LEVEL CURVES OF THE ANGLE FUNCTION OF A POSITIVE DEFINITE SYMMETRIC MATRIX

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Given a real N by N matrix A, write p(A) for the maximum angle by which A rotates any unit vector. Suppose that A and B are positive definite symmetric (PDS) N by N matrices. Then their Jordan product {A, B} := AB + BA is also symmetric, but not necessarily positive definite. If p(A) + p(B) is obtuse, then there exists a special orthogonal matrix S such that {A, SBS^(-1)} is indefinite. Of course, if A and B commute, then {A, B} is positive definite. Our work grows from the following question: if A and B are commuting positive definite symmetric matrices such that p(A) + p(B) is obtuse, what is the minimal p(S) such that {A, SBS^(-1)} indefinite? In this dissertation we will describe the level curves of the angle function mapping a unit vector x to the angle between x and Ax for a 3 by 3 PDS matrix A, and discuss their interaction with those of a second such matrix.

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CONTENTS

CHAPTER 1

INTRODUCTION

Given a real $n \times n$ matrix A, write ϕ_A for the maximum angle by which A rotates any unit vector:

$$\phi_A := \sup_{x \in S^{n-1}} \angle(x, Ax).$$

Here S^{n-1} is the unit sphere in $\mathbb{R}^n$. If Ax is zero, $\angle(x, Ax)$ is regarded as $\frac{\pi}{2}$. It is not difficult to see that a symmetric matrix A is positive definite if and only if $\phi_A < \frac{\pi}{2}$.

Suppose that A and B are positive definite symmetric (PDS) $n \times n$ matrices. Then their Jordan product $\{A, B\} := AB + BA$ is also symmetric, but not necessarily positive definite. In fact,

$$\phi_{\{A,B\}} \leq \phi_A + \phi_B,$$

so if $\phi_A + \phi_B < \frac{\pi}{2}$ then $\{A, B\}$ is positive definite. However, if $\phi_A + \phi_B \geq \frac{\pi}{2}$, then the eigenvalues of A and B alone do not determine whether or not $\{A, B\}$ is positive definite; the relative positions of their eigenvectors also play a role. Speaking roughly, the further the eigenvectors of A are from those of B, the less likely $\{A, B\}$ is to be PDS. Moreover, there is always some "rotation" B_{rot} of B such that $\{A, B_{\text{rot}}\}$ is indefinite. (we use the term indefinite to denote matrices which are neither positive nor negative definite). More precisely, if $\phi_A + \phi_B \geq \frac{\pi}{2}$ then it is possible to find a special orthogonal matrix $S \in \mathrm{SO}_n$ such that $\{A, B^S\}$ is indefinite. Here B^S denotes SBS^{-1}.

When A and B commute, their eigenvectors are the same and $\{A, B\}$ is PDS. This is in some sense the case in which $\{A, B\}$ is the farthest from being indefinite. This dissertation grew out of the following question: if A and B are commuting PDS matrices such that

$\phi_A + \phi_B \geq \frac{\pi}{2}$, what is the "smallest rotation" S such that $\{A, B^S\}$ is indefinite? Of course, for $n \geq 4$ in general S is not a rotation but a product of orthogonal rotations.

In order to state the problem precisely, we define

$$\Phi(A, B) := \inf\{\phi_S : S \in \mathrm{SO}_n \text{ and } \{A, B^S\} \text{ is indefinite }\}.$$

Problem 1 *Compute $\Phi(A, B)$ for commuting PDS matrices A and B.*

There is important related work by Strang [7], who deduced bounds on the extremal eigenvalues of $\{A, B\}$ in answer to a research problem proposed by Taussky-Todd [8]. The second chapter of this thesis reviews his results.

Other related work includes that of Nicholson [6], who (independently of Strang) gave a sufficient condition for $\{A, B\}$ to be positive definite, and Alikakos and Bates [1], who established bounds for all the eigenvalues of $\{A, B\}$. Gustafson [3] gave a trigonometric interpretation of Strang's result, and Fujii, Fujii, Izumino, Kubo and Nakamoto [5] generalized it to non-self adjoint operators. Recently, Conley, Pucci, and Serrin [2] applied it in establishing the domain of validity of a certain version of the maximum principle.

We begin Chapter 3 by proving a proposition that gives ϕ_A for a PDS matrix A in terms of its extremal eigenvalues. We then establish some useful results on ϕ_S for orthogonal matrices S. Next we take an in-depth look at Problem 1 in the 2×2 case. We conclude the chapter with some three dimensional examples.

For any $S \in \mathrm{SO}_3$, the trace of S is given by $1 + 2\cos\phi_S$. Therefore ϕ_S is minimal when the trace of S is maximal. In Chapter 4 we study the trace of S and present formulas for it in different situations pertaining to Problem 1. However, we were unable to solve Problem 1 directly by maximizing these formulas, as they are too complicated. This led us to study the level curves of the angle function $x \mapsto \angle(x, Ax)$ on the unit sphere in $\mathbb{R}^3$ for a PDS matrix A.

Chapter 5 is devoted to these level curves. In the first section we present a series of figures depicting the level curves at different stages both on the unit sphere S^2 and on the plane $\mathcal{P} = \{s \in \mathbb{R}^3 : s_1 + s_2 + s_3 = 1\}$, the s_i being the squares of the standard coordinates. (Matlab was used in obtaining these figures.) Interestingly, on $\mathcal{P}$ the level curves are all parabolas, which we prove in Section 3. On the other hand, their shape on S^2 varies. In Section 2 we give necessary and sufficient conditions for a level curve on S^2 to be a union of circles.

Chapter 6 focuses on level curves of PDS matrices A for small angles. The results are then used to give a geometric solution of a trace maximization problem for two increasing diagonal PDS matrices. We view this problem as a "toy model" of Problem 1.

CHAPTER 2

RESULTS OF STRANG

Throughout this chapter A and B are $n \times n$ symmetric matrices. Suppose that m_A, M_A and m_B, M_B are the extreme eigenvalues of A and B, respectively.

LEMMA 2.1. *For all $x \in \mathbb{R}^n$, there exists a unique vector $Y_A(x)$ such that $|Y_A(x)| \leq 1$, $x \cdot Y_A(x) \geq 0$, and*

$$Ax = m_A x + (M_A - m_A)(x \cdot Y_A(x)) \frac{Y_A(x)}{|Y_A(x)|} \text{ if } Y_A(x) \neq 0.$$

Note: We take $Y_A(x) = 0$ if $Ax - m_A x = 0$.

PROOF. If x is an eigenvector of A of eigenvalue m_A, then $(A - m_A)x = 0$ and $Y_A(x) = 0$. Suppose x is not an eigenvector of eigenvalue m_A. Then $(A - m_A)x \neq 0$. Let us first define a unit vector $y_A(x)$ as follows:

$$y_A(x) = \frac{(A - m_A)x}{|(A - m_A)x|}.$$

Suppose $m_A = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n = M_A$ are the eigenvalues of A. Since A is symmetric, it has an orthonormal eigenbasis $\{v_1, v_2, \cdots, v_n\}$ corresponding to the eigenvalues $\lambda_1, \lambda_2, \cdots, \lambda_n$. Then for some scalars $\alpha_1, \alpha_2, \cdots, \alpha_n$, we have $x = \alpha_1 v_1 + \alpha_2 v_2 + \cdots + \alpha_n v_n$. Hence

$$x \cdot (A - m_A)x = \sum_{i=1}^{n} (\lambda_i - m_A)\alpha_i^2 \geq 0,$$

with equality if and only if $(A - m_A)x = 0$. Since we are assuming that this is not the case, $x \cdot (A - m_A)x$ and $x \cdot y_A(x)$ are positive. For $(A - m_A)x \neq 0$, $M_A - m_A \neq 0$, and so we may define a positive scalar

$$\rho_A(x) = \frac{|(A - m_A)x|^2}{(M_A - m_A)(x \cdot (A - m_A)x)}.$$

Let $Y_A(x) = \rho_A(x) y_A(x)$. Since $\rho_A(x)$ is positive, $|Y_A(x)| = \rho_A(x)$. We now prove $\rho_A(x) \leq 1$. Note that

$$|(A - m_A)x|^2 = \left| \sum_{i=1}^{n} (\lambda_i - m_A) \alpha_i v_i \right|^2 = \sum_{i=1}^{n} (\lambda_i - m_A)^2 \alpha_i^2,$$

$$(M_A - m_A)(x \cdot (A - m_A)x) = \sum_{i=1}^{n} (M_A - m_A)(\lambda_i - m_A) \alpha_i^2.$$

Since $(M_A - m_A) \geq (\lambda_i - m_A)$ for all i,

$$\sum_{i=1}^{n} (M_A - m_A)(\lambda_i - m_A) \alpha_i^2 \geq \sum_{i=1}^{n} (\lambda_i - m_A)^2 \alpha_i^2.$$

Hence $(M_A - m_A)(x \cdot (A - m_A)x) \geq |(A - m_A)x|^2$, so $\rho_A(x) \leq 1$. Since $|Y_A(x)| = \rho_A(x)$, we also have $|Y_A(x)| \leq 1$ and

$$x \cdot Y_A(x) = \rho_A(x)(x \cdot y_A(x)) \geq 0.$$

Finally, we will show that $Ax = m_A x + (M_A - m_A)(x \cdot Y_A(x)) \frac{Y_A(x)}{|Y_A(x)|}$. From the definition of $\rho_A(x)$, we have

$$x \cdot (A - m_A)x = \frac{|(A - m_A)x|^2}{(M_A - m_A)\rho_A(x)}.$$

Note that the dot product of x with $Y_A(x)$ gives

$$x \cdot Y_A(x) = \rho_A(x) \frac{x \cdot (A - m_A)x}{|(A - m_A)x|}.$$

Combining the above two equations, we obtain

$$|(A - m_A)x| = (M_A - m_A)\rho_A(x)(x \cdot Y_A(x)) \frac{1}{|Y_A(x)|}.$$

Substituting this in the definition of $y_A(x)$ and simplifying, we get

$$Ax = m_A x + (M_A - m_A)(x \cdot Y_A(x)) \frac{Y_A(x)}{|Y_A(x)|}.$$

$\square$

Definition 2.2. Given any two symmetric $n \times n$ matrices A and B, let

$$\begin{aligned}\Lambda_m(A,B) &= \inf\{\text{minimum eigenvalue of } \tfrac{1}{2}\{A, B^S\} : S \in \mathrm{O}_n\} \\ \Lambda_M(A,B) &= \sup\{\text{maximum eigenvalue of } \tfrac{1}{2}\{A, B^S\} : S \in \mathrm{O}_n\}.\end{aligned}$$

Since $m_A = \inf\{x \cdot Ax : |x| = 1\}$,

$$\begin{aligned}\Lambda_m(A,B) &= \inf\{x \cdot \tfrac{1}{2}\{A, B^S\}x : S \in \mathrm{O}_n, |x| = 1\} \\ &= \inf\{Ax \cdot B^S x : S \in \mathrm{O}_n, |x| = 1\}.\end{aligned}$$

Similarly,

$$\Lambda_M(A,B) = \sup\{Ax \cdot B^S x : S \in \mathrm{O}_n, |x| = 1\}.$$

By Lemma 2.1, for all $x \in \mathbb{R}^n$ we have

$$Ax = m_A x + (M_A - m_A)(x \cdot Y_A(x)) \frac{Y_A(x)}{|Y_A(x)|}.$$

Since $Y_A(x) = \rho_A(x) y_A(x)$ and $|Y_A(x)| = \rho_A(x)$, the above expression becomes

$$Ax = m_A x + (M_A - m_A)\rho_A(x)(x \cdot y_A(x)) y_A(x).$$

Similarly, we have

$$B^S x = m_B x + (M_B - m_B)\rho_{B^S}(x)(x \cdot y_{B^S}(x)) y_{B^S}(x).$$

Let us write ρ_A, ρ_B for $\rho_A(x), \rho_{B^S}(x)$ and y_A, y_B for $y_A(x), y_{B^S}(x)$. Taking the dot product of Ax and $B^S x$ gives

$$\begin{aligned}Ax \cdot B^S x &= m_A m_B + m_B(M_A - m_A)\rho_A (x \cdot y_A)^2 + m_A(M_B - m_B)\rho_B (x \cdot y_B)^2 \\ &\quad + (M_A - m_A)(M_B - m_B)\rho_A \rho_B (x \cdot y_A)(x \cdot y_B)(y_A \cdot y_B).\end{aligned}$$

Write k_A for $\frac{M_A}{m_A}$ and k_B for $\frac{M_B}{m_B}$, and let $\tilde{k}_A = k_A - 1$ and $\tilde{k}_B = k_B - 1$. Divide both sides of the above expression by $m_A m_B$ and let

$$f(x,S) = \frac{Ax \cdot B^S x}{m_A m_B}.$$

Then

$$(1)\qquad f(x,S)=1+\tilde{k}_A\rho_A(x\cdot y_A)^2+\tilde{k}_B\rho_B(x\cdot y_B)^2+\tilde{k}_A\tilde{k}_B\rho_A\rho_B(x\cdot y_A)(x\cdot y_B)(y_A\cdot y_B)$$

Now consider the function given by

$$(2)\qquad \begin{aligned} F(\gamma_A,\gamma_B,\theta_A,\theta_B,\phi) &= 1+\tilde{k}_A\gamma_A\cos^2\theta_A+\tilde{k}_B\gamma_B\cos^2\theta_B \\ &+\tilde{k}_A\tilde{k}_B\gamma_A\gamma_B\cos\theta_A\cos\theta_B\cos\phi. \end{aligned}$$

Define $V_F(A,B)$ to be the set of values of $F(\gamma_A,\gamma_B,\theta_A,\theta_B,\phi)$ for $\gamma_A,\gamma_B\in[0,1]$, $\theta_A,\theta_B\in[0,\frac{\pi}{2}]$, and $\cos\phi\in\big[\cos(\theta_A+\theta_B),\cos(\theta_A-\theta_B)\big]$. We first prove the following lemma:

Lemma 2.3. $\{f(x,S):x\in\mathbb{R}^n,|x|=1,S\in\mathrm{O}_n\}\subseteq V_F(A,B)$

Proof. This is clear because if we suppose the angle between x and y_A and the angle between x and y_{B^S} to be θ_A and θ_B respectively, then $(x\cdot y_A)=\cos\theta_A$, $(x\cdot y_{B^S})=\cos\theta_B$, and $(y_A\cdot y_{B^S})$ is bounded by $\cos(\theta_A+\theta_B)$ and $\cos(\theta_A-\theta_B)$. □

Proposition 2.4. *The extrema of* $F(\gamma_A,\gamma_B,\theta_A,\theta_B,\phi)$*, for* $\gamma_A,\gamma_B\in[0,1]$*,* $\theta_A,\theta_B\in[0,\frac{\pi}{2}]$*, and* $\cos\phi\in\big[\cos(\theta_A+\theta_B),\cos(\theta_A-\theta_B)\big]$ *are the least and greatest of* $1,k_Ak_B,k_A,k_B$ *and, if* $\left(\frac{cd}{b^2}-\frac{c}{d}-\frac{d}{c}\right)$ *and* $\left(\frac{bd}{c^2}-\frac{b}{d}-\frac{d}{b}\right)$ *(see proof) are in* $[-2,2]$*,*

$$\frac{(k_A+1)^2(k_B+1)^2-(k_A-1)^2(k_B+1)^2-(k_A+1)^2(k_B-1)^2}{8(k_A+1)(k_B+1)}.$$

Proof. Since F is linear in $\cos\phi$ and $\cos\phi\in\big[\cos(\theta_A+\theta_B),\cos(\theta_A-\theta_B)\big]$, for extrema we just need to consider the boundary values of $\cos\phi$. These give two functions, each depending on just $\gamma_A,\gamma_B,\theta_A$ and θ_B. They are

$$\begin{aligned} F^{\pm}(\gamma_A,\gamma_B,\theta_A,\theta_B) &= 1+\tilde{k}_A\gamma_A\cos^2\theta_A+\tilde{k}_B\gamma_B\cos^2\theta_B \\ &\quad+\tilde{k}_A\tilde{k}_B\gamma_A\gamma_B\cos\theta_A\cos\theta_B\cos(\theta_A\pm\theta_B). \end{aligned}$$

Since $F^+(\gamma_A,\gamma_B,\theta_A,-\theta_B)=F^-(\gamma_A,\gamma_B,\theta_A,\theta_B)$, the extrema of $F^-(\gamma_A,\gamma_B,\theta_A,\theta_B)$ for $\theta_A,\theta_B\in[-\frac{\pi}{2},\frac{\pi}{2}]$ are same as that of $F(\gamma_A,\gamma_B,\theta_A,\theta_B,\phi)$. Therefore we will find the extrema of $F^-(\gamma_A,\gamma_B,\theta_A,\theta_B)$ for $\theta_A,\theta_B\in[-\frac{\pi}{2},\frac{\pi}{2}]$.

Since $\cos(\theta_A - \theta_B) = \cos\theta_A \cos\theta_B + \sin\theta_A \sin\theta_B$, we see that $\cos\theta_A \cos\theta_B \cos(\theta_A - \theta_B)$ reduces to $\cos^2\theta_A \cos^2\theta_B + \frac{1}{4}\sin 2\theta_A \sin 2\theta_B$. Now, writing $\frac{1}{2}(\cos 2\theta + 1)$ for $\cos^2\theta$ in the equation for $F^-(\gamma_A, \gamma_B, \theta_A, \theta_B)$, we have

$$
\begin{aligned}
F^-(\gamma_A, \gamma_B, \theta_A, \theta_B) \;&=\; 1 + \tilde{k}_A\gamma_A\tfrac{1}{2}(\cos 2\theta_A + 1) + \tilde{k}_B\gamma_B\tfrac{1}{2}(\cos 2\theta_B + 1) + \\
&\quad\; \tilde{k}_A\tilde{k}_B\gamma_A\gamma_B\tfrac{1}{4}\big\{\cos 2(\theta_A - \theta_B) + \cos 2\theta_A + \cos 2\theta_B + 1\big\}.
\end{aligned}
$$

Since this function is linear in γ_A and γ_B, which lie in $[0,1]$, for extrema we just need to consider the boundary values of γ_A and γ_B. When both γ_A and γ_B are zero, $F^- = 1$. When $\gamma_A = 1$ and $\gamma_B = 0, F^- = 1 + \frac{\tilde{k}_A}{2}(\cos 2\theta_A + 1)$, which yields extrema of 1 and k_A. Similarly, the case $\gamma_A = 0$ and $\gamma_B = 1$ yields extremas of 1 and k_B. All these cases are actually contained in the last and the most interesting case, $\gamma_A = \gamma_B = 1$. Let $G(\theta_A, \theta_B)$ be $F^-(1, 1, \theta_A, \theta_B)$. Setting

$$
\begin{aligned}
a &= 1 + \tfrac{1}{2}\tilde{k}_A + \tfrac{1}{2}\tilde{k}_B + \tfrac{1}{4}\tilde{k}_A\tilde{k}_B = \tfrac{1}{4}(k_A + 1)(k_B + 1), \\
b &= \tfrac{1}{2}\tilde{k}_A + \tfrac{1}{4}\tilde{k}_A\tilde{k}_B = \tfrac{1}{4}(k_A - 1)(k_B + 1), \\
c &= \tfrac{1}{2}\tilde{k}_B + \tfrac{1}{4}\tilde{k}_A\tilde{k}_B = \tfrac{1}{4}(k_B - 1)(k_A + 1), \\
d &= \tfrac{1}{4}\tilde{k}_A\tilde{k}_B = \tfrac{1}{4}(k_B - 1)(k_A - 1),
\end{aligned}
$$

we have

$$G(\theta_A, \theta_B) = a + b\cos 2\theta_A + c\cos 2\theta_B + d\cos 2(\theta_A - \theta_B).$$

The partial derivatives of this equation are

$$
\begin{aligned}
\frac{\partial G}{\partial \theta_A} &= -2b\sin 2\theta_A - 2d\sin 2(\theta_A - \theta_B) \\
\frac{\partial G}{\partial \theta_B} &= -2c\sin 2\theta_B + 2d\sin 2(\theta_A - \theta_B).
\end{aligned}
$$

Clearly, these partials vanish when θ_A and θ_B are both multiples of $\frac{\pi}{2}$. Since $|\theta_A|, |\theta_B| \leq \frac{\pi}{2}$, the choices we have for θ_A and θ_B are 0 and $\pm\frac{\pi}{2}$. Each possibility will result in an extremal value of $1, k_A, k_B$ or $k_A k_B$, the first three of which were already obtained above.

