Twice Differentiable Spectral Functions

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Abstract

A function F on the space of n-by-n real symmetric matrices is called *spectral* if it depends only on the eigenvalues of its argument. Spectral functions are just symmetric functions of the eigenvalues. We show that a spectral function is twice (continuously) differentiable at a matrix if and only if the corresponding symmetric function is twice (continuously) differentiable at the vector of eigenvalues. We give a concise and usable formula for the Hessian.

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1 Introduction

In this paper we are interested in functions F of a symmetric matrix argument that are invariant under orthogonal similarity transformations:

$$F(U^TAU) = F(A), \text{ for all orthogonal } U \text{ and symmetric } A\ .$$

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Every such function can be decomposed as $F(A) = (f \circ \lambda)(A)$, where λ is the map that gives the eigenvalues of the matrix A and f is a symmetric function. (See the next section for more details). We call such functions F *spectral functions* (or just functions of eigenvalues) because de facto they depend only on the spectrum of the operator A. Classical interest in such functions arose from their important role in quantum mechanics [5], [13]. Nowadays they are an inseparable part of optimization [9], and matrix analysis [2, 3]. In modern optimization the key example is "semidefinite programming", where one often encounters problems involving spectral functions like $\log \det(A)$, the largest eigenvalue of A, or the constraint that A must be positive definite.

It turns out that many properties of the spectral function F stem from the same properties of the underlying symmetric function f. Among them are first-order differentiability [7], convexity [6], generalized first-order differentiability [7, 8], analyticity [17], and various second-order properties [16], [15], [14]. It is also worth mentioning the "Chevalley Restriction Theorem", which in this context identifies spectral functions that are polynomials with symmetric polynomials of the eigenvalues. Second-order properties of matrix functions are of great interest for optimization because the application of Newton's method, interior point methods [11], or second-order nonsmooth optimality conditions [12] requires that we know the second-order behaviour of the functions involved in the mathematical model.

The standard reference for the behaviour of the eigenvalues of a matrix subject to perturbations in a particular *direction* is [4]. Second-order properties of eigenvalue functions in a particular direction are derived in [16]. The problem that interests us in this paper is that of when a spectral function is twice differentiable and when its Hessian is continuous. Analyticity is discussed in [17]: thus our result lies in some sense between the results in [6] and [17].

We show that a spectral function is twice (continuously) differentiable at a matrix if and only if the corresponding symmetric function is twice (continuously) differentiable at the vector of eigenvalues. Thus in particular, a spectral function is $\mathcal{C}^2$ if and only if its restriction to the subspace of diagonal matrices is $\mathcal{C}^2$. We also give a concise and easy-to-use formula for the Hessian: the results in [17], for analytic functions, are rather implicit. The paper is self-contained and the results are derived essentially from scratch. In a parallel paper [10] we give an analogous characterization of those spectral functions that have a quadratic expansion at a point (but which may not be twice differentiable).

2 Notation and preliminary results

In what follows S^n will denote the Euclidean space of all $n \times n$ symmetric matrices with inner product $\langle A, B\rangle = \operatorname{tr}(AB)$ and for $A \in S^n$, $\lambda(A) = (\lambda_1(A), ..., \lambda_n(A))$ will be the vector of its eigenvalues ordered in nonincreasing order. By O^n we will denote the set of all $n \times n$ orthogonal matrices. For any vector x in $\mathbb{R}^n$, $\operatorname{Diag} x$ will denote the diagonal matrix with the vector x on the main diagonal, and $\bar{x}$ will denote the vector with the same entries as x ordered in nonincreasing order, that is $\bar{x}_1 \geq \bar{x}_2 \geq \cdots \geq \bar{x}_n$. Let $\mathbb{R}^n_{\downarrow}$ denote the set of all vectors x in $\mathbb{R}^n$ such that $x_1 \geq x_2 \geq \cdots \geq x_n$. Let also the operator $\operatorname{diag}: S^n \to \mathbb{R}^n$ be defined by $\operatorname{diag}(A) = (a_{11}, ..., a_{nn})$. In the whole paper $\{M_m\}_{m=1}^{\infty}$ will denote a sequence of symmetric matrices converging to 0, $\{U_m\}_{m=1}^{\infty}$ will denote a sequence of orthogonal matrices. We describe sets in $\mathbb{R}^n$ and functions on $\mathbb{R}^n$ as *symmetric* if they are invariant under coordinate permutations. Thus $f : \mathbb{R}^n \to \mathbb{R}$ will denote a function, defined on an open symmetric set, with the property

$$f(x) = f(Px) \text{ for any permutation matrix } P \text{ and any } x \in \operatorname{domain} f.$$

