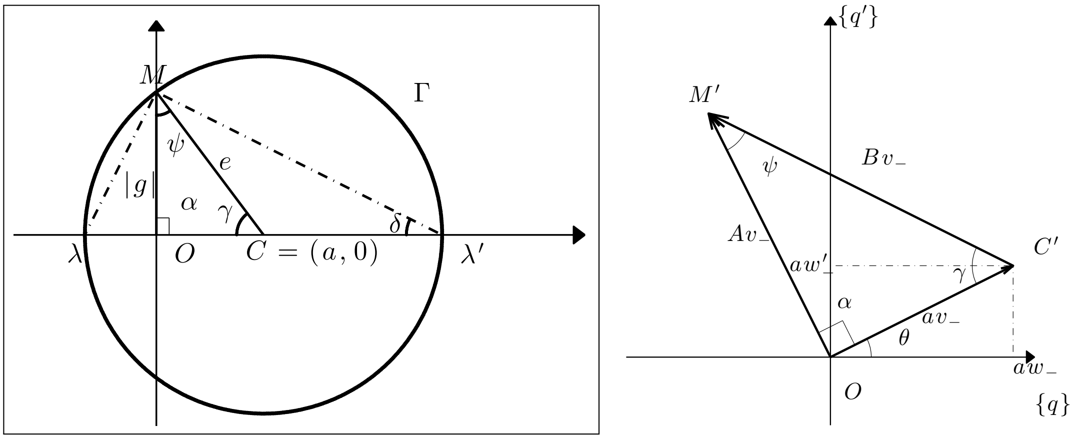
Choosing the pair $\lambda < \lambda'$ at will provides a local optimisation in general. It is well known that a global optimisation can be obtained if we consider a symmetric *positive definite* matrix A with eigenvalues $0 < \lambda_1 \le \ldots \le \lambda_n$ and we couple the extreme pair (λ_1, λ_n). The resulting largest turning angle $\phi(A)$ is called the operator/matrix angle in [Gustafson, 1968].

3.2. $g^2 < 0$, $\alpha = \frac{\pi}{2}$, β **maximum, antieigenvectors.** Letting $\alpha = \frac{\pi}{2}$ when $\lambda\lambda' < 0$ we get the second optimality property yielding the maximisation of the angle β. In the spectral plane we have the following result displayed on Figure 4 (a).

Lemma 3.3. *When $-e^2 < g^2 < 0$, the angle β is maximum at the value ψ with $\sin\psi = \frac{|a|}{e}$, $\cos\psi = \frac{|g|}{e}$ and $\beta = \psi \Leftrightarrow \alpha = \phi = \frac{\pi}{2}$, $\gamma = \frac{\pi}{2} - \psi$.*

Proof. $CH \le CO = |a| > 0$, see Figure 1 (b). The angle β is maximum at the value ψ when the line OM is orthogonal to the spectral axis, and intersects Γ at V . Then $OV^2 + a^2 = e^2$ and $OV = |g|$, $\cos\psi = \frac{|g|}{e} = \sin\gamma$.

□



(a) Spectral plane (b) Invariant plane

FIGURE 4. $\lambda'\lambda < 0$, $\alpha = \frac{\pi}{2}$, $\beta = \psi$ maximum, v_- : antieigenvector

Once more, thanks to the key Corollary 2.3, we are able to transfer the results of Lemma 3.3 about the triangle OMC in the spectral plane to the triangle $OM'C'$ in the invariant plane, see Figure 4 (b). We define w_- and w'_- as the positive square roots of $w_-^2 = \frac{\lambda'}{\lambda'-\lambda}$ and $w'^2_- = -\frac{\lambda}{\lambda'-\lambda}$, after we check that $\lambda'(\lambda'-\lambda) = \lambda'^2 - g^2 > 0$ and $-\lambda(\lambda'-\lambda) = \lambda^2 - g^2 > 0$.

In this case we define the set of four *antieigenvectors* (see Figure 4 (b))

$$D_- = \left\{v_- \ : \ \varepsilon w_- q + \varepsilon' w'_- q',\ \varepsilon = \pm 1,\ \varepsilon' = \pm 1\right\}$$

which are the maximisers for β.

Theorem 3.4. *When $g^2 < 0$, the minimum value $\cos\psi = \frac{|g|}{e}$ is achieved by any v_- in D_- and $\langle v_-, Av_-\rangle = 0$, $\|Av_-\| = \frac{1}{e}\|Fv_-\| = |g|$.*

Proof. When $g^2 < 0$ and $v_- = w_- q + w'_- q'$, $Av_- = \lambda w_- q + \lambda' w'_- q'$ and $\|Av_-\| = |g| = \sqrt{-\lambda\lambda'}$; $Bv_- = e(-w_- q + w'_- q')$ and $\langle Bv_-, Av_-\rangle = -g^2 = |g|^2$. Thus $\cos\angle(Bv_-, Av_-) = \frac{|g|}{e}$, that is $\cos\beta \geq \cos\psi = \frac{|g|}{e}$. Finally $\langle v_-, Av_-\rangle = 0$ and $\frac{1}{|a|}Fv_-$ is orthogonal to Bv_- with length $\frac{e|g|}{|a|}$. □

Remark 3.1. When A is *indefinite*, the spectral coupling of eigenvalues with different sign: $\lambda < 0 < \lambda'$ yields the existence of the vectors v_- in D_- with an orthogonal image Av_-: $\langle v_-, Av_-\rangle = 0$. These vectors which exist only for $\lambda\lambda' < 0$, are out of the scope of [Gustafson, 2012]. They are actually the vectors which are "most turned" by A locally in the invariant plane: their image direction, being orthogonal to, is the "furthest" from, their own direction. This is why they truly deserve to be called *antieigenvectors*. Their dynamics under A is the opposite of that for an eigenvector, whose direction is invariant under the action of A. Therefore, to avoid ambiguity we called the vectors v_+ in D_+ when $g^2 > 0$ *catchvectors*.

The striking similarity between the formulae for v_+ ($g^2 > 0$) and v_- ($g^2 < 0$) suggests that the triple $(\lambda, -\lambda, \lambda')$ is *implicitly* at work when $a \neq 0$. The companion pair $(-\lambda, \lambda')$ is the spectrum of the 2×2 matrix $\tilde{P} = \begin{pmatrix} e & |a| \\ |a| & e \end{pmatrix}$, $\det \tilde{P} = -g^2$. The matrix $\tilde{P}$ is similar to the projection on $\mathbf{M}$ of the *modified* matrix $\tilde{A} = Q\tilde{D}Q^T$: in the original diagonal D of eigenvalues for A, λ is replaced by $-\lambda$ to yield $\tilde{D}$ so that $\|A - \tilde{A}\|_2 = \|D - \tilde{D}\|_2 = 2|\lambda|$. An antieigenvector v_- for A is a catchvector $\tilde{v}_+$ for $\tilde{A}$ and vice-versa, depending on the sign of g^2. The symmetry $\lambda / -\lambda$ entails the symmetry catch-/antieigen- vectors.

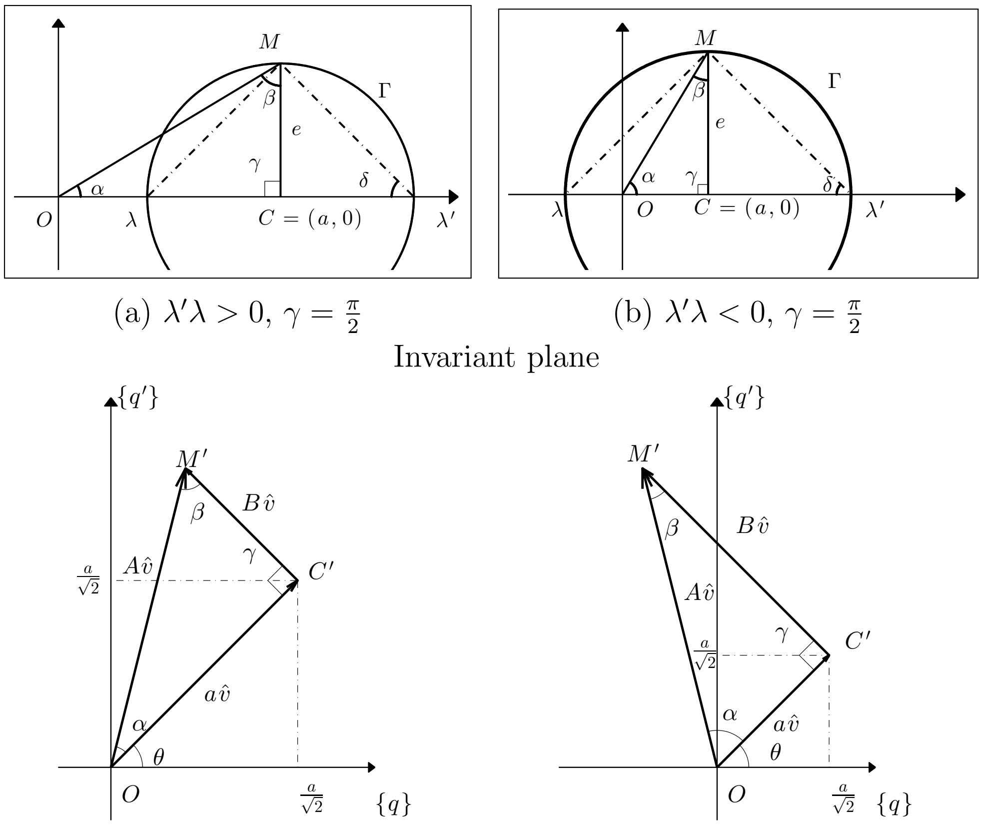
3.3. $\gamma = \frac{\pi}{2}$, **maximal surface, midvectors.** The previous sections have dealt with the orthogonality $\beta = \frac{\pi}{2}$ when $g^2 > 0$ and $\alpha = \frac{\pi}{2}$ when $g^2 < 0$. We turn to the third angle $\gamma = 2\theta$.

When $\gamma = \frac{\pi}{2}$, the third optimality result concerns the surface of the triangles OMC and $OM'C'$. In the spectral plane we have the following result.

Lemma 3.5. *When M describes Γ and $a \neq 0$, the surface of OMC is maximum and equal to $\frac{1}{2}|a|e$ iff $\gamma = \frac{\pi}{2}$.*

Proof. Clear since the surface of OMC is the unsigned area $\frac{1}{2}|a|e \sin\gamma$ with $|a|e = \frac{1}{4}|\lambda'^2 - \lambda^2|$. The maximum is achieved for M at (a, e) so that $OM = \sqrt{a^2 + e^2}$, see Figure 5 (a) and (b). If $a = 0$, OMC is degenerate. □

Spectral plane



(a) $\lambda'\lambda > 0$, $\gamma = \frac{\pi}{2}$ (b) $\lambda'\lambda < 0$, $\gamma = \frac{\pi}{2}$

Invariant plane

(c) $\lambda'\lambda > 0$, $\hat{v}$ midvector (d) $\lambda'\lambda < 0$, $\hat{v}$ midvector

FIGURE 5. Maximal surface, $\gamma = \frac{\pi}{2}$, $g^2 \neq 0$

Now we define the set of four *midvectors* (see Figure 5 (c) and (d))

$$\hat{D} = \left\{ \hat{v} \ : \ \hat{v} = \hat{w}(\varepsilon q + \varepsilon' q'), \ \hat{w} = \frac{1}{\sqrt{2}}, \ \varepsilon = \pm 1, \ \varepsilon' = \pm 1 \right\},$$

and we consider $\gamma = \angle(-au, Bu)$ for $a \neq 0$.