Next we check whether the partial derivatives vanish simultaneously for values of θ_A and θ_B other than 0 and $\pm\frac{\pi}{2}$. Equating them to zero and adding, we obtain

$$b\sin 2\theta_A + c\sin 2\theta_B = 0. \tag{3}$$

We are assuming that either θ_A or $\theta_B \notin \{0, \pm\frac{\pi}{2}\}$. Without loss of generality, assume $\theta_A \notin \{0, \pm\frac{\pi}{2}\}$. Then, $\sin 2\theta_A \neq 0$. Substituting the value of $\sin 2\theta_B$ into the first partial derivative and solving leads to

$$b\cos 2\theta_A + c\cos 2\theta_B = -\frac{bc}{d}. \tag{4}$$

Since $b\sin 2\theta_A = -c\sin 2\theta_B$, we have $b^2(1-\cos^2 2\theta_A) = c^2(1-\cos^2 2\theta_B)$, which leads to

$$b^2 - c^2 = (b\cos 2\theta_A - c\cos 2\theta_B)(b\cos 2\theta_A + c\cos 2\theta_B).$$

Now, substituting the value of $(b\cos 2\theta_A + c\cos 2\theta_B)$ from (4) and simplifying, we obtain

$$b\cos 2\theta_A - c\cos 2\theta_B = -\frac{bd}{c} + \frac{cd}{b}. \tag{5}$$

Solving (4) and (5) gives

$$\cos 2\theta_A = \frac{1}{2}\Big(\frac{cd}{b^2} - \frac{c}{d} - \frac{d}{c}\Big). \tag{6}$$

$$\cos 2\theta_B = \frac{1}{2}\Big(\frac{bd}{c^2} - \frac{b}{d} - \frac{d}{b}\Big). \tag{7}$$

There exist solutions if and only if $\big(\frac{cd}{b^2} - \frac{c}{d} - \frac{d}{c}\big)$ and $\big(\frac{bd}{c^2} - \frac{b}{d} - \frac{d}{b}\big)$ are in $[-2, 2]$.

In order to compute the resulting extrema of F, note that by (3) and (4),

$$\cos 2(\theta_A - \theta_B) = -\cos 2\theta_A\Big(\frac{b}{c}\cos 2\theta_A + \frac{b}{d}\Big) - \frac{b}{c}\sin^2 2\theta_A = -\frac{b}{c} - \frac{b}{d}\cos 2\theta_A.$$

Substituting this value into $G(\theta_A, \theta_B)$ and simplifying using (6) gives

$$G(\theta_A, \theta_B) = a + c\cos 2\theta_B - \frac{bd}{c} = \frac{1}{2}\Big(\frac{bc}{d} - \frac{bd}{c} - \frac{cd}{b}\Big).$$

Finally, substituting in the values of a, b, c and d gives

$$G(\theta_A, \theta_B) = \frac{(k_A+1)^2(k_B+1)^2 - (k_A-1)^2(k_B+1)^2 - (k_A+1)^2(k_B-1)^2}{8(k_A+1)(k_B+1)}.$$

$\square$

Now let $\hat{A} = \left(\begin{smallmatrix} m_A & 0 \\ 0 & M_A \end{smallmatrix}\right)$ and $\hat{B} = \left(\begin{smallmatrix} m_B & 0 \\ 0 & M_B \end{smallmatrix}\right)$. For any unit vector $\hat{x} \in \mathbb{R}^2$ and any $\hat{S} \in \mathrm{O}_2$, define

$$\hat{f}(\hat{x}, \hat{S}) = \frac{\hat{A}\hat{x} \cdot \hat{B}^{\hat{S}}\hat{x}}{m_A m_B}.$$

Lemma 2.5. $\{\hat{f}(\hat{x}, \hat{S}) : \hat{S} \in \mathrm{O}_2, \hat{x} \in \mathbb{R}^2, |\hat{x}| = 1\} \subseteq \{f(x, S) : S \in \mathrm{O}_n, x \in \mathbb{R}^n, |x| = 1\}$.

Proof. Any $\hat{S} \in \mathrm{O}_2$ takes the form $R_\theta = \left(\begin{smallmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{smallmatrix}\right)$ or $R_\theta \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$, and $\left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ commutes with $\hat{B}$, so $\hat{f}(\hat{x}, \hat{S}) = \hat{f}(\hat{x}, R_\theta)$ for some θ.

Given any $\hat{x}$, define $x_1 = \hat{x}_1$, $x_n = \hat{x}_2$, and $x_i = 0$ for $1 < i < n$, and consider the $n \times n$ orthogonal matrix $S = \begin{pmatrix} \cos\theta & & & & -\sin\theta \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ \sin\theta & & & & \cos\theta \end{pmatrix}$. It satisfies $\hat{f}(\hat{x}, \hat{S}) = f(x, S)$.

$\square$

Next we consider $\frac{1}{m_A}\hat{A} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & k_A \end{smallmatrix}\right)$, $\frac{1}{m_B}\hat{B} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & k_B \end{smallmatrix}\right)$, and $\hat{S} = R_\theta$. Verify

$$\frac{1}{m_B}\hat{B}^{\hat{S}} = \begin{pmatrix} \cos^2\theta + k_B \sin^2\theta & (1-k_B)\sin\theta\cos\theta \\ (1-k_B)\sin\theta\cos\theta & \sin^2\theta + k_B\cos^2\theta \end{pmatrix}.$$

Choose any unit vector $\hat{x} = (\sin\phi, \cos\phi) \in \mathbb{R}^2$. Then

$$\frac{\hat{A}\hat{x}}{m_A} = \begin{pmatrix} \sin\phi \\ k_A\cos\phi \end{pmatrix}, \frac{\hat{B}^{\hat{S}}\hat{x}}{m_B} = \begin{pmatrix} (\cos^2\theta + k_B\sin^2\theta)\sin\phi + (1-k_B)\sin\theta\cos\theta\cos\phi \\ (1-k_B)\sin\theta\cos\theta\sin\phi + (\sin^2\theta + k_B\cos^2\theta)\cos\phi \end{pmatrix}.$$

Taking the dot product of these two vectors, we get

$$\begin{aligned} \hat{f}(\hat{x}, \hat{S}) \;=\;& (\cos^2\theta + k_B\sin^2\theta)\sin^2\phi + (1-k_B)\sin\theta\cos\theta\sin\phi\cos\phi + \\ & k_A(1-k_B)\sin\theta\cos\theta\sin\phi\cos\phi + k_A(\sin^2\theta + k_B\cos^2\theta)\cos^2\phi. \end{aligned}$$

Further simplification gives

$$\begin{aligned} \hat{f}(\hat{x}, \hat{S}) \;=\;& (\cos^2\theta\sin^2\phi + \sin\theta\cos\theta\sin\phi\cos\phi) \\ & + k_B(\sin^2\theta\sin^2\phi - \sin\theta\cos\theta\sin\phi\cos\phi) \\ & + k_A(\sin^2\theta\cos^2\phi + \sin\theta\cos\theta\sin\phi\cos\phi) \end{aligned}$$

$$+ k_A k_B(\cos^2\theta\cos^2\phi - \sin\theta\cos\theta\sin\phi\cos\phi).$$

Letting $k_A = \tilde{k}_A + 1$ and $k_B = \tilde{k}_B + 1$ and simplifying, we get

$$\begin{aligned}\hat{f}(\hat{x},\hat{S}) &= 1 + \tilde{k}_A\cos^2\phi + \tilde{k}_B(\cos\theta\cos\phi - \sin\theta\sin\phi)^2 \\ &\quad + \tilde{k}_A\tilde{k}_B\cos\theta\cos\phi(\cos\theta\cos\phi - \sin\theta\sin\phi).\end{aligned}$$

Since $(\cos\theta\cos\phi - \sin\theta\sin\phi) = \cos(\theta+\phi)$, the above expression reduces to

$$\hat{f}(\hat{x},\hat{S}) = 1 + \tilde{k}_A\cos^2\phi + \tilde{k}_B\cos^2(\theta+\phi) + \tilde{k}_A\tilde{k}_B\cos\theta\cos\phi\cos(\theta+\phi). \tag{8}$$

Finally, since ϕ and θ are arbitrary, the extrema of $\hat{f}(\hat{x},\hat{S})$ for $\phi,\theta \in [-\frac{\pi}{2},\frac{\pi}{2}]$ are same as that of the function $G(\theta_A,\theta_B)$ for $\theta_A,\theta_B \in [-\frac{\pi}{2},\frac{\pi}{2}]$. This fact together with Lemmas 2.3 and 2.5 show that extrema of $f(x,S)$ and $\hat{f}(\hat{x},\hat{S})$ are the same. Thus we have established the following theorem:

THEOREM 2.6. *$\Lambda_m(A,B) = \Lambda_m(\hat{A},\hat{B})$ and $\Lambda_M(A,B) = \Lambda_M(\hat{A},\hat{B})$, and values are the extrema of F given by Proposition 2.4.*

CHAPTER 3

ANGLES OF ROTATION OF PDS MATRICES

Recall that the maximum angle by which any $n \times n$ matrix A rotates a non-zero vector x is given by $\phi_A = \sup_{x \in \mathbb{R}^n \setminus \ker A} \angle(x, Ax)$. In this chapter, we first present a method of finding ϕ_A for a PDS matrix A. Then we establish some results regarding orthogonal matrices S and their maximum angles ϕ_S. Any $S \in \mathrm{SO}_n$ has k orthogonal angles of rotation $\theta_1, \theta_2, \cdots, \theta_k$, where $k = \lfloor \frac{n}{2} \rfloor$. Elements of SO_2 take the form $R_\theta = \left(\begin{smallmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{smallmatrix}\right)$, which rotates any vector by the angle θ. Elements of SO_3 also have only one angle of rotation, but describing this angle is not so straightforward as in the two dimensional case. It is usually described by Euler angles or Rodrigues' formula.

In Lemma 3.4, we prove that ϕ_S is $\max_i\{\theta_i\}$ for any $S \in \mathrm{SO}_n$. In Section 3.2 we determine those S such that $\{A, B^S\}$ is indefinite in the two dimensional case. In Section 3.3 we give some examples in three dimensions in which we determine the matrix S with the smallest possible ϕ_S such that $\{A, B^S\}$ is indefinite.

The following proposition, which is equivalent to Kantorovich's Inequality [4], gives the formula for the maximum angle of rotation of a PDS matrix in terms of its extremal eigenvalues.

Proposition 3.1. *Let A be a PDS $n \times n$ matrix with eigenvalues $0 < A_1 \leq A_2 \leq A_3 \leq \cdots \leq A_n$. Then*

$$\cos\phi_A = 2\frac{\sqrt{A_1 A_n}}{A_1 + A_n}, \qquad \sin\phi_A = \frac{A_n - A_1}{A_1 + A_n}.$$

Moreover, $\angle(v, Av) = \phi_A$ if and only if v is scalar multiple of $(v_1\sqrt{A_n} + v_n\sqrt{A_1})$, where v_1 and v_n are unit eigenvectors of A with eigenvalues A_1 and A_n, respectively.

Proof. We may assume that A is a diagonal matrix with $A_{ii} = A_i$. Let ϕ_A be the maximum angle by which A rotates any unit vector. Then

$$\cos\phi_A = \inf_{x\in S^{n-1}} \frac{x\cdot Ax}{|Ax|} = \inf_{x\in S^{n-1}} \frac{\sum x_i^2 A_i}{(\sum x_i^2 A_i^2)^{1/2}}.$$

Thus we want to minimize

$$F(x) := \frac{(x\cdot Ax)^2}{|Ax|^2}$$

subject to $\sum x_i^2 = 1$ by the method of Lagrange multipliers.

Suppose that a unit vector x gives the minimum. Let λ be the Lagrange multiplier. Since

$$\nabla F = 4\frac{(x\cdot Ax)Ax}{|Ax|^2} - 2\frac{(x\cdot Ax)^2 A^2 x}{|Ax|^4}, \qquad \nabla(x\cdot x) = 2x, \tag{9}$$

we have

$$2\frac{(x\cdot Ax)Ax}{|Ax|^2} - \frac{(x\cdot Ax)^2 A^2 x}{|Ax|^4} = \lambda x. \tag{10}$$

Taking the dot product with x on both sides, we get

$$\lambda = \frac{(x\cdot Ax)^2}{|Ax|^2} = \cos^2\phi_A \tag{11}$$

Thus for all i, (10) becomes

$$2\frac{(x\cdot Ax)A_i x_i}{|Ax|^2} - \frac{(x\cdot Ax)^2 A_i^2 x_i}{|Ax|^4} - \cos^2\phi_A x_i = 0.$$

Let $\tilde{A}_i = \frac{(x\cdot Ax)}{|Ax|^2}A_i$. Then for all $i, (\tilde{A}_i^2 - 2\tilde{A}_i + \cos^2\phi_A)x_i = 0$. The quadratic equation $z^2 - 2z + \cos^2\phi_A = 0$ has two roots, $\tilde{A}_\pm$, given by

$$\tilde{A}_\pm = 1 \pm \sin\phi_A. \tag{12}$$

Therefore there are at most two values of $\tilde{A}_i$ such that $x_i \neq 0$. If there is only one such value, then x is an eigenvector of A, so $F(x) = 1$. This is in general not the minimum value of F, so we may assume that there are exactly two distinct values of $\tilde{A}_i$ such that $x_i \neq 0$. Thus we may assume that there are unit eigenvectors $u_\pm$ of A of eigenvalues

$$A_\pm = \frac{|Ax|^2}{(x\cdot Ax)}\tilde{A}_\pm,$$

such that $x = x_+u_+ + x_-u_-$ for some scalars $x_+, x_- \in (0,1)$ with $x_+^2 + x_-^2 = 1$.

Note that $x \cdot Ax = A_+x_+^2 + A_-x_-^2$, which in light of $x_-^2 = 1 - x_+^2$ may be written as

$$x \cdot Ax = (A_+ - A_-)x_+^2 + A_-.$$

Similarly, $|Ax|^2 = A_+^2x_+^2 + A_-^2x_-^2$. Since (11) gives $\sin^2\phi_A = 1 - \frac{(x\cdot Ax)^2}{|Ax|^2}$, we have

$$\sin^2\phi_A = \frac{A_+^2x_+^2 + A_-^2x_-^2 - (A_+x_+^2 + A_-x_-^2)^2}{|Ax|^2} = \frac{(A_+ - A_-)^2x_+^2x_-^2}{|Ax|^2}.$$

Combining this with (12), we get

$$\sin\phi_A = \tilde{A}_+ - 1 = \frac{(A_+ - A_-)x_+x_-}{|Ax|}. \tag{13}$$

On the other hand, since $\tilde{A}_+ = \frac{(x\cdot Ax)}{|Ax|^2}A_+ = \frac{(A_+x_+^2 + A_-x_-^2)}{|Ax|^2}A_+$, we have

$$\sin\phi_A = \tilde{A}_+ - 1 = \frac{(A_+ - A_-)A_-x_-^2}{|Ax|^2}. \tag{14}$$

From (13) and (14),

$$A_-x_- = |Ax|\, x_+.$$

Squaring both sides and simplifying using the fact that $1 - x_+^2 = x_-^2$, we get

$$A_-x_-^2 = A_+x_+^2. \tag{15}$$

It follows that $|Ax|^2 = A_+^2x_+^2 + A_-^2x_-^2 = (A_+ + A_-)A_-x_-^2$. Substituting this value in (14) and simplifying, we get

$$\sin\phi_A = \tilde{A}_+ - 1 = \frac{A_+ - A_-}{A_+ + A_-}.$$

Therefore,

$$\cos\phi_A = \sqrt{1 - \sin^2\phi_A} = 2\frac{\sqrt{A_+A_-}}{A_+ + A_-}.$$

Moreover, (15) together with $1 - x_+^2 = x_-^2$ gives

$$x_\pm = \sqrt{\frac{A_\pm}{A_+ + A_-}}.$$

Clearly, $\cos\phi_A$ is minimal when $A_+ = A_n$ and $A_- = A_1$.

$\square$

Let a be a unit vector such that $\angle(a, Aa) = \phi_A$ for a diagonal PDS matrix A whose entries increase along the diagonal. Suppose $0 < A_1 \leq A_2 \leq \cdots \leq A_n$ are its eigenvalues. Then by Proposition 3.1, there are exactly four choices for a, namely, $\frac{1}{\sqrt{A_1+A_n}}(\pm\sqrt{A_n}, 0, \cdots, 0, \pm\sqrt{A_1})$. Moreover, these choices lie one on each quadrant of the space spanned by e_1 and e_n. Without loss of generality, we may assume a to be the vector on the positive quadrant. We have the following corollary:

COROLLARY 3.2. $\angle(a, e_1) = \frac{\pi}{4} - \frac{\phi_A}{2}$.

PROOF. As discussed, we may take $a = \frac{1}{\sqrt{A_1+A_n}}(\sqrt{A_n}, 0, \cdots, 0, \sqrt{A_1})$. Let the angle between a and e_1 be θ_a, and the angle between e_n and Aa be $\hat{\theta}_a$. It suffices to show that $\theta_a = \hat{\theta}_a$. Note that

$$\cos\theta_a = e_1 \cdot a = \frac{\sqrt{A_n}}{\sqrt{A_1 + A_n}}.$$

On the other hand, since $Aa = \frac{1}{\sqrt{A_1+A_n}}(A_1\sqrt{A_n}, 0, \cdots, 0, A_n\sqrt{A_1})$ and $|Aa| = \sqrt{A_1 A_n}$, we have

$$\cos\hat{\theta}_a = \frac{e_n \cdot Aa}{|Aa|} = \frac{\sqrt{A_n}}{\sqrt{A_1 + A_n}} = \cos\theta_a$$

Hence $\theta_a = \hat{\theta}_a$, so we have $2\theta_a + \phi_A = \frac{\pi}{2}$.

□

3.1. Some Results on SO_n

Recall that for any pair of $n \times n$ PDS matrices A and B, the Jordan product $\{A, B^S\}$ is indefinite for some $S \in \mathrm{SO}_n$ if $\phi_A + \phi_B \geq \frac{\pi}{2}$. The following lemma is well-known.

