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SYMMETRIC AND HERMITIAN MATRICES : A GEOMETRIC PERSPECTIVE ON SPECTRAL COUPLING

CERFACS REPORT TR/PA/15/56

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Abstract. The report develops the presentation begun in [Chatelin and Rincon-Camacho, 2015], of the information processing that can be performed by a general hermitian matrix of order n when two of its distinct eigenvalues are coupled, such as $\lambda < \lambda'$. Setting $a = \frac{\lambda+\lambda'}{2}$ and $e = \frac{\lambda'-\lambda}{2} > 0$, the new spectral information that is provided by coupling is expressed in terms of the ratios $\frac{e}{|a|}$ (if $\lambda\lambda' > 0$) or $\frac{|a|}{e}$ (if $\lambda\lambda' < 0$) and of the product $|a|e$. The information is delivered in geometric form, both metric and trigonometric, associated with various right-angled triangles deriving from optimality conditions on $n-$dimensional vectors. The paper contains a generalisation to indefinite matrices over $\mathbb{R}$ or $\mathbb{C}$ of Gustafson's operator trigonometry which in the matrix case assumes definiteness (mostly over $\mathbb{R}$).

Keywords: Spectral coupling, spectral chaining, hermitian matrix, indefinite symmetric or hermitian, spectral plane, observation angle, perspective angle, catchvector, antieigenvector, middle vector, Euler equation, balance equation, torus in 3D.

1. Composite natural phenomena

1.1. **Introduction.** It is well-known that many natural phenomena are composite: they are produced by the interaction of two (or more) simpler phenomena, where the interaction is in general nonlinear. The coupling of two phenomena is ubiquitous in Physics; electromagnetism, convection-diffusion, plasma fusion, flutter are just a few examples. And it is known that the tighter the coupling, the higher the departure of normality for the matrix resulting from discretisation [Chaitin-Chatelin and Frayssé, 1996, chapter 10]. The theoretical understanding and algorithmic resolution of tightly coupled phenomena remains today a formidable challenge for scientists. A classical path of investigation is to consider the linear coupling $A+tB = A(t)$ by the complex parameter t between two independent phenomena modelled by A and B. Physical examples of such a parameter are given by Reynolds and Péclet numbers, which are real or by the admittance which can be complex. The evolution under t in $\mathbb{C} \cup \{\infty\}$ of the spectrum of $A(t) \in \mathbb{C}^{n\times n}$ is studied in [Chatelin, 2012b, chapter 7]. This approach, known as Homotopic Deviation, puts no restriction on $\|tB\| = |t|\|B\|$, which, by contrast, is classically assumed to be small enough in *perturbation* theory.

In this paper, we propose a different angle of approach to coupling based on two real parameters which are eigenvalues of a single matrix A enjoying a property of *symmetry* that we describe next.

1.2. **Spectral coupling.** 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.* 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. Hence we develop new consequences of the classical spectral theory for symmetric matrices [Parlett, 1998] and

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hermitian matrices [Horn and Johnson, 1985, chapter 4, Chatelin, 2012a, chapter 8] These consequences are almost all derived from the fundamental property that the quadratic form $x^H Ax$ is *real* for $x \in \mathbb{C}^n$. Of special interest are the new informations provided by the simultaneous consideration of *two* eigenelements (values/vectors) rather than a single one in classical theory.

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1.3. **Related work.** The systematic study of spectral coupling that we have developped originates in the pioneering work that Gustafson has pursued in relative isolation for almost five decades [Gustafson, 2012]. His context deals more generally with strongly accretive operators in Hilbert spaces, which admit symmetric or hermitian *positive definite* matrices as particular cases. The work we present is restricted to finite dimension, but deals more generally with *indefinite* matrices.

When referring to his own theory, Gustafson uses several terms such as operator trigonometry, antieigenvalue analysis, introducing the concepts of antieigen(-value/-vector). The reason why his original vocabulary has to be adapted to the context of indefinite matrices will become clear later on. Also, we shall indicate in what sense Gustafson's "antieigenvectors" can be interpreted as the "most turned" vectors by A when the ground field K is $\mathbb{C}$ rather that $\mathbb{R}$.

1.4. **Organisation of the paper.** Section 2 presents the new information provided, in the numerical plane $\mathbb{R}^2$, by the simultaneous consideration of 2 real eigenvalues $\lambda < \lambda'$ for a matrix A which is either symmetric ($A = A^T \in \mathbb{R}^{n\times n}$) or hermitian ($A = A^H \in \mathbb{C}^{n\times n}$). The two isolated eigenvalues are *linked* by the cercle Γ centered at the mean $(\frac{\lambda+\lambda'}{2}, 0)$ with radius $\frac{\lambda'-\lambda}{2}$ drawn in $\mathbb{R}^2$. The proofs involve only *elementary* plane geometry and trigonometry in a triangle. The consideration of two associated orthonormal eigenvectors q and q' in K^n may require to distinguish whether the ground field K is $\mathbb{R}$ or $\mathbb{C}$. Section 3 is devoted to the case $K = \mathbb{R}$ and to trigonometry in the invariant real plane $\mathbb{R}^2$ spanned by q and q' in $\mathbb{R}^n$. Three variational principles are derived in Section 4 by looking at the stationary values of functionals of the type $c : K^n \to \mathbb{R}$ (due to the second author) or $J : K^{n\times p} \to \mathbb{R}$, $1 < p < m$. Next Section 5 presents a geometric interpretation in $\mathbb{R}^3$ of the optimality principles obtained in the complex invariant space $\mathbb{C}^2 \cong \mathbb{R}^4$ (when $K = \mathbb{C}$) with 2 complex dimensions, i.e. 4 real ones. Section 6 illustrates some of the underrated properties of the "middle vectors" that are the linear combinations $zq + z'q'$ with $|z| = |z'| = \frac{1}{\sqrt{2}}$, z, $z' \in \mathbb{C}$. Two examples from Numerical Analysis and Statistics are provided. Section 7 deals with another functional $\nu : \mathbb{R} \times K^n \to \mathbb{R}^+$. The paper closes on Section 8 which wraps up the information processing provided in $\mathbb{R}^2$ by spectral coupling, that is explained by the underlying algebraic structure of $\mathbb{R}^2$ as the ring of bireal numbers.

2. Spectral information processing in a spectral plane

2.1. **Definition.** 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 $K = \mathbb{R}$.

Let us turn to the simultaneous consideration of two distinct eigenvalues $\lambda < \lambda'$ which produces new information (both geometric and trigonometric) best understood if one considers the spectral *plane* $\mathbb{R}^2$ denoted $\mathbf{\Sigma}$ which contains the spectral *line* $\mathbb{R}$ as its real axis.

2.2. **Notation for the eigenvalue pair** $\{\lambda, \lambda'\}$**.** The eigenvalues λ and λ' are the distinct real roots of the quadratic equation

$$\mu^2 - 2a\mu + g^2 = 0, \quad a = \frac{\lambda + \lambda'}{2}, \;\; g^2 = \lambda\lambda' \tag{2.1}$$

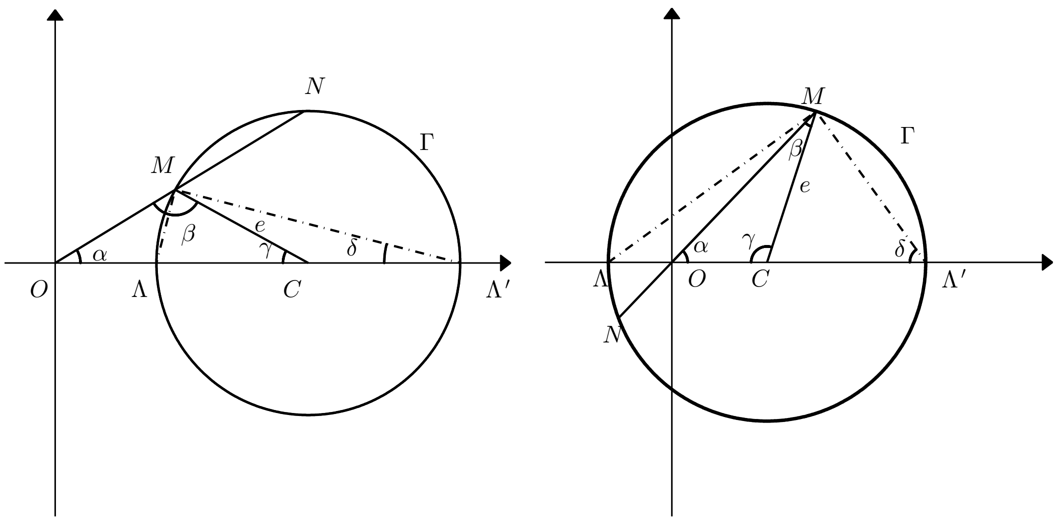
where a is the arithmetic mean. By assumption $a^2 - g^2 = \frac{1}{4}(\lambda - \lambda')^2 > 0$. We set $e = \frac{\lambda' - \lambda}{2} > 0$ and observe that $a^2 = g^2 + e^2 \Leftrightarrow -e^2 \leq g^2 < a^2$. Moreover $g^2 = 0 \Leftrightarrow \lambda$ or $\lambda' = 0$, λ' or $\lambda = 2a$ $\Leftrightarrow e = |a|$.

2.3. **The three pythagorean means of λ and λ', $0 < \lambda < \lambda'$.** To the two positive numbers $0 < \lambda < \lambda'$ are associated three types of mean: arithmetic $a = \frac{\lambda + \lambda'}{2}$, geometric $g = \sqrt{\lambda\lambda'}$, harmonic $h = [\frac{1}{2}(\frac{1}{\lambda} + \frac{1}{\lambda'})]^{-1} = \frac{g^2}{a} = \frac{2\lambda\lambda'}{\lambda + \lambda'}$. The three means which satisfy $0 < \lambda < h < g < a < \lambda'$ are known since Antiquity as the *pythagorean means*.

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

2.4. **The triangle $\mathrm{Tr}(M) = OMC$ in the spectral plane $\boldsymbol{\Sigma}$.** 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 $\Lambda = (\lambda, 0)$ and $\Lambda' = (\lambda', 0)$ and lies in the spectral plane. Depending on the sign of $g^2 = \lambda\lambda'$, the origin O is outside Γ ($g^2 > 0$), on Γ ($g = 0$) or inside Γ ($g^2 < 0$): 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 which necessarily lies in a plane where elementary geometric constructions and trigonometric calculations can be performed.

We first suppose that $g^2 \neq 0$, see Figure 1.



(a) $OC = a > e > 0$ (b) $0 < OC = a < e$

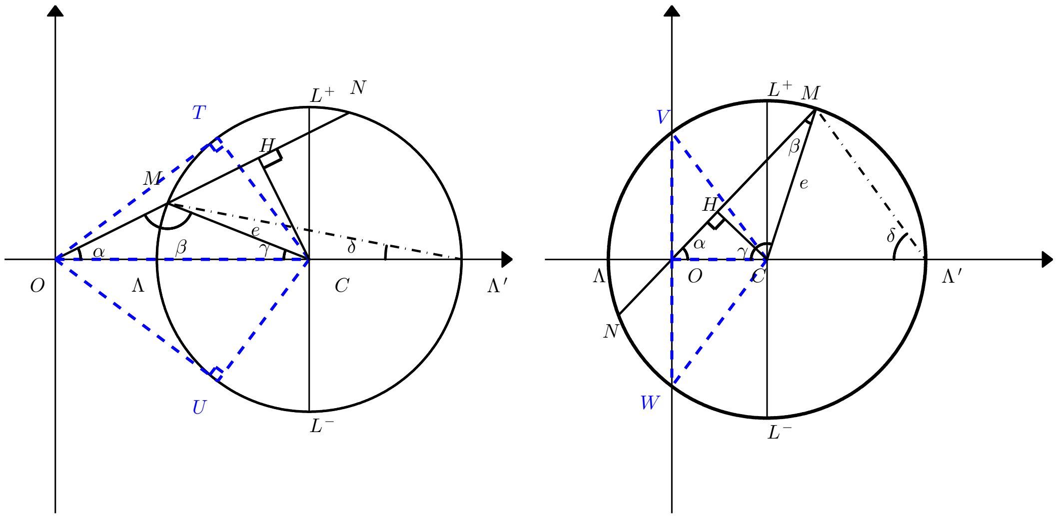
FIGURE 1. $\mathrm{Tr}(M)$ when $g^2 \neq 0$ in $\boldsymbol{\Sigma}$, $a \neq 0$

When O is inside (resp. outside) Γ, an arbitrary line drawn through O intersects Γ in two points M and N always (resp. if the acute angle $\alpha = \angle(OC, OM)$ is not too large). We consider the triangle $\mathrm{Tr}(M) = OMC$ defined for any M on Γ, $M \neq \Lambda$ or Λ', and $a \neq 0$ ($O \neq C$). The role of the dotted right-angled triangle $\Lambda M \Lambda'$ is discussed in Section 2.6 below.

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 $\mathrm{Tr}(M)$ as follows: $\alpha = \angle(OC, OM)$, $\beta = \angle(MC, MO)$ and $\gamma = \angle(CO, CM)$ where the angles vary in $]0, \pi[$ according to $\mathrm{sgn}(g^2)$ as follows:

g^2	$-$	0	$+$
α	$\alpha \in]0, \pi[$		$0 < \alpha < \frac{\pi}{2}$
β	$0 < \beta < \frac{\pi}{2}$		$\beta \in]0, \pi[$
γ	$0 < \gamma < \pi$		

For future reference, we also introduce $\delta = \frac{\gamma}{2} = \angle(\Lambda'\Lambda, \Lambda' M)$, $0 < \delta < \frac{\pi}{2}$. 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) $OC = a > e > 0$ (b) $0 < OC = a < e$

$\sin\alpha = \frac{CH}{a}$ $\sin\beta = \frac{CH}{e}$

FIGURE 2. Trigonometry for α (a) and β (b) in $\boldsymbol{\Sigma}$

If $a = 0$, $O = C$ in case (b) and the triangle is degenerate as the segment OM ($\beta = 0$, $\alpha + \gamma = \pi$).

Lemma 2.1. *(a) When $0 < g^2 < a^2$, $0 < \alpha \leq \phi$ with $\sin\phi = \frac{e}{|a|}$, and $\alpha = \phi < \frac{\pi}{2} \Leftrightarrow \beta = \frac{\pi}{2}$, $\gamma = \frac{\pi}{2} - \phi$.*

(b) When $-e^2 < g^2 < 0$, $\beta \leq \psi$ with $\sin\psi = \frac{|a|}{e}$, and $\beta = \psi \Leftrightarrow \alpha = \frac{\pi}{2}$, $\gamma = \frac{\pi}{2} - \psi$.

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

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

□

When $g^2 > 0$, the circle Γ is seen from the origin O under the angle 2ϕ, hence ϕ is the *(outer) observation angle*. When $g^2 < 0$, $a \neq 0$, the segment $OC \neq 0$ is seen from the circle Γ under the angle β: the maximal angle ψ is called the *(inner) perspective angle*. If $g^2 \to 0^+$ (resp. 0^-) ϕ (resp. ψ) tends to $\frac{\pi}{2}$, hence $\gamma \to 0$. The points T, U (resp. V, W) tend to O and the right-angled triangles tend to collapse into the segment OC.

We observe that $\cos\phi = \frac{g}{|a|}$ or $\cos\psi = \frac{|g|}{e}$ for M at *two* locations on Γ: either T and U ($\beta = \frac{\pi}{2}$, $OT = g$, $g^2 > 0$) or V and W ($\alpha = \frac{\pi}{2}$, $OV = |g|$, $g^2 < 0$).