Lemma 3.6. *The minimum value* 0 *is achieved for* $\cos\gamma$*, $a \neq 0$, at $\hat{v} = \frac{1}{\sqrt{2}}(q + q')$.*

Proof. $\langle au, Bu \rangle = ae\langle u, \tilde{u} \rangle = 0 \Leftrightarrow \theta = \frac{\pi}{4} \Leftrightarrow \cos\theta = \sin\theta = \frac{1}{\sqrt{2}} \Leftrightarrow \gamma = \frac{\pi}{2}$. □

Theorem 3.7. *When $a \neq 0$, the 4 triangles $OM'C'$, $\hat{v} \in \hat{D}$, have the maximal surface $\frac{1}{2}|a|e$.*

Proof. The surface of the triangle OMC is $\Sigma(u) = \frac{1}{2}|a|e \sin\gamma$ which achieves its maximum for $u = \hat{v} \Leftrightarrow \gamma = \frac{\pi}{2}$. □

We leave it to the reader to check that for $\hat{V} = [\hat{v}_+, \hat{v}_-]$ with $\hat{v}_\pm = \frac{1}{\sqrt{2}}(q' \pm q)$, the matrix P in Section 1.2 satisfies $P = \hat{V}^T A \hat{V}$, $\hat{V}^T \hat{V} = I_2$.

If for a symmetric positive definite matrix A we couple the extreme pair (λ_1, λ_n) we can easily deduce that the midvectors associated to the eigenvalues λ_1, λ_n yield the maximum surface $a_* e_* = \frac{1}{4}(\lambda_n^2 - \lambda_1^2)$ for $OM'C'$.

Let us consider in $\mathbb{R}^3$ the vector product of $u = (\cos\theta, \sin\theta, 0)^T$ and $\tilde{u} = (-\cos\theta, \sin\theta, 0)^T$: $u \wedge \tilde{u} = (0, 0, 2\sin\theta\cos\theta = \sin 2\theta)^T$. The quantity $2\Sigma(u)$ measures the vector product $\mathfrak{K} = au \wedge Bu = au \wedge Au = Au \wedge Bu = aeu \wedge \tilde{u}$ which lives in $\mathbf{M}^\perp$. The vector $\mathfrak{K}$ is the vector product of any two adjacent sides in $OM'C'$; it represents the action of the coupling *outside* the invariant plane. Its direction is fixed in $\mathbf{M}^\perp$; if $n = 3$, it is but the third eigendirection. The norm $\|\mathfrak{K}\| = |a|e \sin\gamma$ is called the *influence* of u outside its plane of evolution. In other words, the vertices of $OM'C'$ are submitted to an equal torque as the triangle rotates about O. The torque is nonzero when $OM'C'$ is non degenerate ($u \notin \{\pm q, \pm q'\}$ and $ae \neq 0$). The subtle role of $-\lambda$ shows in the fact that there is disconnection ($\mathfrak{K} = 0$) if the eigenpair is either double ($\lambda = \lambda' = a$) or opposite ($\lambda = -\lambda' = -e$)

When comparing $D_\pm$ and $\hat{D}$, we observe that the vectors $\hat{v}$ are *independent* of the values $\lambda < \lambda'$. These vectors are called *midvectors* since they are the bisectors of the eigenvectors. They have the largest influence $|a|e$: the larger the product $|a|e$, the tighter the bond between the pair (λ, λ') and the rest of the spectrum. Moreover Lemma 2.1 tells us that the maximal *surface* $|a|e$ is precisely the *norm* of $Fu - e^2 u$ for any $u \in (C)$. By comparison the influence of v_+ is eg and that of v_- is $|ag|$.

Remark 3.2. The generic concept of a midvector is absent from Gustafson's theory which focuses on α when $g^2 > 0$. The notion only appears in a statistical setting under the guise of an "inefficient" vector, see Section 5 and [Gustafson, 2012, p. 190].

3.4. **Case $g^2 = \lambda'\lambda = 0$, $|a| = e > 0$.** Let us study the case $|a| = e$. The triangle OMC is isosceles with $\alpha = \beta$, see Figure 6 (a). It is right-angled at C ($\gamma = \frac{\pi}{2}$) with maximal surface $\frac{1}{2}e^2$ if M is at (a, e) and $\hat{\alpha} = \hat{\beta} = \frac{\pi}{4}$ ($\tan\hat{\alpha} = \tan\hat{\beta} = 1$). The triangle OMC is equilateral if $\alpha = \beta = \gamma = \frac{\pi}{3}$, $\delta = \frac{\pi}{6}$, see Figure 6 (b). It is degenerate as OC when $\alpha = \beta = \frac{\pi}{2}$, $\gamma = 0$. Thanks to Corollary 2.3 we can transfer these results on the spectral plane to the invariant plane where now M' describes the segment $[-\lambda', \lambda']$ if $\lambda = 0 < \lambda' = 2a$, see Figure 6 (c) and (d). Let $N' = (2a\cos\theta, 2a\sin\theta)$. It is clear that M' is the orthogonal projection of N' on the vertical axis spanned by q'. Hence $OM' = \|Au\| = 2|a\sin\theta|$. When $\theta = \frac{\pi}{6}$, $\|Au\| = |a|$, confirms that $OM'C'$ is equilateral. If $\lambda = 2a < 0 = \lambda'$, M' corresponds to an orthogonal projection on $\{q\}$.

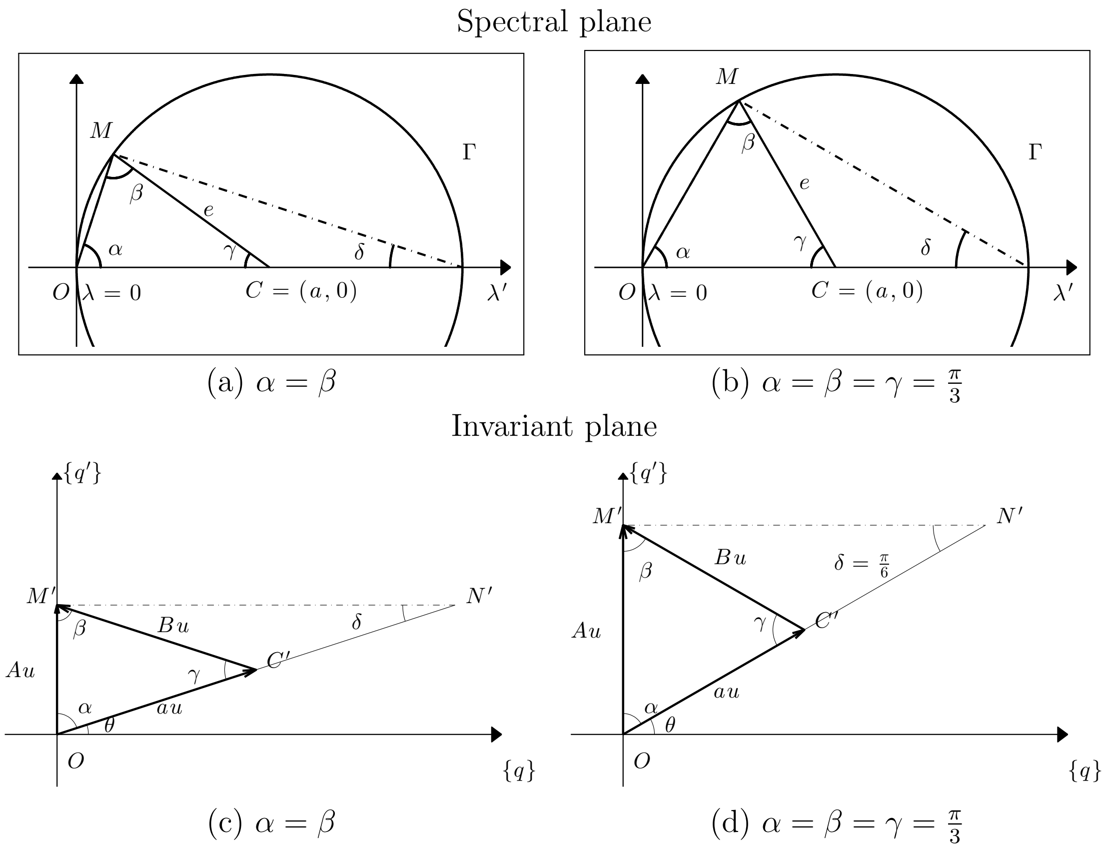


FIGURE 6. $\lambda = 0 < \lambda' = 2a$

3.5. **Summary.** The congruence between the triangles OMC in the spectral plane and $OM'C'$ in the invariant plane is a key property for *symmetric* matrices. It allows the dynamics of eigenvector coupling to be reflected in the spectral plane without any loss of information. The triple nature of the optimal results when $g^2 \neq 0$, $a \neq 0$ is summarised in Figure 7.

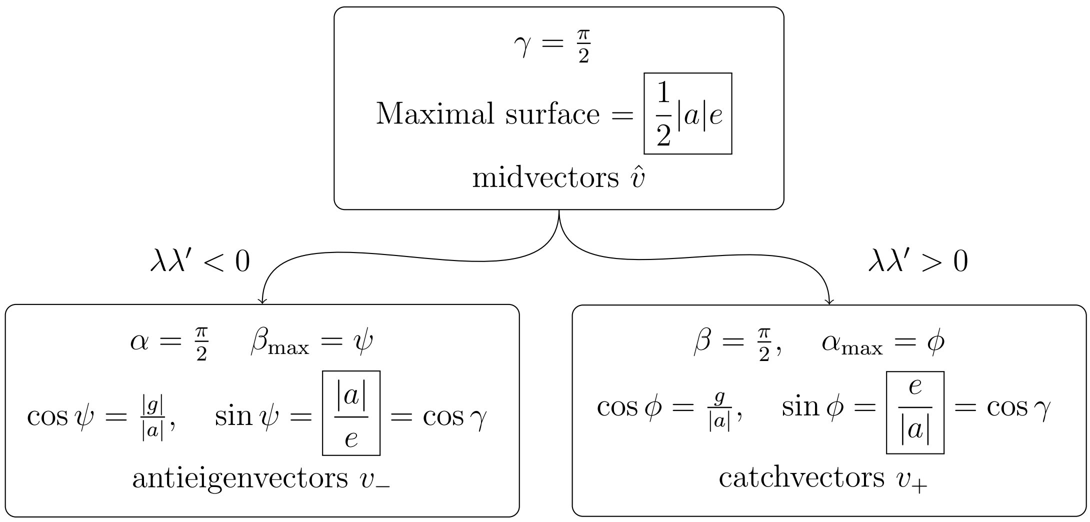


FIGURE 7. Right angles for optimality, $\lambda < \lambda'$, $ag^2 \neq 0$, $K = \mathbb{R}$

From the point of view of information theory, the eigenvectors q and q' define the reference frame in $\mathbf{M} \cong \mathbb{R}^2$ for the dynamics of spectral coupling. They serve to define the midvectors which are independent of $\pm\lambda$ and λ'. The numerical data $|a| = \frac{|\lambda'+\lambda|}{2}$ and $e = \frac{\lambda'-\lambda}{2}$ are sufficient to describe the evolution in $\mathbf{M}$ specific to the pair (λ, λ'). When $ae \neq 0$, the 3 numbers λ, $-\lambda$, λ' are distinct. Thus the primary angle in the data processing is $\gamma = \angle(-au, Bu)$ with

$B = A - aI$ which is well-defined. The associated functional $\cos\gamma$ is 0 for $\gamma = \frac{\pi}{2}$. This signals that triangles with maximal surface are realised by midvectors $\hat{v}$ such that $\hat{\mathfrak{K}} = a\hat{v} \wedge B\hat{v}$ in $\mathbb{R}^3$ has maximal length $|a|e$. Whichever ratio $\frac{e}{|a|}$ or $\frac{|a|}{e}$ is less than 1 yields the value $\cos\gamma$ associated with the optimality of the secondary angles: $\alpha_{\max} = \phi$, $\beta = \frac{\pi}{2}$ or $\beta_{\max} = \psi$, $\alpha = \frac{\pi}{2}$ respectively. Now the associated maximisers, either v_+ or v_-, do depend on the values λ and λ'.