LEMMA 3.3. *Every $S \in \mathrm{SO}_n$ is orthogonally similar to a block diagonal matrix with diagonal entries $R_{\theta_1}, R_{\theta_2}, \cdots, R_{\theta_{\lfloor n/2 \rfloor}}$ if n is even, and $R_{\theta_1}, R_{\theta_2}, \cdots, R_{\theta_{\lfloor n/2 \rfloor}}, 1$ if n is odd.*

LEMMA 3.4. *For $S \in \mathrm{SO}_n$ let $\theta_1, \theta_2, \cdots, \theta_{\lfloor n/2 \rfloor}$ be the orthogonal angles of rotation. Then the maximum angle by which S rotates any vector is $\max_i\{\theta_i\}$.*

Proof. We only give the proof for n even; the odd case is similar. We follow the approach of the proof of Proposition 3.1: we find the minimum of

$$F(y) := y \cdot Sy$$

such that $|y|^2 = 1$.

We may assume that S is block diagonal as in Lemma 3.3. The maximum angle ϕ_S by which S moves any vector is given by

$$\cos \phi_S = \inf_{y \in S^{n-1}} (y \cdot Sy).$$

Let the unit vector $\tilde{y}$ be the minimizer of $y \cdot Sy$. Then

$$\cos \phi_S = \tilde{y} \cdot S\tilde{y} = F(\tilde{y}).$$

It suffices to show that $\phi_S = \theta_i$ for some i.

Let λ be the Lagrange multiplier. Since $\nabla F = 2Sy$ and $\nabla(y \cdot y) = 2y$, we have

$$S\tilde{y} - \lambda\tilde{y} = 0. \tag{16}$$

Taking the dot product with $\tilde{y}$ on both sides, we obtain $\lambda = (\tilde{y} \cdot S\tilde{y}) = F(\tilde{y})$.

Since S is block diagonal, write $\tilde{y}$ as $[\tilde{y}_{11}, \tilde{y}_{12}; \tilde{y}_{21}, \tilde{y}_{22}; \cdots; \tilde{y}_{\lfloor n/2 \rfloor,1}, \tilde{y}_{\lfloor n/2 \rfloor,2}]$. By direct calculation,

$$F(\tilde{y}) = \sum_i (\tilde{y}_{i1}^2 + \tilde{y}_{i2}^2) \cos \theta_i,$$

and (16) becomes

$$\tilde{y}_{ij} \cos \theta_i - \lambda \tilde{y}_{ij} = 0.$$

If $\tilde{y}_{ij} \neq 0$ for some i, then $\lambda = \cos \theta_i$. But $\lambda = \tilde{y} \cdot S\tilde{y} = \cos \phi_S$, so $\phi_S = \theta_i$ for some i. For such i, θ_i is maximal among $\theta_1, \theta_2, \cdots, \theta_{\lfloor n/2 \rfloor}$. Therefore all non-zero components of the minimizer $\tilde{y}$ must correspond to those R_{θ_i} with maximal θ_i.

$\square$

LEMMA 3.5. *Let A and B be two $n \times n$ PDS matrices and let S be in SO_n. The Jordan product $\{A, B^S\}$ is indefinite if and only if there exist non-zero vectors $a, b \in \mathbb{R}^n$ such that $Sb = a$ and $\angle(Aa, SBb) \geq \frac{\pi}{2}$.*

PROOF. If $\{A, B^S\}$ is indefinite, then there exists a non-zero $a \in \mathbb{R}^n$ such that

$$a \cdot \{A, B^S\} a \leq 0.$$

Since A, B and B^S are all symmetric, $a \cdot AB^S a = Aa \cdot B^S a = a \cdot B^S Aa$, so $a \cdot \{A, B^S\} a = 2(Aa \cdot B^S a)$. Let $b = S^{-1} a$. Then $Aa \cdot SBb \leq 0$, so $\angle(Aa, SBb) \geq \frac{\pi}{2}$.

For the converse, use the same argument in the reverse direction.

□

3.2. The 2×2 Case

Throughout this section A and B are 2×2 diagonal PDS matrices. Without loss of generality we may rescale and assume $A = \left(\begin{smallmatrix} 1 & 0 \\ 0 & k \end{smallmatrix}\right)$ and $B = \left(\begin{smallmatrix} 1 & 0 \\ 0 & l \end{smallmatrix}\right)$, where $k = \frac{A_2}{A_1}$ and $l = \frac{B_2}{B_1}$. Let S be in SO_2. Recall that any $S \in \mathrm{SO}_2$ takes the form R_θ, where $\phi_S = \theta$.

We want to find S with the minimum ϕ_S such that the Jordan product $\{A, B^S\}$ is indefinite. This product is given by

$$\{A, B^S\} = \begin{pmatrix} 2(\cos^2\theta + l\sin^2\theta) & (1-l)(1+k)\sin\theta\cos\theta \\ (1-l)(1+k)\sin\theta\cos\theta & 2(k\sin^2\theta + kl\cos^2\theta) \end{pmatrix}.$$

It is indefinite if and only if $\mathrm{Det}\{A, B^S\} \leq 0$. Computation gives

$$\mathrm{Det}\{A, B^S\} = 4lk - \frac{1}{4}\big\{(1-l)^2(1-k)^2\big\}(\sin 2\theta)^2. \tag{17}$$

Hence for $\{A, B^S\}$ to be indefinite, we must have $4lk - \frac{1}{4}\big\{(1-l)^2(1-k)^2\big\}(\sin 2\theta)^2 \leq 0$. Thus $\{A, B^S\}$ is indefinite for some S if and only if

$$16lk \leq (1-l)^2(1-k)^2.$$

This is a corollary of Strang's result proved in Chapter 2.

PROPOSITION 3.6. *The minimum ϕ_S such that $\{A, B^S\}$ is indefinite satisfies*

$$\cos^2\phi_S = \frac{1}{2}\Big(1 + \frac{\sqrt{(l-1)^2(k-1)^2 - 16kl}}{(l-1)(k-1)}\Big).$$

PROOF. The eigenvalues $\lambda_\pm$ of $\{A, B^S\}$ are the roots of

$$\lambda^2 - \lambda\,\mathrm{Tr}\{A, B^S\} + \mathrm{Det}\{A, B^S\} = 0,$$

where $\mathrm{Det}\{A, B^S\}$ is as in (17) and $\mathrm{Tr}\{A, B^S\} = 2(k+1) - 2(l-1)(k-1)\cos^2\theta$. Computation gives

$$\lambda_\pm = (k+l) + (l-1)(k-1)\cos^2\theta \pm C,$$

where

$$C \;=\; \sqrt{(k-l)^2 + (l^2-1)(k^2-1)\cos^2\theta}.$$

Now $\{A, B^S\}$ is indefinite if and only if $\lambda_- \leq 0$, i.e.

$$(k+l) + (l-1)(k-1)\cos^2\theta \leq \sqrt{(k-l)^2 + (l^2-1)(k^2-1)\cos^2\theta}.$$

Squaring on both sides and simplifying gives

$$\cos^4\theta - \cos^2\theta + \frac{4kl}{(l-1)^2(k-1)^2} \leq 0.$$

The boundary values of this inequality are

$$t_\pm = \frac{1}{2}\Big(1 \pm \frac{\sqrt{(l-1)^2(k-1)^2 - 16kl}}{(l-1)(k-1)}\Big).$$

Hence the minimum ϕ_S satisfies

$$\cos^2\phi_S = \frac{1}{2}\Big(1 + \frac{\sqrt{(l-1)^2(k-1)^2 - 16kl}}{(l-1)(k-1)}\Big).$$

□

COROLLARY 3.7. *There exists an angle α such that $\{A, B^{R_\theta}\}$ is indefinite if and only if either $\left|\theta - \frac{\pi}{4}\right| \leq \alpha$ or $\left|\theta - \frac{3\pi}{4}\right| \leq \alpha$.*

Proof. By the last proof, $\{A, B^{R_\theta}\}$ is indefinite if and only if $t_- \leq \cos^2\theta \leq t_+$. Since $t_+ + t_- = 1$, taking $\alpha = \frac{\pi}{4} - \cos^{-1}\sqrt{t_+}$ gives the result.

$\square$

3.3. Some Examples in the 3×3 Case

Definition 3.8. For $\omega \in S^2$ and $\theta \in \mathbb{R}$, let $R(\omega, \theta)$ be the element of SO_3 which rotates by θ counterclockwise around ω.

Fix matrices $A = \begin{pmatrix} A_1 & & \\ & A_2 & \\ & & A_3 \end{pmatrix}$ and $B = \begin{pmatrix} B_1 & & \\ & B_2 & \\ & & B_3 \end{pmatrix}$ such that $0 < A_1 < A_2 < A_3$, the B_i are positive and distinct, and $\phi_A + \phi_B = \frac{\pi}{2}$. We will find $\Phi(A, B)$ in this case. By Lemma 3.5, for S orthogonal $\{A, B^S\}$ is indefinite if and only if there exist non-zero vectors a, b such that $Sb = a$ and $\angle(Aa, SBb) \geq \frac{\pi}{2}$. Recall that for any a, b, A, B, and S,

$$\angle(Aa, SBb) \leq \angle(Aa, a) + \angle(Sb, SBb) \leq \phi_A + \phi_B.$$

Here $\phi_A + \phi_B = \frac{\pi}{2}$, so $\{A, B^S\}$ is indefinite if and only if there exists a with $\angle(a, Aa) = \phi_A$ and b with $\angle(b, Bb) = \phi_B$ such that $\angle(Aa, SBb) = \frac{\pi}{2}$. By Proposition 4.1 of the next chapter, there exists exactly one such S for each such pair (a, b). We write $S_{\max}(a, b)$ for this S.

By Proposition 3.1, there are exactly four distinct unit vectors a satisfying $\angle(a, Aa) = \phi_A$, namely, $\frac{1}{\sqrt{A_1+A_3}}(\pm\sqrt{A_3}, 0, \pm\sqrt{A_1})$. Fix $a = \frac{1}{\sqrt{A_1+A_3}}(\sqrt{A_3}, 0, \sqrt{A_1})$. Similarly, there are exactly four unit vectors b that satisfy $\angle(b, Bb) = \phi_B$. We must deduce which of the four choices of b minimizes $\phi_{S_{\max}(a,b)}$. It is easy to see that $\Phi(A, B)$ is the least of the four choices of $\phi_{S_{\max}}(a, b)$. There are six cases.

The case $B_1 < B_2 < B_3$: By Proposition 3.1, the four unit vectors b that satisfy $\angle(b, Bb) = \phi_B$ are $\frac{1}{\sqrt{B_1+B_3}}(\pm\sqrt{B_3}, 0, \pm\sqrt{B_1})$. We denote them by b_I, b_{II}, b_{III}, and b_{IV}, the subscript indicating their quadrant in the (e_1, e_3) plane. Note that a, Aa, b_i and Bb_i all lie in the (e_1, e_3) plane. By Corollary 3.2, the $\frac{\pi}{4}$ line bisects both $\angle(a, Aa)$ and $\angle(b_I, Bb_I)$. Moreover, the four b_i form a rectangle in standard orientation centered on 0, wider than it is tall, and the four Bb_i form the reflection of the b_i rectangle over the $\frac{\pi}{4}$ line. The situation is shown in Figure 3.1, in which for brevity $[x]$ denotes $\frac{x}{|x|}$.

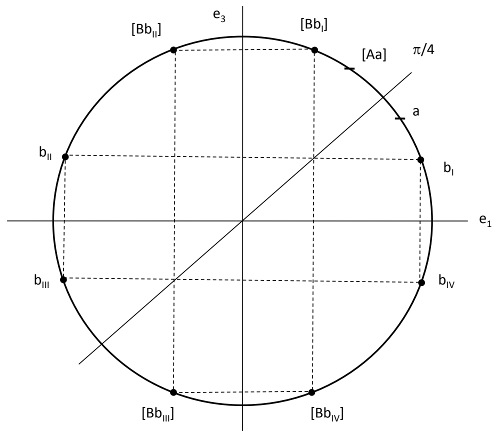

FIGURE 3.1. The case $B_1 < B_2 < B_3$.

It is easy to see that $\phi_{S(a,b)}$ is minimal for $b = b_{IV}$, and that $S(a, b_{IV})$ is rotation by $\angle(a, b_{VI})$ around e_2. Since $\angle(a, Aa) = \phi_A$ and $\angle(b_i, Bb_i) = \phi_B$, the symmetries of the figure yield $\angle(e_1, a) = \frac{\pi}{4} - \frac{1}{2}\phi_A$ and $\angle(b_{IV}, e_1) = \frac{\pi}{4} - \frac{1}{2}\phi_B$. Therefore since $\phi_A + \phi_B = \frac{\pi}{2}$, here $\Phi(A, B) = \frac{\pi}{4}$.

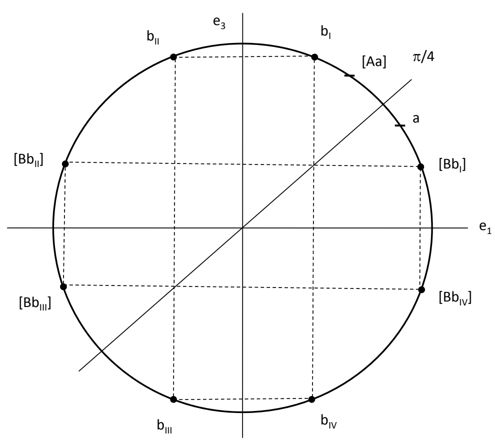

FIGURE 3.2. The case $B_3 < B_2 < B_1$.

The case $B_3 < B_2 < B_1$**:** Here the four choices of b_i are given by the same formula as in the last case, but the rectangle they form is taller than it is wide. Thus the situation is as in the preceding case, with b_i and $[Bb_i]$ exchanged (see Figure 3.2).

A similar argument shows that $\phi_{S_{\max}(a,b_i)}$ is minimal for $i = I$, and $S_{\max}(a, b_I)$ is again a rotation by $\frac{\pi}{4}$ about e_2. So here too, $\Phi(A, B) = \frac{\pi}{4}$. (Both of the first two cases are essentially two dimensional.)

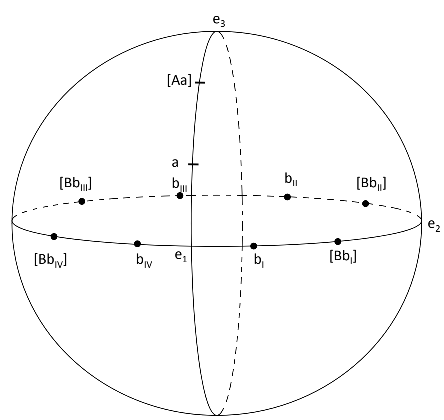

FIGURE 3.3. The case $B_1 < B_3 < B_2$.

The case $B_1 < B_3 < B_2$**:** Here the b_i are $\frac{1}{\sqrt{B_1+B_2}}(\pm\sqrt{B_2}, \pm\sqrt{B_1}, 0)$, on the unit circle in the (e_1, e_2) plane (see Figure 3.3). In contrast to the previous cases, this case is three-dimensional because a and the b_i do not all lie on one plane. Here direct rotation of b_i to a does not give $S_{\max}(a, b_i)$; we must have $[S_{\max}(a, b_i)Bb_i]$ and $[Aa]$ on opposite sides of a on the great circle passing through a and $[Aa]$. Denote this great circle by $\mathrm{GC}(a, Aa)$. $S_{\max}(a, b_i)$ is minimal for b_i equal to either b_I or b_{IV}; we will take $b_i = b_I$. We can factor $S_{\max}(a, b_I)$ as follows. Let

$$S_1 = R(e_3, -\theta_b), \quad S_2 = R(e_1, -\pi/2), \quad S_3 = R(e_2, -\theta_a),$$

where $\theta_a = \angle(e_1, a)$ and $\theta_b = \angle(e_1, b_I)$. One checks that

$$S_{\max}(a, b_I) = S_3 S_2 S_1 = \begin{pmatrix} \cos(\theta_b + \theta_a) & \sin(\theta_b + \theta_a) & 0 \\ 0 & 0 & 1 \\ \sin(\theta_b + \theta_a) & -\cos(\theta_b + \theta_a) & 0 \end{pmatrix},$$

so $\mathrm{Tr}(S_{\max}(a, b_I)) = \cos(\theta_b + \theta_a)$. As in the previous cases, Corollary 3.2 gives $\theta_b + \theta_a = \frac{\pi}{4}$, so $\mathrm{Tr}(S_{\max}(a, b_I)) = \frac{1}{\sqrt{2}}$. Since $\mathrm{Tr}(S) = 1 + 2\cos\phi_S$,

$$\Phi(A, B) = \pi - \cos^{-1}\left(\frac{\sqrt{2} - 1}{2\sqrt{2}}\right).$$

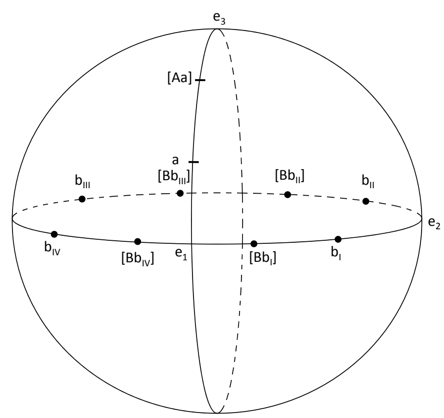

FIGURE 3.4. The case $B_2 < B_3 < B_1$.

The case $B_2 < B_3 < B_1$**:** Here the four choices of b_i are given by the same formula as in the last case. This is similar to the previous case, except that the positions of b_i and $[Bb_i]$ are exchanged (see Figure 3.4). The best choices of b_i are still b_I and b_{IV}. Taking $b_i = b_I$, a similar argument leads to $\mathrm{Tr}(S_{\max}(a, b_I)) = \cos(\theta_a + \theta_b)$. Hence $\Phi(A, B) = \pi - \cos^{-1}\left(\frac{\sqrt{2}-1}{2\sqrt{2}}\right)$.

The case $B_2 < B_1 < B_3$**:** Here the b_i are $\frac{1}{\sqrt{B_2+B_3}}(0, \pm\sqrt{B_3}, \pm\sqrt{B_2})$, on the unit circle in (e_2, e_3) plane (see Figure 3.5). Since we want $[S_{\max}(a, b_i)Bb_i]$ opposite $[Aa]$ on $\mathrm{GC}(a, Aa)$, $S_{\max}(a, b_i)$ is minimal for b_i equal to either b_{III} or b_{IV}; we will take $b_i = b_{IV}$. We can factor

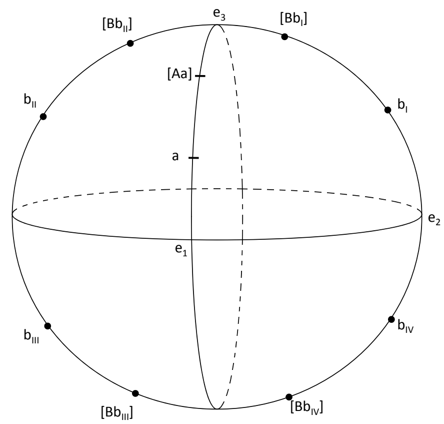

FIGURE 3.5. The case $B_2 < B_1 < B_3$.