We denote the gradient of f by ∇f or f', and the Hessian by $\nabla^2 f$ or f''. In the whole work vectors are understood to be column vectors, unless stated otherwise. Whenever we denote by μ a vector in $\mathbb{R}^n_{\downarrow}$ we make the convention that

$$\mu_1 = \cdots = \mu_{k_1} > \mu_{k_1+1} = \cdots = \mu_{k_2} > \mu_{k_2+1} \cdots \mu_{k_r}, \qquad (k_0 = 0,\ k_r = n).$$

We define a corresponding partition

$$I_1 := \{1, 2, ..., k_1\},\ I_2 := \{k_1 + 1, k_1 + 2, ..., k_2\}, ...,\ I_r := \{k_{r-1} + 1, ..., k_r\},$$

and we call these sets *blocks*. We denote the standard basis in $\mathbb{R}^n$ by $e^1, e^2, ..., e^n$, and e is the vector with all entries equal to 1. We also define corresponding matrices

$$X_l := [e^{k_{l-1}+1}, ..., e^{k_l}], \text{ for all } l = 1, ..., r,$$

For an arbitrary matrix A, A^i will denote its i-th row (a row vector), and $A^{i,j}$ will denote its (i, j)-th entry. Finally, we say that a vector a is *block refined* by a vector b if

$$b_i = b_j \text{ implies } a_i = a_j \text{ for all } i, j.$$

We need the following result.

Lemma 2.1 *Let $f : \mathbb{R}^n \to \mathbb{R}$ be a symmetric function, twice differentiable at the point $\mu \in \mathbb{R}^n_\downarrow$, and let P be a permutation matrix such that $P\mu = \mu$. Then*

(i) $\nabla f(\mu) = P^T \nabla f(\mu)$, *and*

(ii) $\nabla^2 f(\mu) = P^T \nabla^2 f(\mu) P$.

In particular we have the representation

$$\nabla^2 f(\mu) = \begin{pmatrix} a_{11}E_{11} + b_{k_1}J_1 & a_{12}E_{12} & \cdots & a_{1r}E_{1r} \\ a_{21}E_{21} & a_{22}E_{22} + b_{k_2}J_2 & \cdots & a_{2r}E_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ a_{r1}E_{r1} & a_{r2}E_{r2} & \cdots & a_{rr}R_{rr} + b_{k_r}J_r \end{pmatrix},$$

where the E_{uv} are matrices of dimensions $|I_u| \times |I_v|$ with all entries equal to one, $(a_{ij})_{i,j=1}^r$ is a real symmetric matrix, $b := (b_1, ..., b_n)$ is a vector which is block refined by μ, and J_u is an identity matrix of the same dimensions as E_{uu}.

Proof. Just apply twice the chain rule to the equality $f(\mu) = f(P\mu)$ in order to get parts (i) and (ii). To deduce the block structure of the Hessian, consider the block structure of permutation matrices P such that $P\mu = \mu$: then, when we permute the rows and the columns of the Hessian in the way defined by P, it must stay unchanged. ■

Using the notation of this lemma, we define the matrix

$$B := \nabla^2 f(\mu) - \operatorname{Diag} b = (a_{ij}E_{ij})_{i,j=1}^r. \tag{1}$$

Note 2.2 *We make the convention that if the i-th diagonal block in the above representation has dimensions 1×1 then we set $a_{ii} = 0$ and $b_{k_i} = f''_{k_i k_i}(\mu)$. Otherwise the value of b_{k_i} is uniquely determined as the difference between a diagonal and an off-diagonal element of this block. Note also that the matrix B and the vector b depend on the point μ and the function f.*

Lemma 2.3 *For $\mu \in \mathbb{R}^n_\downarrow$ and a sequence of symmetric matrices $M_m \to 0$ we have that*

$$\lambda(\operatorname{Diag} \mu + M_m)^T = \mu^T + \big(\lambda(X_1^T M_m X_1)^T, ..., \lambda(X_r^T M_m X_r)^T\big) + o(\|M_m\|).$$

Proof. Combine Lemma 5.10 in [8] and Theorem 3.12 in [1]. ■

The following is our main technical tool.

Lemma 2.4 *Let $\{M_m\}$ be a sequence of symmetric matrices converging to 0, such that $M_m/\|M_m\|$ converges to M. Let μ be in $\mathbb{R}^n_\downarrow$ and $U_m \to U \in O^n$ be a sequence of orthogonal matrices such that*

$$\text{(2)} \quad \operatorname{Diag}\mu + M_m = U_m\big(\operatorname{Diag}\lambda(\operatorname{Diag}\mu + M_m)\big)U_m^T, \quad \textit{for all} \;\; m = 1, 2, \ldots.$$

Then the following properties hold.

(i) The orthogonal matrix U has the form

$$U = \begin{pmatrix} V_1 & 0 & \cdots & 0 \\ 0 & V_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & V_r \end{pmatrix},$$

where V_l is an orthogonal matrix with dimensions $|I_l| \times |I_l|$ for all l.