4. Variational principles, $K = \mathbb{R}$ or $\mathbb{C}$

Now let us turn to the variational principles that are associated to the catchvectors and antieigenvectors (and possibly to the midvectors) presented in the previous Section with the extension to the ground field $K = \mathbb{C}$, when A is an arbitrary hermitian matrix, $A = A^H \in \mathbb{C}^{n\times n}$.

For any hermitian matrix Y, the ratio $\frac{x^H Y x}{\|x\|\|Yx\|}$ is real in $[-1, 1]$ for any $0 \neq x \in \mathbb{C}^n$. When $x \in \mathbb{R}^n$, the ratio can be interpreted as $\cos\measuredangle(x, Yx)$ thanks to Cauchy's inequality. Because x defines a real direction, the angle $\mathcal{Y}(x) = \measuredangle(x, Yx)$ is a *direction* (or rotation) angle defined mod 2π between the directions spanned by the *real* unit vectors $\frac{x}{\|x\|}$ and $y = \frac{Yx}{\|Yx\|}$. Such a geometric interpretation is not readily available for A hermitian since $x \in \mathbb{C}^n$. In particular the number Arcos $\frac{|\langle x,y\rangle|}{\|x\|\|y\|}$ in $[0, \frac{\pi}{2}]$ which is commonly referred to as angle(x, y) is of an *analytic*, rather than geometric, nature. The question is discussed further in Section 6.

To avoid any ambiguity we use two *distinct* notations to represent an "angle" according to K:

- $K = \mathbb{R}^n$, $\mathcal{Y}(x) = \measuredangle(x, Yx) \in [0, 2\pi]$ with geometric *and* analytic meaning,
- $K = \mathbb{C}^n$, angle$(x, y) \in [0, \frac{\pi}{2}]$ with analytic meaning only.

4.1. **A preparatory Lemma.** Let us start with a preparatory lemma which will allow us to set some of the results of Section 3 in terms of variational principles. Let be given two hermitian matrices Y and Z, the product YZ is hermitian iff Y and Z commute. We consider the real functional

$$c(x) \;=\; \frac{x^H Y Z x}{\|Yx\|\|Zx\|} \in \mathbb{R}, \quad 0 \neq x \in K^n \setminus (\mathrm{Ker}\, Y \cup \mathrm{Ker}\, Z) \tag{4.1}$$

where Y and Z are hermitian and commute: $YZ = ZY$. Thus $|c(x)| = \cos(\mathrm{angle}(Yx, Zx))$ if $K = \mathbb{C}$ or $c(x) = \cos\measuredangle(Yx, Zx)$ if $K = \mathbb{R}$.

Lemma 4.1. *The Euler equation for* (4.1) *is given for* $0 \neq x \in K^n \setminus (\mathrm{Ker}\ Y \cup \mathrm{Ker}\ Z)$, $\langle Yx, Zx\rangle \neq 0$ *by:*

$$\frac{Y^2 x}{\|Yx\|^2} - \frac{2YZx}{\langle Yx, Zx\rangle} + \frac{Z^2 x}{\|Zx\|^2} = 0. \tag{4.2}$$

Proof. When $K = \mathbb{R}$ and $Y = I$, $Z = A$ symmetric positive definite, the proof is easily adapted from that of Theorem 3.2 on p. 36 in [Gustafson, 2012]. For the sake of completeness we present below the proof for the general case YZ hermitian, $K = \mathbb{C}$.

In order to find (4.2), one looks for those x in $\mathbb{C}^n \setminus \{0\}$ which make the directional derivative

$$\frac{dc(x)}{dy}(\varepsilon = 0) = \lim_{\varepsilon\to 0} \frac{1}{\varepsilon}(c(x + \varepsilon y) - c(x)), \quad \varepsilon \in \mathbb{C}, \quad 0 \neq y \in \mathbb{C}^n$$

vanish for all directions $y \in \mathbb{C}^n \setminus \{0\}$. We consider for $\varepsilon > 0$ small enough

$$c(x + \varepsilon y) - c(x) = \frac{(x + \varepsilon y)^H Y Z(x + \varepsilon y)}{\|Y(x + \varepsilon y)\|\|Z(x + \varepsilon y)\|} - \frac{x^H Y Z x}{\|Yx\|\|Zx\|} = \frac{N}{D}, \quad x \notin \mathrm{Ker}\, Y \cup \mathrm{Ker}\, Z$$

with

$$\begin{aligned} N = \quad & (\langle YZx, x\rangle + 2\Re\varepsilon\langle YZy, x\rangle + |\varepsilon|^2\langle YZy, y\rangle)\|Yx\|\|Zx\| \\ & -\langle YZx, x\rangle(\|Yx\|^2 + 2\Re\varepsilon\langle Yx, Yy\rangle + |\varepsilon|^2\|Yy\|^2)^{1/2}(\|Zx\|^2 + 2\Re\varepsilon\langle Zx, Zy\rangle + |\varepsilon|^2\|Zy\|^2)^{1/2} \\ D = \quad & (\|Yx\|^2 + 2\Re\varepsilon\langle Yx, Yy\rangle + |\varepsilon|^2\|Yy\|^2)^{1/2}(\|Zx\|^2 + 2\Re\varepsilon\langle Zx, Zy\rangle + |\varepsilon|^2\|Zy\|^2)^{1/2}\|Yx\|\|Zx\|. \end{aligned}$$

Clearly $D \to (\|Yx\|\|Zx\|)^2$ as $\varepsilon \to 0$. In order to find $\lim_{\varepsilon\to 0} \frac{1}{\varepsilon}N$, we consider limited series expansions in ε for the terms in N to be subtracted:

1) $\|Y(x+\varepsilon y)\| = (\|Yx\|^2 + f(\varepsilon))^{1/2} = \|Yx\| + \frac{1}{2}\frac{1}{\|Yx\|}f(\varepsilon) - \frac{1}{8}\frac{1}{\|Yx\|^3}f^2(\varepsilon) + \ldots = \|Yx\| + r(\varepsilon)$,

2) $\|Z(x+\varepsilon y)\| = (\|Zx\|^2 + g(\varepsilon))^{1/2} = \|Zx\| + \frac{1}{2}\frac{1}{\|Zx\|}g(\varepsilon) - \frac{1}{8}\frac{1}{\|Zx\|^3}g^2(\varepsilon) + \ldots = \|Zx\| + t(\varepsilon)$.

Here $f(\varepsilon) = 2\Re\varepsilon\langle Yx, Yy\rangle + |\varepsilon|^2\|Yy\|^2$ and $g(\varepsilon) = 2\Re\varepsilon\langle Zx, Zy\rangle + |\varepsilon|^2\|Zy\|^2$ are functions which depend on ε taken sufficiently small relative to $\|Yx\|$ and $\|Zx\|$ respectively. Thus

$$\begin{aligned} N &= (\langle YZx, x\rangle + 2\Re\varepsilon\langle YZs, x\rangle + |\varepsilon|^2\langle YZs, s\rangle)\|Ax\|\|Zx\| \\ &\quad -\langle YZx, x\rangle(\|Yx\| + r(\varepsilon))(\|Zx\| + t(\varepsilon)) \\ &= (2\Re\varepsilon\langle YZy, x\rangle + |\varepsilon|^2\langle YZy, y\rangle)\|Yx\|\|Zx\| - \langle YZx, x\rangle(\|Yt\|t(\varepsilon) + \|Zx\|r(\varepsilon)) \\ &= (2\Re\varepsilon\langle YZy, x\rangle + |\varepsilon|^2\langle YZy, y\rangle)\|Yx\|\|Zx\| - \langle YZx, x\rangle(\tfrac{1}{2}\tfrac{\|Yx\|}{\|Zx\|}g(\varepsilon) + \tfrac{1}{2}\tfrac{\|Zx\|}{\|Yx\|}f(\varepsilon)) \\ &= (2\Re\varepsilon\langle YZy, x\rangle + |\varepsilon|^2\langle YZy, y\rangle)\|Yx\|\|Zx\| \\ &\quad -\langle YZx, x\rangle[\tfrac{\|Yx\|}{\|Zx\|}(\Re\varepsilon\langle Zx, Zy\rangle + \tfrac{1}{2}|\varepsilon|^2\|Zy\|^2) + \tfrac{\|Zx\|}{\|Yx\|}(\Re\varepsilon\langle Yx, Yy\rangle + \tfrac{1}{2}|\varepsilon|^2\|Yy\|^2)] \end{aligned}$$

and

$$\begin{aligned} \tfrac{N}{\varepsilon} &= (2\Re\langle YZy, x\rangle + \bar{\varepsilon}\langle YZy, y\rangle)\|Yx\|\|Zx\| \\ &\quad -\langle YZx, x\rangle[\tfrac{\|Yx\|}{\|Zx\|}(\Re\langle Zx, Zy\rangle + \tfrac{1}{2}\bar{\varepsilon}\|Zy\|^2) + \tfrac{\|Zx\|}{\|Yx\|}(\Re\langle Yx, Yy\rangle + \tfrac{1}{2}\bar{\varepsilon}\|Yy\|^2)]. \end{aligned}$$

Finally we have

$$\begin{aligned} \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\frac{N}{D} &= \frac{2\Re\langle YZy, x\rangle}{\|Yx\|\|Zx\|} - \langle YZx, x\rangle\left(\frac{\Re\langle Zx, Zy\rangle}{\|Yx\|\|Zx\|^3} + \frac{\Re\langle Yx, Yy\rangle}{\|Yx\|^3\|Zx\|}\right) \\ &= \frac{1}{\|Yx\|\|Zx\|}\Re\langle y, V\rangle, \quad \text{where } V = 2YZx - \langle YZx, x\rangle\left(\frac{Z^2x}{\|Zx\|^2} + \frac{Y^2x}{\|Yx\|^2}\right) \in \mathbb{C}^n. \end{aligned}$$

The variational calculus imposes that $\Re\langle y, V\rangle = 0$ for any $0 \neq y \in \mathbb{C}^n$. Indeed, if $V^H y = ib$, then $V^H(iy) = -b \in \mathbb{R}$ should also be 0. Therefore $\Re\langle y, V\rangle = 0$ for all $y \neq 0 \Leftrightarrow V = 0 \Leftrightarrow x$ satisfies (4.2).