$S_{\max}(a, b_{IV})$ as follows. Let S_1 rotate around e_3 by $-\frac{\pi}{2}$ so as to put b_{IV} on $\mathrm{GC}(e_1, e_3)$, and let S_2 rotate $S_1 b_{IV}$ to a:

$$S_1 = R(e_3, -\pi/2), \quad S_2 = R(e_2, -\theta),$$

where $\theta = \angle(a, e_1) + \angle(e_1, b)$. Thus

$$S_{\max}(a, b_{IV}) = S_2 S_1 = \begin{pmatrix} 0 & \cos\theta & -\sin\theta \\ -1 & 0 & 0 \\ 0 & \sin\theta & \cos\theta \end{pmatrix},$$

so $\mathrm{Tr}(S_{\max}(a, b_{IV})) = \cos\theta$. As in the earlier cases, $\theta = \theta_a + \theta_b = \frac{\pi}{4}$, so

$$\Phi(A, B) = \pi - \cos^{-1}\left(\frac{\sqrt{2}-1}{2\sqrt{2}}\right).$$

The case $B_3 < B_1 < B_2$**:** Here the four choices of b_i are given by the same formula as in the last case, but the positions of b and $[Bb_i]$ are exchanged (see Figure 3.6). Since we want $[S_{\max}(a, b_i)Bb_i]$ and $[Aa]$ on opposite sides of a on $\mathrm{GC}(a, Aa)$, $S_{\max}(a, b_i)$ is minimal for b_i equal to either b_I or b_{II}. Taking $b_i = b_I$, an argument as above again gives $\Phi(A, B) = \pi - \cos^{-1}\left(\frac{\sqrt{2}-1}{2\sqrt{2}}\right)$.

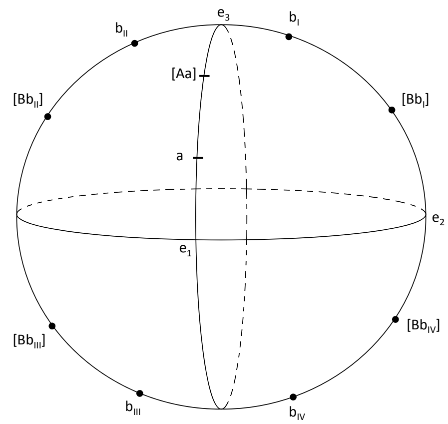

FIGURE 3.6. The case $B_3 < B_1 < B_2$.

CHAPTER 4

THE TRACES OF SOME ORTHOGONAL MATRICES

Throughout this chapter assume that A and B are 3×3 diagonal PDS matrices. Suppose that $\{A, B^S\}$ is indefinite for some $S \in \mathrm{SO}_3$. Recall that in three dimensions, $\mathrm{Tr}(S) = 1 + 2\cos\phi_S$, where ϕ_S is the maximum angle by which S rotates any non-zero vector. Thus in this case, Problem 1 may be solved by computing $\max\{\mathrm{Tr}(S) : \{A, B^S\} \text{ is indefinite}\}$.

Recall that if $\{A, B^S\}$ is indefinite, then by Lemma 3.5 there exist vectors a and b such that $Sb = a$ and $\angle(Aa, SBb) \geq \frac{\pi}{2}$. For the rest of this Chapter, fix arbitrary $a, b \in S^2$, and define

$$\alpha := \angle(a, Aa), \quad \beta := \angle(b, Bb).$$

Note that for any $S \in \mathrm{SO}_3$ such that $Sb = a$,

$$\angle(Aa, SBb) \leq \angle(Aa, a) + \angle(Sb, SBb) = \angle(Aa, a) + \angle(b, Bb) = \alpha + \beta.$$

In Proposition 4.1 we show that there exists a unique $S \in \mathrm{SO}_3$ such that $Sb = a$ and $\angle(Aa, SBb) = \alpha + \beta$. In Proposition 4.2 we show that if $\alpha + \beta > \frac{\pi}{2}$, then there exist exactly two matrices $S \in \mathrm{SO}_3$ such that $Sb = a$ and $\angle(Aa, SBb) = \frac{\pi}{2}$.

Proposition 4.1. *Fix a and b in S^2, and define $\alpha := \angle(a, Aa)$ and $\beta := \angle(b, Bb)$. There exists a unique matrix $S_{\max}(a,b) \in \mathrm{SO}_3$ such that $S_{\max}(a,b)b = a$ and $\angle(Aa, S_{\max}(a,b)Bb) = \alpha + \beta$. Its trace is given by* $\mathrm{Tr}\left(S_{\max}(a,b)\right) =$

$$a \cdot b + \cot\alpha\cot\beta\Big(\frac{a \cdot Bb}{b \cdot Bb} + \frac{b \cdot Aa}{a \cdot Aa} - \frac{Aa \cdot Bb + (b \times Bb)\cdot(a \times Aa)}{(a \cdot Aa)(b \cdot Bb)} - a \cdot b\Big).$$

Proof. Consider the orthonormal bases $\{v_1, v_2, v_3\}$ and $\{w_1, w_2, w_3\}$ of $\mathbb{R}^3$ defined by

$$v_1 = b, \quad v_3 = \frac{b \times Bb}{|b \times Bb|}, \quad v_2 = v_3 \times v_1,$$

$$w_1 = a, \quad w_3 = \frac{a \times Aa}{|a \times Aa|}, \quad w_2 = w_3 \times w_1.$$

We want to find an orthogonal matrix S such that $Sb = a$ and $\angle(Aa, SBb) = \alpha + \beta$. Clearly SBb must lie in $\mathrm{Span}\{a, Aa\} = \mathrm{Span}\{w_1, w_2\}$. Since $v_1 = b$ and $Sb = a$, we have $Sv_1 = w_1$. Thus $SBb \in \mathrm{Span}\{w_1, w_2\}$ if and only if $Sv_2 \in \mathrm{Span}\{w_1, w_2\}$. Since $v_2 \perp v_1$, we have $Sv_2 \perp Sv_1 = w_1$. Therefore $Sv_2 = \pm w_2$.

By the definition of the orthonormal basis $\{w_1, w_2, w_3\}$, Aa lies on the first quadrant of the (w_1, w_2) plane. Thus for $\angle(Aa, SBb)$ to be maximal, SBb must be on the fourth quadrant of the (w_1, w_2) plane, so $Sv_2 = -w_2$.

Since $|b \times Bb| = |Bb| \sin\beta$ and $(b \times Bb) \times b = Bb - b\,|Bb| \cos\beta$, we have $v_2 = v_3 \times v_1 = \left(\frac{Bb}{|Bb|\cos\beta} - b\right)\cot\beta$. Using $|Bb|\cos\beta = b \cdot Bb$ and applying the same argument to the w_i gives

$$v_2 = \left(\frac{Bb}{b \cdot Bb} - b\right)\cot\beta, \qquad w_2 = \left(\frac{Aa}{a \cdot Aa} - a\right)\cot\alpha. \tag{18}$$

Summarizing, we have $v_1 \cdot Sv_1 = a \cdot b$ and

$$v_2 \cdot Sv_2 = -\left(\frac{Bb}{b \cdot Bb} - b\right) \cdot \left(\frac{Aa}{a \cdot Aa} - a\right)\cot\alpha\cot\beta.$$

Also note that $Sv_3 = Sv_1 \times Sv_2 = -w_1 \times w_2 = -w_3$. Thus

$$v_3 \cdot Sv_3 = -\frac{b \times Bb}{|Bb|\sin\beta} \cdot \frac{a \times Aa}{|Aa|\sin\alpha} = -\frac{(b \times Bb)\cdot(a \times Aa)}{(a \cdot Aa)(b \cdot Bb)}\cot\alpha\cot\beta.$$

Finally, since $\mathrm{Tr}(S) = v_1 \cdot Sv_1 + v_2 \cdot Sv_2 + v_3 \cdot Sv_3$, we have

$$\mathrm{Tr}(S) = a \cdot b + \cot\alpha\cot\beta\Big(\frac{a \cdot Bb}{b \cdot Bb} + \frac{b \cdot Aa}{a \cdot Aa} - \frac{Aa \cdot Bb + (b \times Bb)\cdot(a \times Aa)}{(a \cdot Aa)(b \cdot Bb)} - a \cdot b\Big).$$

Since Sv_i is determined for $1 \le i \le 3$, S is unique.

$\square$

Proposition 4.2. *Maintain a, b, α and β as in Proposition 4.1, and assume that $\alpha + \beta > \frac{\pi}{2}$. Then there exist exactly two matrices $S \in \mathrm{SO}_3$ such that $Sb = a$ and $\angle(Aa, SBb) = \frac{\pi}{2}$. Their traces are given by*

$$\mathrm{Tr}(S) = a \cdot b + \cot^2\alpha\cot^2\beta\Big\{\Big(\frac{a \cdot Bb}{b \cdot Bb} + \frac{b \cdot Aa}{a \cdot Aa} - \frac{Aa \cdot Bb + (b \times Bb)\cdot(a \times Aa)}{(a \cdot Aa)(b \cdot Bb)} - a \cdot b\Big)$$

$$\pm\Delta\Big|\big(a-\frac{Aa}{a\cdot Aa}\big)\cdot\big(\frac{b\times Bb}{b\cdot Bb}\big)-\big(b-\frac{Bb}{b\cdot Bb}\big)\cdot\big(\frac{a\times Aa}{a\cdot Aa}\big)\Big|\Big\},$$

where $\Delta=\sqrt{\tan^2\alpha\tan^2\beta-1}$. *(Note that* $\tan^2\alpha\tan^2\beta\geq 1$ *precisely when* $\alpha+\beta\geq\frac{\pi}{2}$*.)*

Proof. Define orthonormal bases $\{v_1,v_2,v_3\}$ and $\{w_1,w_2,w_3\}$ of $\mathbb{R}^3$ as in the last proof. Then v_2 and w_2 are as in (18). Inverting these equations gives

$$Aa=|Aa|\,(w_1\cos\alpha+w_2\sin\alpha),\qquad Bb=|Bb|\,(v_1\cos\beta+v_2\sin\beta).$$

Here we want to find an orthogonal matrix S such that $Sb=a$ (i.e., $Sv_1=w_1$) and $\angle(Aa,SBb)=\frac{\pi}{2}$. Since $Sv_2\in\mathrm{Span}\{w_2,w_3\}$, for some non-zero scalars γ_2 and γ_3 we can write $Sv_2=\gamma_2w_2+\gamma_3w_3$. Therefore

$$SBb=|Bb|\,(w_1\cos\beta+\gamma_2w_2\sin\beta+\gamma_3w_3\sin\beta). \tag{19}$$

Note that $\gamma_2^2+\gamma_3^2=1$, or $\gamma_3=\pm\sqrt{1-\gamma_2^2}$. Now we want $SBb\cdot Aa=0$. Since

$$SBb\cdot Aa=|Bb|\,|Aa|\,(\cos\alpha\cos\beta+\gamma_2\sin\alpha\sin\beta),$$

we must have

$$\gamma_2=-\cot\alpha\cot\beta,\qquad \gamma_3=\pm\cot\alpha\cot\beta\sqrt{\tan^2\alpha\tan^2\beta-1}.$$

Denote $\sqrt{\tan^2\alpha\tan^2\beta-1}$ by Δ, so $\gamma_3=\pm\Delta\cot\alpha\cot\beta$.

To compute $\mathrm{Tr}(S)=\sum_{i=1}^3 v_i\cdot Sv_i$, note that $v_1\cdot Sv_1=b\cdot a$ and $v_2\cdot Sv_2=\gamma_2(v_2\cdot w_2)+\gamma_3(v_2\cdot w_3)$. Since $v_2=(\frac{Bb}{b\cdot Bb}-b)\cot\beta$, $w_2=(\frac{Aa}{a\cdot Aa}-b)\cot\alpha$, and $w_3=(\frac{a\times Aa}{a\cdot Aa})\cot\alpha$,

$$v_2\cdot Sv_2=\Big\{\gamma_2\Big(\frac{Bb}{b\cdot Bb}-b\Big)\cdot\Big(\frac{Aa}{a\cdot Aa}-a\Big)+\gamma_3\Big(\frac{Bb}{b\cdot Bb}-b\Big)\cdot\Big(\frac{a\times Aa}{a\cdot Aa}\Big)\Big\}\cot\alpha\cot\beta.$$

Further simplification leads to

$$\begin{aligned} v_2\cdot Sv_2 \;&=\; \Big\{\frac{a\cdot Bb}{b\cdot Bb}+\frac{b\cdot Aa}{a\cdot Aa}-\frac{Aa\cdot Bb}{(a\cdot Aa)(b\cdot Bb)}-a\cdot b\\ &\qquad \pm\Delta\Big(\frac{Bb}{b\cdot Bb}-b\Big)\cdot\Big(\frac{a\times Aa}{a\cdot Aa}\Big)\Big\}\cot^2\alpha\cot^2\beta.\end{aligned}$$

Finally, we want $v_3\cdot Sv_3$. Note that $Sv_3=Sv_1\times Sv_2$. Recall that $Sv_1=a$ and $Sv_2=\gamma_2w_2+\gamma_3w_3$. Hence we must find the scalar triple products $v_3\cdot(a\times Aa)$ and $v_3\cdot(a\times w_3)$.

Since $v_3 = \frac{b\times Bb}{b\cdot Bb}\cot\beta$, the first triple product becomes $\frac{(b\times Bb)\cdot(a\times Aa)}{(a\cdot Aa)(b\cdot Bb)}\cot\alpha\cot\beta$. Similarly, since $a\times w_3 = (a-\frac{Aa}{a\cdot Aa})\cot\alpha$, the second triple product becomes $(a-\frac{Aa}{a\cdot Aa})\cdot(\frac{b\times Bb}{b\cdot Bb})\cot\alpha\cot\beta$. Hence substituting the values of γ_2 and γ_3, we get

$$v_3\cdot Sv_3 = \Big\{\frac{(b\times Bb)\cdot(a\times Aa)}{(a\cdot Aa)(b\cdot Bb)} \pm \Delta\Big(a-\frac{Aa}{a\cdot Aa}\Big)\cdot\Big(\frac{b\times Bb}{b\cdot Bb}\Big)\Big\}\cot^2\alpha\cot^2\beta,$$

where the choice of sign for Δ must be same as that for $v_2\cdot Sv_2$. Combining all three components, we obtain the desired formula for $\mathrm{Tr}(S)$.

Since the Sv_i are determined by the choice of sign of γ_3, there are exactly two choices of S.

□

We denote the two choices of S given by $\pm\Delta$ in Proposition 4.2 by $S_\perp^\pm(a,b)$, respectively. Define $S_\perp(a,b) := S_\perp^+(a,b)$. Note that in the limiting case $\Delta = 0, \alpha+\beta = \frac{\pi}{2}$ and $S_\perp^+(a,b) = S_\perp^-(a,b) = S_{\max}(a,b)$.

PROPOSITION 4.3. $\Phi(A,B) = \min\{\phi_{S_\perp(a,b)} : \alpha+\beta \geq \frac{\pi}{2}\}$.

PROOF. Clearly the left side is less than or equal to the right. To prove the converse, suppose that $\{A, B^S\}$ is indefinite. Then by Lemma 3.5 $Sb_1 = a_1$ and $\angle(Aa_1, SBb_1) \geq \frac{\pi}{2}$ for some (a_1,b_1), so $\angle(Aa_1, B^Sa_1) \geq \frac{\pi}{2}$. Since both A and B^S are PDS, if a_2 is an eigenvector of A we have $\angle(Aa_2, SBS^{-1}a_2) < \frac{\pi}{2}$. Thus by the connectedness of S^2, there exists a_3 such that $\angle(Aa_3, B^Sa_3) = \frac{\pi}{2}$, so S is one of $S_\perp^\pm(a_3, S^{-1}a_3)$. Since $\mathrm{Tr}(S_\perp^+(a,b)) \geq \mathrm{Tr}(S_\perp^-(a,b))$, we have $\phi_S \geq \phi_{S_\perp(a_3,S^{-1}a_3)}$. The result follows.

□

Thus in three dimensions, Problem 1 amounts to maximizing the function $\mathrm{Tr}(S_\perp(a,b))$ given in Proposition 4.2 over all $a,b\in S^2$ with $\alpha+\beta\geq\frac{\pi}{2}$. It would be interesting to prove the following conjecture.

CONJECTURE 4.4. *The minimum of* $\phi_{S_\perp(a,b)}$ *over all* (a,b) *with* $\alpha+\beta\geq\frac{\pi}{2}$ *occurs for some* (a,b) *with* $\alpha+\beta=\frac{\pi}{2}$.

CHAPTER 5

LEVEL CURVES OF THE ANGLE FUNCTION OF A PDS MATRIX A

In this chapter we discuss the level curves of the angle function $x \mapsto \angle(x, Ax)$ of A on the unit sphere in $\mathbb{R}^3$ for a PDS matrix A. We may assume without loss of generality that $A = \left(\begin{smallmatrix} A_1 & 0 & 0 \\ 0 & A_2 & 0 \\ 0 & 0 & A_3 \end{smallmatrix}\right)$, where $0 < A_1 \leq A_2 \leq A_3$. Recall that ϕ_A is the maximum angle by which the matrix A rotates any non-zero vector x. Thus $\angle(x, Ax) \leq \phi_A$ for all $x \in \mathbb{R}^3$.

Since A is positive definite, $\phi_A < \frac{\pi}{2}$. It follows that the level curves of $x \mapsto \angle(x, Ax)$ are the same as those of

$$F(x) := \cos^2\big(\angle(x, Ax)\big) = \frac{(\sum_i A_i x_i^2)^2}{(\sum_i x_i^2)(\sum_i A_i^2 x_i^2)}. \tag{20}$$

Let us denote the level curve $F = \gamma$ by $\mathcal{L}(A, \gamma)$. Writing s_i for x_i^2, this curve has equation

$$\Big(\sum_i A_i s_i\Big)^2 - \gamma\Big(\sum_i s_i\Big)\Big(\sum_i A_i^2 s_i\Big) = 0. \tag{21}$$

Since $|x| = 1$, we must have $s_1 + s_2 + s_3 = 1$ and $s_i \geq 0$ for all i. Thus we seek solutions of (21) on the standard simplex $\mathcal{T}$, which is contained in the plane $\mathcal{P}$:

$$\mathcal{T} := \big\{s \in \mathbb{R}^3 : s_1 + s_2 + s_3 = 1, s_i \geq 0\big\}, \qquad \mathcal{P} := \{s : s_1 + s_2 + s_3 = 1\}.$$

We may write (21) as $s^T M_A(\gamma) s = 0$, where $M_A(\gamma)$ is the symmetric matrix

$$\begin{pmatrix} A_1^2(1-\gamma) & A_1A_2 - \frac{\gamma}{2}(A_1^2 + A_2^2) & A_1A_3 - \frac{\gamma}{2}(A_1^2 + A_3^2) \\ A_1A_2 - \frac{\gamma}{2}(A_1^2 + A_2^2) & A_2^2(1-\gamma) & A_2A_3 - \frac{\gamma}{2}(A_2^2 + A_3^2) \\ A_1A_3 - \frac{\gamma}{2}(A_1^2 + A_3^2) & A_2A_3 - \frac{\gamma}{2}(A_2^2 + A_3^2) & A_3^2(1-\gamma) \end{pmatrix}.$$

We wish to find all $s \in \mathcal{T}$ such that $s^T M_A(\gamma) s = 0$. Let λ_1, λ_2, and λ_3 be the eigenvalues of $M_A(\gamma)$, and let $\{u_1, u_2, u_3\}$ be an orthonormal eigenbasis corresponding to these eigenvalues, respectively. Thus for some scalars α_1, α_2 and α_3, we can write $s = u_1\alpha_1 + u_2\alpha_2 + u_3\alpha_3$. This leads to

$$s^T M_A(\gamma)s = \alpha_1^2\lambda_1 + \alpha_2^2\lambda_2 + \alpha_3^2\lambda_3.$$

When the λ_i are all positive or all negative, the only solution of $s^T M_A(\gamma)s = 0$ is $s = 0$. Towards the end of this chapter we will show that if the determinant of $M_A(\gamma)$ is not zero, then $M_A(\gamma)$ has exactly one negative eigenvalue. This can be proven using a factorization of $M_A(\gamma)$. Therefore $s^T M_A(\gamma)s = 0$ defines a cone $\mathcal{M}(A, \gamma)$, and the solution of (21) is the conic $\mathcal{P} \cap \mathcal{M}(A, \gamma)$.