(ii) If $i \in I_l$ then

$$\lim_{m\to\infty} \frac{1 - \sum_{p\in I_l} (U_m^{i,p})^2}{\|M_m\|} = 0.$$

(iii) If i and j do not belong to the same block then

$$\lim_{m\to\infty} \frac{(U_m^{i,j})^2}{\|M_m\|} = 0.$$

(iv) If $i \in I_l$ then

$$V_l^i \left(\operatorname{Diag}\lambda(X_l^T M X_l)\right) (V_l^i)^T = M^{i,i}.$$

(v) If $i, j \in I_l$, and $p \notin I_l$ then

$$\lim_{m\to\infty} \frac{U_m^{i,p} U_m^{j,p}}{\|M_m\|} = 0.$$

(vi) For any indices $i \neq j$ such that $i, j \in I_l$,

$$\lim_{m\to\infty} \frac{\sum_{p\in I_l} U_m^{i,p} U_m^{j,p}}{\|M_m\|} = 0.$$

(vii) For any indices $i \neq j$ such that $i, j \in I_l$,

$$V_l^i \big(\operatorname{Diag} \lambda(X_l^T M X_l)\big)(V_l^j)^T = M^{i,j}.$$

(viii) For any three indices i, j, p in distinct blocks,

$$\lim_{m\to\infty} \frac{U_m^{i,p} U_m^{j,p}}{\|M_m\|} = 0.$$

(ix) For any two indices i, j such that $i \in I_l$, $j \in I_s$, where $l \neq s$,

$$\lim_{m\to\infty} \left(\mu_{k_l} \frac{\sum_{p\in I_l} U_m^{i,p} U_m^{j,p}}{\|M_m\|} + \mu_{k_s} \frac{\sum_{p\in I_s} U_m^{i,p} U_m^{j,p}}{\|M_m\|} \right) = M^{i,j}.$$

Proof.

(i) After taking the limit in equation (2) we are left with

$$(\operatorname{Diag} \mu) U = U (\operatorname{Diag} \mu).$$

The described representation of the matrix U follows.

(ii) Let us denote

$$h_m = \big(\lambda(X_1^T M_m X_1)^T, ..., \lambda(X_r^T M_m X_r)^T\big)^T. \tag{3}$$

We use Lemma 2.3 in equation (2) to obtain

$$\operatorname{Diag} \mu + M_m = U_m (\operatorname{Diag} \mu) U_m^T + U_m (\operatorname{Diag} h_m) U_m^T + o(\|M_m\|),$$

and the equivalent form

$$U_m^T (\operatorname{Diag} \mu) U_m + U_m^T M_m U_m = \operatorname{Diag} \mu + \operatorname{Diag} h_m + o(\|M_m\|).$$

We now divide both sides of these equations by $\|M_m\|$ and rearrange:

$$\frac{\operatorname{Diag} \mu - U_m (\operatorname{Diag} \mu) U_m^T}{\|M_m\|} = -\frac{M_m}{\|M_m\|} + \frac{U_m (\operatorname{Diag} h_m) U_m^T}{\|M_m\|} + o(1), \tag{4}$$

and

$$\text{(5)} \qquad \frac{\operatorname{Diag}\mu - U_m^T(\operatorname{Diag}\mu)U_m}{\|M_m\|} = \frac{U_m^T M_m U_m}{\|M_m\|} - \frac{\operatorname{Diag} h_m}{\|M_m\|} - o(1).$$

Notice that the right hand sides of these equations converge to a finite limit as m increases to infinity. If we call the matrix limit of the right hand side of the first equation L, then clearly the limit of the second equation is $-U^T LU$.

We are now going to prove parts (ii) and (iii) together inductively, by dividing the orthogonal matrix U_m into the same block structure as U. We begin by considering the first row of blocks of U_m.

Let i be an index in the first block, I_1. Then the limit of the (i,i)-th entry in the matrix at the left hand side of equation (4) is

$$\text{(6)} \quad \lim_{m\to\infty} \frac{\left(\mu_{k_1}\left(1 - \sum_{p\in I_1} (U_m^{i,p})^2\right) - \sum_{s=2}^r \mu_{k_s} \sum_{p\in I_s} (U_m^{i,p})^2\right)}{\|M_m\|} = L^{i,i}.$$

Now recall that

$$L^{i,i} = -M^{i,i} + V_1^i(\operatorname{Diag}\lambda(X_1^T M X_1))(V_1^i)^T,$$

and because V_1 is an orthogonal matrix, notice that

$$\begin{aligned}
\sum_{i\in I_1} L^{i,i} &= -\operatorname{tr}(X_1^T M X_1) + \sum_{i\in I_1} V_1^i(\operatorname{Diag}\lambda(X_1^T M X_1))(V_1^i)^T \\
&= -\operatorname{tr}(X_1^T M X_1) + \sum_{i\in I_1} \lambda_i(X_1^T M X_1) \sum_{j\in I_1} (V_1^{j,i})^2 \\
&= -\operatorname{tr}(X_1^T M X_1) + \sum_{i\in I_1} \lambda_i(X_1^T M X_1) \\
&= 0.
\end{aligned}$$