□

By making appropriate choices for Y and Z, we shall obtain below an Euler equation corresponding to either catchvectors ($g^2 > 0$) or antieigenvectors ($g^2 < 0$).

4.2. **Catchvectors.** When we choose $Z = A$ and $Y = I$, equation (4.1) becomes

$$c(x) = \frac{x^H Ax}{\|x\|\|Ax\|} = \cos(\text{angle}(x, Ax)) \in \mathbb{R},\ 0 \neq x \in K^n \setminus \text{Ker } A \tag{4.3}$$

and its corresponding Euler equation (4.2) is

$$A^2x - 2\frac{\|Ax\|^2}{\langle x, Ax\rangle}Ax + \left(\frac{\|Ax\|}{\|x\|}\right)^2 x = 0 \tag{4.4}$$

for $\langle x, Ax\rangle \neq 0$, $x \in \mathbb{C}^n \setminus \text{Ker } A$.

In order to solve (4.4) we set $\frac{\|Ax\|^2}{\langle x, Ax\rangle} = k(x) = k$ and $\left(\frac{\|Ax\|}{\|x\|}\right)^2 = l(x) = l > 0$. Then with $A = QDQ^H$, $y = Q^H x$, $\|y\| = \|x\|$, (4.4) can be written

$$(D^2 - 2kD + lI)y = 0, \quad y = (y_i) \in \mathbb{C}^n,$$

that is, with $D = \mathrm{diag}(\mu_i)$:

$$(\mu_i^2 - 2k\mu_i + l)y_i = 0, \quad i = 1, \dots, n. \tag{4.5}$$

We consider the quadratic equation $\mu_i^2 - 2k\mu_i - l = 0$ whose coefficients k and l depend on $x = Qy$. Observe that the discriminant is $k^2 - l = \|Ax\|^2 \left(\frac{\|Ax\|^2}{\langle x, Ax\rangle^2} - \frac{1}{\|x\|^2} \right)$: its sign is that of $(\|x\|\|Ax\| - |\langle x, Ax\rangle|) \geq 0$ by Cauchy's inequality. Eq. (4.4) is obviously satisfied when x is an eigenvector: $Ax = \lambda x$. Let us assume that x and Ax are independent. Eq. (4.5) entails $y_j = 0$ for all j such that $\mu_i^2 - 2k\mu_i + l \neq 0$ and vice versa.

Since at most two different μ_j, μ_j' can satisfy $\mu_i^2 - 2k\mu_i + l = 0$, $i = 1, \dots, n$, for any given $x = Qy$, a vector x which is a solution of (4.4) is a linear combination of at most two eigenvectors q_j and q_j': $x = y_j q_j + y_j' q_j'$. Moreover this shows explicitly why the quadratic equation (1.1) and the matrix A are intimately connected through spectral coupling. Thus, if $\lambda < \lambda'$ are the two distinct roots $\{\mu_j, \mu_j'\}$ of the quadratic equation, x is a solution of (4.4) iff $k(x) = a = \frac{\lambda' + \lambda}{2}$ and $l(x) = g^2 = \lambda\lambda'$, $0 \leq g^2 < a^2$.

Let q, q' be two orthonormal eigenvectors associated with $\lambda < \lambda'$ which span the invariant subspace $\mathbf{M}$ with 4 real dimensions when $K = \mathbb{C}$. The unit sphere (S) in $\mathbb{R}^4$ passing through q and q' consists of vectors $u = zq + z'q'$, $|z|^2 + |z'|^2 = 1$. When are the conditions $k(u) = a$, $l(u) = g^2 > 0$ satisfied for $u \in (S)$?

Proposition 4.2. *The solutions of Euler's equation* (4.4) *which are not eigenvectors are the catchvectors* $v_+ = e^{i\xi} w_+ q + e^{i\xi'} w_+' q'$, $\xi, \xi' \in [0, 2\pi[$ *corresponding to all couplings* $\lambda < \lambda'$ *such that* $g^2 = \lambda\lambda' > 0$. *They yield the critical value* $c(v_+) = \frac{g}{a} = \mathrm{sgn}(a)\cos\phi$.

Proof. For $u = zq + z'q'$, $\|u\| = 1$, set $|z|^2 = \tau$, $|z'|^2 = 1 - \tau$. $k(u) = a \Leftrightarrow 2\frac{\lambda^2\tau + \lambda'^2(1-\tau)}{\lambda\tau + \lambda'(1-\tau)} = \lambda + \lambda'$ entails $\tau = \frac{\lambda'}{\lambda + \lambda'} = w_+^2$ and $1 - \tau = \frac{\lambda}{\lambda + \lambda'} = w_+'^2$, hence $u = v_+$. One checks that $l(v_+) = g^2 > 0$. The conclusion follows from $c(v_+) = \frac{\langle v_+, Av_+\rangle}{\|Av_+\|}$, $\langle v_+, Av_+\rangle = \frac{g^2}{a} = h \neq 0$. Thus $|c(v_+)| = \cos\phi$. □

Corollary 4.3. *If A is positive definite, the extreme coupling* $\{\lambda_1 = \lambda_{\min}, \lambda_n = \lambda_{\max}\}$ *yields the global minimum (resp. maximum)* $\cos\phi(A) = \frac{2\sqrt{\lambda_1\lambda_n}}{\lambda_1 + \lambda_n}$ *(resp.* $\sin\phi(A) = \frac{\lambda_n - \lambda_1}{\lambda_n + \lambda_1}$*).*

Proof. Clear. □

When $K = \mathbb{R}$, this is one of the major theorems in Gustafson's approach. Diverse applications are presented in [Gustafson, 2012, chapters 4 to 8]. When $K = \mathbb{C}$ the global minimum for $c(x)$ equals $\frac{g_*}{a_*} = c(v_{+,*})$, a value which, coincidentally, equals $\cos\phi(A)$ displayed in the spectral plane by the triangle OMC with the choice (λ_1, λ_n), see Figure 3 (a).

4.3. **Antieigenvectors.** When A is *indefinite*, Section 3.2 with $K = \mathbb{R}$ suggests to choose $Z = A$, $Y = B$, so that $c(x) = \cos\measuredangle(Bx, Ax)$ reduces to $\cos\beta$ when x belongs to the invariant plane $\mathbf{M}$. Thus, in this case equation (4.1) becomes

$$c(x) \;=\; \frac{x^H ABx}{\|Ax\|\|Bx\|} \in \mathbb{R}, \quad 0 \neq x \in \mathbb{C}^n \setminus (\mathrm{Ker}\ A \cup \mathrm{Ker}\ B) \tag{4.6}$$

and the Euler equation is

$$A^2x - 2\frac{\|Ax\|^2}{\langle Bx, Ax\rangle} ABx + \left(\frac{\|Ax\|}{\|Bx\|}\right)^2 B^2x = 0, \tag{4.7}$$

for $\langle Bx, Ax\rangle \neq 0$. We set $k'(x) = \frac{\|Ax\|^2}{\langle Bx, Ax\rangle}$, $l'(x) = (\frac{\|Ax\|}{\|Bx\|})^2$. Using $A = QDQ^H$, $B = Q(D - aI)Q^H$, $y = Q^Hx$, $\|y\| = \|x\|$, equation (4.7) can be written

$$[D^2 - 2k'(D^2 - aD) + l'(D - aI)^2]y = 0, \quad y = (y_i) \in \mathbb{C}^n,$$

with $D = \mathrm{diag}(\mu_i)$:

$$[(1-2k'+l')\mu_i^2 + 2a(k'-l')\mu_i + l'a^2]y_i = 0, \ \ i = 1, \dots, n,$$

We consider now the quadratic equation

$$(1-2k'+l')\mu_i^2 - 2a(l'-k')\mu_i + l'a^2 = 0. \tag{4.8}$$

The discriminant is $4a^2(k'^2 - l') = 4a^2\|Ax\|^2\left(\frac{\|Ax\|^2}{\langle Ax,Bx\rangle^2} - \frac{1}{\|Bx\|^2}\right)$: its sign is that of $(\|Ax\|\|Bx\| - |\langle Ax, Bx\rangle|) \geq 0$ by Cauchy's inequality. We assume that $2k' \neq 1 + l'$ so that (4.8) has degree 2. Hence at most two different μ_j, μ_j' satisfy $\mu_i^2 - 2K\mu_i + L = 0$, $i = 1, \dots, n$, $K = \frac{a(l'-k')}{(1-2k'+l')}$, $L = \frac{l'a^2}{(1-2k'+l')}$, for any given $x = Qy$, a vector x which is a solution of (4.7) is a linear combination of at most two eigenvectors q_j and q_j': $x = y_j q_j + y_j' q_j'$. Thus, if we denote $\lambda < \lambda'$ the two distinct roots $\{\mu_j, \mu_j'\}$ of the quadratic equation, x is a solution of (4.7) iff $K(x) = a$ and $L(x) = g^2$, $g^2 = \lambda\lambda' < 0$. We have the following result.

Proposition 4.4. *When A is indefinite, the solutions of Euler's equation* (4.7) *which are not eigenvectors are the antieigenvectors $v_- = e^{i\xi}w_-q + e^{i\xi'}w'_-q'$, $\xi, \xi \in [0, 2\pi[$ corresponding to all couplings $\{\lambda, \lambda'\}$ such that $\lambda < 0 < \lambda'$, $g^2 < 0$, and $\lambda' \neq -\lambda$. They yield the critical value $c(v_-) = \cos\psi < 1$.*

Proof. 1) Let $u = e^{i\xi}q$, $Au = \lambda u$, $Bu = -eu$, $\langle Bu, Au\rangle = -\lambda e$ and (4.7) is obviously satisfied: $(\lambda^2 - 2\lambda^2 + \lambda^2)q = 0$.

2) When $u \in (S)$ is not an eigenvector, u may satisfy (4.7) iff $K(u) = a$ and $L(u) = g^2$ together with $2k'(u) \neq 1 + l'(u)$. This is always possible when $g^2 < 0$ if $e^2 > -g^2 \Leftrightarrow a \neq 0 \Leftrightarrow \lambda' \neq -\lambda$.

When $g^2 < 0$, it is easy to check that $u = zq + z'q'$ should be such that $\tau = |z|^2 = \frac{\lambda'}{\lambda'-\lambda} = w_-^2$. Therefore u is any of the antieigenvectos v_- which satisfy $\langle Av_-, Bv_-\rangle = -g^2 < 0$. Direct computation shows that the antieigenvectors are the only solutions which are not eigenvectors.

3) $c(v_-) = \frac{v_-^H BAv_-}{\|Bv_-\|\|Av_-\|} = -\frac{g^2}{e|g|} = \frac{|g|}{e} = \cos\psi < 1$ for $a \neq 0$, which is the algebraic version of the geometric condition $O \neq C$, that is $OMC \neq OM$.

□

We shall go back to the exceptional case $a = 0$ later in Section 4.5.