We will see that this conic is in fact a parabola for all values of γ, and obtain a formula for this parabola. In the next section we graph $\mathcal{T} \cap \mathcal{M}(A, \gamma)$ for some A and γ, and map the result back to S^2 to obtain $\mathcal{L}(A, \gamma)$. Note that each point in $\mathcal{T}$ corresponds to exactly one point in each octant of S^2.

5.1. The Level Curves

PDS matrices fall into several categories, with qualitatively different level curves. For each case, we will give pictures (created with Matlab) of the level curves for certain values of γ on $\mathcal{T}$ and on S^2.

Recall Proposition 3.1, and write $\phi(C_1, C_2)$ for ϕ_C when $C = \begin{pmatrix} C_1 & \\ & C_2 \end{pmatrix}$. The level curves show a qualitative transition when γ is $\cos^2\phi(A_1, A_2), \cos^2\phi(A_2, A_3)$, or $\cos^2\phi(A_1, A_3)$ (note that $\phi(A_1, A_3)$ is ϕ_A). We display the level curves at each of these values, as well as at some intermediate values. When $\gamma = 1$, the parabola touches all three vertices of $\mathcal{T}$ and the level curve on S^2 consists of the six points $\pm e_1, \pm e_2$ and $\pm e_3$.

The case $A_1 = A_2 < A_3$. Here the parabola $\mathcal{P} \cap \mathcal{M}(A, \gamma)$ is degenerate and is either two parallel lines or a single "double" line. The level curves have a transition only at $\gamma = \cos^2\phi_A$. For $\gamma < \cos^2\phi_A$, $\mathcal{T} \cap \mathcal{M}(A, \gamma)$ and $\mathcal{L}(A, \gamma)$ are empty. For $\gamma = \cos^2\phi_A$, $\mathcal{T} \cap \mathcal{M}(A, \gamma)$ is a line segment, and $\mathcal{L}(A, \gamma)$ is a pair of opposite latitude lines with respect to the poles $\pm e_3$, one in the northern and one in the southern hemisphere. For $\gamma > \cos^2\phi_A$, $\mathcal{T} \cap \mathcal{M}(A, \gamma)$ consists of two parallel line segments, and $\mathcal{L}(A, \gamma)$ is two pairs of latitude lines. For $\gamma = 1$, $\mathcal{T} \cap \mathcal{M}(A, \gamma)$

consists of e_3 and the line segment $\overline{e_1e_2}$. We illustrate the situation for $A = \left(\begin{smallmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{smallmatrix}\right)$ in Figures 5.1 and 5.2.

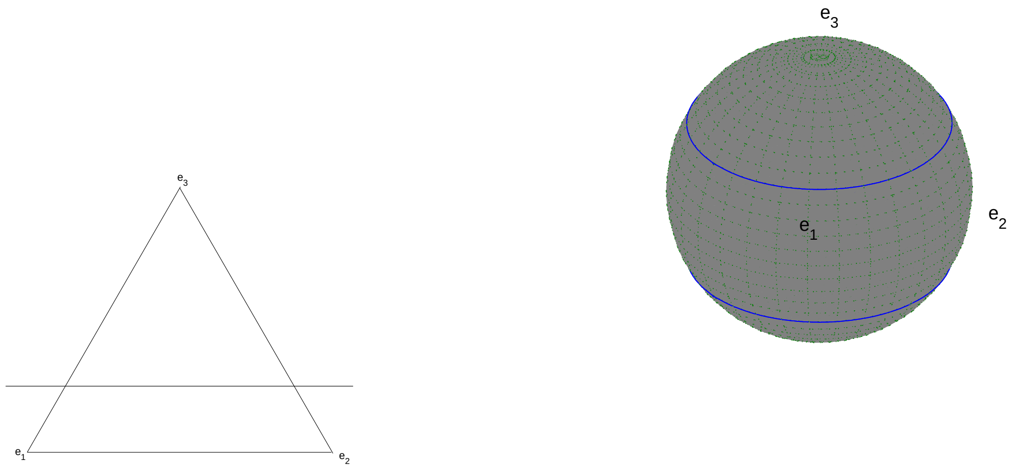

FIGURE 5.1. $A = \begin{pmatrix} 1 & & \\ & 1 & \\ & & 3 \end{pmatrix}, \gamma = \frac{3}{4} = \cos^2 \phi_A$

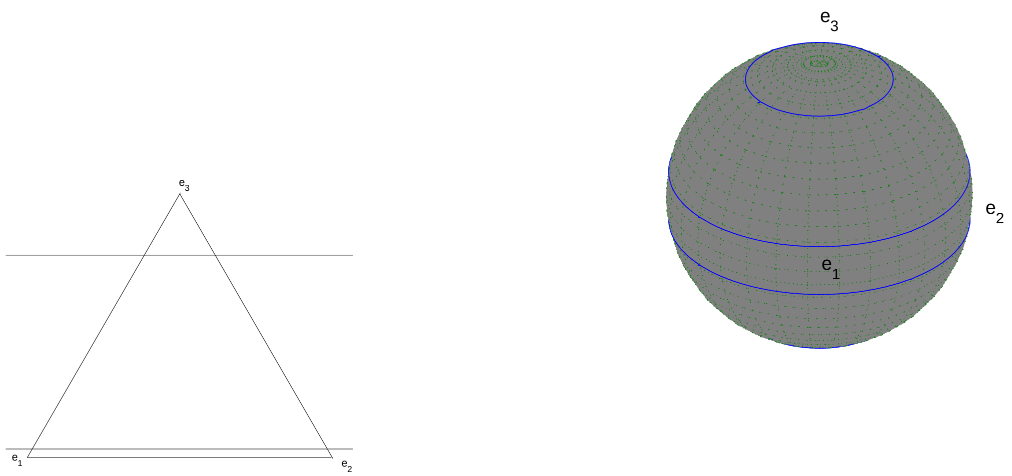

FIGURE 5.2. $A = \begin{pmatrix} 1 & & \\ & 1 & \\ & & 3 \end{pmatrix}, \ \gamma = \frac{9}{10} > \cos^2 \phi_A$

The case $A_1 < A_2 = A_3$. This is similar to the previous case. Here too the level curves have a transition only at $\gamma = \cos^2 \phi_A$. The only difference is that $\mathcal{L}(A, \gamma)$ consists of latitude lines with $\pm e_1$ as the poles, as $\mathcal{T} \cap \mathcal{M}(A, \gamma)$ consists of line segments parallel to $\overline{e_2 e_3}$. Figures are omitted since they are as in the previous case with e_1 and e_3 exchanged.

The case $1 < \frac{A_2}{A_1} < \frac{A_3}{A_2}$. Here $\phi(A_1, A_2) < \phi(A_2, A_3) < \phi(A_1, A_3) = \phi_A$. We present the level curves for these angles and some intermediate values. Take as an example $A = \left(\begin{smallmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 5 \end{smallmatrix}\right)$. By Proposition 3.1, $\phi(1,2) \approx 20°, \phi(2,5) \approx 25°$, and $\phi(1,5) = \phi_A \approx 42°$. The corresponding

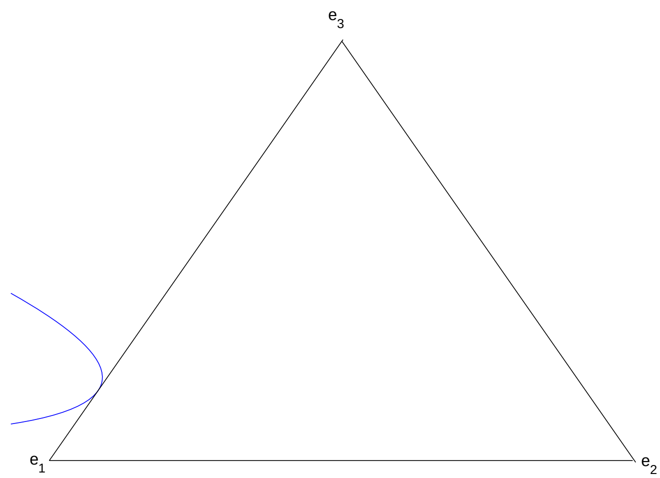

FIGURE 5.3. $A = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 5 \end{pmatrix}$, $\gamma = \frac{5}{9} = \cos^2 \phi_A$

γ values are $\frac{8}{9}, \frac{40}{49}$, and $\frac{5}{9}$ respectively. For $\gamma < \frac{5}{9}$, $\mathcal{L}(A, \gamma)$ is empty. At $\gamma = \frac{5}{9}$, the parabola is tangent to $\overline{e_1 e_3}$ (Figure 5.3). Thus the level curve on the sphere at this stage consists of four points, a point on each of the four quadrants of the great circle $\mathrm{GC}(e_1, e_3)$.

For $\frac{5}{9} < \gamma < \frac{40}{49}$, the parabola intersects $\overline{e_1 e_3}$ but not $\overline{e_2 e_3}$ or $\overline{e_1 e_2}$. Hence $\mathcal{L}(A, \gamma)$ consists of four roughly oval curves; see Figure 5.4.

At $\gamma = \frac{40}{49}$ the parabola is tangent to $\overline{e_2 e_3}$. The corresponding four points on $\mathrm{GC}(e_2, e_3)$ are saddle points of the angle function of A; see Figure 5.5.

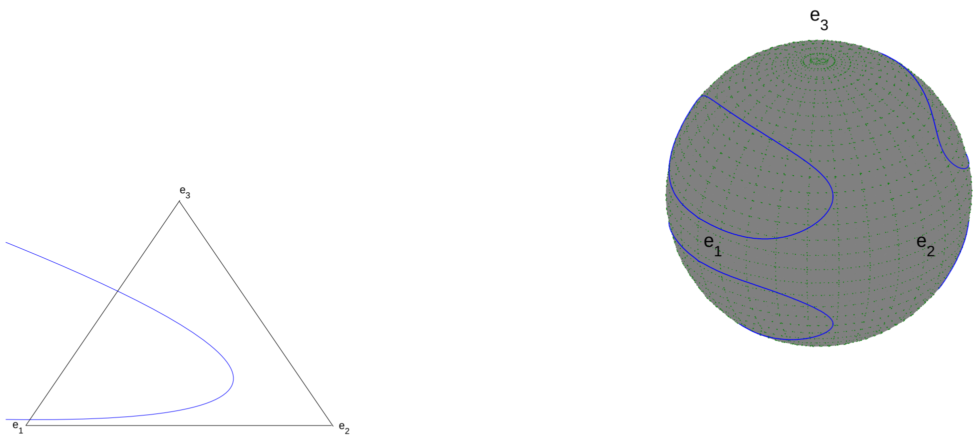

FIGURE 5.4. $A = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 5 \end{pmatrix}$, $\cos^2 \phi_A = \frac{5}{9} < \gamma < \frac{40}{49}$

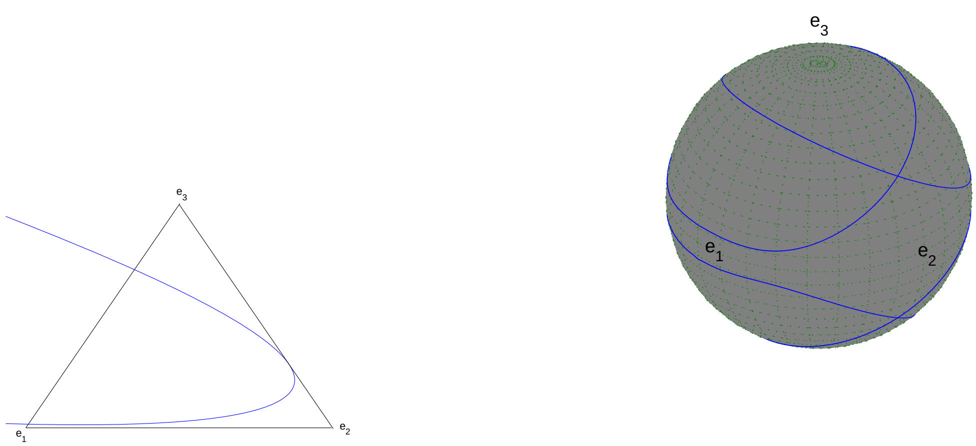

FIGURE 5.5. $A = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 5 \end{pmatrix}$, $\gamma = \frac{40}{49}$

For $\frac{40}{49} < \gamma < \frac{8}{9}$, the parabola intersects $\overline{e_1 e_2}$ and $\overline{e_2 e_3}$, but not $\overline{e_1 e_2}$; see Figure 5.6.

At $\gamma = \frac{8}{9}$, the parabola is tangent to $\overline{e_1 e_2}$, giving the four saddle points of the angle function on $\mathrm{GC}(e_1, e_2)$; see Figure 5.7.

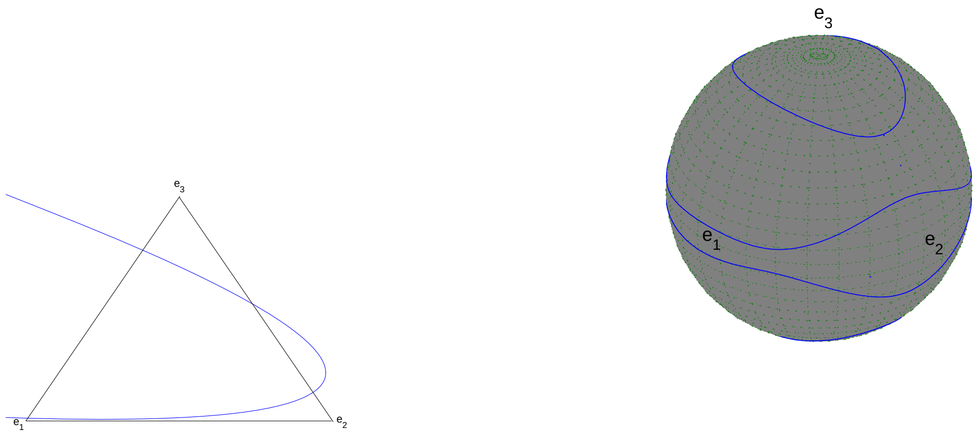

FIGURE 5.6. $A = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 5 \end{pmatrix}$, $\frac{40}{49} < \gamma < \frac{8}{9}$

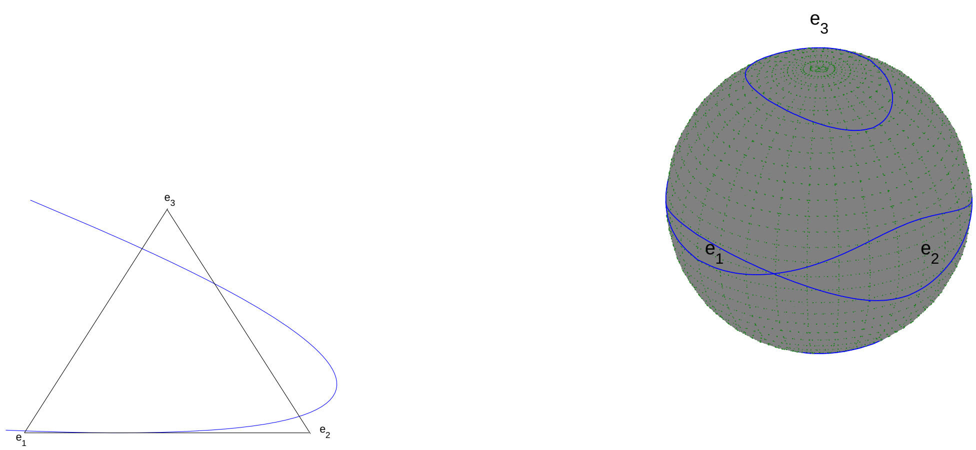

FIGURE 5.7. $A = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 5 \end{pmatrix}$, $\gamma = \frac{8}{9}$

For $\frac{8}{9} < \gamma < 1$, the parabola intersects all three sides of $\mathcal{T}$ in two points. Hence $\mathcal{L}(A, \gamma)$ consists of six roughly oval curves, around $\pm e_1, \pm e_2$ and $\pm e_3$; see Figure 5.8.

Finally, at $\gamma = 1$ the parabola touches all three vertices of the triangle; see Figure 5.9.

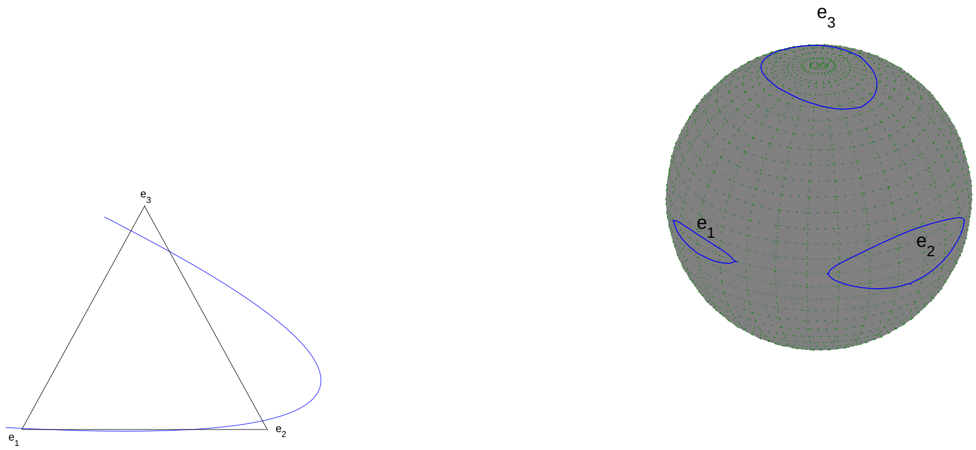

FIGURE 5.8. $A = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 5 \end{pmatrix}$, $\frac{8}{9} < \gamma < 1$

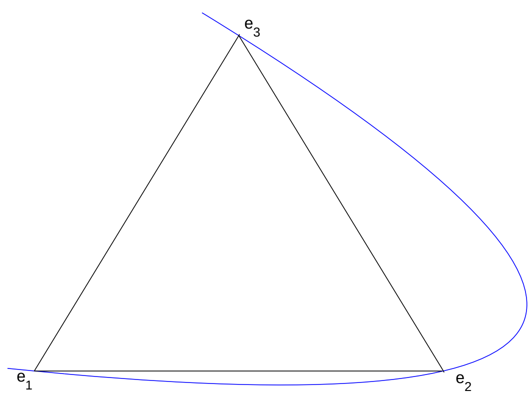

FIGURE 5.9. $A = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 5 \end{pmatrix}$, $\gamma = 1$

We remark that the angle function of A on S^2 is minimal at $\pm e_1, \pm e_2$ and $\pm e_3$, maximal at the four points on $\mathrm{GC}(e_1, e_3)$ corresponding to Figure 5.3, and has saddles at the eight points on $\mathrm{GC}(e_1, e_2)$ and $\mathrm{GC}(e_2, e_3)$ arising from Figures 5.5 and 5.7. It follows from the proof of Proposition 3.1 that it has no other critical points. A contour map is given in Figure 5.10.