We now sum equation (6) over all i in I_1 to get

$$\lim_{m\to\infty} \frac{\left(\mu_{k_1}\left(|I_1| - \sum_{i,p\in I_1} (U_m^{i,p})^2\right) - \sum_{s=2}^r \mu_{k_s} \sum_{i\in I_1,\, p\in I_s} (U_m^{i,p})^2\right)}{\|M_m\|} = 0.$$

Notice here, that the coefficients in front of the μ_{k_l}, $l = 1, 2, ..., r$ in the numerator sum up to zero. That is,

$$|I_1| - \sum_{i,p \in I_1} \left(U_m^{i,p}\right)^2 - \sum_{s=2}^{r} \sum_{i \in I_1,\, p \in I_s} \left(U_m^{i,p}\right)^2 = 0.$$

So let us choose a number α such that

$$(\mu + \alpha e)_{k_1} > 0 > (\mu + \alpha e)_{k_1+1},$$

and add α to every coordinate of the vector μ thus "shifting" it. The coordinates of the shifted vector that are in the first block are strictly bigger than zero, and the rest are strictly less than zero. By our comment above, the last limit remains true if we "shift" μ in this way. If we rewrite the last limit for the "shifted" vector, because all summands are positive, we immediately see that we must have

$$\lim_{m \to \infty} \frac{|I_1| - \sum_{i,p \in I_1} \left(U_m^{i,p}\right)^2}{\|M_m\|} = 0$$

and

$$\lim_{m \to \infty} \frac{\sum_{i \in I_1,\, p \in I_s} \left(U_m^{i,p}\right)^2}{\|M_m\|} = 0, \quad \text{for all } \ s = 2, .., r.$$

The first of these limits can be written as

$$\lim_{m \to \infty} \frac{\sum_{i \in I_1} \left(1 - \sum_{p \in I_1} \left(U_m^{i,p}\right)^2\right)}{\|M_m\|} = 0,$$

and because all the summands are positive, we conclude that

$$\lim_{m \to \infty} \frac{1 - \sum_{p \in I_1} \left(U_m^{i,p}\right)^2}{\|M_m\|} = 0, \quad \text{for all } i \in I_1.$$

The second of the limits implies immediately that

$$\lim_{m \to \infty} \frac{\left(U_m^{i,p}\right)^2}{\|M_m\|} = 0, \ \text{ for any } i \in I_1,\, p \notin I_1.$$

Thus we proved part (ii) for $i \in I_1$ and part (iii) for the cases specified above.

Here is a good place to say a few more words about the idea of the proof. As we said, we divide the matrix U_m into blocks complying with the block structure of the vector μ (exactly as in part (i) for the matrix U). We proved part (ii) and (iii) for the elements in the first row of blocks of this division. What we are going to do now is prove the same thing for the first *column* of blocks. In order to do this we fix an index i in I_1 and consider the (i,i)-th entry in the matrix at the left hand side of equation (5), and take the limit:

$$\lim_{m\to\infty} \frac{\mu_{k_1}\left(1-\sum_{p\in I_1}\left(U_m^{p,i}\right)^2\right)-\sum_{s=2}^r \mu_{k_s}\sum_{p\in I_s}\left(U_m^{p,i}\right)^2}{\|M_m\|}$$

$$= -(U^T L U)^{i,i}. \tag{7}$$

Using also the block-diagonal structure of the matrix U, we again have

$$\sum_{i\in I_1}(U^T L U)^{i,i} = \sum_{i\in I_1} L^{i,i} = 0.$$

So we proceed just as before in order to conclude that

$$\lim_{m\to\infty} \frac{1-\sum_{p\in I_1}\left(U_m^{p,i}\right)^2}{\|M_m\|} = 0, \quad \text{for all } i \in I_1,$$

and

$$\lim_{m\to\infty} \frac{\left(U_m^{p,i}\right)^2}{\|M_m\|} = 0, \quad \text{for any } i \in I_1,\ p \notin I_1. \tag{8}$$

We are now ready for the second step of our induction. Let i be an index in I_2. Then the limit of the (i,i)-th entry in the matrix at the left hand side of equation (4) is

$$\lim_{m\to\infty}\frac{1}{\|M_m\|}\Bigg(-\mu_{k_1}\sum_{p\in I_1}\left(U_m^{i,p}\right)^2+\mu_{k_2}\Big(1-\sum_{p\in I_2}\left(U_m^{i,p}\right)^2\Big)-$$
$$\sum_{s=3}^{r}\mu_{k_s}\sum_{p\in I_s}\left(U_m^{i,p}\right)^2\Bigg) = L^{i,i}.$$