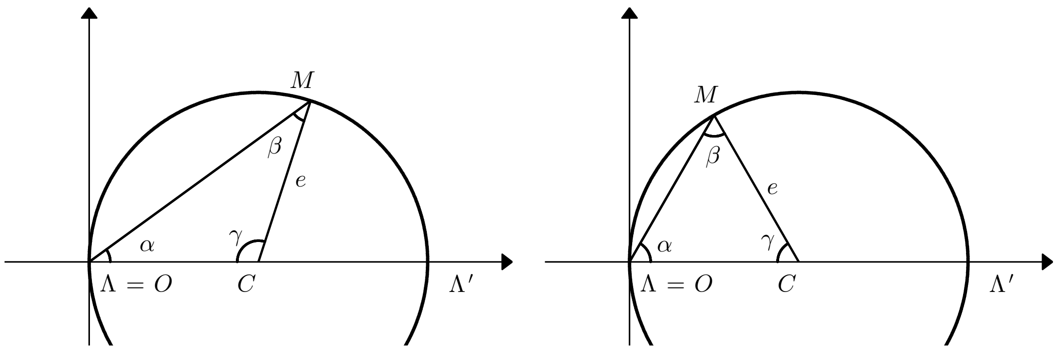
By contrast the value $\frac{e}{|a|}$ (resp. $\frac{|a|}{e}$) is fixed, independently of the location of M on Γ. Of course the number can be interpreted as the maximum value $\sin\phi$ (resp. $\sin\psi$) only if $\mathrm{Tr}(M)$ is *right-angled* at M (resp. O), that is when M is at T or U (resp. V or W).

Lemma 2.2. *When M describes Γ and $a \neq 0$, the surface of $\mathrm{Tr}(M)$ is maximum and equal to $\frac{1}{2}|a|e$ when $\gamma = \frac{\pi}{2}$.*

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

Let $\hat{\alpha}$ denote $\angle(OC, OL^+)$ and $\hat{\beta} = \angle(L^+C, L^+O)$, then $\tan\hat{\alpha} = \frac{e}{|a|} = \frac{1}{\tan\hat{\beta}}$. When $g^2 > 0$ (resp. < 0) the angles $\hat{\alpha}$ and ϕ (resp. $\hat{\beta}$ and ψ) are related by $\hat{\alpha} = \tan^{-1}\sin\phi$ (resp. $\hat{\beta} = \tan^{-1}\sin\psi$).

We now suppose that $g^2 = 0$, see Figure 3 where $\Lambda = O$.

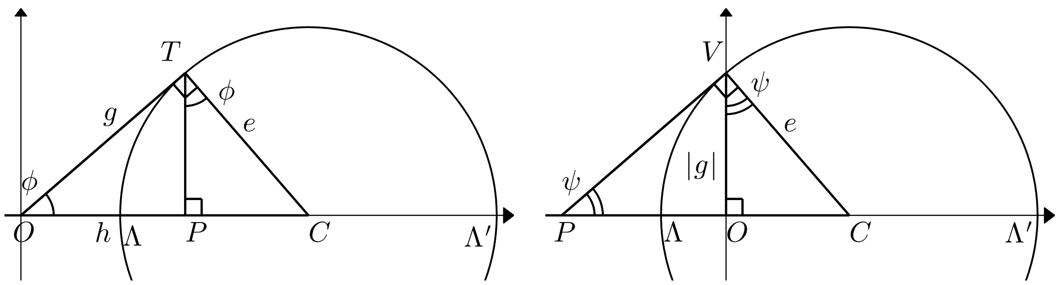


(a) $\lambda = 0$, $\alpha = \beta \neq \gamma$ (b) $\lambda = 0$, $\alpha = \beta = \gamma = \frac{\pi}{3}$

FIGURE 3. $\mathrm{Tr}(M)$ when $g^2 = 0$, $|a| = e > 0$

When $|a| = e$, the triangle OMC is isosceles with $\alpha = \beta$. It is right-angled if M is at L^+ or L^-: $\hat{\alpha} = \hat{\beta} = \frac{\pi}{4}$ ($\tan\hat{\alpha} = \tan\hat{\beta} = 1$) and equilateral if $\alpha = \beta = \gamma = \frac{\pi}{3}$, $\delta = \frac{\pi}{6}$. It is degenerate as OC when $\alpha = \beta = \frac{\pi}{2}$, $\gamma = 0$.

2.5. **Similar triangles when α or $\beta = \frac{\pi}{2}$, $g^2 \neq 0$.** We suppose that $\alpha = \phi$, $\beta = \frac{\pi}{2}$ for $g^2 > 0$ or $\alpha = \frac{\pi}{2}$, $\beta = \psi$ for $g^2 < 0$, see Figure 4. The location of the generic point M is either T or U (resp. V or W) if $g^2 > 0$ (resp. $g^2 < 0$).



(a) $OC = a > e$, $\alpha = \phi$ (b) $0 < OC = a < e$, $\beta = \psi$

FIGURE 4. Similar right-angled triangles for $g^2 \neq 0$

When $|a| > e$, let P inside Γ be the projection of T or U on the spectral axis. The triangles OTC and CPT are similar, with ratio $\frac{|a|}{e} > 1$. Moreover $\cos\phi = \frac{g}{|a|} = \frac{OP}{g}$, hence $OP = h = \frac{g^2}{|a|}$, $PT = \frac{ge}{|a|}$.

When $|a| < e$, let the tangent to Γ at V intersect the real axis at P outside Γ. The triangles OVC and VPC are also similar with ratio $\frac{e}{PC}$, with $PC = PO + |a|$ and $PO = \frac{-g^2}{|a|}$, hence $PC = \frac{1}{|a|}(-g^2 + a^2) = \frac{e^2}{|a|}$ yields the value $\frac{e}{PC} = \frac{|a|}{e} < 1$.

2.6. **Homothetic triangles for $\delta \in]0, \frac{\pi}{2}[$, $a \neq 0$.** We assume that $a \neq 0$, $e > 0$ so that the triangle $\mathrm{Tr}(M) = OMC$ is not degenerate. When M describes the upper half of Γ, δ varies in $]0, \frac{\pi}{2}[$. And we associate to M, parametrised by δ, the rotating frame OX, OY where $\angle(OX, \mathbb{R}) = \delta$, see Figure 5 where $a > e$ ($\Rightarrow g^2 > 0$).

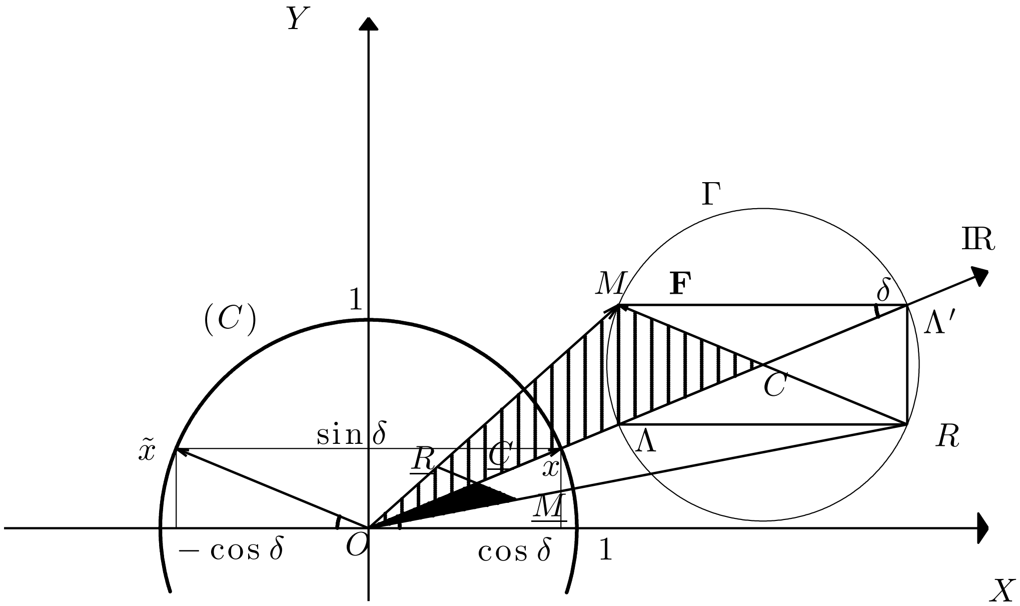


FIGURE 5. $\mathrm{Tr}(M)$ and $\mathrm{Tr}(\underline{M})$, $a > e$, $g^2 > 1$

Let $x = x(\delta) = (\cos\delta, \sin\delta)^T$, $\|x\| = 1$, $D = \mathrm{diag}(\lambda, \lambda')$, $J = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$ and $K = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. $\vec{OC} = ax \neq 0$ by assumption, $\vec{OM} = (\lambda\cos\delta, \lambda'\sin\delta) = Dx$, $\tilde{x} = x(\pi - \delta)$. $\vec{OR} = \vec{OC} + \vec{CR} = \vec{OC} - \vec{CM} = \mathring{D}x$, where $\mathring{D} = \mathrm{diag}(\lambda', \lambda) = KDK$ is similar to D. The triangle $\mathrm{Tr}(R) = ORC$ is associated with $\mathring{D}$, that is with the pair (λ', λ) in *reverse* order.

It is clear that the rectangle $\mathbf{F} = \Lambda M \Lambda' R$ displayed on Figure 5 has sides parallel to the rotating axes OX and OY. Its diagonals are two diameters of Γ forming the angle $\gamma = 2\delta$. The rectangle reduces to a square iff $\gamma = \frac{\pi}{2} \Leftrightarrow \delta = \frac{\pi}{4} \Leftrightarrow x(\frac{\pi}{4}) = \hat{x} = \frac{1}{\sqrt{2}}(1,1)^T$. The geometric figure $\mathbf{F}$ enables an easy construction of the companion triangle $\mathrm{Tr}(\underline{M}) = O\underline{MC}$ based on $\vec{O\underline{M}} = D^{-1}x$. The meaning of the quantities referring to D^{-1} which are underlined is clear from context. For example, since $g^2 = \lambda\lambda'$, $\underline{g}^2 = \frac{1}{\lambda}\frac{1}{\lambda'} = \frac{1}{g^2}$.

Lemma 2.3. *$\vec{O\underline{C}} = \underline{a}x = \frac{1}{g^2}\vec{OC}$, $\underline{\vec{CM}} = -\frac{1}{g^2}\vec{CM} = \frac{1}{g^2}\vec{CR}$, $\bar{\gamma} + \gamma = \pi$.*

Proof. $\underline{a} = \frac{1}{2}(\frac{1}{\lambda} + \frac{1}{\lambda'}) = \frac{a}{g^2} = \frac{1}{h}$, $D^{-1} = \mathrm{diag}(\frac{1}{\lambda}, \frac{1}{\lambda'}) = \frac{1}{g^2}\mathrm{diag}(\lambda', \lambda) = \frac{1}{g^2}\mathring{D}$, $(D^{-1} - \underline{a}I_2)x = -\frac{e}{g^2}Jx = -\frac{1}{g^2}(e\tilde{x}) = \underline{\vec{CM}}$. Since $\vec{CM}$ and $\underline{\vec{CM}}$ are parallel with *opposite* directions, $\gamma + \underline{\gamma} = \pi$. □

Corollary 2.4. *The triangles $O\underline{RC}$ and $O\underline{MC}$ are derived from the triangles OMC and ORC by the homothety $(O, \frac{1}{g^2})$. They are symmetrically placed with respect to the real axis $\mathbb{R}$ iff $\delta = \frac{\pi}{4}$ $\Leftrightarrow x(\frac{\pi}{4}) = \hat{x}$.*

Proof. Clear from Lemma 2.3. When $\delta = \frac{\pi}{4}$, $\hat{x} = \frac{1}{\sqrt{2}}(1,1)^T$ spans the principal bisector of the frame OXY. □

Corollary 2.4 establishes a remarkably simple dynamical connection between D and D^{-1} which is elegantly formulated on triangles in plane geometry, provided that $\lambda' \neq -\lambda$. When $\lambda' = -\lambda = e$, C and $\underline{C}$ coalesce into O: the triangles become the segments OM and $O\underline{M}$.

Proposition 2.5. *When $g^2 = -e^2$, the geometric transformation $M \to \underline{M}$ in $\mathbf{\Sigma}$ is the inversion $\overline{OM} \cdot \overline{O\underline{M}} = 1$ with respect to the unit cercle $(C) = (O, 1)$.*

Proof. $\vec{OM} = Dx = e\tilde{x}$ and $O\vec{\underline{M}} = D^{-1}x = -\frac{1}{g^2}Dx = \frac{1}{e}\tilde{x}$. For $x = x(\delta)$, $0 \leq \delta \leq \frac{\pi}{2}$, M and $\underline{M}$ belong to the positive axis generated by $\tilde{x} = x(\pi - \delta)$ and satisfy $\overline{OM} \cdot \overline{O\underline{M}} = 1$. If $\delta = 0$ (resp. $\frac{\pi}{2}$) $\tilde{x} = -x$ (resp. x). □

2.7. **An epistemological pause.** The above analysis relies only on the knowledge of a pair (λ, λ') of real eigenvalues for A. It is therefore valid for *real root* coupling for equations defined by polynomials or functions enjoying at least 2 distinct real roots.

The rest of the report explores what additional information is provided by the fact that A is a linear map over K^n with an orthogonal eigenbasis.

3. The invariant plane $\mathbf{M}$ spanned by q and q'

3.1. **Generalities.** Let q and q' be an orthonormal pair of eigenvectors associated with λ and λ': $\|q\| = \|q'\| = 1$ and $\langle q, q' \rangle = q'^H q = 0$. The subspace $\mathbf{M}$ of complex (resp. real) linear combinations of q and q' is a complex (resp. real) plane invariant under the action of A when $K = \mathbb{C}$ (resp. $\mathbb{R}$). Therefore $\mathbf{M}$ lives in $\mathbb{R}^4$ (resp. $\mathbb{R}^2$): the real interpretation of $\mathbf{M}$ differs whether $K = \mathbb{C}$ or $\mathbb{R}$. We suppose in this Section that A is symmetric, hence $\mathbf{M}$ is isomorphic to the real plane $\mathbb{R}^2$. The treatment of A hermitian is deferred to Sections 4 and 5.

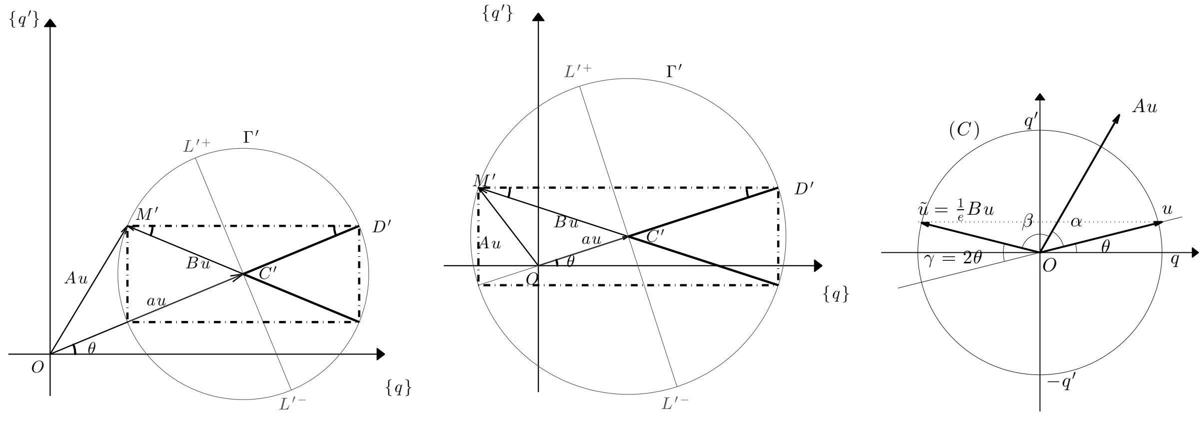
3.2. $K = \mathbb{R}$: **the triangle $OM'C'$ in the invariant 2D-plane $\mathbf{M}$.** We consider the real combination $u = u(\theta) = (\cos\theta)q + (\sin\theta)q'$, with unit norm $\|u\| = 1$, $\theta \in [0, 2\pi[$. When θ varies in $[0, 2\pi[$, the vector u describes, in the invariant plane $\mathbf{M}$, the unit circle (C) centered at O and passing through the eigenvectors $\pm q$, $\pm q'$.

We define $B = A - aI$, a matrix which commutes with A: $F = AB = BA = A^2 - aA$.

Lemma 3.1. *$\|Bu\| = e$, $B^2u = e^2u$ and $\|Fu - e^2u\| = |a|e$ for any $u \in (C)$.*

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

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 $\text{Tr}(u) = OM'C'$, see Figure 6 (a) when $a > e$ and (b) when $a < e$ which displays the circle Γ' centered at C' with radius e. In order that $\text{Tr}(u)$ be non degenerate ($C' \neq O$), we assume below that $a \neq 0$ when $g^2 < 0$.