4.4. **Midvectors.**

Section 3.3 with $K = \mathbb{R}$ suggests to use $Y = -I$, $a \neq 0$, $Z = B = A - aI$ in order to obtain the midvectors through (4.1). However the corresponding Euler equation for this choice cannot yield the midvectors $\hat{v} = \frac{1}{\sqrt{2}}(e^{i\xi}q + e^{i\xi'}q')$, $\xi, \xi' \in [0, 2\pi[$ because (4.2) is not defined for $x = \hat{v}$ since $\langle \hat{v}, B\hat{v}\rangle = \frac{e}{2}\langle e^{i\xi}q + e^{i\xi'}q', -e^{i\xi}q + e^{i\xi'}q'\rangle = 0$. It turns out that these vectors can be characterised in another way when A is invertible.

Proposition 4.5. *When A is invertible, the solutions $x \in K^n$, $\|x\| = 1$ distinct from eigenvectors, of the equation*

$$A^2x - 2\frac{\langle x, Ax\rangle}{\|x\|^2}Ax + \frac{\langle x, Ax\rangle}{\langle x, A^{-1}x\rangle}x = 0 \tag{4.9}$$

are midvectors $\hat{v}$ associated with all couplings $\lambda < \lambda'$ such that $\lambda \neq -\lambda' \Leftrightarrow a \neq 0$.

Proof. 1) It is easily checked that $\langle \hat{v}, A\hat{v}\rangle = \frac{1}{2}(\lambda + \lambda') = a$. Because $\lambda\lambda' \neq 0$, $A^{-1}\hat{v} = \frac{1}{\sqrt{2}}(\frac{1}{\lambda}e^{i\xi}q + \frac{1}{\lambda'}e^{i\xi'}q')$ is well-defined, thus $\frac{\langle \hat{v}, A\hat{v}\rangle}{\langle \hat{v}, A^{-1}\hat{v}\rangle} = \frac{a}{a}g^2 = g^2$ when $a \neq 0$. The equality $(A^2 - 2aA + g^2I)\hat{v} = 0$ follows.

2) Direct computation shows that the midvectors $\hat{v}$ are the only solutions in (S) which are not eigenvectors.

□

The case $a = 0$ is studied in Section 4.5. The equation (4.9) is called the *balance equation* since its (non eigenvector) solutions are the midvectors $\hat{v}$ independently of the nonzero values $\lambda < \lambda' \neq -\lambda$ because the balance equation is defined only if A^{-1} exists. However the above formula for $\hat{v}$ is well defined even if $\lambda\lambda' = 0$ or $\lambda' = -\lambda$, since it does *not* depend on λ and λ'.

If we set $y = A^{-1}x$, Eq. (4.9) takes the remarkable form:

$$\frac{A^3 y}{\langle A^3 y, y\rangle} - 2\frac{A^2 y}{\langle A^2 y, y\rangle} + \frac{Ay}{\langle Ay, y\rangle} = 0.$$

This expresses a linear combination between the 3 vectors Ay, A^2y, A^3y computed from any given $y \neq 0$.

Moreover, the midvectors can be **indirectly** related to the preparatory Lemma 4.1 when A is *definite* thanks to the square root $Y = A^{1/2}$ (resp. $(-A)^{1/2}$) when A is positive (resp. negative) definite. We suppose below that A is positive definite, so that $\langle x, Ax\rangle = \|A^{1/2}x\|^2 > 0$ for $x \neq 0$. Then with $Y = A^{1/2}$, $Z = A^{-1/2}$, $YZ = I$, equation (4.1) becomes

$$c(x) = \frac{\|x\|^2}{\|x\|_A \|x\|_{A^{-1}}} \in \mathbb{R}, \quad x \in \mathbb{C}^n \setminus \mathrm{Ker}\, A$$

where $\|x\|_A = \langle x, Ax\rangle^{1/2} = \|A^{1/2}x\|$ denotes the elliptic norm defined by A. The corresponding Euler equation (4.2) takes the form

$$\frac{Ax}{\langle x, Ax\rangle} - 2\frac{x}{\|x\|^2} + \frac{A^{-1}x}{\langle x, A^{-1}x\rangle} = 0. \qquad (4.10)$$

Multiplying (4.10) by A, we rewrite it in the equivalent form

$$A^2 x - 2\frac{\langle x, Ax\rangle}{\|x\|^2} Ax + \frac{\langle x, Ax\rangle}{\langle x, A^{-1}x\rangle} x = 0,$$

which is precisely the balance equation (4.9) of Proposition 4.5. Thus we have the following result.

Proposition 4.6. *When A is positive definite,* (4.9) *is the Euler equation associated with* $\min_{x\neq 0} \frac{\|x\|^2}{\|x\|_A \|x\|_{A^{-1}}}$ *which represents either*

$$\min_{0\neq x\in\mathbb{R}^n} \cos\measuredangle(A^{-1/2}x, A^{1/2}x) \;\; \textit{or} \;\; \min_{0\neq x\in\mathbb{C}^n} \cos\mathrm{angle}(A^{-1/2}x, A^{1/2}x). \qquad (4.11)$$

The solutions of the Euler equation (4.10) *which are not eigenvectors are the midvectors* $\hat{v} = \frac{1}{2}(e^{i\xi}q + e^{i\xi'}q')$, $\xi, \xi' \in [0, 2\pi[$ *corresponding to all couplings* $\lambda < \lambda'$ *such that* $g^2 = \lambda\lambda' > 0$. *They yield the critical value* $c(\hat{v}) = \frac{g}{a} = \mathrm{sgn}(a)\cos\phi$

Proof. It is easy to check that $\|\hat{v}\|_A^2 = \frac{\lambda+\lambda'}{2} = a$ and $\|\hat{v}\|_{A^{-1}}^2 = \frac{\lambda+\lambda'}{2\lambda\lambda'} = \frac{a}{g^2}$. □

Clearly, we can see that the global minimum is achieved for the extreme pair $\{\lambda_1 = \lambda_{\min}, \lambda_n = \lambda_{\max}\}$ and a pair of associated midvectors at the value $\frac{2\sqrt{\lambda_1\lambda_n}}{\lambda_1+\lambda_n} = \cos\phi(A)$.

We observe that when coupling $\lambda < \lambda'$, $g^2 = \lambda\lambda' > 0$, the critical value of the functional (4.3) ($\frac{g}{a} = \mathrm{sgn}(a)\cos\phi$) is the same as that of (4.11). It turns out that some of the real variational approach of Section 4.4 on vectors x in $\mathbb{R}^n$, $\|x\| = 1$, can be extended to rectangular matrices X in $\mathbb{R}^{n\times p}$, $1 \leq p \leq n$, such that $X^T X = I_p$ which define, when A is symmetric positive definite, the positive functional $X \to J_p(X) = \det[(X^T AX)(X^T A^{-1}X)]$ for which a *maximum* is sought. We obtain a generalisation of Proposition 4.6 which involves spectral *chaining*, that is the simultaneous consideration of p spectral couplings, $p < n$. For more, see Section 4.6 in [Chatelin and Rincon-Camacho, 2015b].

All this points to a relation between catchvectors and midvectors which is applied to Numerical Analysis in Section 5.4 and to Statistics in Section 5.5.

4.5. **The exceptional case** $a = 0$**.** Because $a^2 = e^2 + g^2$, the case $a = 0$ may occur only for $g^2 = -e^2 < 0$, $\lambda' = -\lambda = e = |g|$: $\pm e$ are eigenvalues of $A = B$. Moreover, Lemma 2.1 entails $A^2u = e^2u$ for $u \in \mathbf{M}$, $\|u\| = 1$. Therefore $A^2_{\restriction\mathbf{M}} = e^2I_2$: $\mathbf{M}$ is an *eigensubspace* for A^2 associated with $e^2 = -g^2 > 0$. Let us look at what the equations (i) (4.9) and (ii) (4.7) have to tell us when $a = 0$.

(i) If $a = 0$ and $x = \hat{v} \in \hat{D}$, the coefficient of $\hat{v}$ in (4.9) takes the indeterminate form $a\frac{g^2}{a}$. In the limit $a \to 0$, Eq (4.9) becomes $A^2\hat{v} + g^2\hat{v} = 0$ which represents a particular case of $A^2u + g^2u = 0$ valid for any $u \in \mathbf{M}$.

(ii) If $a = 0$, $A = B$ and (4.7) becomes tautologic: $A^2x - 2A^2x + A^2x \equiv 0$, with $k' = l' = 1$. So that (4.8) yields also $0 \equiv 0$, Neither (4.7) nor (4.9) convey any information about $c(x) = \frac{x^HA^2x}{\|Ax\|^2} = \frac{\|Ax\|^2}{\|Ax\|^2} \equiv 1$ for $Ax \neq 0$. We observe that, when $\lambda' = -\lambda = e$, $w_-^2 = w_-'^2 = \frac{1}{2}$ so that $D_- = \hat{D}$. And $v_- = \hat{v}$ yields the *maximal* value $c(v_-) = 1$ which actually holds for all $x \in \mathbb{C}^n \setminus \operatorname{Ker} A$. The global tautology is beyond the reaches of the spectral plane where the triangle OMC is reduced to the segment CM ($\alpha + \gamma = \pi$, $\beta = 0$).

Unless otherwise stated, we assume below that $ae \neq 0$, so that $\mathbf{M}$ is not an eigenspace for A^2, and OMC is not degenerate into OC or CM.

5. More on midvectors, $K = \mathbb{R}$ or $\mathbb{C}$

We observe that the variational principles related to the midvectors presented in Section 4.4, when A is definite, do not indicate how one could extend from $K = \mathbb{R}$ to $\mathbb{C}$ the maximal surface property ($\Sigma(\hat{v}) = \max_{u\in(C)} \Sigma(u) = \frac{1}{2}|a|e$) described in Section 3.3. However, Lemma 3.5 remains valid since the spectrum of a hermitian matrix is real. Thus, given $\lambda < \lambda'$, any midvector in $\hat{D}$ contains the spectral information which defines in the spectral plane the triangle OMC with maximal surface $\frac{1}{2}|a|e$, see Figure 5. We shall see in Section 5.4 that in numerical analysis, equality in the well-known Wielandt, Kantorovich and Greub-Rheinboldt inequalities are attained by the midvectors when coupling the extreme pair $\{\lambda_1 = \lambda_{\min}, \lambda_n = \lambda_{\max}\}$, [Horn and Johnson, 1985, pp. 441-445, 452]. This Section shows why the reason for these results can be traced to spectral coupling. By considering α, β, γ, we understand the nD-geometry which underlies inequalities in $\mathbb{R}^+$.

5.1. **Midvectors as bisectors.** When coupling $\lambda < \lambda'$, clearly the midvectors $\hat{v} \in \hat{D}$ are the bisectors of the angle between the eigenvectors directions $\{q\}$ and $\{q'\}$. If $K = \mathbb{R}$, this can be seen geometrically, $\hat{v} = \varepsilon \cos\frac{\pi}{4}q + \varepsilon' \cos\frac{\pi}{4}q'$, $\varepsilon = \pm 1$, $\varepsilon' = \pm 1$ and $\measuredangle(q, \hat{v}) = \measuredangle(\hat{v}, q') = \frac{\pi}{4}$, see Figure 8. If $K = \mathbb{C}$, the analytic definition only remains valid (angle$(q, \hat{v})$ = angle$(\hat{v}, q') = \frac{\pi}{4}$).