Analogously as above we have

$$\sum_{i\in I_2} L^{i,i} = 0,$$

so summing the above limit over all i in I_2 we get

$$\lim_{m\to\infty} \frac{1}{\|M_m\|}\Bigg(-\mu_{k_1} \sum_{i\in I_2,\, p\in I_1} \left(U_m^{i,p}\right)^2 + \mu_{k_2}\Big(|I_2| - \sum_{i,p\in I_2} \left(U_m^{i,p}\right)^2\Big) - \sum_{s=3}^{r} \mu_{k_s} \sum_{i\in I_2,\, p\in I_s} \left(U_m^{i,p}\right)^2 \Bigg) = 0.$$

We know from (8) that

$$\lim_{m\to\infty} \frac{\sum_{i\in I_2,\, p\in I_1} \left(U_m^{i,p}\right)^2}{\|M_m\|} = 0.$$

So now we choose a number α such that

$$(\mu + \alpha e)_{k_2} > 0 > (\mu + \alpha e)_{k_2+1}$$

and as before exchange μ with its shifted version. Just as before we conclude that

$$\lim_{m\to\infty} \frac{1 - \sum_{p\in I_2} \left(U_m^{i,p}\right)^2}{\|M_m\|} = 0, \ \text{ for all } i \in I_2,$$

and

$$\lim_{m\to\infty} \frac{\left(U_m^{i,p}\right)^2}{\|M_m\|} = 0, \ \text{ for any } i \in I_2,\ p \notin I_2.$$

We repeat the same steps for the second column of blocks in the matrix U_m and so on inductively until we exhaust all the blocks. This completes the proof of parts (ii) and (iii).

(iv) For the proof of this part, one needs to consider the (i,i)-th entry of the right hand side of equation (4). Because the diagonal of the left hand side converges to zero (by (ii) and (iii)), taking the limit proves the statement in this part.

(v) This part follows immediately from part (iii).

(vi) Taking the limit in equation (4) gives

$$\lim_{m\to\infty} -\sum_{s\neq l} \mu_{k_s} \frac{\sum_{p\in I_s} U_m^{i,p} U_m^{j,p}}{\|M_m\|} - \mu_{k_l} \frac{\sum_{p\in I_l} U_m^{i,p} U_m^{j,p}}{\|M_m\|} = L^{i,j},$$

where $L^{i,j}$ is the (i,j)-th entry of the limit of the right hand side of equation (4). Note that the coefficients of μ_{k_s} again sum up to zero:

$$\sum_{s\neq l} \sum_{p\in I_s} U_m^{i,p} U_m^{j,p} + \sum_{p\in I_l} U_m^{i,p} U_m^{j,p} = 0,$$

because U_m is an orthogonal matrix. Now by part (v) we have

$$0 = \lim_{m\to\infty} -\sum_{s\neq l} \frac{\sum_{p\in I_s} U_m^{i,p} U_m^{j,p}}{\|M_m\|} = \lim_{m\to\infty} \frac{\sum_{p\in I_l} U_m^{i,p} U_m^{j,p}}{\|M_m\|},$$

as required, and moreover $L^{i,j} = 0$.

(vii) The statement of this part is the detailed way of writing the fact, proved in the previous part, that $L^{i,j} = 0$.

(viii) This part follows immediately from part (iii). (In fact the expression in part (viii) is identical to the one in part (v), re-iterated with different index conditions for later convenience.)

(ix) We again take the limit of the (i,j)-th entry of the matrices on both sides of equation (4).

$$\lim_{m\to\infty} \Bigg(-\sum_{t\neq l,s} \mu_{k_t} \frac{\sum_{p\in I_t} U_m^{i,p} U_m^{j,p}}{\|M_m\|} - \mu_{k_l} \frac{\sum_{p\in I_l} U_m^{i,p} U_m^{j,p}}{\|M_m\|} - \mu_{k_s} \frac{\sum_{p\in I_s} U_m^{i,p} U_m^{j,p}}{\|M_m\|} \Bigg) = L^{i,j}.$$

By part (viii) we have that all but the l-th and the s-th summand above converge to zero. On the other hand

$$\begin{aligned} L^{i,j} &= \lim_{m\to\infty} \Big(-\frac{M_m}{\|M_m\|} + \frac{U_m(\operatorname{Diag} h_m)U_m^T}{\|M_m\|} \Big)^{i,j} \\ &= -M^{i,j} + U^i \Big(\lim_{m\to\infty} \frac{\operatorname{Diag} h_m}{\|M_m\|} \Big) (U^j)^T \\ &= -M^{i,j}, \end{aligned}$$

because U^i and U^j are rows in different blocks and $(\mathrm{Diag}\, h_m)/\|M_m\|$ converges to a diagonal matrix. $\blacksquare$

Now we have all the tools to prove the main result of the paper.