(a) $a > e$ (b) $0 < a < e$ (c) $0 \leq \theta \leq \frac{\pi}{2}$

FIGURE 6. $\mathrm{Tr}(u)$ as a function of θ when $K = \mathbb{R}$

The point $M' = (r, r')$ in the basis $\{q, q'\}$ is the meeting point on Γ' of Au and Bu, $\|Bu\| = C'M' = e$.

Lemma 3.2. *The point $M' = (r, r')$ describes the ellipse of equation $\left(\frac{r}{\lambda}\right)^2 + \left(\frac{r'}{\lambda'}\right)^2 = 1$ iff $g^2 \neq 0$. If $g^2 = 0$ (resp. $a = 0$), the ellipse is reduced to a segment (resp. a circle with radius e).*

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 $\lambda\lambda' \neq 0$. If $g^2 = 0$, $\lambda = 0 < \lambda'$, $r = 0$ and $r' \in [-\lambda', \lambda']$ (say). If $a = 0$, $\lambda' = -\lambda = e$

□

One can check readily on Figure 6 (a) and (b) that $\gamma = \angle(C'O, C'M') = 2\theta = 2\angle(D'O, D'M') = 2\delta$ as ordinary angles in $]0, \pi[$; the geometric meaning of the dotted rectangles follows from Section 2.6 and Figure 5. On Figure 6 (c) we see that $\angle(-u, \tilde{u}) = 2\theta$. The restriction $\theta \in [0, \frac{\pi}{2}]$ is sufficient to display the complete geometric evolution of $\mathrm{Tr}(u)$. Therefore we may restrict θ to describe the first quadrant for simplicity.

3.3. **When $\delta = \theta$ in $]0, \frac{\pi}{2}[$.** We may compare the triangle $\mathrm{Tr}(M) = OMC$ parameterised by δ and the triangle $\mathrm{Tr}(u) = OM'C'$ parameterised by θ.

Corollary 3.3. *The equality $\delta = \theta$ in $]0, \frac{\pi}{2}[$ yields the congruence* $\mathrm{Tr}(M) = \mathrm{Tr}(u)$.

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 $]0, \frac{\pi}{2}[$: $\gamma = 2\theta = 2\delta \in]0, \pi[$. Observe that $x(\delta) = (\cos\delta, \sin\delta)^T$ in OXY is equivalent to $u(\theta) = (\cos\theta, \sin\theta)^T$ in $\{q, q'\}$ □

When M' describes its ellipse once in $\mathbf{M}$, θ varies in $[0, 2\pi[$. This entails that the corresponding point M describes its circle Γ *twice* in the spectral plane.

3.4. **Local optimisation in M.** The key Corollary 3.3 allows us to transfer the results of Section 2 about $\mathrm{Tr}(M)$ to the triangle $\mathrm{Tr}(u)$. The optimality properties $\alpha \leq \phi$ ($g^2 > 0$), $\beta \leq \psi$ ($g^2 < 0$) are valid for the corresponding ordinary angles $\alpha = \angle(u, Au)$, $\beta = \angle(Bu, Au)$ 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 4 vectors $v_+ = \varepsilon w_+ q + \varepsilon' w'_+ q'$, with $\varepsilon = \pm 1$, $\varepsilon' = \pm 1$, and $D_+ = \{v_+\}$.

When $g^2 < 0$, we define analogously 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 four vectors $v_- = \varepsilon w_- q + \varepsilon' w'_- q'$, with $\varepsilon = \pm 1$, $\varepsilon' = \pm 1$ and $D_- = \{v_-\}$.

Theorem 3.4. *i) When $g^2 > 0$, the minimum value $\cos\phi = \frac{g}{|a|}$ is achieved by any v_+ in D_+ and $\langle Bv_+, Av_+\rangle = 0$, $\|Av_+\| = \frac{1}{e}\|Fv_+\| = g$.*

ii) 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. 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 $\cos\angle(v_+, Av_+) = \frac{g}{a}$. Therefore $|\cos\alpha| \geq \cos\phi = \frac{g}{|a|}$. Moreover $\langle Bv_+, Av_+\rangle = 0$ as expected. The vector $\frac{1}{|a|}Fv_+$ is orthogonal to v_+ with length $PT = PU = \frac{eg}{|a|}$.

ii) 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 $PV = PW = \frac{e|g|}{|a|}$. $\square$

3.5. **Catchvectors and antieigenvectors.** When A is *indefinite*, the spectral coupling of eigenvalues with different sign: $\lambda < 0 < \lambda'$ yields the existence of 4 vectors v_- with an orthogonal image Av_-: $\langle v_-, Av_-\rangle = 0$. These vectors are the "most turned" vectors by A locally in $\mathbf{M}$: their image direction being orthogonal, it is the "furthest" from their own direction. Such vectors, which can exist only when A is *indefinite*, 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. To avoid ambiguity the vectors v_+ in D_+ when $g^2 > 0$ are called *catchvectors.*

Remark 3.1. Because the theory of Gustafson assumes that A is positive definite, all spectral couplings are realised by positive eigenvalues with $a > 0$, and $g^2 = \lambda\lambda' > 0$ is the rule. Therefore $\cos\alpha$ is bounded from below by $\frac{g}{a} > 0$. Because we put no other assumption on $A \in \mathbb{R}^{n\times n}$ than symmetry, we are led to depart from Gustafson's nomenclature. When A is indefinite, it becomes necessary to distinguish between catch- and antieigen- vectors.

But it turns out that our work differs from Gustafson's theory on some more fundamental grounds. Because of the basic assumption that A is symmetric positive definite, his theory focuses mainly on the *specific angle* $\alpha = \angle(u, Au)$ maximum for (λ_1, λ_n); it ignores the key role of the triangles $\mathrm{Tr}(M)$ in the spectral plane $\mathbf{\Sigma}$ and $\mathrm{Tr}(u)$ in the invariant plane $\mathbf{M} \subset \mathbb{R}^n$, and of the information brought by their *three* angles α, β, $\gamma = \frac{\theta}{2} = \frac{\delta}{2}$. The full extent to which we have developed Gustafson's seminal ideas will be unravelled as we proceed.

3.6. **Middle vectors.** The previous section has 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 $\gamma = 2\theta$. We define $\hat{w} = \frac{1}{\sqrt{2}}$ and $\hat{v} = \hat{w}(\varepsilon q + \varepsilon' q')$, $\hat{D} = \{\hat{v}, \varepsilon \text{ and } \varepsilon' = \pm 1\}$.

Lemma 3.5. *The minimum value $\langle au, Bu\rangle = 0$ is achieved, for $a \neq 0$, at $\hat{v} = \frac{1}{\sqrt{2}}(q + q')$.*

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

Theorem 3.6. *When $a \neq 0$, the 4 triangles $\mathrm{Tr}(\hat{v})$, $\hat{v} \in \hat{D}$, have the maximal surface $\frac{1}{2}|a|e$.*

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

The quantity $2\Sigma(u)$ is called the *influence* of u. It is nonzero when $\mathrm{Tr}(u)$ is non degenerate ($u \notin \{\pm q, \pm q'\}$ or $a \neq 0$).

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 *middle vectors* (or *midvectors*) since they are the bisectors of the eigenvectors. They have the largest influence $|a|e$, which is the surface of any of the two *rectangles* with diagonal OL^+ or OL^-, see Figure 2. Moreover Lemma 3.1 tells us that the maximal *surface* $|a|e$ is precisely the *norm* of $Fu - e^2u$ for any $u \in (C)$.

Remark 3.2. The generic concept of a middle vector is absent from Gustafson's theory. It only appears in a statistical setting under the guise of an "inefficient" vector, see Section 6.2 and [Gustafson, 2012, p. 190].

3.7. A **is positive definite.** Let A be symmetric positive definite with eigenvalues $0 < \lambda_1 \leq \ldots \leq \lambda_n$. Choosing the extreme pair (λ_1, λ_n) we set $a_* = \frac{\lambda_1+\lambda_n}{2} > 0$, $e_* = \frac{\lambda_n-\lambda_1}{2}$, $g_* = \sqrt{\lambda_1\lambda_n}$.

Lemma 3.7. *For any coupling $\lambda < \lambda'$ which is not extreme the following inequalities hold: $\frac{e}{a} < \frac{e_*}{a_*} < 1 \Leftrightarrow \frac{g}{a} > \frac{g_*}{a_*} > 0$, $ae < a_*e_*$.*

Proof. First, $\frac{e}{a} < \frac{e_*}{a_*} < 1 \Leftrightarrow \lambda_1\lambda(\frac{\lambda_n}{\lambda_1} - \frac{\lambda'}{\lambda}) > 0$. Since $\frac{g}{a} = \frac{\sqrt{a^2-e^2}}{a} = \sqrt{1-(\frac{e}{a})^2}$, we get $\frac{g}{a} > \frac{g_*}{a_*} > 0$. Second, $a < a_*$ and $e < e_*$ entail $ae < a_*e_*$. □

Corollary 3.8. *The maximum turning angle $\phi(A)$ satisfies $\cos\phi(A) = \frac{g_*}{a_*}$, $\sin\phi(A) = \frac{e_*}{a_*}$. The associated middle vectors have the highest influence $a_*e_* = \frac{1}{4}(\lambda_n^2 - \lambda_1^2)$.*

Proof. Direct consequence of Lemma 3.7. The weights $w_{+,*}$, $w'_{+,*}$ of the catchvectors $v_{+,*}$ satisfy $\frac{w_{+,*}}{w'_{+,*}} = \sqrt{\frac{\lambda_n}{\lambda_1}} = \mathrm{cond}(A^{1/2})$, where $\mathrm{cond}(A) = \sup_{\lambda'>\lambda} \frac{\lambda'}{\lambda}$ is the condition number of A expressed with the euclidean norm $\|\cdot\|$. The middle vectors are the bisectors of any two orthonormal eigenvectors q_*, q'_* for λ_1 and λ_n: $\hat{v}_* = \frac{1}{\sqrt{2}}(\varepsilon q_* + \varepsilon' q'_*)$, ε and $\varepsilon' = \pm 1$. □

For future reference we denote $\gamma(A)$ the trigonometric complement of $\phi(A)$: $\phi(A) + \gamma(A) = \frac{\pi}{2} = \beta(A)$.

3.8. **A difference between $\mathbf{Tr}(M)$ and $\mathbf{Tr}(u)$.** Despite their congruence when $a \neq 0$, the triangles $\mathrm{Tr}(M)$ and $\mathrm{Tr}(u)$ do not process spectral information in an identical way. In the spectral plane $\mathbf{\Sigma}$, the axis OC is fixed whereas in $\mathbf{M}$, only O is fixed: C' describes the circle $|a|(C)$.

We saw in Section 2 that $\mathrm{Tr}(M)$ can be right-angled at the vertex M ($g^2 > 0$) or O ($g^2 < 0$) and C ($g^2 \neq 0$) for M at *two* locations on Γ, namely (T, U) or (V, W) and (L^+, L^-). By comparison $\mathrm{Tr}(u)$ can be right-angled at M' ($g^2 > 0$) or O ($g^2 < 0$) and C' ($g^2 \neq 0$) when u belongs to the sets D_+ or D_- and $\hat{D}$. And each set consists of *four* vectors leading to *eight* right-angled triangles (2 triangles per vector).

4. Variational principles

In this Section, A is an arbitrary hermitian matrix, $A = A^H \in \mathbb{C}^{n\times n}$ where the ground field is $K = \mathbb{C}$ which can be specialised to be $\mathbb{R}$ (A symmetric).

For any hermitian matrix Y, the ratio $\frac{x^HYx}{\|x\|\|Yx\|}$ 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 5.1.

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

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

4.1. **A preparatory lemma (M.M. Rincon-Camacho).** Let be given two hermitian matrices Y and Z, the product YZ is hermitian iff Y and Z commute. We consider the real functional

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

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:*

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

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 adapt below the proof to the general case Y, Z and YZ hermitian and indefinite, $K = \mathbb{C}$.

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

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

with

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

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

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

and

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

Finally we have

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

The variational calculus imposes that $\Re\langle y,V\rangle = 0$ for any $0\neq y\in\mathbb{C}^n$. Indeed, if $V^Hy = ib$, 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).

□

4.2. **The catchvectors: $Y = I$, $Z = A$.** When we choose $Z = A$ and $Y = I$, the Euler equation (4.2) becomes

$$A^2x - 2\frac{\|Ax\|^2}{\langle x,Ax\rangle}Ax + \left(\frac{\|Ax\|}{\|x\|}\right)^2 x = 0 \tag{4.3}$$

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

In order to solve (4.3) 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 $A = QDQ^H$, $y = Q^Hx$, $\|y\| = \|x\|$, (4.3) can be written

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

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

$$(\mu_i^2 - 2k\mu_i + l)y_i = 0, \quad i = 1,\dots,n. \tag{4.4}$$

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. (4.3) is obviously satisfied when x is an eigenvector: $Ax = \lambda x$. Let us assume that x and Ax are independent. Eq. (4.4) entails $y_j = 0$ for all j such that $\mu_i^2 - 2k\mu_i + l\neq 0$ and vice versa. We denote $\lambda < \lambda'$ the two distinct roots $\{\mu_j,\mu_j'\}$ of the quadratic equation. The corresponding multiplicities are m, m' and the associated eigensubspaces are $\mathcal{M}$, $\mathcal{M}'$ with $\dim\mathcal{M} = m$, $\dim\mathcal{M}' = m'$. As before, $a = \frac{\lambda+\lambda'}{2}$, $g^2 = \lambda\lambda'$.

Lemma 4.2. *Let X, X' be arbitrary normalised eigenvectors in $\mathcal{M}$, $\mathcal{M}'$. Any vector $x = X+X'$ in $\mathcal{M}\oplus\mathcal{M}'$, $\|x\| = \sqrt{2}$, is a solution of* (4.3) *iff $k(x) = a$ and $l(x) = g^2$, $0\leq g^2 < a^2$.*

Proof. By definition, $\lambda = \mu_j$, $j\in J_m = \{1,\dots,m\}$ and $\lambda' = \mu_{j'}$, $j'\in J_{m'} = \{1,\dots,m'\}$, and the pair $\{\mu_j,\mu_{j'}\}$ solves the quadratic equation $r^2 - 2ar + g^2 = (r-\mu_j)(r-\mu_{j'}) = 0$. It follows that for $k = a$ and $l = g^2 > 0$, Eq. (4.4) is satisfied for $i\in J_m\cup J_{m'}$, letting $y_i\in\mathbb{C}$ be arbitrary. For i outside $J_m\cup J_{m'}$, it is clear that $\mu_i^2 - 2k\mu_i + l\neq 0$, imposing that $y_i = 0$. Let q_i be the columns of $Q = [q_1,\dots,q_n]$ which are eigenvectors for A. Then $x = Qy = \sum_{j\in J_m} y_jq_j + \sum_{j'\in J_{m'}} y_{j'}q_{j'} = X + X'$. □

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 4.3. *The solutions of Euler's equation* (4.3) *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 $c(v_+) = \frac{g}{a} = \operatorname{sgn}(a)\cos\phi$.*

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 $c(v_+) = \frac{\langle v_+,Av_+\rangle}{\|Av_+\|}$, $\langle v_+,Av_+\rangle = \frac{g^2}{a} = h$. Thus $|c(v_+)| = \cos\phi$.

□

Corollary 4.4. *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. 1) The case $K = \mathbb{R}$ is clear. Each of the 4 catchvectors $v_{+,*} = \varepsilon w_{+,*}q + \varepsilon' w'_{+,*}q'$ is rotated by A by the maximal turning angle $\phi(A)$ which shows in $\mathrm{Tr}(v_{+,*})$ and equals $\mathcal{A}(\hat{v})$. This is one of the major theorems in Gustafson's approach. Diverse applications are presented in [Gustafson, 2012, chapters 4 to 8].

2) The proof is also clear when $K = \mathbb{C}$ but the interpretation differs. The global minimum for $c(x)$ equals $\frac{g_*}{a_*} = c(v_{+,*})$, a value which, coincidentally, equals $\cos\phi(A)$ displayed in $\mathbf{\Sigma}$ by $\mathrm{Tr}(T)$ and $\mathrm{Tr}(U)$ with the choice (λ_1, λ_n).