When A is invertible, A and A^{-1} share the same eigenvectors. Let us assume first that λ and λ' are positive and $K = \mathbb{R}$ or $\mathbb{C}$. If we consider the catchvectors v_+ and $\mathring{v}_+$ respectively associated with the arbitrary couplings (λ, λ') for A and $(\frac{1}{\lambda'}, \frac{1}{\lambda})$ for A^{-1}, we have that the midvectors bisect the angle between the directions of the catchvectors v_+ and $\mathring{v}_+$.

Proposition 5.1. *When λ and λ' are positive, the catchvectors v_+ and $\mathring{v}_+$ are symmetrically placed with respect to the corresponding midvectors $\hat{v}$. They envelop the same observation angle $0 \leq \phi < \frac{\pi}{2}$.*

Proof. Without loss of generality, we may assume that $v_+ = wq + w'q'$ in D_+ and $\hat{v} = \frac{1}{\sqrt{2}}(q + q')$ in $\hat{D}$. By inversion, the catchvector $\mathring{v}_+$ is defined by $\mathring{w} = (\lambda'(\frac{1}{\lambda'} + \frac{1}{\lambda}))^{-1/2} = \sqrt{\frac{\lambda}{\lambda' + \lambda}} = w'$ and $\mathring{w}' = w$. Thus $\mathring{v}_+ = w'q + wq'$ is the symmetric of v_+ with respect to the (real or complex) axis spanned by $\hat{v}$. It is colinear with the image Av_+. Indeed $Av_+ = \lambda wq + \lambda' w'q' = \sqrt{\lambda\lambda'}\mathring{v}_+ = g\mathring{v}_+$. □

5.2. **Midvectors and catchvectors.** As announced at the end of Section 4.4, the coupling of $\lambda < \lambda'$, $\lambda'\lambda > 0$ yields, when A is positive definite, a relation between the catchvectors and the midvectors given by the

Lemma 5.2. *Let $\hat{v}$ be a midvector, and $h = \frac{g^2}{a}$ be the harmonic mean. Then $v_+ = \sqrt{h}A^{-1/2}\hat{v}$ is a catchvector, $Av_+ = \sqrt{h}A^{1/2}\hat{v}$ and $\langle A^{-1/2}\hat{v}, A^{1/2}\hat{v}\rangle = \frac{1}{h}\langle v_+, Av_+\rangle = 1 = \|\hat{v}\|^2$.*

Proof. By straightforward calculation: $\langle v_+, Av_+\rangle = h$.

□

If A is symmetric ($K = \mathbb{R}$), direction angles are well-defined. Since $\cos\measuredangle(A^{1/2}\hat{v}, \hat{v}) = \cos\measuredangle(A^{-1/2}\hat{v}, \hat{v}) = \frac{\sqrt{\lambda'}+\sqrt{\lambda}}{2\sqrt{a}}$, then $\measuredangle(v_+, \hat{v}) = \measuredangle(\hat{v}, Av_+)$, the midvector $\hat{v}$ bisects the angle $\phi = \measuredangle(v_+, Av_+)$, see the triangle $OM'C'$ on Figure 8 (a): $OP' = h$.

Lemma 5.2 indicates a non trivial algebraic connection between the roots of the quadratic equations (4.4) and (4.9) which are not eigenvectors and are defined by pairs of *positive* eigenvalues (λ, λ') in the associated invariant (real or complex) plane $\mathbf{M}$.

5.3. **Midvectors and antieigenvectors.** The global connection in Lemma 5.2 based on $A^{1/2}$ for A definite is replaced by a necessarily *local* one when A is indefinite. We restrict A to be 2×2: $A_0 = A_{\restriction \mathbf{M}}$ and $B_0 = A_0 - aI_2 : \mathbf{M} \to \mathbf{M}$.

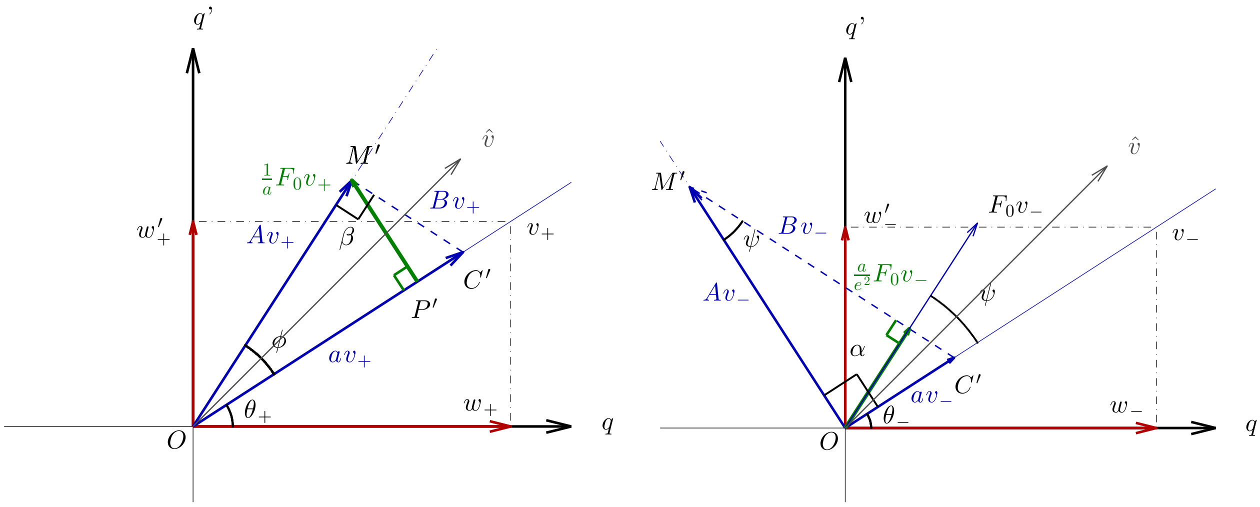
When $\lambda < 0 < \lambda'$, A_0 is indefinite as well as B_0. However, the eigenvalues of $F_0 = A_0B_0$ are positive, being $\{-e\lambda, e\lambda'\}$. Observe the resurgence of $-\lambda$.

The relation between antieigenvectors v_- and midvectors $\hat{v}$ when $\lambda < 0 < \lambda'$ is given by the following *local* analogue of Lemma 5.2 based on F_0:

Proposition 5.3. *When $g^2 < 0$, let $\hat{v}$ be a midvector. Then $v_- = |g|F_0^{-1/2}\hat{v}$ is an antieigenvector, $F_0v_- = |g|F_0^{1/2}\hat{v}$ and $\langle F_0^{-1/2}\hat{v}, F_0^{1/2}\hat{v}\rangle = -\frac{1}{g^2}\langle v_-, F_0v_-\rangle = 1 = \|\hat{v}\|^2$.*

Proof. Straightforward calculation. See the triangle $OM'C'$ on Figure 8 (b) valid when $K = \mathbb{R}$: $\hat{v}$ bisects $\psi = \measuredangle(v_-, F_0v_-)$ and v_-, Av_- are orthogonal ($\alpha = \frac{\pi}{2}$).

□



(a) $g^2 > 0$, $a > 0$, , $\beta = \frac{\pi}{2}$ (b) $g^2 < 0$, $a > 0$, $\alpha = \frac{\pi}{2}$

FIGURE 8. Midvectors as bisectors in $\mathbf{M}$ when $K = \mathbb{R}$

We observe that when $a = 0$, $e = |g|$ and $F_0 = e^2I$. Therefore $\hat{v} = v_-$. Thus is established the following

Corollary 5.4. *The midvectors $\hat{v}$ satisfy $\hat{v} = \frac{1}{g}(aA_0)^{1/2}v_+ = (\frac{1}{h}A_0)^{1/2}v_+$ when $g^2 > 0$ and $\hat{v} = \frac{1}{|g|}F_0^{1/2}v_-$ when $g^2 < 0$.*

Since F_0 depends on the local parameter $a = \frac{\lambda+\lambda'}{2}$, it is clear that the *global* optimisation expressed in Proposition 4.6 can only be replaced by the following *local* one:

$$\min_{u\in\mathbf{M},u\neq 0} \frac{\|u\|^2}{\|u\|_{F_0}\|u\|_{F_0^{-1}}} = \cos\psi = \frac{|g|}{e}$$

where $\psi = \measuredangle(F_0^{-1/2}\hat{v},\, F_0^{1/2}\hat{v}) = \measuredangle(v_-, F_0 v_-)$, if $K = \mathbb{R}$.

5.4. **Numerical Analysis.** Here we consider the case where A is a positive definite hermitian matrix with eigenvalues $0 < \lambda_1 \leq \ldots \leq \lambda_n$. A relation between the maximal turning angle $\phi(A)$ and the Wielandt angle θ_W related to the condition number of a matrix has been given in [Gustafson, 1999]. However considering the *three* angles α, β, γ sheds more light on the geometrical picture. Here we consider the coupling of the extremal pair of eigenvalues $\{\lambda_1, \lambda_n\}$, with $\hat{D}_*$ the corresponding set of midvectors.

The condition number of $A^{\frac{1}{2}}$ in the euclidean norm is $\mathrm{cond}(A^{\frac{1}{2}}) = \sqrt{\frac{\lambda_n}{\lambda_1}} = \cot\angle(q, v_{+,*}) = \cot\theta_+$. The angle θ_W appearing in Wielandt's inequality is defined in the first quadrant by $\cot(\frac{\theta_W}{2}) = \mathrm{cond}(A^{\frac{1}{2}})$ so that $\theta_+ = \frac{\theta_W}{2}$ and $\theta_W = \frac{\pi}{2} - \phi(A) = \gamma(A)$, see Figure 9. Thus, Wielandt's inequality for any pair of orthogonal vectors $x, y \in K^n$ and $A^{\frac{1}{2}}$ is given by

$$\frac{|\langle A^{\frac{1}{2}}x, A^{\frac{1}{2}}y\rangle|}{\|A^{\frac{1}{2}}x\|\|A^{\frac{1}{2}}y\|} = \frac{\langle x, Ay\rangle}{\|x\|_A\|y\|_A} \leq \cos\theta_W = \cos\gamma(A) = \sin\phi(A) = \frac{\lambda_n - \lambda_1}{\lambda_n + \lambda_1}. \tag{5.1}$$

The angles $\gamma(A)$ and $\phi(A)$ are complementary, thus if the turning angle $\phi(A)$ is large the angle $\theta_W = \gamma(A)$ is small which indicates that the matrix A is ill-conditioned.

The equality is attained if x and y are precisely orthogonal midvectors in $\hat{D}_*$. The case $K = \mathbb{R}$ is illustrated in Figure 9 with $\hat{v}_1 = \frac{1}{\sqrt{2}}(q_n + q_1)$ and $\hat{v}_2 = \frac{1}{\sqrt{2}}(q_n - q_1)$, where q_1 and q_n are eigenvectors associated with the eigenvalues λ_1 and λ_n of A. Figure 9 shows the complementarity between $\gamma(A)$ and $\phi(A)$. The smaller the angle $\gamma(A) = \measuredangle(A^{\frac{1}{2}}\hat{v}_1, A^{\frac{1}{2}}\hat{v}_2) = \measuredangle(Av_{+,1}, Av_{+,2})$, the closer the vectors $A^{\frac{1}{2}}\hat{v}_1$, and $A^{\frac{1}{2}}\hat{v}_2$ are to be dependent.