3 Twice differentiable spectral functions

In this section we prove that a symmetric function f is twice differentiable at the point $\lambda(A)$ if and only if the corresponding spectral function $f \circ \lambda$ is twice differentiable at the matrix A.

Recall that the Hadamard product of two matrices $A = [A^{i,j}]$ and $B = [B^{i,j}]$ of the same size is the matrix of their elementwise product $A \circ B = [A^{i,j}B^{i,j}]$. Let the symmetric function $f : \mathbb{R}^n \to \mathbb{R}$ be twice differentiable at the point $\mu \in \mathbb{R}^n_{\downarrow}$, where

$$\mu_1 = \cdots = \mu_{k_1} > \mu_{k_1+1} = \cdots = \mu_{k_2} > \mu_{k_2+1} \cdots \mu_{k_r}, \qquad (k_0 = 0,\ k_r = n).$$

We define the vector $b(\mu) = (b_1(\mu), ..., b_n(\mu))$ as in Lemma 2.1. Specifically, for any index i, (say $i \in I_l$ for some $l \in \{1, 2, ..., r\}$) we define

$$b_i(\mu) = \begin{cases} f''_{ii}(\mu), & \text{if } |I_l| = 1. \\ f''_{pp}(\mu) - f''_{pq}(\mu), & \text{for any } p \neq q \in I_l. \end{cases}$$

Lemma 2.1 guarantees that the second case of this definition doesn't depend on the choice of p and q. We also define the matrix $\mathcal{A}(\mu)$:

$$\mathcal{A}^{i,j}(\mu) = \begin{cases} 0, & \text{if } \ i = j. \\ b_i(\mu), & \text{if } \ i \neq j \text{ but } i, j \in I_l. \\ \frac{f'_i(\mu) - f'_j(\mu)}{\mu_i - \mu_j}, & \text{else }. \end{cases} \tag{9}$$

For simplicity, when the argument is understood by the context, we will write just b_i and $\mathcal{A}^{i,j}$. The following lemma is Theorem 1.1 in [7].

Lemma 3.1 *Let $A \in S^n$ and suppose $\lambda(A)$ belongs to the domain of the symmetric function $f : \mathbb{R}^n \to \mathbb{R}$. Then f is differentiable at the point $\lambda(A)$ if and only if $f \circ \lambda$ is differentiable at the point A. In that case we have the formula*

$$\nabla(f \circ \lambda)(A) = U\big(\mathrm{Diag}\, \nabla f(\lambda(A))\big)U^T,$$

for any orthogonal matrix U satisfying $A = U\big(\mathrm{Diag}\, \lambda(A)\big)U^T$.

We recall some standard notions about twice differentiability. Consider a function F from S^n to $\mathbb{R}$. Its gradient at any point A (when it exists) is a linear functional on the Euclidean space S^n, and thus can be identified with an element of S^n, which we denote $\nabla F(A)$. Thus ∇F is a map from S^n to S^n. When this map is itself differentiable at A we say F is *twice differentiable* at A. In this case we can interpret the Hessian $\nabla^2 F(A)$ as a symmetric, bilinear function from $S^n \times S^n$ into $\mathbb{R}$. Its value at a particular point $(H, Y) \in S^n \times S^n$ will be denoted $\nabla^2 F(A)[H, Y]$. In particular, for fixed H, the function $\nabla^2 F(A)[H, \cdot]$ is again a linear functional on S^n, which we consider an element of S^n, for brevity denoted by $\nabla^2 F(A)[H]$. When the Hessian is continuous at A we say F is *twice continuously differentiable* at A. In that case the following identity holds:

$$\nabla^2 F(A)[H, H] = \frac{d^2}{dt^2} F(A + tH)\bigg|_{t=0}.$$

The next theorem is a preliminary version of our main result.

Theorem 3.2 *The symmetric function $f : \mathbb{R}^n \to \mathbb{R}$ is twice differentiable at the point $\mu \in \mathbb{R}^n_{\downarrow}$ if and only if $f \circ \lambda$ is twice differentiable at the point* $\operatorname{Diag} \mu$. *In that case the Hessian is given by*

$$\nabla^2 (f \circ \lambda)(\operatorname{Diag} \mu)[H] \;=\; \operatorname{Diag}\big(\nabla^2 f(\mu)(\operatorname{diag} H)\big) + \mathcal{A} \circ H. \tag{10}$$

Hence

$$\nabla^2 (f \circ \lambda)(\operatorname{Diag} \mu)[H, H] = \nabla^2 f(\mu)[\operatorname{diag} H, \operatorname{diag} H] + \langle \mathcal{A}, H \circ H \rangle.$$