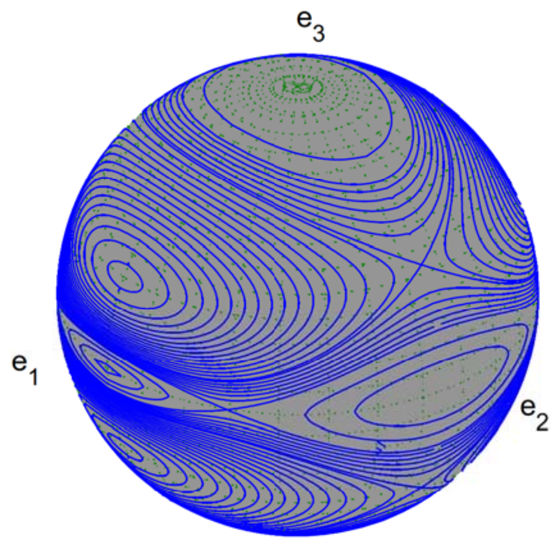

FIGURE 5.10. Contour map for $A = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 5 \end{pmatrix}$

The case $1 < \frac{A_3}{A_2} < \frac{A_2}{A_1}$. Here we have $\phi(A_2, A_3) < \phi(A_1, A_2) < \phi(A_1, A_3) = \phi_A$. We give some level curves for $A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}$.

By Proposition 3.1, $\phi(2,3) \approx 12°, \phi(1,2) \approx 20°$, and $\phi(1,3) = \phi_A = 30°$. The corresponding γ values are $\frac{24}{25}, \frac{8}{9}$, and $\frac{3}{4}$ respectively. For $\gamma < \frac{3}{4}$, there is no level curve. At $\gamma = \frac{3}{4}$, the parabola is tangent to $\overline{e_1 e_3}$ and so $\mathcal{L}(A, \gamma)$ consists of four points, a point on each of the four quadrants of $\mathrm{GC}(e_1, e_3)$. For $\frac{3}{4} < \gamma < \frac{8}{9}$, the situation is similar to that in Figure 5.4.

At $\gamma = \frac{8}{9}$, the parabola is tangent to $\overline{e_1 e_2}$ and the angle function has saddle points on $\mathrm{GC}(e_1, e_2)$; see Figure 5.11.

For $\frac{8}{9} < \gamma < \frac{24}{25}$, the parabola intersects $\overline{e_1 e_2}$ in two points but does not intersect $\overline{e_2 e_3}$; see Figure 5.12.

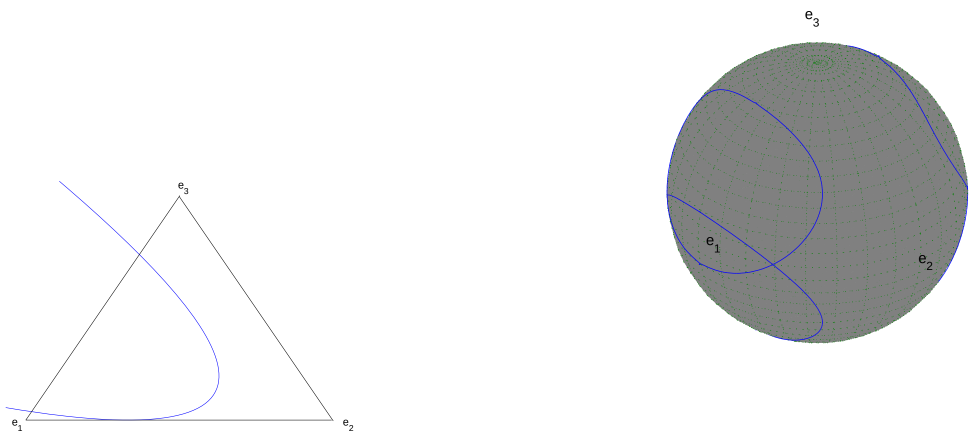

FIGURE 5.11. $A = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 3 \end{pmatrix}$, $\gamma = \frac{8}{9}$

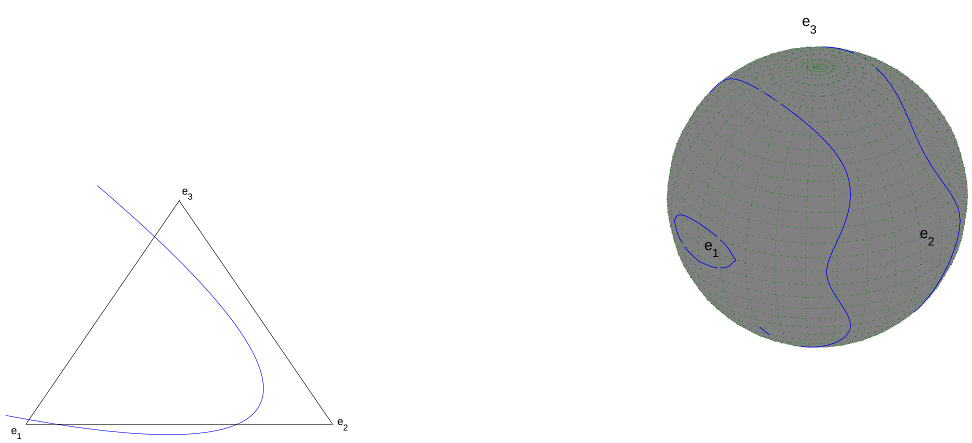

FIGURE 5.12. $A = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 3 \end{pmatrix}$, $\frac{8}{9} < \gamma < \frac{24}{25}$

At $\gamma = \frac{24}{25}$, the parabola is tangent to $\overline{e_2 e_3}$, yielding the saddle points of the angle function on $\mathrm{GC}(e_2, e_3)$; see Figure 5.13.

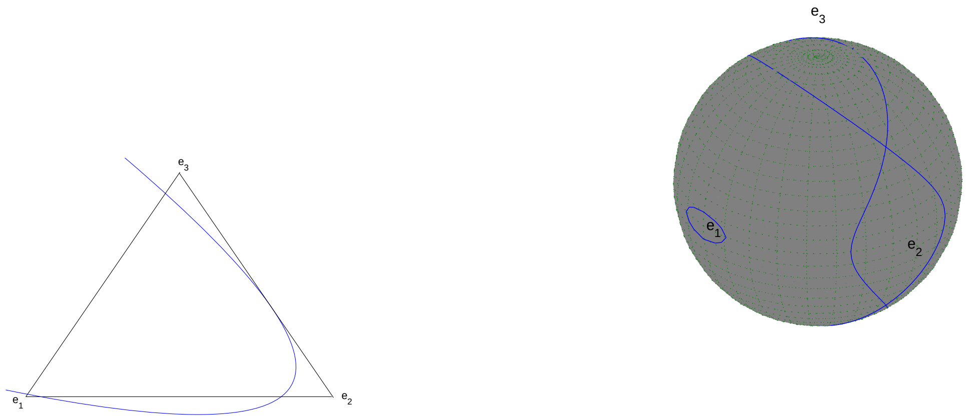

FIGURE 5.13. $A = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 3 \end{pmatrix}$, $\gamma = \frac{24}{25}$

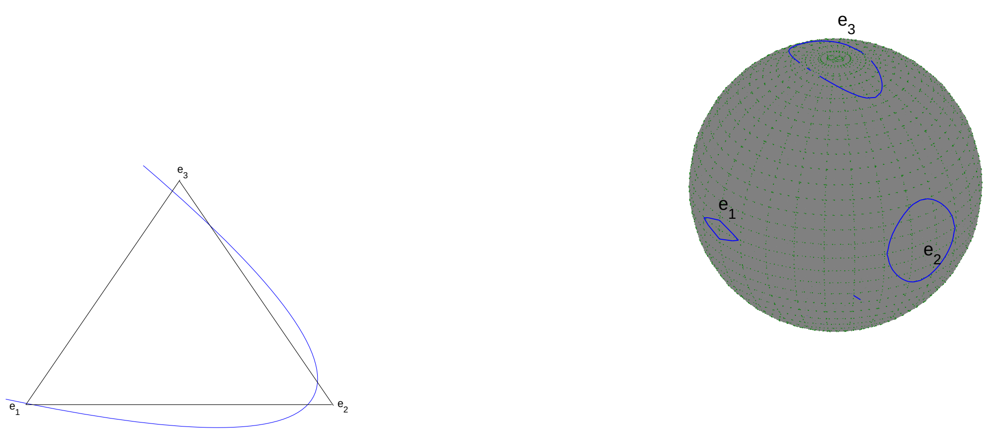

FIGURE 5.14. $A = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 3 \end{pmatrix}$, $\frac{24}{25} < \gamma < 1$

For $\frac{24}{25} < \gamma < 1$, the situation is roughly as in Figure 5.8; see Figure 5.14. Figure 5.15 gives a contour map of the angle function.

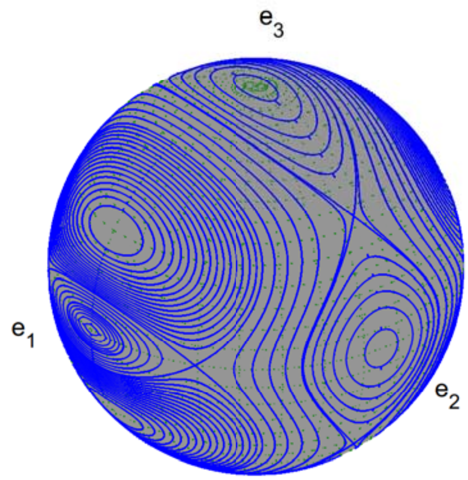

FIGURE 5.15. Contour map for $A = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 3 \end{pmatrix}$

The case $1 < \frac{A_2}{A_1} = \frac{A_3}{A_2}$**.** Here $\phi(A_1, A_2) = \phi(A_2, A_3) < \phi(A_1, A_3) = \phi_A$. Consider as an example the matrix $A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{pmatrix}$. By Proposition 3.1, $\phi(1, 2) = \phi(2, 4) \approx 20°$ and $\phi(1, 4) = \phi_A \approx 37°$. The corresponding γ values are $\frac{8}{9}$ and $\frac{16}{25}$. For $\gamma < \frac{16}{25}$, there are no level curves. For $\gamma = \frac{16}{25}$, the parabola is tangent to $\overline{e_1e_3}$ and the situation is as in Figure 5.3.

For $\frac{16}{25} < \gamma < \frac{8}{9}$, the parabola intersects only the side $\overline{e_1e_3}$ and the situation is as in Figure 5.4.

At $\gamma = \frac{8}{9}$, the parabola is tangent to both $\overline{e_1e_2}$ and $\overline{e_2e_3}$, and so $\mathcal{L}(A, \gamma)$ contains all eight saddle points of the angle function; see Figure 5.16. In the next section we will prove that this level curve is in fact a union of four circles.

For $\frac{8}{9} < \gamma < 1$, the situation is as in Figures 5.8 and 5.14. Figure 5.17 gives a contour map.

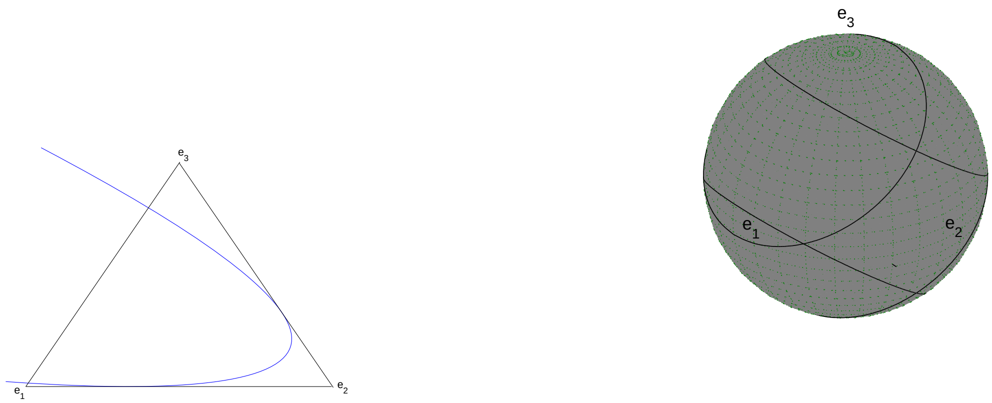

FIGURE 5.16. $A = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 4 \end{pmatrix}$, $\gamma = \frac{8}{9}$

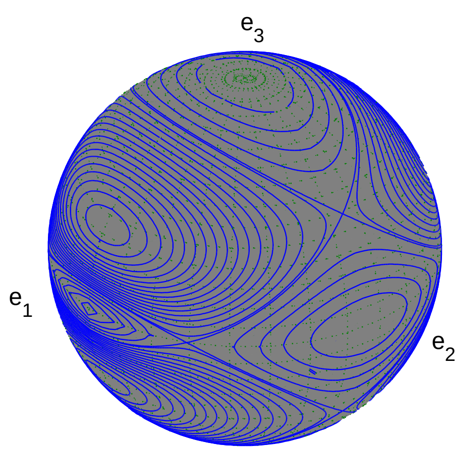

FIGURE 5.17. Contour map for $A = \begin{pmatrix} 1 & & \\ & 2 & \\ & & 4 \end{pmatrix}$

5.2. Level Curves Containing Circles

Proposition 5.1. *The level curve $\mathcal{L}(A,\gamma)$ is a union of circles if and only if either the ratios $\frac{A_2}{A_1}$ and $\frac{A_3}{A_2}$ are equal and $\gamma = \cos^2\phi(A_1,A_2) = \cos^2\phi(A_2,A_3)$, or A has repeated eigenvalues and $\gamma \geq \cos^2\phi_A$.*

Proof. Suppose that $\mathcal{L}(A,\gamma)$ contains a circle. If n is any vector normal to this circle, then the equation of the circle (on S^2) is $x \cdot n = N$ for some constant N. Note that since A is diagonal, $x \cdot Mn = N$ must also be contained in $\mathcal{L}(A,\gamma)$ for any M in $\left\{\begin{pmatrix} \pm1 & & \\ & \pm1 & \\ & & \pm1 \end{pmatrix}\right\} \cong \mathbb{Z}_2^3$. It follows that the product of all $x \cdot Mn = N$ with $M \in \mathbb{Z}_2^3$ and Mn distinct must divide the equation of $\mathcal{L}(A,\gamma)$. Since $\mathcal{L}(A,\gamma)$ is quartic in x, this implies that at least one entry of n is zero. There are two cases.

Suppose first that two entries of n are zero. In this case the circles are centered on $\pm e_1$, $\pm e_2$ or $\pm e_3$. Thus they correspond to line segments parallel to one side of the triangle $\mathcal{T}$ in s-space. This occurs only when A has repeated eigenvalues, in which case the level curve on $\mathcal{T}$ consists of a single line if $\gamma = \cos^2\phi_A$ and a pair of lines if $\gamma > \cos^2\phi_A$. On the sphere it consists of two circles if $\gamma = \cos^2\phi_A$ and four circles if $\gamma > \cos^2\phi_A$.

Now suppose that only one entry of n is zero. Here by symmetry $\mathcal{L}(A,\gamma)$ contains four congruent circles, so since it is quartic it must be exactly the union of these circles.

Assume first that the second entry of n is zero. Then the normals of the four circles are $n = (\pm n_1, 0, \pm n_3)$, so the equation of $\mathcal{L}(A,\gamma)$ is

$$0 = \prod_{\epsilon_1,\epsilon_3=\pm1} (x_1\epsilon_1 n_1 + x_3\epsilon_3 n_3 - N) = \left(s_1 n_1^2 + s_3 n_3^2 - N^2\right)^2 - 4 s_1 s_3 n_1^2 n_2^2,$$

where $s_i = x_i^2$ for all i. Expanding and simplifying, we obtain

$$N^4 - 2N^2 n_1^2 s_1 - 2N^2 n_3^2 s_3 + (s_1 n_1^2 - s_3 n_3^2)^2 = 0. \tag{22}$$

Set $k = \frac{A_2}{A_1}$ and $l = \frac{A_3}{A_2}$. We may assume that $A = \begin{pmatrix} 1 & & \\ & k & \\ & & l \end{pmatrix}$. Recall that $\mathcal{L}(A,\gamma)$ is

$$(s_1 + ks_2 + ls_3)^2 - \gamma(s_1 + k^2 s_2 + l^2 s_3) = 0,$$

where $s_2 = 1 - s_1 - s_3$. Expanding and simplifying gives

$$(23) \qquad \begin{aligned} &k^2(1-\gamma) - \big(\gamma(1+k) - 2k\big)(1-k)s_1 \\ &-\big(2k - \gamma(k+l)\big)(k-l)s_3 + \big((1-k)s_1 - (k-l)s_3\big)^2 = 0. \end{aligned}$$

Since (22) and (23) have the same solutions, they are proportional. We may replace (n, N) by (cn, cN) for any scalar c, so we may assume that

$$\begin{aligned} N^4 &= k^2(1-\gamma), \\ 2N^2 n_1^2 &= \big(\gamma(1+k) - 2k\big)(1-k), \\ 2N^2 n_3^2 &= \big(2k - \gamma(k+l)\big)(k-l), \\ n_1^2 &= 1-k, \\ n_3^2 &= k-l. \end{aligned}$$

The last four of these give

$$(24) \qquad N^2 = \frac{\gamma(1+k) - 2k}{2} = \frac{2k - \gamma(k+l)}{2},$$

so $\gamma = \frac{4k}{1+2k+l}$. Using (24) and $N^4 = k^2(1-\gamma)$, we arrive at $l = k^2$. Hence the ratios of the eigenvalues of A are equal and

$$\gamma = \frac{4k}{(1+k)^2} = \cos^2\phi(1,k).$$

If n_1 or n_3 is the zero coordinate instead of n_2, the above argument shows that l is k^{-1} or $\sqrt{k}$, respectively, contradicting the assumption that $A_1 \le A_2 \le A_3$.

□

5.3. The Equation of the Parabola

For convenience, let us define $\vec{1} := (1,1,1)$, $\vec{A} := (A_1, A_2, A_3)$ and $\vec{A}^2 := (A_1^2, A_2^2, A_3^2)$. Then the equation $s^T M_A(\gamma)s = 0$ of $\mathcal{M}(A,\gamma)$ may be written as

$$(\vec{A}\cdot s)^2 = \gamma(\vec{1}\cdot s)(\vec{A}^2\cdot s).$$

The plane $\mathcal{P}$ is defined by $\vec{1}\cdot s = 1$, so the equation of $\mathcal{P}\cap\mathcal{M}(A,\gamma) \subset \mathcal{P}$ is

$$(25) \qquad (\vec{A} \cdot s)^2 = \gamma(\vec{A}^2 \cdot s).$$

For A_1, A_2 and A_3 distinct, $\vec{A} \cdot s$ and $\vec{A}^2 \cdot s$ are independent linear coordinates on $\mathcal{P}$, so (25) defines a parabola. Define vectors

$$l = \vec{A} - \tfrac{1}{3}(\vec{A} \cdot \vec{1})\vec{1}, \qquad n = \vec{1} \times \vec{l} = \vec{1} \times \vec{A}.$$

Since only the square of $\vec{A} \cdot s$ appears in (25), the axis of the parabola is perpendicular to $\vec{A}$. Since it is in $\mathcal{P}$, the axis is parallel to $\vec{n}$. Note that the axial direction is independent of γ.