In [Horn and Johnson, 1985, p. 444], Kantorovich's inequality is derived from Wielandt's inequality (5.1). However, Kantorovich's inequality

$$\frac{\|x\|^2}{\|x\|_A\|x\|_{A^{-1}}} \geq \frac{2\sqrt{\lambda_1\lambda_n}}{\lambda_1 + \lambda_n} = \cos\phi(A) \tag{5.2}$$

is equally a direct consequence of Proposition 4.6 where equality is attained if x is any midvector $\hat{v}$ in $\hat{D}_*$. In Figure 9 the geometrical meaning of the angles $\phi(A)$ and $\theta_W = \gamma(A)$ when $K = \mathbb{R}$ is illustrated: $\frac{\|\hat{v}\|^2}{\|\hat{v}\|_A\|\hat{v}\|_{A^{-1}}} = \cos\measuredangle(A^{-1/2}\hat{v}, A^{1/2}\hat{v}) = \cos\phi(A)$. See also [Gustafson, 2012, p.188].

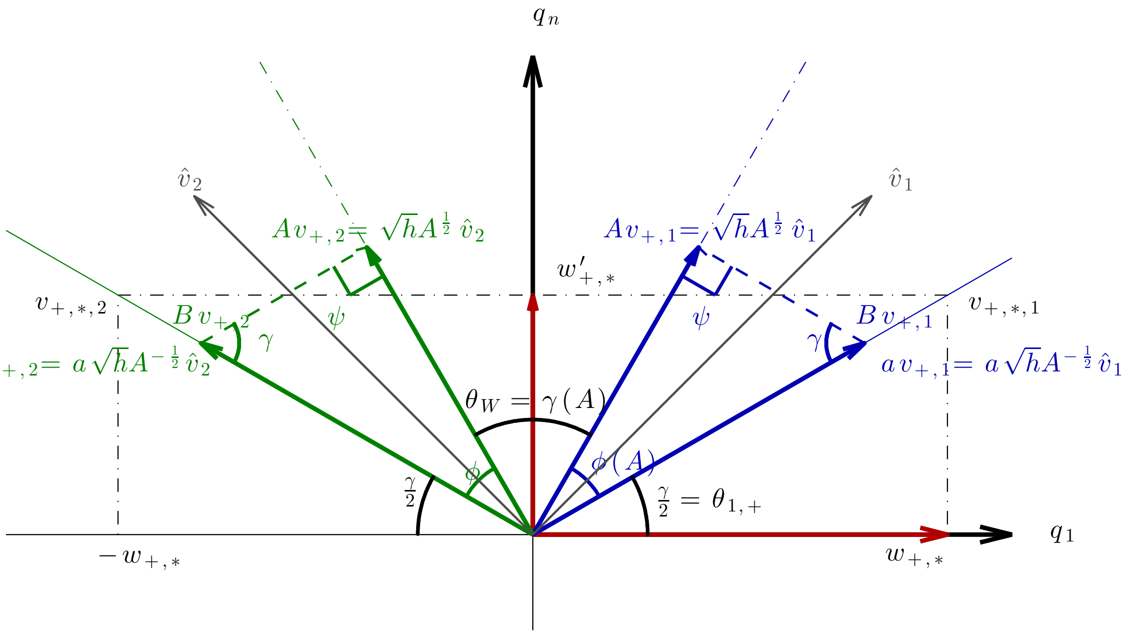


FIGURE 9. A midvector pair in $\hat{D}_*$, $K = \mathbb{R}$

The Greub-Rheinboldt inequality was introduced in 1959 as a generalisation of the Kantorovich inequality (5.2) [Horn and Johnson, 1985, Chapter 7, Problem 10, p. 452]. Let us assume that the commuting matrices Y and Z in Section 4.1 are positive definite such that $A = YZ$. If the eigenvalues of Y and Z, ordered by increasing magnitude, are denoted by y_i and z_i, $i = 1$ to n, then $\lambda_i = y_i z_i$ are the eigenvalues of $A = YZ$. Then the Greub-Rheinboldt inequality can be written

$$c(x) = \frac{x^H YZx}{\|Yx\|\|Zx\|} \geq 2\frac{\sqrt{\lambda_1\lambda_n}}{\lambda_1 + \lambda_n} = \cos\phi(A). \tag{5.3}$$

Greub and Rheinboldt tell us that the (analytic) angle between the directions Yx and Zx may equal, at its maximum, the turning angle $\phi(A)$ for the matrix product $A = YZ$. This is but an easy consequence of Corollary 4.3. Following [Gustafson, 2004, Theorem 1] with $y = Zx$, $c(x) = \frac{y^H YZ^{-1}y}{\|YZ^{-1}y\|\|y\|} \geq \cos\phi(YZ^{-1}) \geq \cos\phi(A)$ since the eigenvalues $\frac{y_i}{z_i}$ for YZ^{-1} may not be ordered by magnitude. We discuss the final remark in Horn and Johnson (Problem 10): when is equality achieved in (5.3)? Given a catchvector $v_+ \in D_{+*}$ for A, the equality $v_+^H Av_+ = \frac{g^2}{a} = h$ requires that $\|Yv_+\|\|Zv_+\| = \|v_+\|\|Av_+\| = g$ for $A = YZ$. Computation shows that necessarily one factor is rI, the other $\frac{1}{r}A$ with $r > 0$ arbitrary: $r = 1$ is precisely the choice made in Section 4.2. Other choices for Y and Z cannot yield other maximisers, but can achieve equality.

5.5. **Statistics.** When $K = \mathbb{R}$ some of the matrix identities that are used in statistics and econometrics [Gustafson, 2002, 2012, chapter 6], [Wang and Chow, 1994] can benefit from the light provided by Sections 4.4 and 5.2. As a consequence of Lemma 5.2 we get, for A positive definite, the equality:

$$\cos\measuredangle(A^{-1/2}\hat{v}, A^{1/2}\hat{v}) = \cos\measuredangle(v_+, Av_+) = \frac{g}{a}, \tag{5.4}$$

see Figure 9. This equality finds an interesting application in Statistics for the measure of the efficiency of least squares proposed in [Bloomfield and Watson, 1975] as

$$\min J_p(X)^{-1} = [\det(XAX)(XA^{-1}X)]^{-1},\ X^TX = I_p,\ p \leq \left\lfloor\frac{n}{2}\right\rfloor$$

where A is the noise covariance matrix. Bloomfield and Watson have shown that the worst regressors consist of pairs of *midvectors* associated to the nested sequence of p eigenvalue pairs

(λ_1, λ_n), $(\lambda_2, \lambda_{n-1})$, ... $(\lambda_p, \lambda_{n-p})$ for the covariance matrix. On the other hand [Gustafson, 2002, pp. 147-150] and [Gustafson, 2012, Theorem 6.1, p. 93] relate the worst regressors to *catchvectors*. Equality (5.4) is the reason why the two points of view are equivalent. For more along these lines, the reader is referred to [Chatelin and Rincon-Camacho, 2015b, Section 4.6]. The potential domains of application are many, from econometrics to computational inverse problems and machine learning.

6. The 4D-invariant subspace when $K = \mathbb{C}$

6.1. **Angles between complex lines in real geometry.** When x and y are nonzero *complex* vectors, the angle between the complex directions that they define is a subject that is rarely treated, even in advanced textbooks on linear algebra [Scharnhorst, 2001]. Since $\mathbb{C}^n \cong \mathbb{R}^{2n}$ two complex lines define two real planes in a space of at least 4 real dimensions. Generically *two* Jordan (canonical) real angles are necessary to specify the relative position of two arbitrary real planes [Jordan, 1875]. In the present context where A is hermitian, there is a vast geometric simplification. One can show that the two Jordan angles are *equal* [Kwietniewski, 1902, Maruyama, 1950, Wong, 1977, Theorem 1.7.4]. See also [Gustafson, 2012, chap. 9, Section 9.2, p. 186].

6.2. **Angles between real planes in M.** We consider the coupling $\lambda < \lambda'$ and the associated 4D-subspace $\mathbf{M}$ spanned by the respective eigenvectors q and q'. Any $u = zq + z'q'$ belongs to the unit sphere in 4 dimensions $(S) = \{(z, z'), |z|^2 + |z'|^2 = 1, z, z' \in \mathbb{C}\}$. When u is not an eigenvector and $a \neq 0$, the three complex vectors au, Au, Bu define three real planes all passing through O. It is not an easy matter to interpret in 4D the angles α, β and γ which are Jordan canonical angles between the 3 planes. It is clear that the *triangle* $OM'C'$ which lies in the 2D-plane $\mathbf{M}$ when $K = \mathbb{R}$ and the trigonometric information it provides (Fig. 2) have no general counterparts when $K = \mathbb{C}$. Hence no known trigonometric interpretation is available to us in 4D. However, the properties of the triangle OMC in the spectral plane (Fig. 1) cover both cases $K = \mathbb{R}$ *and* $\mathbb{C}$. Therefore a 2D-trigonometric interpretation involving ordinary angles remains available in the spectral plane.

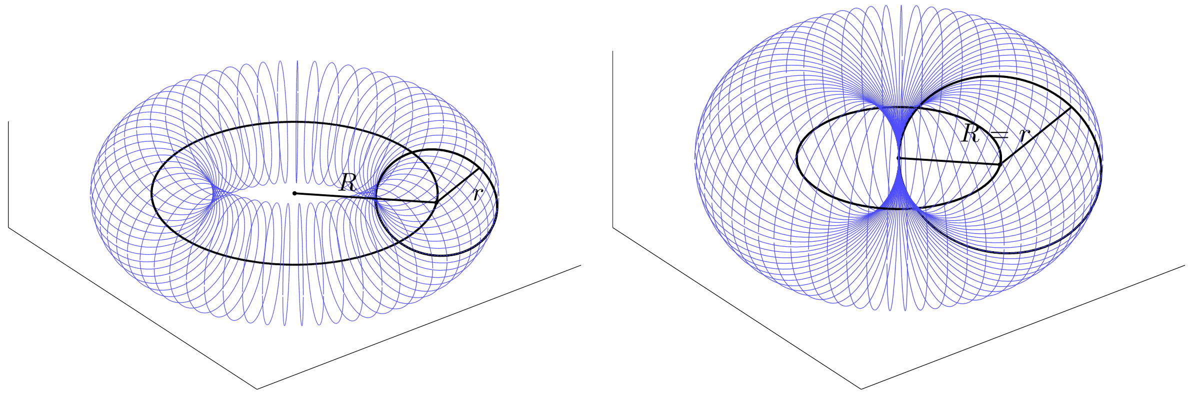
6.3. **The distinguished sets $D_\pm$, $\hat{D}$ in $\mathbb{R}^3$.** We recall that the cartesian product of two circles $S^1 \times S^1 \subset \mathbb{C}^2$ is homeomorphic, in topology, to a torus in $\mathbb{R}^3$. The three distinguished subsets $D_\pm$, $\hat{D}$ of the unit sphere $(S) = S^3 \subset \mathbb{R}^4$, which signal *orthogonality* in $\mathbf{M} \subset \mathbb{C}^n$ between 2 of the 3 complex vectors u, Au, Bu, can therefore be interpreted as *tori* in $\mathbb{R}^3$. Indeed

i) $D_+ = w_+ S^1 \times w'_+ S^1$, $1 > w_+^2 > w_+'^2 > 0$, $g^2 > 0$,

ii) $D_- = w_- S^1 \times w'_- S^1$, $w_-^2 \neq w_-'^2$ in $]0, 1[$, $g^2 < 0$,

iii) $\hat{D} = \hat{w} S^1 \times \hat{w} S^1$, $\hat{w} = \frac{1}{\sqrt{2}}$.