Proof. It is easy to see that f must be twice differentiable at the point μ whenever $f \circ \lambda$ is twice differentiable at $\operatorname{Diag} \mu$ because by restricting $f \circ \lambda$ to the subspace of diagonal matrices we get the function f. So the interesting case is the other direction. Let f be twice differentiable at the point $\mu \in \mathbb{R}^n_{\downarrow}$ and suppose on the contrary that either $f \circ \lambda$ is not twice differentiable at the point $\operatorname{Diag} \mu$, or equation (10) fails. Define a linear operator Δ by

$$\Delta(H) := \operatorname{Diag}\big((\nabla^2 f(\mu)(\operatorname{diag} H)\big) + \mathcal{A} \circ H.$$

(Lemma 3.1 tells us that $f \circ \lambda$ is at least differentiable around $\operatorname{Diag} \mu$.) So, for this linear operator Δ there is an $\epsilon > 0$ and a sequence of symmetric matrices $\{M_m\}_{m=1}^{\infty}$ converging to 0 such that

$$\frac{\|\nabla (f \circ \lambda)(\operatorname{Diag} \mu + M_m) - \nabla (f \circ \lambda)(\operatorname{Diag} \mu) - \Delta(M_m)\|}{\|M_m\|} > \epsilon$$

for all $m = 1, 2, \ldots$. Without loss of generality we may assume that the sequence $\{M_m\}_{m=1}^{\infty}$ is such that $M_m/\|M_m\|$ converges to a matrix M, because some subsequence of $\{M_m\}_{m=1}^{\infty}$ surely has this property. Let $\{U_m\}_{m=1}^{\infty}$ be a sequence of orthogonal matrices such that

$$\operatorname{Diag}\mu + M_m = U_m\big(\operatorname{Diag}\lambda(\operatorname{Diag}\mu + M_m)\big)U_m^T, \quad \text{for all} \quad m = 1, 2, \ldots.$$

Without loss of generality we may assume that $U_m \to U \in O^n$, or otherwise we will just take subsequences of $\{M_m\}_{m=1}^{\infty}$ and $\{U_m\}_{m=1}^{\infty}$. The above inequality shows that for every m there corresponds a pair (or more precisely at least one pair) of indices (i, j) such that

$$\frac{|\big(\nabla(f \circ \lambda)(\operatorname{Diag}\mu + M_m) - \operatorname{Diag}\nabla f(\mu) - \Delta(M_m)\big)^{i,j}|}{\|M_m\|} > \frac{\epsilon}{n}. \tag{11}$$

So at least for one pair of indices, call it again (i, j), we have infinitely many numbers m for which (i, j) is the corresponding pair, and because if necessary we can again take a subsequence of $\{M_m\}_{m=1}^{\infty}$ and $\{U_m\}_{m=1}^{\infty}$ we may assume without loss of generality that there is a pair of indices (i, j) for which the last inequality holds for all $m = 1, 2, \ldots$. Define the symbol h_m again by equation (3). Notice that using Lemma 3.1, Lemma 2.3, and the fact that ∇f is differentiable at μ, we get

$$\begin{aligned}
\nabla(f \circ \lambda)(\operatorname{Diag}\mu + M_m) &= U_m\big(\operatorname{Diag}\nabla f(\lambda(\operatorname{Diag}\mu + M_m))\big)U_m^T \\
&= U_m\big(\operatorname{Diag}\nabla f(\mu + h_m + o(\|M_m\|))\big)U_m^T \\
&= U_m(\operatorname{Diag}(\nabla f(\mu) + \nabla^2 f(\mu)h_m + o(\|M_m\|)))U_m^T \\
&= U_m(\operatorname{Diag}\nabla f(\mu))U_m^T + U_m(\operatorname{Diag}(\nabla^2 f(\mu)h_m))U_m^T + o(\|M_m\|).
\end{aligned} \tag{12}$$

We consider three cases. In every case we are going to show that the left hand side of inequality (11) actually converges to zero, which contradicts the assumption.

Case I. If $i = j$, then using equation (12) the left hand side of inequality (11) is less that or equal to

$$\frac{|U_m^i\big(\operatorname{Diag}\nabla f(\mu)\big)(U_m^i)^T - f_i'(\mu)|}{\|M_m\|} + \frac{|U_m^i\big(\operatorname{Diag}\nabla^2 f(\mu)h_m\big)(U_m^i)^T - \big(\nabla^2 f(\mu)(\operatorname{diag}M_m)\big)_i|}{\|M_m\|} + o(1).$$

We are going to show that each summand approaches zero as m goes to infinity. Assume that $i \in I_l$ for some $l \in \{1, ..., r\}$. Using the fact that the vector μ block refines the vector $\nabla f(\mu)$ (Lemma 2.1, part (i)) the first term can be written as

$$\frac{1}{\|M_m\|}\left| f'_{k_l}(\mu)\Big(1 - \sum_{p\in I_l} \big(U_m^{i,p}\big)^2\Big) - \sum_{s: s\neq l} f'_{k_s}(\mu) \sum_{p\in I_s} \big(U_m^{i,p}\big)^2 \right|.$$

We apply now Lemma 2.4 parts (ii) and (iii) to the last expression.