Now $\{\vec{1}, l, n\}$ is an orthogonal basis of $\mathbb{R}^3$, and $\{l, n\}$ is an orthogonal basis of the space of vectors parallel to $\mathcal{P}$. Therefore $l \cdot s$ and $n \cdot s$ are orthogonal coordinates of $\mathcal{P}$. We will find constants L, M and N so that (25) takes the form

$$(l \cdot s - L)^2 = Mn \cdot s - N.$$

To do this, write $\vec{A}$ and $\vec{A}^2$ in terms of $\vec{1}, l$, and n, use $\vec{1} \cdot s = 1$, and complete the square appropriately. One arrives at

$$L = \frac{\gamma}{2}\frac{l \cdot \vec{A}^2}{l \cdot l} - \frac{\vec{A} \cdot \vec{1}}{3}, \quad M = \gamma\frac{n \cdot \vec{A}^2}{n \cdot n},$$

$$N = \frac{\gamma}{3}\frac{l \cdot \vec{A}^2}{l \cdot l}(\vec{A} \cdot \vec{1}) - \gamma\frac{\vec{1} \cdot \vec{A}^2}{\vec{1} \cdot \vec{1}} - \frac{\gamma^2}{4}\Big(\frac{l \cdot \vec{A}^2}{l \cdot l}\Big)^2.$$

These constants enable us to read off the vertex and axis of the parabola: they are $\big(L, \frac{N}{M}\big)$ and $(l \cdot s) = L$.

5.4. Factorization of $M_A(\gamma)$ and Its Eigenvalues

Here we exhibit a factorization property of the symmetric matrix $M_A(\gamma)$ and use it to prove that when determinant of this matrix is not zero, it has exactly one negative eigenvalue. In fact, when $M_A(\gamma)$ is expressed in the basis $\{\vec{1}, \vec{A}, \vec{A}^2\}$, it factors as a product of two Vandermonde matrices and a diagonal matrix. To explain, let Y be the Vandermonde matrix $Y = \left(\begin{smallmatrix} 1 & A_1 & A_1^2 \\ 1 & A_2 & A_2^2 \\ 1 & A_3 & A_3^2 \end{smallmatrix}\right)$. Then for A_1, A_2, and A_3 distinct

$$Y^{-1} = \begin{pmatrix} \frac{A_2A_3}{(A_1-A_3)(A_1-A_2)} & -\frac{A_1A_3}{(A_2-A_1)(A_3-A_2)} & \frac{A_1A_2}{(A_2-A_3)(A_1-A_3)} \\ -\frac{A_3+A_2}{(A_1-A_3)(A_1-A_2)} & \frac{A_1+A_3}{(A_2-A_1)(A_3-A_2)} & -\frac{A_1+A_2}{(A_2-A_3)(A_1-A_3)} \\ \frac{1}{(A_1-A_3)(A_1-A_2)} & -\frac{1}{(A_2-A_1)(A_3-A_2)} & \frac{1}{(A_2-A_3)(A_1-A_3)} \end{pmatrix}.$$

One checks that

$$Y^{-1}M_A(\gamma) = \begin{pmatrix} -\frac{\gamma}{2} & & \\ & 1 & \\ & & -\frac{\gamma}{2} \end{pmatrix} \begin{pmatrix} A_1^2 & A_2^2 & A_3^2 \\ A_1 & A_2 & A_3 \\ 1 & 1 & 1 \end{pmatrix},$$

and so

$$\operatorname{Det} M_A(\gamma) = \operatorname{Det} Y^{-1}M_A(\gamma)Y = -\frac{\gamma^2}{4}(A_1 - A_2)^2(A_2 - A_3)^2(A_1 - A_3)^2 < 0.$$

Since $\operatorname{Tr} M_A(\gamma) = (1-\gamma)(a_1^2 + a_2^2 + a_3^2) \geq 0$, it must be that $M_A(\gamma)$ has one negative and two positive eigenvalues. Therefore the solution set $\mathcal{M}(A, \gamma)$ of $s^T M_A(\gamma)s = 0$ is a cone.

CHAPTER 6

INTERACTIONS BETWEEN THE SETS OF LEVEL CURVES OF TWO PDS MATRICES

Recall that in light of Proposition 4.3, Problem 1 amounts to maximizing the function $\mathrm{Tr}(S_\perp(a,b))$ given in Proposition 4.2 over all $a, b \in S^2$ with $\alpha + \beta \geq \frac{\pi}{2}$. Although we needed $\min \phi_{S_\perp(a,b)}$ for the solution of Problem 1, we could not make progress as calculations were prohibitively complicated. Instead, we look at $\min \phi_{S_{\max}(a,b)}$ by studying the interactions between the sets of level curves of two PDS matrices.

Throughout this chapter, suppose that A and B are 3×3 increasing diagonal PDS matrices with distinct eigenvalues. We work exclusively on S^2. We consider the level curves of the angle functions of A and B for fixed small angles α and β, respectively, as described in Chapter 5.

Recall from the previous chapter that the level curves change qualitatively when the angles are either $\phi(A_1, A_2), \phi(A_2, A_3)$ or $\phi(A_1, A_3) = \phi_A$. Choose α smaller than both $\phi(A_1, A_2)$ and $\phi(A_2, A_3)$. Similarly, choose β smaller than both $\phi(B_1, B_2)$ and $\phi(B_2, B_3)$. For such α, we saw that $\mathcal{L}(A, \cos^2 \alpha)$ consists of oval shaped structures around $\pm e_1, \pm e_2$ and $\pm e_3$.

Consider the portion of $\mathcal{L}(A, \cos^2 \alpha)$ around e_1 (see Figure 5.8). Let us call this component of the level curve $\mathcal{C}(A, \alpha)$. Note that $\mathcal{C}(A, \alpha)$ is symmetric about both $\mathrm{GC}(e_1, e_2)$ and $\mathrm{GC}(e_1, e_3)$. Let $a_\pm$ be the points on the intersection of $\mathrm{GC}(e_1, e_3)$ and $\mathcal{C}(A, \alpha)$ closest to e_1 in the northern and southern hemisphere, respectively (see Figure 6.1). Define $b_\pm$ similarly. In this chapter we prove that the minimum of $\phi_{S_{\max}(a,b_-)}$ as a ranges over $\mathcal{C}(A, \alpha)$ occurs at a_+. The precise statement is given below in Theorem 6.1. Its proof takes most of Chapter 6.

THEOREM 6.1. *The minimum of* $\phi_{S_{max}(a,b_-)}$ *as* a *ranges over* $\mathcal{C}(A,\alpha)$ *is* $\angle(a_+, b_-)$ *and occurs at* a_+.

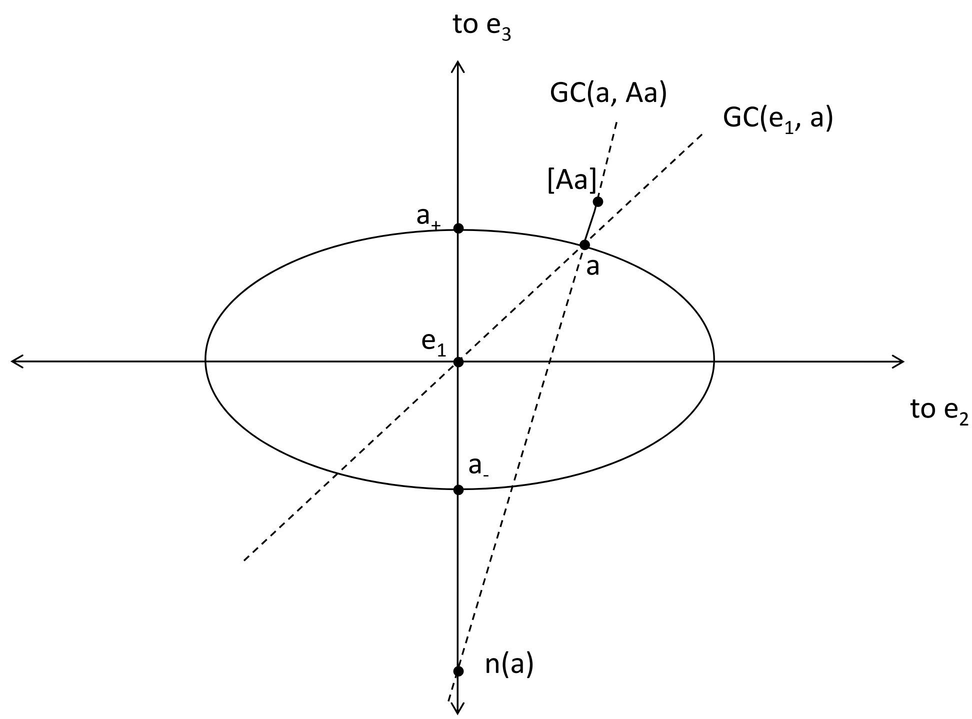

FIGURE 6.1. Polar projection of region of sphere near e_1.

Recall that $\angle(a, Aa) = \alpha$ for all a on $\mathcal{C}(A,\alpha)$. We use again the notation $[x] = \frac{x}{|x|}$ in figures. If a lies on either $\mathrm{GC}(e_1, e_3)$ or $\mathrm{GC}(e_1, e_2)$, then $[Aa]$ also does so. Suppose that a does not lie on either $\mathrm{GC}(e_1, e_3)$ or $\mathrm{GC}(e_1, e_2)$. Without loss of generality, we may assume a to be a point on the first octant of S^2 for the remainder of this chapter. A polar projection of the region of S^2 near e_1 is shown in Figure 6.1. The dotted line segments represent $\mathrm{GC}(e_1, a)$ and $\mathrm{GC}(a, Aa)$, as labeled.

Any two distinct great circles intersect each other at exactly two points. Consider the points of intersection of $\mathrm{GC}(e_1, e_3)$ and $\mathrm{GC}(a, Aa)$. Since $\mathrm{GC}(e_1, e_3)$ has axis e_2 and

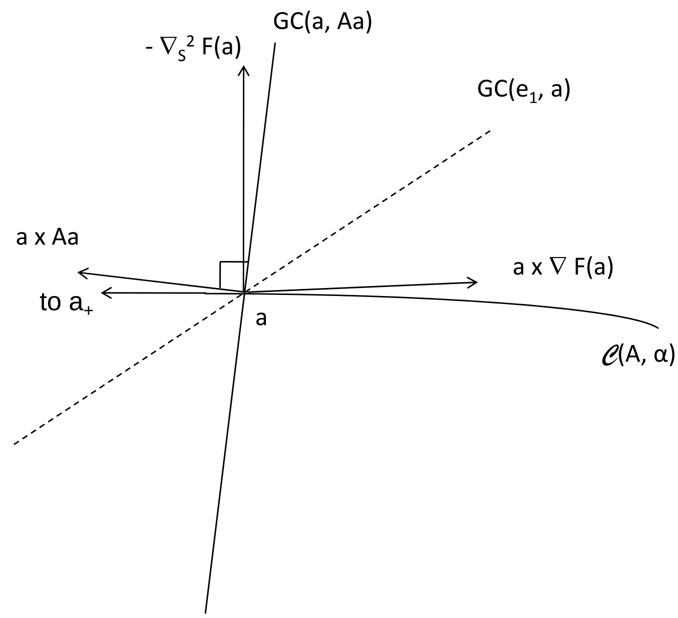

FIGURE 6.2. Polar projection at a.

GC(a, Aa) has axis $a \times Aa$, these points of intersection are along $\pm e_2 \times (a \times Aa) = \pm(A_2 - A)a$. Let $n(a) = [(A_2 - A)a]$.

LEMMA 6.2. *$n(a)$ is always between e_1 and $-e_3$ on $GC(e_1, e_3)$.*

PROOF. By definition $n(a)$ is along $\begin{pmatrix} (A_2-A_1)a_1 \\ 0 \\ (A_2-A_3)a_3 \end{pmatrix}$. Since A is increasing diagonal with distinct eigenvalues, the third component of $n(a)$ is negative, and the first component is positive. $\square$

By the above lemma, GC(a, Aa) is always "steeper" than GC(e_1, a), as shown in Figure 6.1.

Next, recall from Chapter 5 that $F(u) = \cos^2 \angle(u, Au)$, and $F = \cos^2 \alpha$ defines the level curve $\mathcal{L}(A, \cos^2 \alpha)$. Let $\nabla_{S^2} F$ be the projection of this vector to the tangent plane of the sphere at a. It is perpendicular to $\mathcal{C}(A, \alpha)$ at a and points inward from the oval, in the direction of decreasing $\angle(a, Aa)$. A polar projection near a is shown in Figure 6.2. Note that

$a \times \nabla F$ is tangent to $\mathcal{C}(A, \alpha)$ at a and points away from a_+. The next proposition justifies the fact that in the drawing, $-\nabla_{S^2} F(a)$ is to the left of $\mathrm{GC}(a, Aa)$.

PROPOSITION 6.3. *The great circle through a that is perpendicular to $\mathcal{C}(A, \alpha)$ passes through $GC(e_1, e_3)$ strictly between $n(a)$ and $-e_3$.*

PROOF. We first prove the following identity: $-\nabla F \cdot (a \times Aa) > 0$. By (9),

$$a \times \nabla F = 4 \frac{a \cdot Aa}{|Aa|^2}(a \times Aa) - 2 \frac{(a \cdot Aa)^2}{|Aa|^4}(a \times A^2 a).$$

Since $Aa \cdot (a \times Aa) = 0$, we have

$$Aa \cdot (a \times \nabla F) = -2 \frac{(a \cdot Aa)^2}{|Aa|^4} \big\{ Aa \cdot (a \times A^2 a) \big\}.$$

Now $A^2 a = (A_1^2 a_1, A_2^2 a_2, A_3^2 a_3)$, so $a \times A^2 a = \begin{pmatrix} a_2 a_3 (A_3^2 - A_2^2) \\ a_1 a_3 (A_1^2 - A_3^2) \\ a_1 a_2 (A_2^2 - A_1^2) \end{pmatrix}$. Thus

$$\begin{aligned} Aa \cdot (a \times A^2 a) &= a_1 a_2 a_3 \big\{ A_1 (A_3^2 - A_2^2) + A_2 (A_1^2 - A_3^2) + A_3 (A_2^2 - A_1^2) \big\}. \\ &= a_1 a_2 a_3 (A_3 - A_2)(A_2 - A_1)(A_1 - A_3). \end{aligned}$$

Since $A_1 < A_2 < A_3$, this quantity is negative, so $Aa \cdot (a \times \nabla F)$ and hence $-\nabla F \cdot (a \times Aa)$ are positive, proving the identity.

Using $a \cdot (a \times Aa) = 0$ and $a \cdot a = 1$, we obtain

$$\{(a \times Aa) \times a\} \cdot (a \times \nabla F) = -\nabla F \cdot (a \times Aa).$$

Since $a \times Aa$ is perpendicular to $\mathrm{GC}(a, Aa)$ at a, $(a \times Aa) \times a$ is parallel to $\mathrm{GC}(a, Aa)$ at a. Thus the angle measured counterclockwise from $(a \times Aa) \times a$ to $\nabla_{S^2} F$ is positive. This together with Lemma 6.2 proves the Proposition. □

Hence for any a on $\mathcal{C}(A, \alpha)$, $\mathrm{GC}(a, Aa)$ is "between" $\mathrm{GC}(e_1, a)$ and the normal on the sphere to $\mathcal{C}(A, \alpha)$. Next we prove following lemma:

LEMMA 6.4. *As a moves towards a_+ on $\mathcal{C}(A, \alpha)$, $n(a)$ moves monotonically towards $-e_3$.*

Proof. Since $n(a)$ is along $\begin{pmatrix} (A_2-A_1)a_1 \\ 0 \\ (A_2-A_3)a_3 \end{pmatrix}$, $\left|\frac{n_3}{n_1}\right|$ is proportional to the ratio $\left|\frac{(A_2-A_3)a_3}{(A_2-A_1)a_1}\right|$. As A is fixed, the ratio $\left|\frac{n_3}{n_1}\right|$ is proportional to $\frac{a_3}{a_1}$. Hence as a moves towards a_+ on $\mathcal{C}(A,\alpha)$, $n(a)$ moves monotonically towards $-e_3$ if and only if $\frac{a_3}{a_1}$ is strictly increasing, or equivalently, $\frac{s_3}{s_1} = \frac{a_3^2}{a_1^2}$ is strictly increasing.

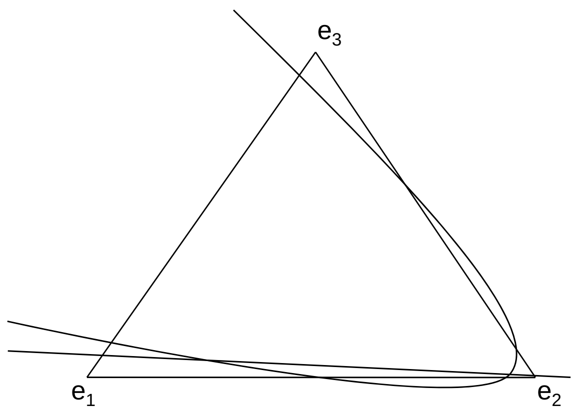

Figure 6.3. Schematic diagram.

Suppose $\frac{s_3}{s_1}$ is not strictly increasing. Then for some point a on $\mathcal{C}(A,\alpha)$, there exists a second point $\tilde{a}$ on $\mathcal{C}(A,\alpha)$, between a and a_+, such that $\frac{\tilde{s_3}}{\tilde{s_1}} = \frac{s_3}{s_1}$. Note that $\frac{x_3}{x_1} = \frac{a_3}{a_1}$ defines $\mathrm{GC}(a,e_2)$ on the sphere, and $\frac{s_3}{s_1} = \frac{a_3^2}{a_1^2}$ defines the line segment passing through s and e_2 in the triangle $\mathcal{T}$. Since $\alpha < min\{\phi(A_1,A_2),\phi(A_2,A_3)\}$, this line segment intersects the parabola corresponding to $\mathcal{C}(A,\alpha)$ at s and also at a point corresponding to a point on the oval on S^2 around e_2 (see Figure 6.3). Since $\frac{\tilde{s_3}}{\tilde{s_1}} = \frac{s_3}{s_1}$, the line segment also passes through $\tilde{s}$. This is a contradiction as a line segment intersects a parabola at most twice. $\square$

Define $\mathrm{Lat}_b(a)$ to be the latitude line through a with b as a pole, the path of a through all rotations about b. As a corollary to Proposition 6.3, we prove following lemma:

LEMMA 6.5. *Consider the acute arc of* $\mathrm{Lat}_{n(a)}(a)$ *from* a *to* $GC(e_1, e_3)$. *Near* a, *this arc is on the outside of* $\mathcal{C}(A, \alpha)$ *(see Figure 6.4).*

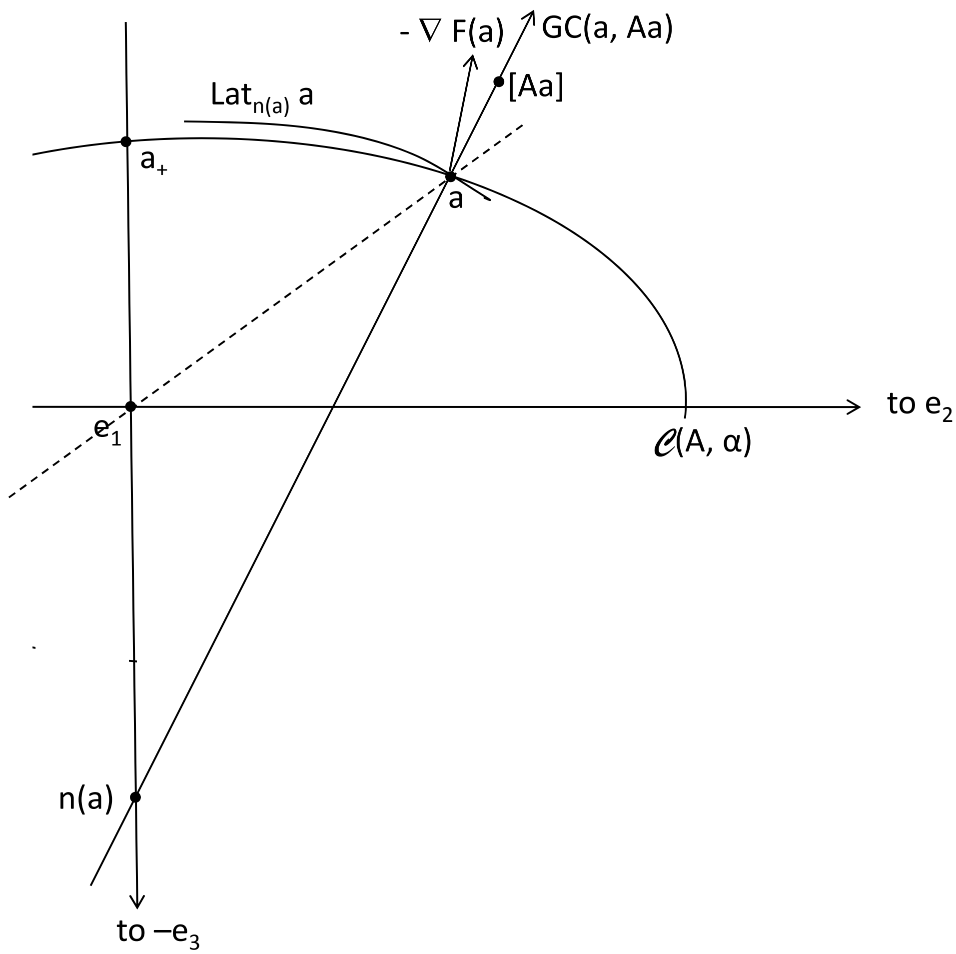

FIGURE 6.4. Polar projection at a.