In case i) or ii) with $a \neq 0$ the radii w and w' are distinct and yield a *ring* torus. And in case ii) with $\lambda = -\lambda'$ or iii) the equal radii $\frac{1}{\sqrt{2}}$ yield a *horn* torus, see Figure 10.



(a) i) or ii) $a \neq 0$
$R = w'_-$ and $r = w_-$ if $w'_- > w_-$
$R = w_\pm$ and $r = w'_\pm$ if $w'_\pm < w_\pm$

(b) iii) or ii) $a = 0$
$R = r = \hat{w} = \frac{1}{\sqrt{2}}$

FIGURE 10. Distinguished tori in $\mathbb{R}^3$ when $K = \mathbb{C}$

6.4. **Invariance and derived optimality.** Because of the difference in dimension, the transfer of information from the 4D invariant subspace $\mathbf{M}$ to the 2D spectral plane is not as conservative as it is when $K = \mathbb{R}$: it provides only an *image* of the 4D real evolution.

The dimension reduction has an important impact on the functional $\frac{1}{e}\langle x, Bx\rangle$ when $x \in \mathbb{C}^n$, $\|x\| = 1$. Whereas it is still true that $\langle \hat{v}, B\hat{v}\rangle = 0$ implies that $\cos\gamma = 0$, i.e. the triangle OMC has maximal surface, this $\mathbb{R}^2-$property tells us nothing about the geometric configuration in $\mathbb{R}^4$. This is confirmed by the fact that the balance equation (4.9) which characterises $\hat{v}$ in $\hat{D}$ when $\det A \neq 0$ does not express a variational principle in $\mathbb{C}^n$ when A is indefinite. And when it does (A definite, Proposition 4.6), the functional cannot be interpreted in terms of a planar surface. Accordingly, there is no analogue to the connexion vector $\mathfrak{K}(u)$ when u is considered in $\mathbb{R}^4$ (no vector product). But it remains true that, if $a = 0$, $\mathbf{M}$ is the complex eigenplane for A^2 associated with e^2.

When the ground field is complex, the above theory allows us to state the following

Theorem 6.1. *When $ae \neq 0$, the triangle OMC in the spectral plane carries exact information about local evolution in the invariant subspace $\mathbf{M}$ in the following 3 orthogonality cases*

$$(i)\langle x, Ax\rangle = 0, \quad (ii)\langle Bx, Ax\rangle = 0, \quad (iii)\langle x, Bx\rangle = 0$$

when $0 \neq x \in \mathbb{C}^n \setminus Ker\ A \cup Ker\ B$. More precisely, the following 3 statements hold:

(i) OMC is right-angled at O, that is $\alpha = \frac{\pi}{2}$ when $g^2 < 0$: this signals that x is an antieigenvector v_- in D_-, $\|Av_-\| = |g|$ and $\frac{\langle Bv_-, Av_-\rangle}{\|Bv_-\|\|Av_-\|} = \frac{|g|}{e} = \cos\psi$ is minimum when $x \in \mathbf{M}$.

(ii) OMC is right-angled at M, that is $\beta = \frac{\pi}{2}$ when $g^2 > 0$: this signals that x is a catchvector $v_+ \in D_+$, $\|Av_+\| = g$ and $\frac{\langle v_+, Av_+\rangle}{\|v_+\|\|Av_+\|} = \frac{g}{|a|} = \cos\phi$ is minimum when $x \in \mathbf{M}$.

(iii) OMC is right-angled at C, that is $\gamma = \frac{\pi}{2}$ when $g^2 \neq 0$: this signals that x is a mid vector $\hat{v}$ in $\hat{D}$, $\|A\hat{v}\| = \sqrt{a^2 + e^2}$.

Proof. Clear from the above discussion. We recall that the ordinary ϕ or ψ are not readily related to the Jordan canonical angles between 2 complex lines in at least 4 real dimensions. □

A comparison between Corollary 2.3 for $K = \mathbb{R}$ and Theorem 6.1 for $K = \mathbb{C}$ indicates that the price for greater freedom in real evolution, from 2 to 4D, is paid by a global loss in geometric intelligibility. However, more can be said in the complex case. We first turn to Lemma 2.1 which remains valid for $K = \mathbb{C}$. We recall that $B = A - aI$, $F = AB$, and we define $G = \frac{1}{e}F - eI$.

Proposition 6.2. *For any u in $\mathbf{M}$, $\|u\| = 1$, the norms of the colinear vectors $\frac{1}{a}Bu$ and $\frac{1}{e}Gu$ are invariant with value $\frac{e}{|a|}$ and $\frac{|a|}{e}$ respectively.*

Proof. Direct consequence of Lemma 2.1 where $\cos\theta$ and $\sin\theta$ are replaced by z and z'. The $\mathbb{R}$-dependent vectors $f_1(u) = \frac{1}{a}Bu = \frac{e}{a}\tilde{u}$ and $f_2(u) = \frac{1}{e}Gu = \frac{a}{e}\tilde{u}$ describe the spheres $\frac{e}{|a|}(S)$ and $\frac{|a|}{e}(S)$ respectively.

□

The relation $a^2 = g^2 + e^2$ entails one of the two possibilities: (i) $g^2 > 0$, $(\frac{g}{a})^2 + (\frac{e}{a})^2 = 1$ and $\cos\phi = \frac{g}{|a|}$, (ii) $g^2 < 0$, $(\frac{|g|}{e})^2 + (\frac{a}{e})^2 = 1$, and $\cos\psi = \frac{|g|}{e}$.

The complexification of the ground field has put into full light the difference in signification for the ratios between $|a|$, e and $|g|$. Both ratios $\frac{e}{|a|}$ and $\frac{|a|}{e}$ are *new* invariants for $\mathbf{M}$ which represent $\|f_1(u)\|$ and $\|f_2(u)\|$ as u describes the unit sphere. By contrast, only *one* of the ratios $\frac{g}{|a|}$ or $\frac{|g|}{e}$ can be achieved on the distinguished subset D_+ or D_- inside $\mathbf{M}$. Proposition 6.2 tells us that there is much more geometric signification for $\frac{e}{|a|}$ or $\frac{|a|}{e}$ than the simple sine interpretation they may acquire from optimisation of the quadratic forms $x^H Ax$ $(g^2 > 0)$ or $x^H ABx$ $(g^2 < 0)$. For example, the end points of $f_1(u)$ and $f_2(u)$ are inverse in the unit sphere (S) centered at O.

6.5. **Confinement to the real 2D-subspace of M.** When the components z and z' for u in $\mathbf{M}$ are kept *real*, $u_R = \cos\theta\, q + \sin\theta\, q'$ describes the unit circle in the real plane $\mathbf{M}_R$ which is the real 2D-subspace of the complex invariant plane $\mathbf{M}$. In this section, all underscripts R refer to the *real* evolution in $\mathbf{M}$ under A which is clearly confined to the plane $\mathbf{M}_R$. It follows readily that the real analysis presented in Section 2 and 3 applies when u_R and $\mathbf{M}_R$ replace the former u and $\mathbf{M}$. This is true in particular for Figures 3 (b), 4 (b), 5 and 6 (c-d). The triangle $OM'C'$ provides an exact image for the real version of the complex evolution.

The result remains valid in any rotated plane $e^{i\xi}\mathbf{M}_R$ associated with $e^{i\xi}u_R = e^{i\xi}\cos\theta\, q + e^{i\xi}\sin\theta q'$, where z and z' are $\mathbb{R}$-dependent. This dependence between z and z' is precisely the reason why there exists an exact 2D-image. Such a representation vanishes when z and z' are $\mathbb{R}$-independent.

7. Conclusion and perspective

The report has advanced our understanding of the dynamics of a general hermitian matrix A by structural coupling associated with $\lambda < \lambda'$ in the following directions:

1) The matrix A need not be definite, so that the spectral distributions $\lambda < 0 < \lambda'$, $\lambda = 0$ or $\lambda' = 0$ are acceptable.

2) In addition to λ and λ', the value $-\lambda$ also plays a role. This is a surprising fact when $a \neq 0$, $\lambda' \neq -\lambda$ and $-\lambda$ may or may not be an eigenvalue of A.

3) When $a \neq 0$, the matrices $B = A - aI$ and $AB - A^2 - aA$ play a significant role. For example the $\mathbb{R}$-dependent vectors $f_1(u) = \frac{1}{a}Bu$ and $f_2(u) = \frac{1}{e^2}ABu - I$ have inverse constant norms $\frac{e}{|a|}$ and $\frac{|a|}{e}$ for any normalised u in the invariant (real or complex) plane $\mathbf{M}$ (isomorphic to $\mathbb{R}^2$ or $\mathbb{R}^4$). This leads to geometric *inversion* in the unit (real or complex) circle.

4) The real (resp. complex) evolution in $\mathbb{R}^2$ for $K = \mathbb{R}$ (resp. $\mathbb{R}^4$ when $K = \mathbb{C}$) can be exactly (resp. partly) interpreted by the geometry/trigonometry of a *triangle* expressing that $Bu = Au - au$ in $\mathbf{M}$.

5) *Each* of the 3 ordinary angles α, β, γ in the triangle has its own *raison d'être*. It is unexpected that their being right angles signals three kinds of optimal property taking place in K^n. For example, the fact $\gamma = \frac{\pi}{2}$ is achieved by midvectors having the remarkable property that they do *not* depend on the chosen couple (λ, λ'). They are the common midvectors for all matrices with varying spectra and fixed eigenbasis.

6) There exists a unique generic variational principle in $K^n (K = \mathbb{R}$ or $\mathbb{C})$ which can be specialised into the three different principles expressing orthogonality between lines $(K = \mathbb{R})$ or planes $(K = \mathbb{C})$ in the invariant subspace inside K^n.

The report only represents a first step towards a systematic treatment of spectral coupling for a general hermitian matrix. Many questions remain open which suggest future directions for research. Spectral chaining is one new direction. It was presented by invitation at the AMS Regional Meeting at CSU Fullerton, CA in October 2015 [Chatelin and Rincon-Camacho, 2015a]. The other direction currently under investigation is, for $K = \mathbb{C}$, the confinement of u to $\mathbb{R} \times \mathbb{C}$ so that the connection vector $\mathfrak{K}(u) = au \wedge Bu$ can be defined. More generally, we aim at furthering our understanding of the *differences* between $K = \mathbb{R}$ and $\mathbb{C}$.

Acknowledgement: The work of M. M. Rincon-Camacho has been supported by a grant from Total, Direction Scientifique.

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