□

4.3. **The antieigenvectors:** $Z = A$ **indefinite,** $Y = A - aI = B$**.** When A is *indefinite*, Section 3 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 $\mathbf{M}$. The Euler equation becomes

$$A^2x - 2\frac{\|Ax\|^2}{\langle Bx, Ax\rangle}ABx + \left(\frac{\|Ax\|}{\|Bx\|}\right)^2 B^2x = 0 \tag{4.5}$$

for $\langle Bx, Ax\rangle \neq 0$, $x \in \mathbb{C}^n \setminus (\mathrm{Ker}\ A \cup \mathrm{Ker}\ B)$. We set $k_1(x) = \frac{\|Ax\|^2}{\langle Bx,Ax\rangle}$, $l(x) = (\frac{\|Ax\|}{\|x\|})^2$ unchanged. Using $B = A - aI$, we rewrite (4.5) under the equivalent form $A^2x - 2KAx + Lx = 0$ where $K = \frac{l-k_1}{1-2k_1+l}$ and $L = \frac{la^2}{1-2k_1+l}$ depend on x by means of $k_1(x)$ and $l(x)$ which are assumed to satisfy $2k_1 \neq 1 + l$.

Proposition 4.5. *When A is indefinite, the solutions of Euler's equation* (4.5) *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 $\lambda < 0 < \lambda'$, $g^2 < 0$. They yield the critical value $c(v_-) = \cos\psi$.*

Proof. 1) Let $u = e^{i\xi}q$, $Au = \lambda u$, $Bu = -eu$, $\langle Bu, Au\rangle = -\lambda e$ and (4.5) is obviously satisfied: $(\lambda^2 - 2\lambda^2 + \lambda^2)q = 0$.

2) When $u \in (S)$ is not an eigenvector, u may satisfy (4.5) iff $K(u) = a$ and $L(u) = g^2$. 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_-. Direct computation shows that the antieigenvectors are the only solutions which are not eigenvectors.

3) $c(v_-) = \frac{v_-^H BAv_-}{\|Bv_-\|\|Av_-\|} = -\frac{g^2}{e|g|} = \frac{|g|}{e} = \cos\psi > 0$ for $a \neq 0$. □

When, $K = \mathbb{C}$, we still denote D_+ (resp. D_-) the set of catchvectors (resp. antieigenvectors) whose cardinality is now that of the continuum. It is clear that Theorem 3.4 remains valid in a weak form. If only expresses a *coincidence* between $|c(v_+)|$ and $\cos\phi$ or $c(v_-)$ and $\cos\psi$.

4.4. **The midvectors.** The choice $Y = -I$, $a \neq 0$, $Z = B = A - aI$ and the corresponding Euler equation cannot yield the middle vectors $\hat{v} = \frac{1}{\sqrt{2}}(e^{i\xi}q + e^{i\xi'}q')$, $\xi, \xi' \in [0, 2\pi[$ 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. Indeed, the following result holds when $\det A \neq 0$:

Proposition 4.6. *When A is invertible, the solutions $x \in K^n$, distinct from eigenvectors, of the equation*

$$A^2x - 2\frac{\langle x, Ax\rangle}{\|x\|^2}Ax + \frac{\langle x, Ax\rangle}{\langle x, A^{-1}x\rangle}x = 0 \tag{4.6}$$

are midvectors $\hat{v}$ associated with all couplings $\lambda < \lambda'$.

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 $a \neq 0$. When $a = 0$, the indeterminate ratio is defined at $g^2 < 0$ by continuity.

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

□

The equation (4.6) is called the *balance equation* since its (non eigenvector) solutions are the middle vectors $\hat{v}$ independently of the nonzero values λ and $\lambda' \neq -\lambda$.

It is noteworthy that the balance equation is defined only if A^{-1} exists. However $\hat{v}$ is well-defined for any g^2 in $]-e^2, a^2[$, which includes 0 for $a \neq 0$, hence $\hat{v}$ satisfies $\langle a\hat{v}, B\hat{v}\rangle = 0$. Moreover the balance equation, which provides the middle vectors, does not indicate how one could extend from $K = \mathbb{R}$ to $\mathbb{C}$, the property that $\Sigma(\hat{v}) = \max_{u\in(C)} \Sigma(u) = \frac{1}{2}|a|e$ since we have no more triangles at hand.

Again, a weak form of Theorem 3.6 remains valid when $K = \mathbb{C}$.

Proposition 4.7. *Given $\lambda < \lambda'$, any middle vector in $\hat{D}$ contains the spectral information which defines in $\mathbf{\Sigma}$ the triangles* $\mathrm{Tr}(L^+)$ *and* $\mathrm{Tr}(L^-)$ *with maximal surface $\frac{1}{2}|a|e$.*

And this is but one of the many properties of the middle vectors. For example, when A is invertible, the middle vector $\hat{v}$, common to A and A^{-1}, suggests to look for some connection with 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 shall assume first that λ and λ' are positive and $K = \mathbb{R}$ or $\mathbb{C}$.

Proposition 4.8. (M. M. Rincon-Camacho) *When λ and λ' are positive, the catchvectors v_+ and $\mathring{v}_+$ are symmetrically placed with respect to the corresponding middle vectors $\hat{v}$. 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 $Av_+ = \lambda wq + \lambda' w'q' = \sqrt{\lambda\lambda'}\mathring{v}_+ = g\mathring{v}_+$. If we set $A_0 = A_{\restriction \mathbf{M}}$, $A_0^{1/2}$ is well-defined and $\mathring{v}_+ = \frac{1}{\sqrt{a}} A_0^{1/2}\hat{v}$, $v_+ = \frac{g}{\sqrt{a}} A_0^{-1/2}\hat{v}$. □

Proposition 4.8 indicates a non trivial algebraic connection between the roots of the quadratic equations (4.3) and (4.6) which are not eigenvectors and are defined by pairs of *positive* eigenvalues (λ, λ') in the associated invariant (real or complex) plane $\mathbf{M}$. The connection is based on the square roots of the 2×2 (symmetric or hermitian) matrices $A_0 = A_{\restriction \mathbf{M}}$ and A_0^{-1}. The presentation of the complete picture ($g^2 > 0$ and $a < 0$, or $g^2 < 0$) is deferred to Section 4.7.

4.5. A **is positive definite:** $Y = A^{1/2}$**,** $Z = A^{-1/2}$**.** We restrict our attention in this Section to the case where all eigenvalues are positive, so that middle vectors are connected to catchvectors only.

Corollary 4.9. *Let $\hat{v}$ be a middle vector, 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. [Rincon-Camacho, 2015a]. By straightforward calculation: $\langle v_+, Av_+\rangle = h$. □

It is clear that the normalised solutions of (4.6) and (4.3) are in 1-to-1 correspondence. They consist of the n eigenvectors, and of all distinguished sets $\hat{D}$ and D_+ created by spectral coupling which satisfy $D_+ = (hA)^{1/2}\hat{D}$.

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 $\measuredangle(v_+, \hat{v}) = \measuredangle(\hat{v}, Av_+)$ and v_+, $F_0 v_+$ are orthogonal ($\beta = \frac{\pi}{2}$), the middle vector $\hat{v}$ bisects the angle $\phi = \measuredangle(v_+, Av_+)$, see $\mathrm{Tr}(v_+) = OT'C'$ on Figure 7 (a).

Interestingly, 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 $Y = A^{1/2}$, $Z = A^{-1/2}$, Eq. (4.2) takes the form

$$\frac{Ax}{\langle x, Ax\rangle} - 2\frac{x}{\|x\|^2} + \frac{A^{-1}x}{\langle x, A^{-1}x\rangle} = 0. \tag{4.7}$$

Multiplying (4.7) by A, we rewrite it in the equivalent form

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

which is precisely the balance equation (4.6) of Proposition 4.6. The corresponding functional is $c(x) = \frac{\|x\|^2}{\|x\|_A\|x\|_{A^{-1}}}$ where $\|x\|_A = \langle x, Ax\rangle^{1/2} = \|A^{1/2}x\|$ denotes the elliptic norm defined by A.

We just have proved the

Proposition 4.10. *When A is positive definite,* (4.6) *is the Euler equation associated with $\min_{x\neq 0} \frac{\|x\|^2}{\|x\|_A\|x\|_{A^{-1}}}$ which represents either*

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

The global minimum is achieved for the extreme pair $\{\lambda_1 = \lambda_{\min}, \lambda_n = \lambda_{\max}\}$ and a pair of associated middle vectors at the value $\frac{2\sqrt{\lambda_1\lambda_n}}{\lambda_1+\lambda_n} = \cos\phi(A)$.

The middle vectors associated with a positive definite matrix play an essential role in the successful analysis of many matrix techniques used in Statistics and Numerical Analysis. Some aspects of their role are illustrated in Section 6. The reader can find below a generalisation of Proposition 4.10 to the case A symmetric where $x \in \mathbb{R}^n$ is replaced by $X \in \mathbb{R}^{n\times p}$, $p < n$ which is supported by the simultaneous consideration of p spectral couplings, called spectral chaining.

4.6. **Spectral chaining.** Let A be symmetric positive definite, $X \in \mathbb{R}^{n\times p}$, $1 \leq p \leq n$ and consider the positive functional

$$J_p(X) = \det[(X^TAX)(X^TA^{-1}X)], \quad X^TX = I_p, \quad 1 \leq p \leq n, \tag{4.8}$$

which is the determinant of the product of the two Gram matrices $G(A) = X^TAX$ and $G(A^{-1}) = X^TA^{-1}X$ when X runs over all orthonormal matrices of rank p. We denote $\{u_i\}$, $i = 1$ to p, the set of orthogonal eigenvectors of $G(A)$ and $G(A^{-1})$: $U = [u_1, \dots, u_p]$ is orthogonal such that $U^TG(A)U = N = \mathrm{diag}(n_i)$, where $\{n_i\}$ are the eigenvalues of $G(A)$. Similarly N' is the diagonal form of $G(A^{-1})$ We may use the underscript X for $G_X(\cdot)$ and U_X to stress their dependence on X. Let $P_X = XX^T$ denote the orthogonal projection on the range $\mathrm{Im}X$ and define the commutator $L = P_XA - AP_X = [P_X, A]$. Then, $J_p(X) = \det(I_p - X^TLA^{-1}X) = \det(I_p + X^TA^{-1}LX)$ suggests an implicit role of $L \neq 0$ when $J_p(X) > 1$. It is proved in [Rincon-Camacho, 2015b] that the identity $J_p(X) = \det(I_n + A^{-1}L)$ which appears on p. 122 of [Bloomfield and Watson, 1975] is erroneous.

Lemma 4.11. *Any stationary value for $J_p(X)$ is achieved iff the orthonormal vectors $s_i = Xu_i$, $i = 1$ to p, are either chosen among the solutions of the balance equation* (4.6) *for A, when $p < n$, or arbitrary when $p = n$.*

Proof. We adapt the Lagrangian approach devised in Section 2 of [Bloomfield and Watson, 1975]. Since $J_p(X)$ is positive and ln is monotone increasing, we may consider the functional $\ln J_p(X) = \ln\det(X^TAX) + \ln\det(X^TA^{-1}X)$. To the constraint $X^TX = I_p$ is associated Λ, the upper triangular matrix of $p\frac{p+1}{2}$ Lagrange multipliers: if $(X^TX)_{ij} = c_{ij}$, $\sum_{i=1}^p(\sum_{j\leq i} c_{ij}\lambda_{ij}) = \mathrm{tr}((X^TX)\Lambda)$. The Lagrangian is taken under the form $\mathcal{L}(X, \Lambda) = \ln J_p(X) - 2\mathrm{tr}[(X^TX - I_p)\Lambda]$. Matrix calculus tells us that, given the map $G : X \in \mathbb{R}^{n\times p} \mapsto X^TAX \in \mathbb{R}^{p\times p}$, $A \in \mathbb{R}^{n\times n}$, the Jacobean is $\frac{\partial}{\partial X}G = X^T(A + A^T)$, and when A is invertible, $\frac{\partial}{\partial A}\det A = (\det A)(A^{-1})^T$. Using

$\frac{\partial}{\partial X}\ln(X^TAX) = 2(X^TAX)^{-1}AX$ and $\frac{\partial}{\partial X}\mathrm{tr}(X^TX\Lambda) = X(\Lambda+\Lambda^T)$, the condition $\frac{\partial}{\partial X}\mathcal{L}(X,\Lambda) = 0$ yields:

$$AX(X^TAX)^{-1} + A^{-1}X(X^TA^{-1}X)^{-1} = X(\Lambda + \Lambda^T). \tag{4.9}$$

Premultiplication by X^T implies $2I_p = \Lambda + \Lambda^T$ for $X^TX = I_p$. Hence

$$AX(X^TAX)^{-1} + A^{-1}X(X^TA^{-1}X)^{-1} = 2X, \tag{4.10}$$

an equation which generalises Eq. (4.7) on x to the orthonormal $n \times p$ matrix X. Premultiplication of (4.10) by X^TA gives $X^TA^2X(X^TAX)^{-1} = 2X^TAX - (X^TA^{-1}X)^{-1}$ symmetric. This shows that the symmetric matrices X^TA^2X, X^TAX and $X^TA^{-1}X$ of order p *commute*. Hence they enjoy a common orthonormal eigenbasis $\{u_i\}$, $i = 1$ to $p < n$ in $\mathbb{R}^p$. Since $G(A)U = UN$ and $G(A^{-1})U = UN'$, post multiplication of (4.10) by U yields, for $S = XU$, the equation

$$ASN^{-1} + A^{-1}SN'^{-1} = 2S. \tag{4.11}$$

The column vectors of S are $s_i = Xu_i$ in $\mathbb{R}^n$ such that $s_i^TAs_i = u_i^TG(A)u_i = n_i$, $s_i^TA^{-1}s_i = n_i'$, $\|s_i\| = 1$. They satisfy Eq. (4.7), an equivalent form of the balance equation (4.6). Eq. (4.6) has exactly n^2 normalised independent solutions if the n eigenvalues of A are *simple*, consisting of the n eigenvectors and $n(n-1)$ middle vectors. The $\{s_i\}$ are necessarily p orthonormal vectors chosen among these solutions when $p < n$. If $p = n$, then $J_n(X) = 1$ for all orthogonal X and $\mathrm{Im}\ X = \mathrm{Im}\ S$: $P_S = SS^T = P_X$.

□

Lemma 4.11 tells us that X is a critical matrix for (4.8) iff X and the eigenvector matrix U_X for $G_X(\cdot)$ are *linked* by $S = XU_X$ where S solves (4.11) and $\mathrm{Im}\ X = \mathrm{Im}\ S$: $P_S = SS^T = XX^T$. If S consists of eigenvectors for A, then clearly $X = S$ with $U_S = I_p$. So that $J_p(X) = 1$: no coupling is involved. Only *middle vectors* in S can provide larger values for J_p when $p < n$, indicating coupling.

For $p < n$, a p-chain C_p is a set of p spectral couplings (λ, λ'), $\lambda < \lambda'$. To each pair of eigenvectors (q, q') is associated the pair of middle vectors $\hat{v} = \frac{1}{\sqrt{2}}(q + q')$ and $\hat{v}' = \frac{1}{\sqrt{2}}(q - q')$. If $C_p = \cup_{i=1}^p(\lambda_i, \lambda_i')$, $\lambda_i < \lambda_i'$ we set $\hat{V} = [\hat{v}_1, \ldots, \hat{v}_p]$. Midvectors in $\hat{V} = XU$ are called critical for (4.8). More generally we consider $V \in \mathbb{R}^{n\times p}$ where each column vector v_i is arbitrary in M_i; $\|v_i\| = 1$.

Lemma 4.12. *The condition $\bar{V} = X\Omega$, $\Omega \in O(p)$ entails $p \le m = \lfloor \frac{n}{2} \rfloor$, and Ω is an eigenbasis for G_X.*

Proof. By assumption, $\bar{v}_i$ in the invariant subspace $\mathbf{M}_i$ is orthogonal to $\oplus_{j=1}^{i-1}\mathbf{M}_j$, $i \ge 2$, so that $\bar{v}_i^TA\bar{v}_j = 0$. Since $\dim \oplus_i \mathbf{M}_i = n - 2p$, there cannot exist more than m independent vectors. Since $G_V(\cdot)$ is diagonal and $X = V\Omega^T$, $X^TAX = \Omega(V^TAV)\Omega^T$. □

It follows that the 2^p critical mid vector matrices $\hat{V}$ resulting from 2^p binary choices define 2^p classes of critical matrices $X = \hat{V}\Omega^T$, Ω arbitrary in $O(p)$, which are equivalent to $\hat{V}$ by isometry of order p. Each class is isomorphic to $\mathbb{R}^{p\frac{p-1}{2}}$ for $2 \le p \le m$. If $p = 1$, we get back Proposition 4.10.