PROOF. By Proposition 6.3, GC(a, Aa) is "between" GC(e_1, a) and the normal on the sphere to $\mathcal{C}(A, \alpha)$. Since GC(a, Aa) is perpendicular to $\mathrm{Lat}_{n(a)}(a)$, it must cross $\mathcal{C}(A, \alpha)$ at a from lower right to upper left as shown in Figure 6.4. $\square$

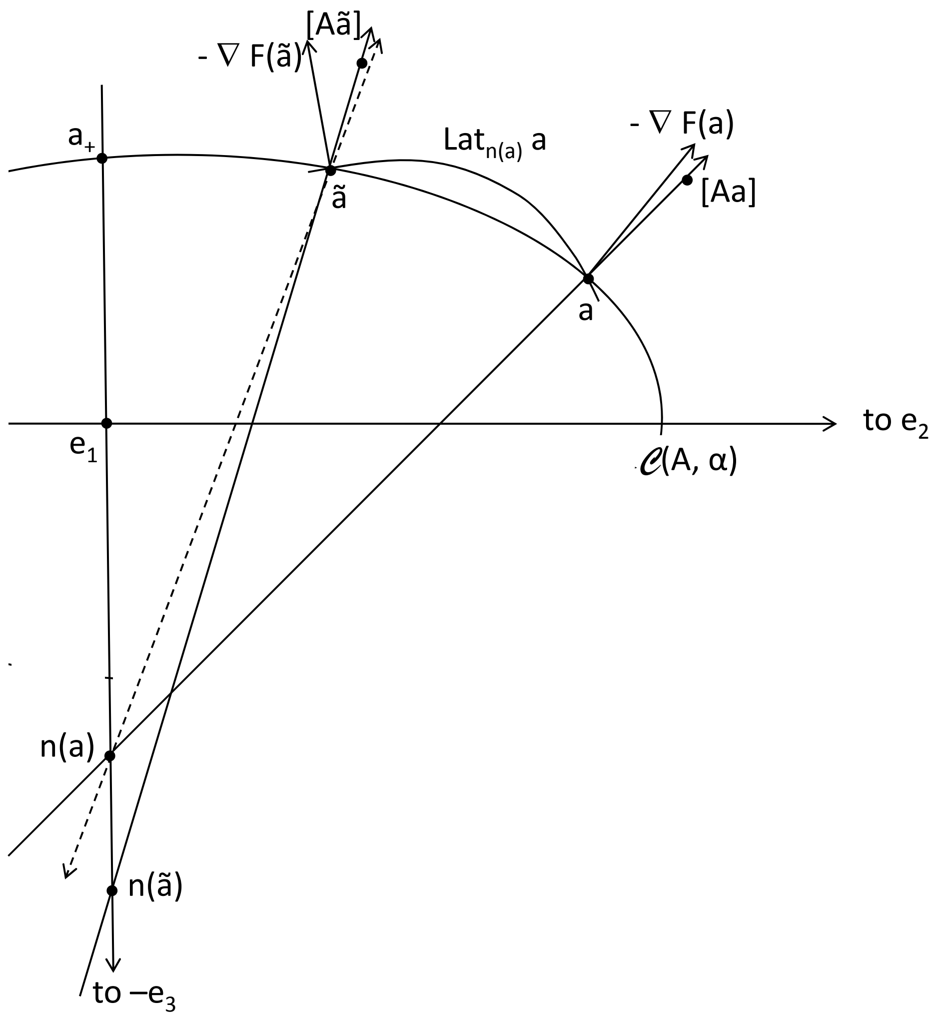

FIGURE 6.5. Polar projection at e_1.

LEMMA 6.6. $\mathrm{Lat}_{n(a)}(a)$ *never crosses* $\mathcal{C}(A,\alpha)$ *between* a_+ *and* a.

PROOF. We prove this by contradiction. Suppose that $\mathrm{Lat}_{n(a)}(a)$ crosses $\mathcal{C}(A,\alpha)$ at a point $\tilde{a}$ between a_+ and a from above. By Lemma 6.4, $n(\tilde{a})$ is between $n(a)$ and $-e_3$. Let $\tilde{S}$ be the rotation around $n(a)$ such that $\tilde{a} = \tilde{S}a$. Then $[\tilde{S}Aa]$ lies on $\mathrm{GC}(\tilde{a}, n(a))$. Note that $\mathrm{GC}(\tilde{a}, n(a))$ is perpendicular to $\mathrm{Lat}_{n(a)}(a)$, and $\nabla_{S^2}F(\tilde{a})$ is perpendicular to the tangent to $\mathcal{C}(A,\alpha)$ at $\tilde{a}$. Thus the angle measured counterclockwise from the tangent to $\mathcal{C}(A,\alpha)$ at $\tilde{a}$ to $\mathrm{GC}(\tilde{a}, n(a))$ is obtuse (see Figure 6.5). This contradicts Proposition 6.3. Hence $\mathrm{Lat}_{n(a)}(a)$ never crosses $\mathcal{C}(A,\alpha)$ from above between a and a_+. Therefore it never crosses $\mathcal{C}(A,\alpha)$

between a and a_+ at all, as it starts out above at a by Lemma 6.5. The argument is similar if it is ever tangent to $\mathcal{C}(A, \alpha)$ between a and a_+. $\square$

Thus the situation is as shown below in Figure 6.6.

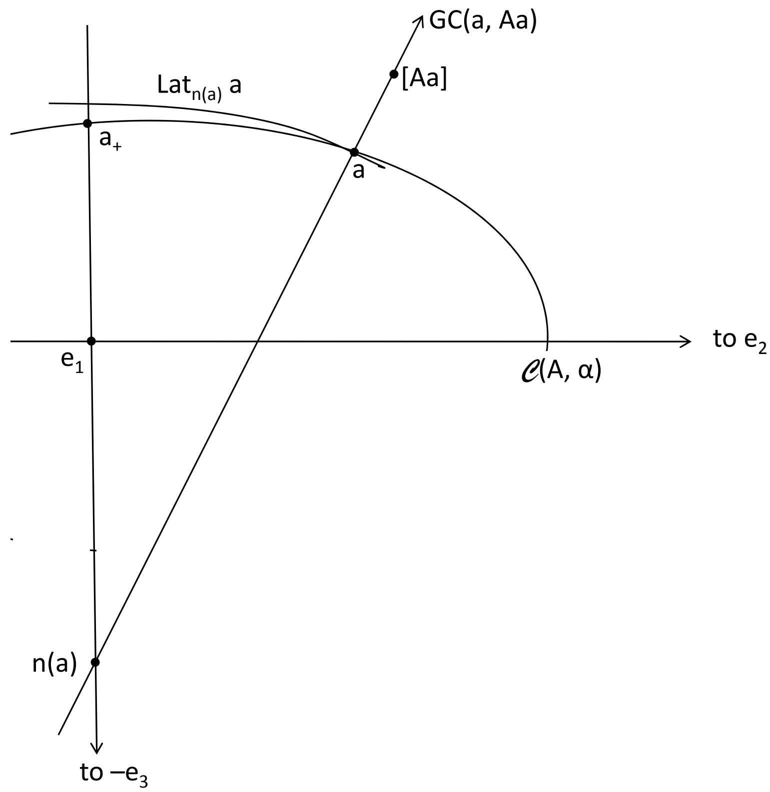

FIGURE 6.6. Polar projection at e_1.

We need two elementary results before proving Theorem 6.1.

LEMMA 6.7. *Let $S_1, S_2 \in \mathrm{SO}_3$ have perpendicular axes of rotation. Then*

$$\cos^2\left(\frac{\phi_{S_1S_2}}{2}\right) = \cos^2\left(\frac{\phi_{S_1}}{2}\right)\cos^2\left(\frac{\phi_{S_2}}{2}\right).$$

PROOF. Without loss of generality, we may assume $S_1 = R(e_3, \phi_{S_1})$ and $S_2 = R(e_2, -\phi_{S_2})$. Computation gives $\mathrm{Tr}(S_1S_2) = (1 + \cos\phi_{S_1})(1 + \cos\phi_{S_2}) - 1$. On the other hand $\mathrm{Tr}(S_1S_2) = 1 + 2\cos\phi_S$. The result follows. $\square$

Corollary 6.8. *Let $S_1, S_2 \in \mathrm{SO}_3$ be two matrices with perpendicular axes of rotation. Let $S = S_1 S_2$, then $\phi_S \geq \max\{\phi_{S_1}, \phi_{S_2}\}$.*

Proof of Theorem 6.1. Consider the point b_- on the intersection of $\mathcal{C}(B, \beta)$ and $\mathrm{GC}(e_1, e_3)$ between e_1 and $-e_3$. Recall that $S_{\max}^{-1}(a, b_-)$ is the orthogonal matrix that moves a to b_- such that $[S_{\max}^{-1}(a, b_-)Aa]$ lies on $\mathrm{GC}(e_1, e_3)$, opposite $[Bb_-]$ from b_- (see Figure 6.7).

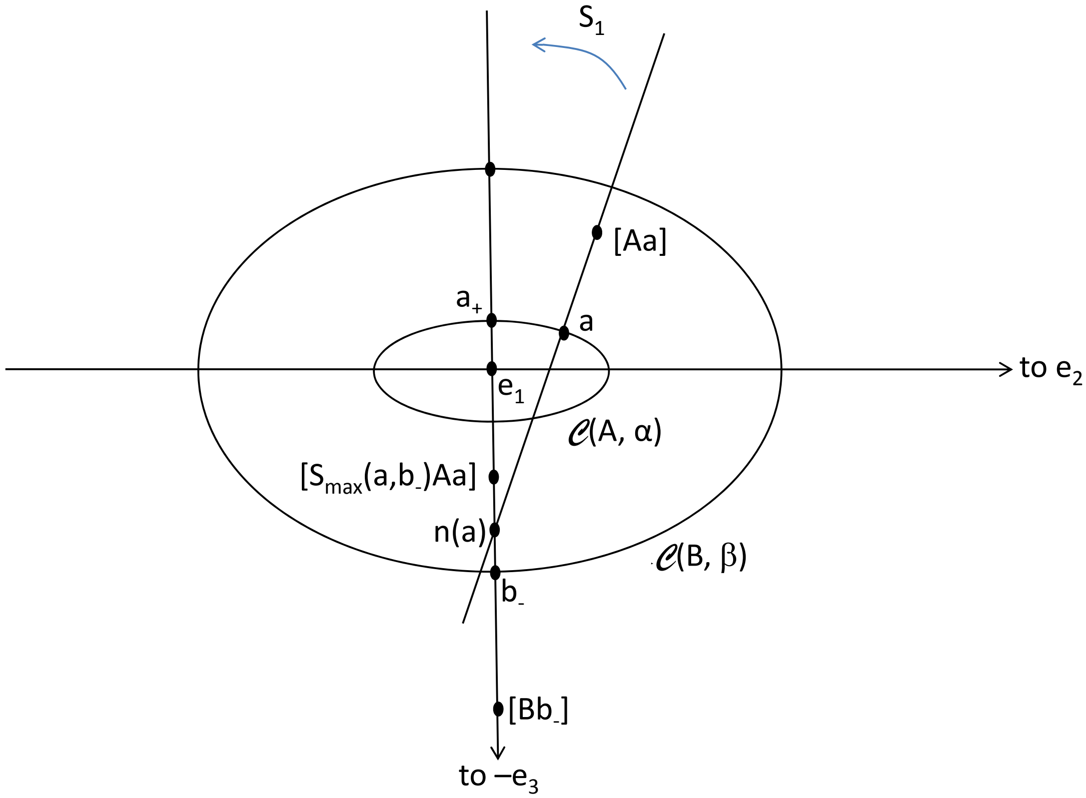

Figure 6.7. Polar projection of region of sphere near e_1.

Note that $\phi_{S_{\max}(a_+, b_-)} = \angle(a_+, b_-)$. By Corollary 3.2, $\angle(a_+, e_1) \leq \frac{\pi}{4} - \frac{\phi_A}{2}$ and $\angle(e_1, b_-) \leq \frac{\pi}{4} - \frac{\phi_B}{2}$, so both $\angle(a_+, e_1)$ and $\angle(e_1, b_-)$ are less than or equal to $\frac{\pi}{4}$. Therefore $\angle(a_+, b_-) \leq \frac{\pi}{2}$.

First suppose that a is a point on $\mathcal{C}(A, \alpha)$ in the first octant of S^2 (i.e., the first quadrant in Figure 6.7). We factor $S_{\max}^{-1}(a, b_-)$ as $S_2 S_1$, where S_1 and S_2 are the following rotations:

S_1 rotates $\mathrm{GC}(a, Aa)$ to $\mathrm{GC}(e_1, e_3)$ counterclockwise (hence by an acute angle) about $n(a)$, and S_2 moves $[S_1 a]$ to b_- about e_2 so that $[S_2 S_1 Aa]$ is opposite $[Bb_-]$ on $\mathrm{GC}(e_1, e_3)$.

By Lemma 6.6, since $\mathrm{Lat}_{n(a)}(a)$ never crosses $\mathcal{C}(A, \alpha)$ between a and a_+, $S_1 a$ is above a_+ on $\mathrm{GC}(e_1, e_3)$ (see Figure 6.6). Thus the distance between $S_1 a$ and b_- is greater than the distance between a_+ and b_- along $\mathrm{GC}(e_1, e_3)$, so $\phi_{S_2} > \angle(a_+, b_-)$. By Corollary 6.8, $\phi_{S_{\max}(a,b_-)} \geq \max\{\phi_{S_1}, \phi_{S_2}\}$. Therefore $\phi_{S_{\max}(a,b_-)} > \angle(a_+, b_-)$.

Next, suppose a is on the part of $\mathcal{C}(A, \alpha)$ in the fourth quadrant (Figure 6.8). We factor $S_{\max}^{-1}(a, b_-)$ as $S_2 S_1$, where S_1 and S_2 are the following rotations: S_1 rotates $\mathrm{GC}(a, Aa)$ to $\mathrm{GC}(e_1, e_3)$ counterclockwise (hence by an obtuse angle) about $n(a)$, and S_2 rotates $[S_1 a]$ to

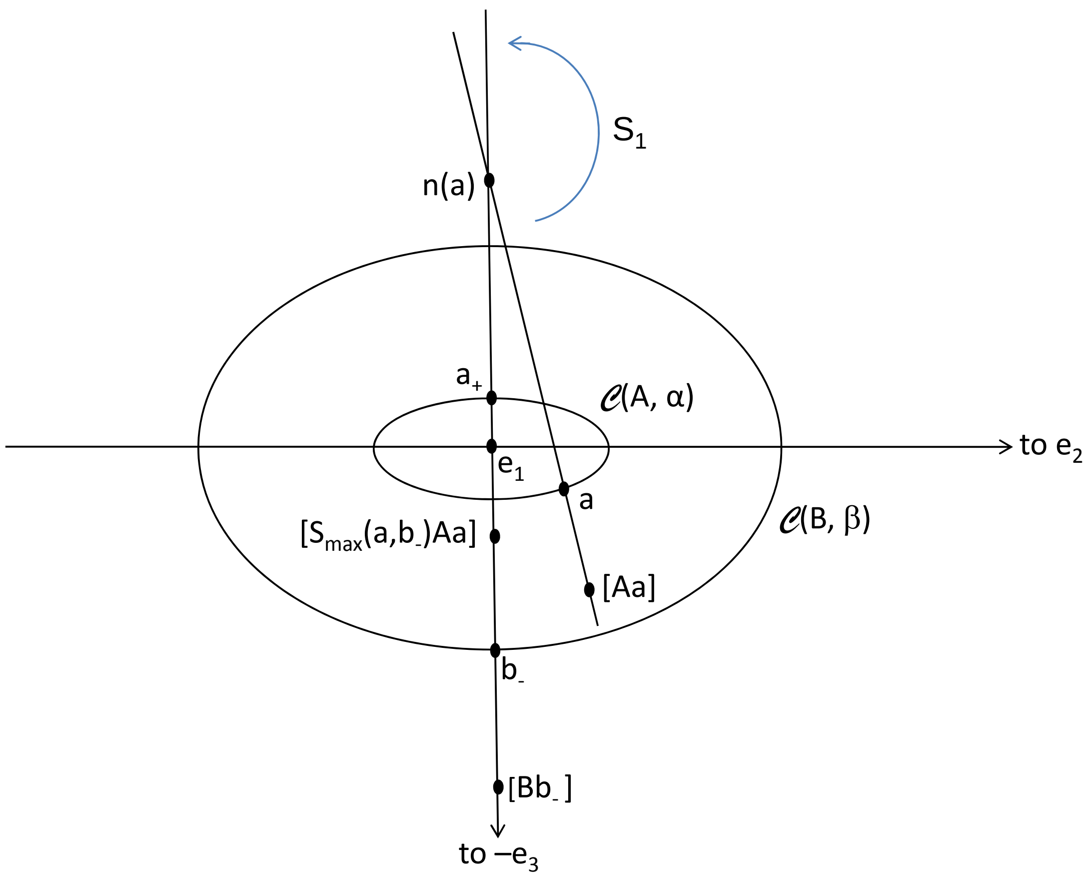

FIGURE 6.8. Polar projection of region of sphere near e_1.

b_- about e_2 so that $[S_2S_1Aa]$ is opposite $[Bb_-]$ on $\mathrm{GC}(e_1, e_3)$. Since $\phi_{S_1} > \frac{\pi}{2}$, by Corollary 6.8 $\phi_{S_{\max}(a,b_-)} > \frac{\pi}{2}$.

The proof is similar if a is on the second or the third quadrant. $\square$

We conclude with a conjecture similar in spirit to Conjecture 4.4.

CONJECTURE 6.9. *The minimum of* $\phi_{S_{\max}(a,b)}$ *on* $\mathcal{C}(A,\alpha) \times \mathcal{C}(B,\beta)$ *occurs at* (a_+, b_-) *and* (a_-, b_+).

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