Corollary 4.13. *Let $\hat{V} = XU$ be associated with C_p, $p \le m$. Then $J_p(X) = \prod_{C_p} \frac{(\lambda+\lambda')^2}{4\lambda\lambda'} = \prod_{C_p} \frac{1}{\cos^2\phi} > 1$ is a stationary value.*

Proof. For $p \le m$, the choice of one middle vector $\hat{v}$ in each invariant subspace $\mathbf{M}$ for (λ, λ') in C_p yields a set of $p < n$ orthonormal eigenvectors such that $\Rightarrow G_{\hat{V}}(A) = \mathrm{diag}(\frac{1}{2}(\lambda + \lambda'))$, $G_{\hat{V}}(A^{-1}) = \mathrm{diag}(\frac{1}{2}(\frac{1}{\lambda} + \frac{1}{\lambda'}))$.

Thus, by Lemma 4.11, $J_p(X) = \prod_{C_p}(\hat{v}^TA\hat{v})(\hat{v}^TA^{-1}\hat{v}^T)$ where $\frac{1}{2}(\lambda + \lambda')\frac{1}{2}(\frac{1}{\lambda} + \frac{1}{\lambda'}) = \frac{1}{\cos^2\phi} > 1$. □

Definition 4.1. If $p \le m = \lfloor \frac{n}{2} \rfloor$, the nested p-chain C_p^* is defined by the choice $(\lambda_i, \lambda_{n+1-i})$, $i = 1$ to p. A set of p nested midvectors is denoted $\hat{V}_{*p}$. The underscript p may be skipped when the context is clear.

Proposition 4.14. *When $p \le m$ the nested p-chain C_p^* provides the global maximum value $\bar{J}_p = \max(J_p(X), X^T X = I_p)$.*

Proof. Clear by induction on p, $1 \le p \le m = \lfloor \frac{n}{2} \rfloor$. The case $p = 1$ is covered by Proposition 4.10. For $p \ge 2$, let X_p be defined by $C_p^* : XU = \hat{V}_{*p} = [\hat{V}_{*p-1}, \hat{v}_p]$. We define $\mathbf{E}_p = \oplus_{i=1}^{p} \mathbf{M}_i$ where $\mathbf{M}_i$ is spanned by $\{q_i, q_{n+1-i}\}$; $\mathbf{V}_p = \mathbf{E}_p^{\perp}$ is a subspace of dimension $n - 2p$. Then $\bar{J}_p = \bar{J}_{p-1} \frac{1}{\cos^2 \phi_p}$ where ϕ_p is the turning angle associated with the matrix $\tilde{A}_p = A_{\restriction \mathbf{V}_{p-1}}$ of order $n - 2(p-1)$ with extreme eigenvalues $(\lambda_p, \lambda_{n+1-p})$. Clearly $\mathbf{V}_m$ is reduced to $\{0\}$ (resp. $\{q_{m+1}\}$) with dimension 0 (resp. 1) if n is even (resp. odd) yielding $\phi_{m+1} = 0$. The sequence of nested turning angles is non increasing in $[0, \frac{\pi}{2}[$: $\frac{\pi}{2} > \phi(A) = \phi_1 \ge \ldots \ge \phi_p \ge \ldots \ge \phi_m \ge \phi_{m+1} = 0$. ☐

According to [Bloomfield and Watson, 1975], the nested midvectors $\hat{V}_*$ maximise equally $\mathrm{tr}(LL^T) \le \frac{1}{4} \sum_{i=1}^{p} (\lambda_i - \lambda_{n+1-i})^2$, $p \le m$, where the functional $X \mapsto \mathrm{tr}(LL^T) = \|L\|_F^2$ measures by how much X fails to be an invariant subspace for A when $X^T X = I_p$. If we define the nested p-chain spread $\varepsilon_* = (e_i) \in \mathbb{R}^p$, the Frobenius norm $\|L\|_F$ is bounded above by $\|\varepsilon_*\|_2$ which is an absolute measure of the chaining potential of A: the larger the spread, the greater the potential. A relative measure is obtained by replacing each e_i by $\frac{e_i}{g_i} = \tan \phi_i$.

It is clear that the above induction on midvectors for $1 \le p \le m$ cannot be carried any further since $\tilde{A}_{m+1} = 0$ (resp. λ_{m+1}) if n is even (resp. odd).

We set $q = \min(p, n-p)$ with $1 \le q \le m$ for $1 \le p < n$. If $1 \le p \le m$ then $n - 1 \ge n - p \ge n - m = m$ (resp. $m + 1$) if n is even (resp. odd).

Theorem 4.15. *For $1 \le p < n$, $J_p(X) \le \bar{J}_q$.*

Proof. The case $p \le m$ is treated in Proposition 4.14. We examine the case $m < p < n$.

Let $\hat{V}_*$ of rank m be associated with C_m^*, $\hat{V}_* = XU$. Assume first that n is even. To construct $X = SU^T$ of rank $p = m + 1$ which decreases $J_{m+1}(X)$ minimally, we define $S = [\hat{v}_1, \ldots, \hat{v}_{m-1}, q_m, q_{m+1}]$ so that $\bar{J}_{m+1} = \bar{J}_{m-1} = \prod_{i=1}^{m-1} \frac{1}{\cos^2 \phi_i}$ proves $q = m - 1$. After $m - 1$ such steps, we get $S = [\hat{v}_1, q_2, \ldots, q_{n-1}]$ of rank $p = n - 1$. And $\bar{J}_1 = \bar{J}_{n-1} = J_1(\hat{v}_1) = \frac{1}{\cos^2 \phi_1}$ proves $q = 1$.

When n is odd, the global maximum $\bar{J}_m = \bar{J}_{m+1}$ is achieved with $X = \hat{V} U_X^T$ of rank m and $X = [\hat{V}, q_{m+1}] U_X^T$ of rank $m + 1$. ☐

In conclusion, we indicate that (4.8) can be interpreted as a quantification, by means of its determinant, of the effect of replacing the Gram matrix $G(I_n) = X^T X = I_p$ by the product $G(A)G(A^{-1})$, that is replacing X by $A^{1/2}X$ and $A^{-1/2}X$. The functional J_p measures the intensity of the chaining. Only middle vectors for A and A^{-1} can produce a stationary value larger than 1. The reader may check easily that if $J_p(X)$ in (4.8) is replaced either by $\det G(A)$ or by $\det G(A^{-1})$, the stationary values are obtained for those X whose p column vectors are chosen among the eigenvectors q_i of A and A^{-1} only. The role of the middle vectors emerges in full light with the *product* $G(A)G(A^{-1})$ for $1 \le p \le m$. To contrast with eigenvectors: $q^T A q = \lambda$, $q^T A^{-1} q = \frac{1}{\lambda}$ are inverse whereas $\hat{v}^T A \hat{v} = \frac{1}{2}(\lambda + \lambda') = a$ and $\hat{v}^T A^{-1} \hat{v} = \frac{1}{2}(\frac{1}{\lambda} + \frac{1}{\lambda'}) = \frac{a}{g^2} = \frac{1}{h}$ multiply as $\frac{a^2}{g^2} = \frac{1}{\cos^2 \phi} > 1$ if $\lambda < \lambda'$. The maximal measure of geometric development is realised by means of the m nested midvectors through $\hat{V}_*$. It realises the full extent of the chaining potential which resides in A. When the rank p exceeds m (n even) or $m + 1$ (n odd), midvectors are gradually replaced by eigenvectors and a refolding takes place which decouples what had been previously coupled ($p \le m$). Moreover $\bar{J}_q$ is expressed in terms of turning angles

$\phi_i = \angle(v_{i+}, Av_{i+})$, $1 \le q \le m$, where the directions v_{i+} and Av_{i+} have been derived from the midvector $\hat{v}_i$ in Corollary 4.9, revealing an unsuspected symmetry.

Alternatively, one could consider the functional $X \mapsto T_p(X) = \mathrm{tr}(X^TAX - (X^TA^{-1}X)^{-1}) = \mathrm{tr}(G(A) - (G(A^{-1}))^{-1})$ based on the trace of a *difference* for $X^TX = I_p$, see [Rincon-Camacho, 2015a]. Both functionals J_p and T_p have been studied by several statisticians [Bloomfield and Watson, 1975, Rao, 1985] in the decade 1975-1985 to quantify the inefficiency of least squares. In the above presentation, we made explicit the roles of spectral chaining and geometry which underlie the inequalities, roles which have mostly remained implicit in the statistical literature to-date. It appears that geometry is an ally to decipher the tension between evolution by assimilation and invariance by conservation which is at work through multiple couplings forming a chain.

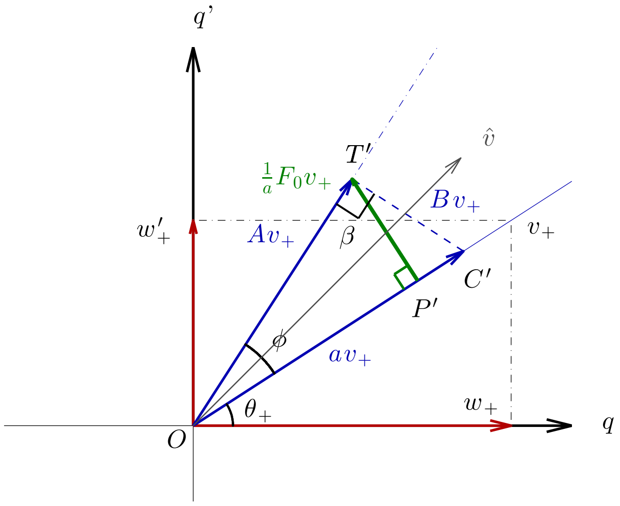
4.7. **Local optimisation when A is indefinite.** When A is indefinite so is the sign of $g^2 = \lambda\lambda'$. We restrict A to be 2×2: $A_0 = A_{\restriction \mathbf{M}}$ and $B_0 = A_0 - aI_2 : \mathbf{M} \to \mathbf{M}$.

When $0 < \lambda < \lambda'$, the results of Corollary 4.9 apply readily to A_0. When $\lambda < \lambda' < 0$, $(-A_0)$ is positive definite and $(-A_0)^{1/2}$ is well-defined, a and $h = \frac{g^2}{a}$ should be replaced by $-a$ and $-h$. In other words $\frac{1}{h}A_0$ is positive definite for $g^2 > 0$. 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 $\{-e\lambda, e\lambda'\}$.

The relation between antieigenvectors v_- and middle vectors $\hat{v}$ when $\lambda < 0 < \lambda'$ is given by

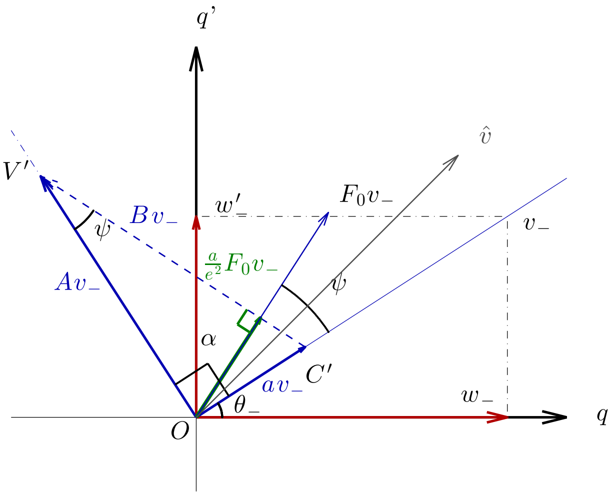
Proposition 4.16. *When $g^2 < 0$, let $\hat{v}$ be a middle vector. Then $v_- = |g|F_0^{-1/2}\hat{v}$ is an antieigenvector, $F_0v_- = |g|F_0^{1/2}\hat{v}$ and $\langle F_0^{-1/2}\hat{v}, F_0^{1/2}\hat{v}\rangle = -\frac{1}{g^2}\langle v_-, F_0v_-\rangle = 1 = \|\hat{v}\|^2$.*

Proof. Straightforward calculation. See $\mathrm{Tr}(v_-) = OV'C'$ on Figure 7 (b) valid when $K = \mathbb{R}$: $\hat{v}$ bisects $\psi = \measuredangle(v_-, F_0v_-)$ and v_-, Av_- are orthogonal ($\alpha = \frac{\pi}{2}$). □



(a) $g^2 > 0$, $a > 0$

observation angle ϕ, $\beta = \frac{\pi}{2}$



(b) $g^2 < 0$, $a > 0$

perspective angle ψ, $\alpha = \frac{\pi}{2}$

FIGURE 7. $\mathrm{Tr}(v_+)$ (a) and $\mathrm{Tr}(v_-)$ (b) 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 4.17. *The middle vectors $\hat{v}$ 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 4.10 can only be replaced by the following *local* one:

$$\max_{u\in \mathbf{M},\ \|u\|=1} (u^T F_0 u)(u^T F_0^{-1} u) = \frac{1}{\cos^2\psi}, \quad \text{where } \psi = \measuredangle(F_0^{-1/2}\hat{v}, F_0^{1/2}\hat{v}) = \measuredangle(v_-, F_0 v_-) \text{ if } K = \mathbb{R}.$$

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

5.1. **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].

5.2. **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* $\mathrm{Tr}(u)$ which lies in the 2D-plane $\mathbf{M}$ when $K = \mathbb{R}$ and the trigonometric information it provides (Fig. 6 and 7) 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 $\mathrm{Tr}(M)$ in the spectral plane cover both cases $K = \mathbb{R}$ *and* $\mathbb{C}$. Therefore a 2D-trigonometric interpretation involving ordinary angles remains available in the spectral plane $\mathbf{\Sigma}$, see Section 5.5.

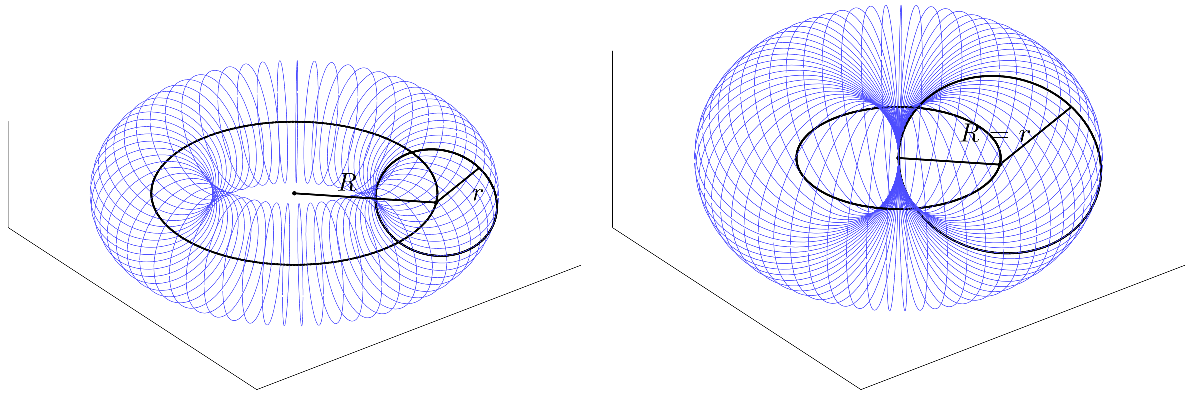
5.3. **The distinguished sets $D_\pm$, $\hat{D}$ in $\mathbb{R}^3$.** We recall that the cartesian product of two circles $S^1 \times S^1 \subset \mathbb{C}^2$ is homeomorphic, in topology, to a torus in $\mathbb{R}^3$. The three distinguished subsets $D_\pm$, $\hat{D}$ of the unit sphere $(S) = S^3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

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

ii) $D_- = w_- S^1 \times w'_- S^1$, $w'_- = \sqrt{1 - w_-^2}$, $g^2 < 0$,

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 8



(a) i) or ii) $a \neq 0$

$R = w'_{\pm}$ and $r = w_{\pm}$ if $w'_{\pm} > w_{\pm}$

$R = w_{\pm}$ and $r = w'_{\pm}$ if $w'_{\pm} < w_{\pm}$

(b) iii) or ii) $a = 0$

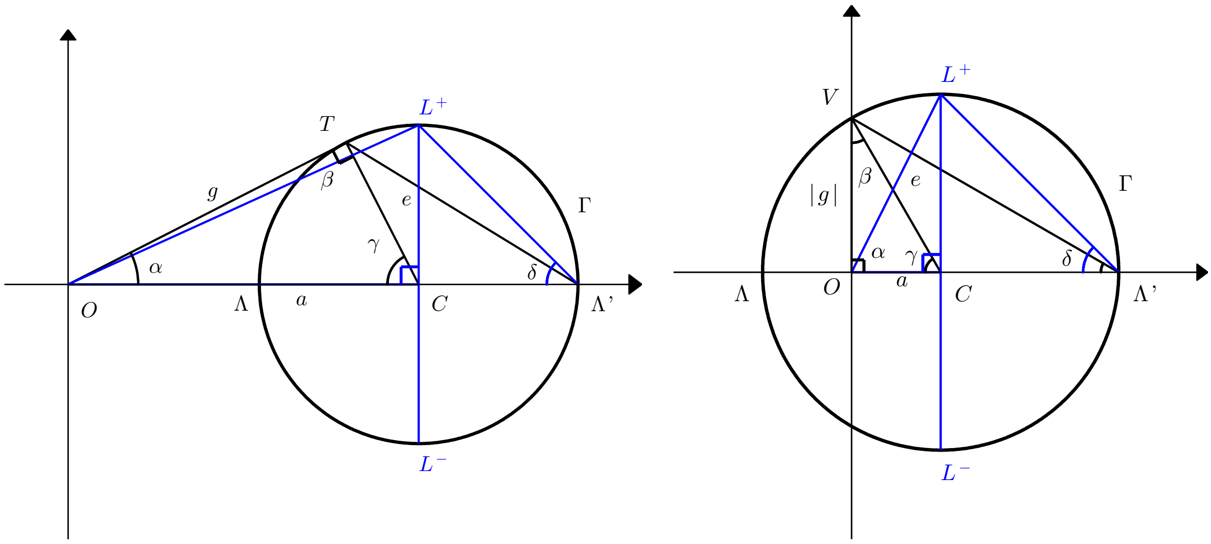
$R = r = \hat{w} = \frac{1}{\sqrt{2}}$

FIGURE 8. Distinguished tori in $\mathbb{R}^3$ when $K = \mathbb{C}$

5.4. **The locus of the end-point for** Au**,** $u \in (S)$**.** Let $\vec{OM'} = Au$, $u \in (S)$, we denote $M' = (s, s')$ with $s, s' \in \mathbb{C}$. Since $Au = \lambda z q + \lambda' z' q'$ when $g^2 \neq 0$, the point M' describes the quadratic surface $\frac{|s|^2}{\lambda^2} + \frac{|s'|^2}{\lambda'^2} = 1$ in $\mathbb{R}^4$. If $g^2 = 0$, $\lambda = 0 < \lambda'$ (say), $Au = \lambda' z' q'$ and $M' = (0, s')$ describes the disk $0 \times \{s', |s'| \leq \lambda'\}$. Observe that the segment $[-\lambda', \lambda']$ when $K = \mathbb{R}$ becomes a disk when $K = \mathbb{C}$.

It follows readily that the endpoints of Av_+ or Av_- describe the homothetic tori gD_+ or $|g|D_-$ for $g^2 \neq 0$. If $g^2 = 0$, $\|Av_+\| = \|Av_-\| = 0$: the endpoints coalesce with the origin O.

5.5. **The full trigonometric information is given by Tr**(M)**.** We show how the spectral plane is a complete source of information when $K = \mathbb{C}$. The angles, the distances and the weights describing the catchvectors (if $g^2 > 0$), the antieigenvectors (if $g^2 < 0$) or the middle vectors can be easily constructed by ruler and compass in the spectral plane. Given two eigenvalues $\lambda < \lambda'$ and their relative position with respect to the origin O, we construct the circle Γ (linking curve between λ and λ') of radius e and center C with coordinates $(a, 0)$.



(a) $g^2 > 0$ (b) $g^2 < 0$

β or $\gamma = \frac{\pi}{2}$ α or $\gamma = \frac{\pi}{2}$

FIGURE 9. Sequential optimisation in the spectral plane, $g^2 \neq 0$

The information corresponding to the catchvectors and antigeigenvectors contained in the spectral plane is given by the black triangles in Figure 9 (a) and (b) respectively. If $g^2 > 0$ (resp. $g^2 < 0$), we draw the tangent to the circle Γ (resp. the vertical line) passing through O which intersects Γ at the point T (resp. V) and we obtain simultaneously the angles $\alpha = \angle(OC, OT) = \phi$ and $\beta = \angle(TC, TO) = \frac{\pi}{2}$ (resp $\alpha = \angle(OC, OV) = \frac{\pi}{2}$ and $\beta = \angle(VC, VO) = \psi$). Here we consider only the points T (if $g^2 > 0$) and V (if $g^2 < 0$) but analogous results are obtained if we use the points U and W in Figure 2. Then, the angle γ is obtained as follows: $\gamma = \angle(CO, CT) = \frac{\pi}{2} - \phi$ (resp. $\gamma = \angle(CO, CV) = \frac{\pi}{2} - \psi$) if $g^2 > 0$ (resp. $g^2 < 0$), which is such that $\cos\gamma = \frac{e}{|a|}$ and $\sin\gamma = \frac{g}{|a|}$ (resp. $\cos\gamma = \frac{|a|}{e}$ and $\sin\gamma = \frac{|g|}{e}$). Finally, the angle δ is such that: $\delta = \frac{\gamma}{2} = \angle(\Lambda'\Lambda, \Lambda'M)$ (resp. $\delta = \frac{\gamma}{2} = \angle(\Lambda'\Lambda, \Lambda'V)$). Since the values $\cos\gamma$ and $\sin\gamma$ are known, by trigonometric identities we obtain that: $\cos\delta = \sqrt{\frac{\lambda'}{2|a|}} = w_+$ and $\sin\delta = \sqrt{\frac{\lambda}{2|a|}} = w'_+$ (resp. $\cos\delta = \sqrt{\frac{\lambda'}{2e}} = w_-$ and $\sin\delta = \sqrt{\frac{-\lambda}{2e}} = w'_-$) if $g^2 > 0$ (resp. $g^2 < 0$). Thus, the weights $w_\pm$, $w'_\pm$ describing the sets $D_\pm$ in both the invariant plane $\mathbf{M}$ if $K = \mathbb{R}$ and the 4D-invariant subspace $\mathbf{M}$ if $K = \mathbb{C}$, are also found in the spectral plane.

In the case of middle vectors the information corresponds to the blue triangles with maximal surface $\frac{1}{2}|a|e$ in Figure 9 (a) and (b). We draw the vertical line passing through C which intersects Γ at $L^+ = (a, e)$ and $L^- = (a, -e)$. In this case, $\gamma = \frac{\pi}{2}$ and $\delta = \frac{\pi}{4}$. Thus, the unique weight $\hat{w} = \frac{1}{\sqrt{2}}$ describing the set $\hat{D}$ is given by $\cos\delta = |\sin\delta| = \frac{1}{\sqrt{2}}$.

When $|a| \neq e \Leftrightarrow g^2 \neq 0$, there exist two mutually exclusive optimal configurations: in one of them, α or $\beta = \frac{\pi}{2}$ according to the sign of g^2, in the other $\gamma = \frac{\pi}{2}$. This 2-fold optimisation can be described as *sequential*, see Figure 9. When $|a| = e \Leftrightarrow g^2 = 0$, $\alpha = \beta$, it is possible to get the *common* value $\alpha = \beta = \gamma = \frac{\pi}{3}$, lesser than $\frac{\pi}{2}$ but achieved by all three angles.

6. MORE ON MIDDLE VECTORS WHEN A IS POSITIVE DEFINITE

6.1. **Numerical Analysis.** As indicated in Remark 3.1, the consideration of the *three* angles α, β, γ sheds more light on the geometrical picture related to the well-known Wielandt and Kantorovich inequalities for a nonsingular matrix described in [Horn and Johnson, 1985, p. 441-445]. 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]. The condition number of $A^{\frac{1}{2}}$ in the euclidean norm is $\mathrm{cond}(A^{\frac{1}{2}}) = \frac{\sqrt{\lambda_n}}{\sqrt{\lambda_1}} = \cot\angle(q, v_{+,*}) = \cot\theta_+$. 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 $\theta_+ = \frac{\theta_W}{2}$. Proposition 4.10 in Section 4.4, tells us that $\alpha \leq \phi(A)$, hence $\theta_W = \frac{\pi}{2} - \phi(A) = \gamma(A)$. Thus, Wielandt's inequality for any pair of orthogonal vectors $x, y \in K^n$ and $A^{\frac{1}{2}}$ is given by

$$\text{(6.1)} \qquad \frac{|\langle A^{\frac{1}{2}}x, A^{\frac{1}{2}}y\rangle|}{\|A^{\frac{1}{2}}x\|\|A^{\frac{1}{2}}y\|} = \frac{\langle x, Ay\rangle}{\|x\|_A\|y\|_A} \leq \cos\theta_W = \cos\gamma(A) = \sin\phi(A).$$

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 middle vectors in $\hat{D}_*$. The case $K = \mathbb{R}$ is illustrated in Figure 10 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 10 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 parallel.

In [Horn and Johnson, 1985, p. 444], Kantorovich's inequality −which goes back to [Frucht, 1943]− is derived from Wielandt's inequality (6.1). However, Kantorovich's inequality is equally a direct consequence of Proposition 4.10:

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

where equality is attained if x is any middle vector $\hat{v}$ in $\hat{D}_*$. In Figure 10 the geometrical meaning of the angles $\phi(A)$ and $\theta_W = \gamma(A)$ when $K = \mathbb{R}$ is illustrated: $\frac{\|\hat{v}\|^2}{\|\hat{v}\|_A\|\hat{v}\|_{A^{-1}}} = \cos\measuredangle(A^{-1/2}\hat{v}, A^{1/2}\hat{v}) = \cos\phi(A)$.

6.2. **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 Section 4.5. The usual assumption in statistics is that $p \leq m$. As a consequence of Corollary 4.9 we get

$$\text{(6.2)} \qquad \cos\measuredangle(A^{-1/2}\hat{v}, A^{1/2}\hat{v}) = \cos\measuredangle(v_+, Av_+) = \frac{g}{a},$$

see Figure 10. A direct application is provided by the statistical efficiency RE of a general linear regression model with noise covariance matrix A of order n and $p \leq m = \lfloor \frac{n}{2} \rfloor$ real parameters. The lower bound in $\prod_{i=1}^{p} \cos^2\phi_i \leq RE \leq 1$ is achieved by the most inefficient regressor. It is known in the Statistics literature as the Durbin-Bloomfield-Watson-Knott inequality. Using $X \in \mathbb{R}^{n\times p}$, the problem is equivalent to (4.8) treated in Section 4.6. With the notation therein, the worst regressors are $X = \hat{V}_*\Omega$, for all $\Omega \in O(p)$.

It is shown in [Rincon-Camacho, 2015b] that (6.2) provides the missing step to elucidate the worst case of statistical efficiency in the geometric interpretation of [Gustafson, 2002, pp. 147-150], [Gustafson, 2012, theorem 6.2, pp. 102-103]. The equality (6.2) tells us that the worst efficiency is characterised *equally* by the catchvectors v_+ by means of $\phi = \measuredangle(v_+, A_+)$ or by the middle vectors $\hat{v}$ through $\measuredangle(A^{-1/2}\hat{v}, A^{1/2}\hat{v})$ which correspond to the p-nested chain C_p^*, $p \leq m$ (see Section 4.6). These middle vectors have been introduced as "inefficient" vectors in [Gustafson, 2002, 2012]. For a detailed insight into statistics, see [Rincon-Camacho, 2015b]. The potential domains of application are many, from econometrics to computational inverse problems and machine learning.

Another measure of relative efficiency has been proposed in [Rao, 1985] which is based on the functional X, $X^TX = I_p \mapsto T_p(X) = \mathrm{tr}(X^TAX - (X^TA^{-1}X)^{-1})$, $1 \leq p \leq m$. With this measure, the worst efficiency $\sum_{C_p^*}(\sqrt{\lambda_{n+1-i}} - \sqrt{\lambda_i})^2$ is obtained when $X = SU$, $U \in O(p)$, and the columns of S are p nested *catchvectors* for $A^{-1/2}$, see [Rincon-Camacho, 2015a]. For $p = 1$, the inequality

$$\max_{\|x\|=1}\left(\langle Ax, x\rangle - \frac{1}{\langle A^{-1}x, x\rangle}\right) \leq (\sqrt{\lambda_n} - \sqrt{\lambda_1})^2$$

is due to [Shisha and Mond, 1967]. The following remark is in order. When performed by means of J or T, the study of the inefficiency of least squares offers a convincing quantitative agreement which is *not geometric*. The inefficient critical matrices for J and T are derived from midvectors for A and catchvectors for $A^{-1/2}$ respectively. We recall that, for the same A, $V_+ = A^{-1/2}\hat{V}H^{1/2}$, $H = \text{diag}(h)$ (Corollary 4.9). Understanding the role of this geometric discrepancy calls for further investigation.

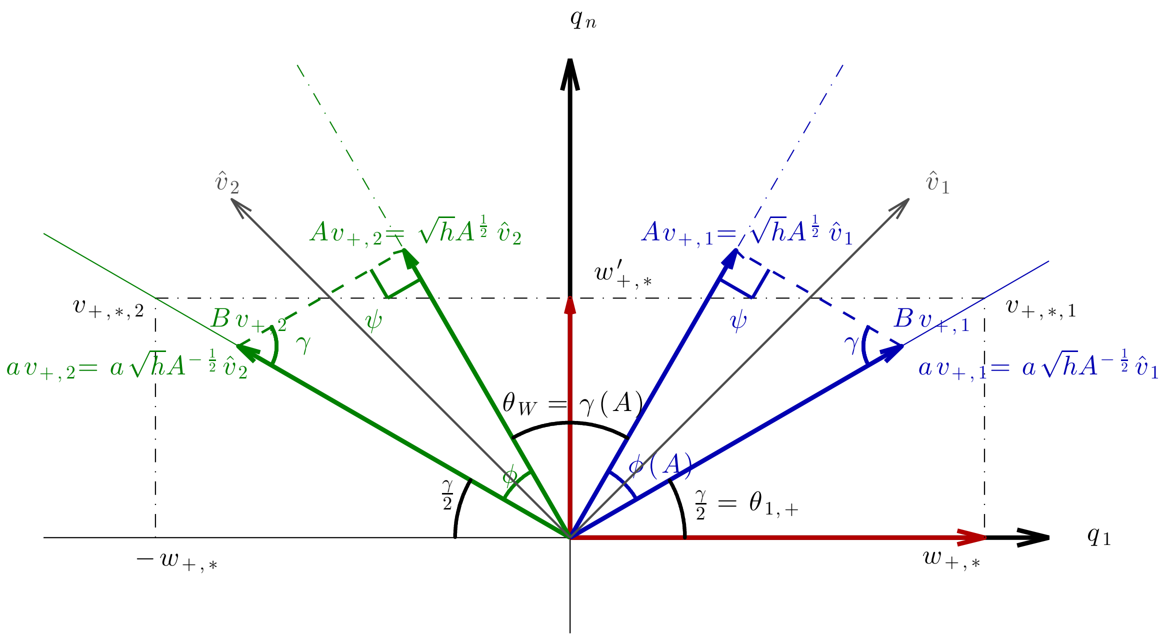


FIGURE 10. A middle vector pair in $\hat{D}_*$, $K = \mathbb{R}$

7. A trigonometric aspect for $K = \mathbb{C}^n$

7.1. The source of Gustafson's theory. Assuming that A is symmetric positive definite in $\mathbb{R}^{n\times n}$, Gustafson added to the functional:

$$x \in \mathbb{R}^n,\ \|x\| = 1 \mapsto c(x) = \frac{x^T Ax}{\|Ax\|} \in \mathbb{R}^+$$

the companion functional:

$$(\eta, x) \in \mathbb{R}^+ \times \mathbb{R}^n,\ \|x\| = 1 \mapsto n(\eta, x) = \|(\eta A - I)x\| \in \mathbb{R}^+.$$

This led him in 1968 to the remarkable theorem

$$\max_{\|x\|=1}\min_{\eta>0} n(\eta, x) = \min_{\eta>0}\max_{\|x\|=1} n(\eta, x) = \frac{\lambda_n - \lambda_1}{\lambda_1 + \lambda_n} < 1, \tag{7.1}$$

where $0 < \lambda_1 < \lambda_n$ are the extreme eigenvalues of A. Since $\cos\phi(A) = \frac{2\sqrt{\lambda_1\lambda_n}}{\lambda_1+\lambda_n} = \frac{g_*}{a_*}$, it becomes clear that the value of (7.1) is but $\sin\phi(A) = \frac{e_*}{a_*}$ where $\phi(A)$ denotes the maximal turning angle for A [Gustafson, 1968]. Actually (7.1) is a by-product of Gustafson's much more encompassing work on perturbation theory of semi-groups, see Chapter 1 in [Gustafson, 2012]. And Gustafson insists repeatedly that one has no trigonometry unless one has a cosine *and* a sine.

Our purpose in this Section is to examine how we can get a trigonometry in the general case A hermitian indefinite over $K = \mathbb{C}$. This we do by first considering the functional:

$$(\eta, x) \in \mathbb{R} \times \mathbb{C}^n,\ \|x\| = 1 \mapsto \nu(\eta, x) = \|(\eta YZ - I)x\|^2 \tag{7.2}$$

where Y and Z are two commuting hermitian matrices, $S = YZ = ZY$.

7.2. **The partial derivative $\frac{\partial\nu}{\partial\eta}(\eta, x) = 0$, $\|x\| = 1$.** We write

$$\nu(\eta, x) = \langle \eta YZx - x, \eta YZx - x\rangle = \|YZx\|^2\eta^2 - 2\langle x, YZx\rangle\eta + 1, \quad \text{for} \quad \|x\| = 1.$$

Then $\frac{\partial\nu}{\partial\eta} = 2(\|YZx\|^2\eta - \langle x, YZx\rangle) = 0$ iff η equals $\eta_0(x) = \frac{\langle x, YZx\rangle}{\|YZx\|^2}$ defined for x such that $YZx \neq 0$. We set $\jmath(x) = \frac{\langle Yx, Zx\rangle}{\|YZx\|}$, $|\jmath(x)| \in [0, 1]$.

Lemma 7.1. *For x fixed in K^n, $\|x\| = 1$, the condition $\frac{\partial\nu}{\partial\eta} = 0$ at (η_0, x) entails that $\nu_0(x) = \nu(\eta_0, x) = 1 - \jmath^2(x)$, $0 \le \nu_0(x) \le 1$.*

Proof. Clear: set $\eta_0 = \frac{\jmath(x)}{\|YZx\|}$ in $\nu(\eta, x)$. We get $\nu_0(x) = 1 - (\frac{x^H YZx}{\|YZx\|})^2$, $\|x\| = 1$, $YZx \neq 0$, that is $1 - \jmath^2(x)$.

□

When can we relate $\jmath(x)$, the cosine of angle (x, Sx) to that of one of the three angles of interest α, β or γ in $\mathbf{\Sigma}$? In other words, when is it that $\|YZx\| = \|Yx\|\|Zx\|$?

When Y is proportional to I, the answer is obvious:

- $Y = I$, $Z = A$ yield $\jmath(x) = \cos\alpha$,
- $Y = -I$, $Z = B$ yield $\jmath(x) = \cos\gamma$.

When $Y = B$, $Z = A$, $F = BA$, the answer is given by the

Lemma 7.2. *For any $u \in (S) \subset \mathbf{M}$, $\jmath(u) = \cos\beta$.*

Proof. We have to show that $\|BAu\| = \|Bu\|\|Au\|$ for $u \in (S)$. With $Au = e^{i\xi}\lambda q + e^{i\xi'}\lambda' q'$, we get $BAu = e(-e^{i\xi}\lambda q + e^{i\xi'}\lambda' q')$, hence $\|BAu\| = e\|Au\|$, $e = \|Bu\|$. □

7.3. **The trigonometric aspect $\zeta : \|x\| = 1 \mapsto \zeta(x) \in [0, \frac{\pi}{2}]$.** Let $\mathbf{S}$ be the unit sphere in $\mathbb{C}^n$ we consider the two connected functions $\mathbf{S} \to [0, 1]$ defined respectively by $\kappa : x \in \mathbf{S} \mapsto \kappa(x) = |\jmath(x)|$ and $\sigma : x \in \mathbf{S} \mapsto \sigma(x) = \sqrt{\nu_0(x)}$. The two functions are *connected* by the relation

$$\kappa^2(x) + \sigma^2(x) = 1 \quad \text{for all} \quad x \quad \text{in } \mathbf{S}. \tag{7.3}$$

In the plane $\mathbb{R}^2$, the numbers κ and σ in $[0, 1]$ define ζ in $[0, \frac{\pi}{2}]$ such that $\kappa = \cos\zeta$ and $\sigma = \sin\zeta$. See Figure 11.

Definition 7.1. The function $\zeta : \mathbf{S} \to [0, \frac{\pi}{2}]$ is called aspect of $x \in \mathbb{C}^n$. It is defined by the identities $\kappa(x) = \cos\zeta(x) = |\jmath(x)|$ and $\sigma(x) = \sin\zeta(x) = \sqrt{\nu_0(x)}$.

The concept of *aspect* is an *emerging* one: it captures the essence of the identity (7.3) which *links* $\kappa(x)$ and $\sigma(x)$: $\zeta(x)$ is the ordinary angle in the quarter plane defined by points on the unit circle with nonnegative components $(\kappa(x), \sigma(x))$, see Figure 11. It provides the geometric meaning of an angle in $\mathbb{R}^2$ to the analytic variable $\zeta(x) = \text{angle}(x, Sx) \in [0, \frac{\pi}{2}]$ when $x \in \mathbb{C}^n$. By comparison, it is an easy matter, when $x \in \mathbb{R}^n$ to relate $\zeta(x)$ to $\mathcal{S}(x) = \measuredangle(x, Sx) \in [0, 2\pi]$.

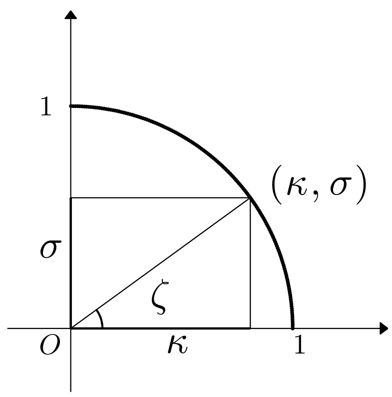


FIGURE 11. The aspect ζ of $x \in \mathbb{C}^n$

7.4. **Three applications of Lemma 7.1.** We address the three possibilities that $u \in D_\pm$, $\hat{D}$ in $\mathbf{M} \subset \mathbb{C}^n$.

Proposition 7.3. *The distinguished sets yield the following results where $u \in (S)$:*
i) $v_+ \in D_+ \Rightarrow \eta_0(v_+) = \frac{1}{a}$, $\nu_0(u) = \frac{e^2}{a^2} = \sin^2\phi$,
ii) $v_- \in D_- \Rightarrow \eta_0(v_-) = \frac{1}{e^2} > 0$, $\nu_0(u) = \frac{a^2}{e^2} = \sin^2\psi$,
iii) $\hat{v} \in \hat{D} \Rightarrow \eta_0(\hat{v}) = 0$, $\nu_0(u) = 1$.

Proof. i) $\eta_0(v_+) = \frac{1}{a}$ follows from $v_+^H A v_+ = \frac{g^2}{a}$ and $\|Av_+\| = g$; $\nu_0(u) = \|(\frac{1}{a}A - I)u\|^2 = \frac{1}{a^2}\|Bu\|^2$.
ii) $\eta_0(v_-) = \frac{1}{e^2}$ follows from $v_-^H F v_- = -g^2 > 0$ and $\|Fv_-\|^2 = -g^2e^2$; $\nu_0(u) = \|(\frac{1}{e^2}F - I)u\|^2 = \frac{a^2e^2}{e^4} = \frac{a^2}{e^2}$.
iii) $\eta_0(\hat{v}) = 0$ follows from $\langle \hat{v}, B\hat{v}\rangle = 0$; $\nu_0(u) = \|-u\| = 1$.

□

It is clear that even though $\nu_0(u)$ is constant at the optimal value for any $u \in (S)$, the aspect ζ emerges only for vectors in the corresponding distinguished set. When this occurs, ζ can be identified with any of the angles α, β, γ in $\mathbf{\Sigma}$ provided one of them is $\frac{\pi}{2}$.

To proceed toward a min-max equality, it is useful to introduce a 2×2 hermitian matrix H with eigenvalues $h < h'$, and to consider $n(\eta, x) = \sqrt{\nu(\eta, x)}$

Lemma 7.4. *i) If $hh' > 0$, then*

$$\max_{x \in \mathbb{C}^2,\, \|x\|=1} \min_{\eta \in \mathbb{R}} \|(\eta H - I_2)x\| = \min_\eta \|\eta H - I_2\| = \frac{h' - h}{|h' + h|}.$$

ii) If $h < 0 < h'$ and $h + h' = 0$, then

$$\max_{x \in \mathbb{C}^2,\, \|x\|=1} \min_{\eta \in \mathbb{R}} \|(\eta H - I_2)x\| = \min_\eta \|\eta H - I_2\| = 1.$$

Proof. i) $\|\eta H - I_2\| = \max(|\eta h - 1|, |\eta h' - 1|)$. The minimal value for $\eta \in \mathbb{R}$ is achieved when the two quantities to be compared are equal, hence $\eta_0 = \frac{2}{h+h'}$, yielding the right-hand side equality at $\frac{h'-h}{|h'+h|} > 0$.

We turn to $\min_\eta \|(\eta H - I_2)x\|$ with $H = Q \begin{pmatrix} h & 0 \\ 0 & h' \end{pmatrix} Q^H$, $\|x\| = 1$. We set $\Delta_0 = \mathrm{diag}(h, h')$, $n(\eta, x) = \|(\eta H - I_2)x\| = \|(\eta A_0 - I_2)Q^H x\|$, $y = Q^H x = (y_1, y_2)^T \in \mathbb{C}^2$, $Y(\eta, y) = ((\eta h - 1)y_1, (\eta h' - 1)y_2)^T$ and $n^2(\eta, x) = N(\eta, y) = \|Y(\eta, y)\|^2 = (\eta h - 1)^2 y_1^2 + (\eta h' - 1)^2 y_2^2$. Thus $N(\eta, y) = \mathbf{A}\eta^2 - 2\mathbf{B}\eta + 1$ with $\mathbf{A}(y) = h^2 y_1^2 + h'^2 y_2^2 = \|\Delta_0 y\|^2 > 0$, $\mathbf{B}(y) = hy_1^2 + h'y_2^2 = \langle y, \Delta_0 y\rangle$. It follows that $N(\eta, y) \geq 0$ for $\eta \in \mathbb{R}$, $y \in \mathbb{C}^2$. The 0 value is achieved if $\mathbf{B}^2 = \mathbf{A} \Leftrightarrow x$ is an eigenvector. When x is not an eigenvector, $N(\eta, y)$ is positive and minimum for y fixed if η solves $\frac{\partial N}{\partial \eta} = 0$, that is $\eta_1(y) = \frac{\mathbf{B}}{\mathbf{A}}$. Hence $\min_\eta N(\eta, y) = N(\eta_1, y) = N_1(y) = 1 - \frac{\mathbf{B}^2}{\mathbf{A}} = n_1^2(x) = \min_\eta \|(\eta H - I_2)x\|^2$. Therefore $\left(\max_{\|y\|=1}(1 - \frac{\mathbf{B}^2}{\mathbf{A}}) < 1\right) = 1 - \min_{\|y\|=1}\left(\frac{\langle y, \Delta_0 y\rangle}{\|\Delta_0 y\|}\right)^2 = 1 - \frac{4hh'}{(h'+h)^2} = \left(\frac{h'-h}{h'+h}\right)^2$ is achieved for $y_+ = (e^{i\xi}w_+, e^{i\xi'}w'_+)^T = Q^H v_+$, $v_+ \in D_+$. Note that

$$\eta_1(y_+) = \frac{\langle y_+, \Delta_0 y_+\rangle}{\|\Delta_0 y_+\|^2} = \frac{\langle v_+, Hv_+\rangle}{\|Hv_+\|^2} = \frac{2hh'}{(h+h')hh'} = \eta_0.$$

ii) $\|\eta H - I_2\| = \max(|\eta h' - 1|, |\eta h' + 1|) \geq 1$ since $h' = -h > 0$. The minimal value 1 is achieved for $\eta = 0$. On the other hand, let $x \in \hat{D}$, then $|y_1| = |y_2| = \frac{1}{\sqrt{2}}$ and $\mathbf{B} = \langle y, \Delta_0 y\rangle = \frac{1}{\sqrt{2}}(h + h') = 0$. Thus $1 - \frac{\mathbf{B}^2}{\mathbf{A}} = 1$.

□

Example 7.1. We illustrate Lemma 7.4 i) on $H = \begin{pmatrix} 0.5 & -0.3 \\ -0.3 & 0.5 \end{pmatrix}$ with eigenvalues $0 < h = 0.2 < h' = 0.8$ and $Q = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$. For $x = \cos\theta q + \sin\theta q'$, $y = Q^T x = (\cos\theta, \sin\theta)^T$: the point (η, x) is coded in $\mathbb{R}^2$ as $\eta y = (\eta\cos\theta, \eta\sin\theta)$. See on Figure 12 (a) a sample of 5 circles with increasing radius η. With $a = \frac{1}{2}$, $e = 0.3$, $w_+ = \sqrt{0.8} \sim 0.89$, $w'_+ = \sqrt{0.2} \sim 0.45$, $\eta_1(y_+) = \eta_0 = 2$, $n(2, x) = \frac{0.3}{0.5} = 0.6 = \sin\phi(H)$ where $\phi(H)$ is the turning angle, finally $\tan\theta_+ = \frac{w'_+}{w_+} = \sqrt{\frac{h}{h'}} = \sqrt{0.25} = 0.5$. See Figure 12 (b).

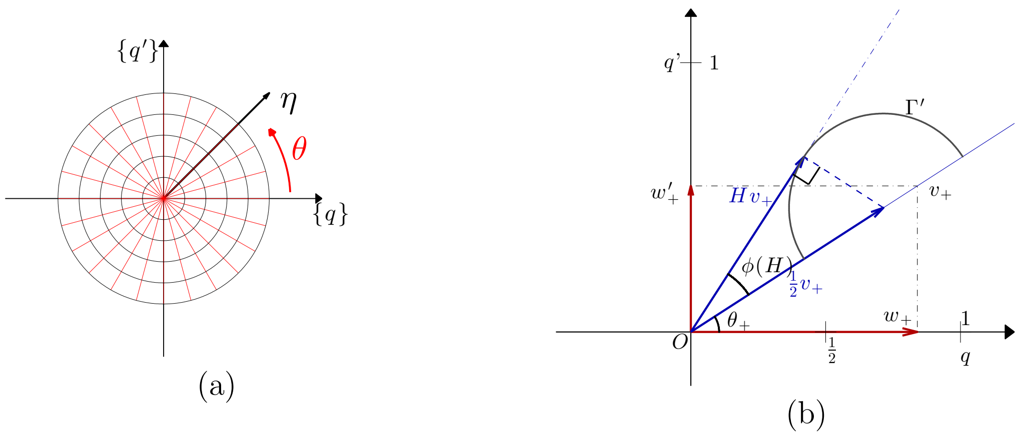


FIGURE 12. (a) Code for $(\eta, x) \cong (ny) \in \mathbb{R}^2$ (b) triangle $\mathrm{Tr}(v_+)$ in $\mathbb{R}^2$

Figure 13 displays for $\eta > 0$ the corresponding functional $n(\eta, x) = \|(\eta H - I_2)x\|$, $x \in \mathbb{R}^2$, $\|x\| = 1$ for $0 \le \eta \le 4$ and $\theta \in [0, 2\pi]$ in three views: (a) (resp. (b), (c)) displays the surface $(\eta y, n(\eta, x))$ in 3D (resp. (b) the 2D view from above, (c) the side view along $\theta_+ \sim 0.46365$).

The saddle points correspond to $\eta_1(y_+) = \eta_0$: they are the intersection of the critical value η_1 (in black) and the angle θ_+ (in red) which defines the 4 catchvectors $v_+ = \varepsilon\cos\theta_+ \, q + \varepsilon' \sin\theta_+ \, q'$, $\varepsilon, \varepsilon' = \pm 1$ in D_+, see Figure 13 (a) and (b). We observe that for η_1 fixed at $\eta_1(y)$, the value $n(\eta_1(y), y) = \sqrt{1 - \left(\frac{\langle y, \Delta_0 y\rangle}{\|\Delta_0 y\|}\right)^2} = \sin\angle\left(y, \frac{\Delta_0 y}{\|\Delta_0 y\|}\right) \le \sin\phi(H) = 0.6$ and for θ_+ fixed, $n(\eta, v_+)$ describes the piecewise convex curve depending on η with minimum value at $\eta_1(y_+) = \eta_0 = 2$, displayed in red on Figure 13 (c).

$\triangle$

We recall that $A_0 = A_{\restriction \mathbf{M}}$, $B_0 = A_0 - aI_2$, $F_0 = A_0 B_0$.

Corollary 7.5. *Let be given a coupling $\lambda < \lambda'$, $g^2 = \lambda\lambda'$. For $u \in (S) \subset \mathbf{M}$, the following min-max equalities hold:*

i) if $g^2 > 0 \Leftrightarrow |a| > e$, (7.4) $\Leftrightarrow$

$$\max_u \min_\eta \|(\eta A - I)u\| = \min_\eta \max_u \|(\eta A - I)u\| = \min_\eta \|(\eta A - I)_{\restriction \mathbf{M}}\| = \|\frac{1}{a}A_0 - I_2\| = \frac{e}{a} = \sin\phi,$$

ii) if $g^2 < 0 \Leftrightarrow |a| < e$, (7.5) $\Leftrightarrow$

$$\max_u \min_\eta \|(\eta F - I)u\| = \min_\eta \max_u \|(\eta F - I)u\| = \min_\eta \|(\eta F - I)_{\restriction \mathbf{M}}\| = \|\frac{1}{e^2}F_0 - I_2\| = \frac{|a|}{e} = \sin\psi,$$

iii) if $g^2 \neq 0$, (7.6) $\Leftrightarrow$

$$\max_u \min_\eta \|(\eta B - I)u\| = \min_\eta \max_u \|(\eta B - I)u\| = \min_\eta \|(\eta B - I)_{\restriction \mathbf{M}}\| = \min_\eta \|\eta B_0 - I_2\|$$

$$= \|I_2\| = 1 = \sin\frac{\pi}{2}.$$

Proof. (7.4) and (7.5) follow from Lemma 7.4 i) since $\lambda\lambda' > 0$ for A_0 and $-e\lambda\lambda' > 0$ for F_0 (with eigenvalues $\{-e\lambda, e\lambda'\}$). And (7.6) follows from Lemma 7.4 ii) since the eigenvalues of B_0 are $\{-e, e\}$ with zero mean: $-e + e = 0$.

□

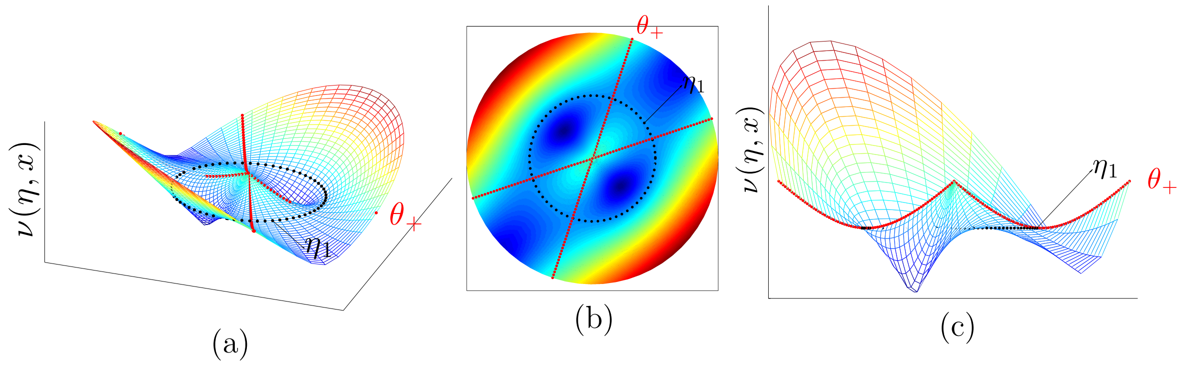


FIGURE 13. $n(\eta, x) = \|(\eta H - I_2)x\|$ (a) Surface (b) Top view (c) Side view θ_+

When A is positive definite (7.1) is a direct consequence of (7.4).

The following general remark is in order. Given the coupling (λ, λ') characterised by $(a = \frac{\lambda+\lambda'}{2}, e = \frac{\lambda'-\lambda}{2})$, the maximal value $\sin\phi$ if $g^2 > 0$ (resp. $\sin\psi$ if $g^2 < 0$) is the *ratio* $\frac{e}{|a|}$ (resp. $\frac{|a|}{e}$) related to a 2 or 4D-optimisation process in $\mathbf{M} \subset K^n$, whereas the maximal surface of the rectangle with diagonal $OL^+ = \sqrt{a^2 + e^2}$ is the *product* $|a|e$. Moreover, the ratios can be equally related to a 3 or 5D min-max optimisation process taking place in $\mathbb{R} \times \mathbf{M}$, $\mathbf{M} \subset K^n$, leading to constant values in $\mathbf{M}$. Note that $g^2 = 0 \Leftrightarrow \frac{e}{|a|} = \frac{|a|}{e} = 1$ and $|a|e = e^2$.

8. Conclusion and perspective on spectral information processing

8.1. **Summary.** We have seen that the simultaneous consideration of the eigenelements (λ, q) and (λ', q') for hermitian matrices opens new vistas about their spectral theory, a domain considered so-far as almost completely researched. Spectral information is processed in a way which mixes analysis, elementary plane geometry and trigonometry in a most elegant and rich fashion. The added value is that the proofs are embarrassingly simple! If A invertible admits d distinct eigenvalues, $2 \le d \le n$, there are $d\frac{d-1}{2}$ eigenvalue pairs $\lambda < \lambda'$ which produce $d(d-1)$ new informations in the form of the ratios $\frac{e}{|a|}$ $(g^2 > 0)$ or $\frac{|a|}{e}$ $(g^2 < 0)$ and the products $|a|e$. Most interestingly, the information process resulting from spectral coupling is delivered under various geometric forms, metric and trigonometric, derived from various right-angled triangles. To the matrix A, each coupling implicitly adds the two auxiliary matrices $B = A - aI$ and $F = AB = BA$ providing optimal *orthogonality*: $\langle v_+, Fv_+\rangle = 0$ in D_+ if $g^2 > 0$, $\langle v_-, Av_-\rangle = 0$ in D_- if $g^2 < 0$ and $\langle \hat{v}, B\hat{v}\rangle = 0$ in $\hat{D}$. Therefore six (resp. four) distinguished aspects are associated with any given coupling such that $g^2 \neq 0$ (resp. $= 0$), according to the table

<table>
<tr><td>g^2</td><td>$-$</td><td>$+$</td><td>0</td></tr>
<tr><td rowspan="3">α, β, γ</td><td>$\frac{\pi}{2}, \psi, \frac{\pi}{2} - \psi$</td><td>$\phi, \frac{\pi}{2}, \frac{\pi}{2} - \phi$</td><td>$\frac{\pi}{2}, \frac{\pi}{2}, 0$</td></tr>
<tr><td colspan="2">and</td><td>and</td></tr>
<tr><td colspan="2">$\hat{\alpha}, \hat{\beta}, \frac{\pi}{2}$</td><td>$\frac{\pi}{4}, \frac{\pi}{4}, \frac{\pi}{2}$</td></tr>
</table>

Why is it that the visionary insight of Gustafson −dating back from almost half a century− has attracted so little attention outside the matrix statistics community? A possible answer is that it *explains* more elegantly a body of well-known techniques which had already been proved to work by more familiar arguments −both in theory and practice −. The work is regarded by many as a nice confirmation of established facts. Only a handful of scientists have been receptive to its implicit potential for advancing our knowledge about the natural information processing realised through hermitian matrices.

8.2. **Spectral information processing in the bireal plane.** It has been proved elsewhere [Chatelin, 2016] that the way the information is optimally processed, either in the spectral plane or in the invariant plane if $K = \mathbb{R}$ is the result of an underlying multiplication in $\mathbb{R}^2$, known as *bireal* (Cockle 1848) which *differs* from the complex one (Cardano 1545). In $\mathbb{C}$, the non real unit is the imaginary number $i = \sqrt{-1}$, $i^2 = -1$. By contrast, in the ring ${}^2\mathbb{R}$ of bireal numbers, the non real unit is the unipotent number $\mathbf{u}$, $\mathbf{u}^2 = 1$ ($\mathbf{u} \neq \pm 1$). Thus if $z = x + \mathbf{u}y$, $z \times z' = (x + y\mathbf{u}) \times (x' + y'\mathbf{u}) = xx' + yy' + (x'y + xy')\mathbf{u}$, and $z^* = x - y\mathbf{u}$ [Rincon-Camacho and Latre, 2013]. Note that the above use of the term "unipotent" *departs* from the conventional one in abstract algebra where $(\mathbf{u} - 1)^n = 0$. The indefinite quadratic form $z \times z^* = x^2 - y^2 \in \mathbb{R}$ is nonzero for $|x| \neq |y|$ only: the algebra ${}^2\mathbb{R} = \mathbb{R} \oplus \mathbf{u}\mathbb{R}$ has a ring structure with zerodivisors equipped with the *hyperbolic* measure $\sqrt{|x^2 - y^2|}$ which is not a norm in the mathematical sense. By comparison $\mathbb{C} = \mathbb{R} \oplus i\mathbb{R}$ has a field structure equipped with the modulus $\sqrt{x^2 + y^2}$ which is the true *euclidean* norm $|x + iy| = \|z\|$. This may be the reason why $\mathbb{C}$ is the preferred structure to equip $\mathbb{R}^2$ in modern Calculus. But this choice narrows dramatically our understanding of natural information processing. Such a narrowing is amply documented in [Chatelin, 2016], under its two-fold aspect, algebraic and analytic.

8.3. **Bireal roots of the characteristic polynomial.** Because the n eigenvalues of A hermitian are *real* its characteristic polynomial has real coefficients. As such it can be regarded as an element in $\mathbb{C}[X]$ as well as in ${}^2\mathbb{R}[X]$. We know that the first choice provides no additional information to the real spectrum. But the second choice does provide new *bireal* eigenvalues! This follows readily from

$$\begin{aligned} 0 &= \mu^2 - 2a\mu + g^2 = (\mu - \lambda)(\mu - \lambda') \text{ for } \mu \in \mathbb{R} \text{ or } \mathbb{C}, \\ &= (\mu - (a + e\mathbf{u})) \times (\mu - (a - e\mathbf{u})) \text{ for } \mu \in^2 \mathbb{R}. \end{aligned}$$

In other words the real eigenpair (λ, λ') is complemented by the bireal eigenpair ($\sigma = a + e\mathbf{u}$, $\sigma^* = a - e\mathbf{u}$) which are represented on Figures 2 and 9 by the points L^+ and L^- of Γ, if one agrees to equip the spectral plane $\mathbf{\Sigma} = \mathbb{R}^2$ with the bireal ring structure ${}^2\mathbb{R}$.

Of course, it is not surprising that a polynomial of degree n may have *more* than n roots in a ring, rather than the n roots classically expected in an algebraically closed field such as $\mathbb{C} \supset \mathbb{R}$.

When $K = \mathbb{R}$ there is more to the bireal story. Bireal eigenvectors $\mathbf{x} = x_1 + x_2\mathbf{u}$, x_1 and $x_2 \in \mathbb{R}^n$ can be defined by $A\mathbf{x} = (a + \varepsilon e\mathbf{u})\mathbf{x}$, $\varepsilon = \pm 1$. Thus $(A - aI)x_1 = Bx_1 = ex_2$, $Bx_2 = ex_1$: both x_1 and x_2 satisfy $B^2x = e^2x$ in $\mathbf{M} \subset \mathbb{R}^n$. An application of Lemma 3.1 yields the key result that, in *bireal* arithmetic, σ and σ^* are double and enjoy the *same* bireal eigenplane $\mathbf{M} \oplus \mathbf{M}\mathbf{u} = \mathbf{V}$ in $({}^2\mathbb{R})^2$ with 4 real dimensions. Since x_1 and x_2 can vary arbitrarily on (C), the eigenspace $\mathbf{V}$ has the structure $S^1 \times S^1$ which can be represented in $\mathbb{R}^3$ by a horn torus.

Spectral theories for *symmetric* matrices *differ* significantly when they are carried in real or bireal arithmetic, whereas they are *identical* in real and complex arithmetic.

Now, the real invariant plane $\mathbf{M}$ itself can be thought of algebraically as the ring ${}^2\mathbb{R}$. If one sets $q \cong 1$, $q' \cong \mathbf{u}$, then the two middle vectors $\hat{v}_1 = \frac{1}{\sqrt{2}}(q + q') = \sqrt{2}\frac{1+\mathbf{u}}{2}$ and $\hat{v}_2 = \frac{1}{\sqrt{2}}(q - q') = \sqrt{2}\frac{1-\mathbf{u}}{2}$ are zerodivisors: $\hat{v}_1 \times \hat{v}_2 = \frac{1}{2}(1 - \mathbf{u}^2) = 0$. They are proportional to the idempotent numbers $\mathbf{e}_\pm = \frac{1}{2}(1 \pm \mathbf{u})$ which satisfy $\mathbf{e}_\pm^2 = \mathbf{e}_\pm$; thus $\hat{v}^2 = \sqrt{2}\hat{v}$ for $\hat{v} \in \hat{D}$. In the idempotent basis $\{\mathbf{e}_+, \mathbf{e}_-\}$ the bireal multiplication is performed *componentwise*. Let

$z = x + y\mathbf{u} = \frac{x+y}{2}\mathbf{e}_+ + \frac{x-y}{2}\mathbf{e}_- = X\mathbf{e}_+ + Y\mathbf{e}_-$, then $z \times z' = (X\mathbf{e}_+ + Y\mathbf{e}_-) \times (X'\mathbf{e}_+ + Y'\mathbf{e}_-) = XX'\mathbf{e}_+ + YY'\mathbf{e}_-$.

"And what if $K = \mathbb{C}$?" will rightly ask the curious reader. Just like ${}^2\mathbb{R}$ can replace $\mathbb{C}$ for multiplication in $\mathbb{R}^2$, in the four real dimensions of $\mathbb{R}^4 \cong \mathbb{C}^2$, the classical noncommutative field $\mathbb{H}$ of quaternions can be replaced by the commutative ring of bicomplex numbers ${}^2\mathbb{C} = \mathbb{C} \oplus \mathbf{u}\mathbb{C}$, where $\mathbf{u}$ is now a 4D-unipotent vector ($\mathbf{u}^2 = 1$, $\mathbf{u} \neq \pm 1$). It follows that σ and σ^* are double bireal eigenvalues in ${}^2\mathbb{C}$ with eigenspace $\mathbf{V}$ in $({}^2\mathbb{C})^2$ with 8 real dimensions. The structure of $\mathbf{V}$ is now $S^3 \times S^3$. For more on bicomplex multiplication, see [Cockle, 1848, Segre, 1892, Price, 1991, Rincon-Camacho and Latre, 2013].

8.4. **Bireals for hydrodynamics.** Some physicists with a strong mathematical leaning are aware of the computational potential that resides in the inconspicuous ring of 2D-bireal numbers. The book [Lavrentiev and Chabat, 1980] , a classic in hydrodynamics, devotes its whole chapter 2 more generally to the three families of algebraic structures that can equip the real plane. It also compares the properties of functions in 2 real variables which are analytic with respect to the complex or the bireal multiplication, the latter being useful to model supersonic flows, see chapter 4 of the same book. It is possible that the information carried by spectral coupling could bring new insights into computational fluid dynamics. The matter is investigated elsewhere [Chatelin, 2016].

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