We now concentrate on the second term above. Using the notation of equation (1) (that is, $\nabla^2 f(\mu) = B + \mathrm{Diag}\, b$) this term is less than or equal to

$$\begin{aligned} &\frac{|U_m^i\big(\mathrm{Diag}\,(Bh_m)\big)(U_m^i)^T - \big(B(\mathrm{diag}\, M_m)\big)_i|}{\|M_m\|} \\ &\qquad + \frac{|U_m^i\big(\mathrm{Diag}\,((\mathrm{Diag}\, b)h_m)\big)(U_m^i)^T - \big((\mathrm{Diag}\, b)(\mathrm{diag}\, M_m)\big)_i|}{\|M_m\|}. \end{aligned} \tag{13}$$

As m approaches infinity, we have that $U_m^i \to U^i$. We define the vector h to be:

$$h := \lim_{m\to\infty} \frac{h_m}{\|M_m\|} = \big(\lambda(X_1^T M X_1)^T, ..., \lambda(X_r^T M X_r)^T\big)^T.$$

So taking limits, expression (13) turn into:

$$\begin{aligned} &|U^i\big(\mathrm{Diag}\,(Bh)\big)(U^i)^T - \big(B(\mathrm{diag}\, M)\big)_i| \\ &\qquad + |U^i\big(\mathrm{Diag}\,((\mathrm{Diag}\, b\big)h))(U^i)^T - \big((\mathrm{Diag}\, b)(\mathrm{diag}\, M)\big)_i|. \end{aligned}$$

We are going to investigate each absolute value separately and show that they are both actually equal to zero. For the first, we use the block structure of the matrix B (see Lemma 2.1) and the block structure of the vector h to obtain

$$(Bh)_j = \sum_{s=1}^{r} a_{qs} \mathrm{tr}\,(X_s^T M X_s), \quad \text{when } j \in I_q.$$

Using the fact that $i \in I_l$ and that V_l is orthogonal we get

$$\begin{aligned}
U^i\big(\mathrm{Diag}\,(Bh)\big)(U^i)^T &= \big(V_l^i X_l^T\big)\big(\mathrm{Diag}\,(Bh)\big)\big(X_l(V_l^i)^T\big) \\
&= V_l^i\big(X_l^T(\mathrm{Diag}\,(Bh))X_l\big)(V_l^i)^T \\
&= \Big(\sum_{s=1}^{r} a_{ls}\mathrm{tr}\,(X_s^T M X_s)\Big)\Big(\sum_{s=1}^{|I_l|}(V_l^{i,s})^2\Big) \\
&= \sum_{s=1}^{r} a_{ls}\mathrm{tr}\,(X_s^T M X_s) \\
&= (B\mathrm{diag}\,M)_i,
\end{aligned}$$

which shows that the first absolute value is zero. For the second absolute value, we use the block structure of the vector b, to write

$$(\mathrm{Diag}\,b)h = \big(b_{k_1}\lambda(X_1^T M X_1)^T, ..., b_{k_r}\lambda(X_r^T M X_r)^T\big)^T.$$

In the next to the last equality below we use part (iv) of Lemma 2.4:

$$\begin{aligned}
U^i\big(\mathrm{Diag}\,((\mathrm{Diag}\,b)h)\big)(U^i)^T &= \big(V_l^i X_l^T\big)\big(\mathrm{Diag}\,((\mathrm{Diag}\,b)h)\big)\big(X_l(V_l^i)^T\big) \\
&= V_l^i\big(X_l^T(\mathrm{Diag}\,((\mathrm{Diag}\,b)h))X_l\big)(V_l^i)^T \\
&= V_l^i\big(\mathrm{Diag}\,b_{k_l}\lambda(X_l^T M X_l)\big)(V_l^i)^T \\
&= b_{k_l}M^{i,i} \\
&= \big((\mathrm{Diag}\,b)(\mathrm{diag}\,M)\big)_i.
\end{aligned}$$

We can see now that the second absolute value is also zero.

Case II. If $i \neq j$ but $i, j \in I_l$ for some $l \in \{1, 2, ...r\}$, then using equation (12) the left hand side of inequality (11) becomes

$$\frac{|U_m^i\big(\mathrm{Diag}\,\nabla f(\mu)\big)(U_m^j)^T + U_m^i\big(\mathrm{Diag}\,(\nabla^2 f(\mu)h_m)\big)(U_m^j)^T - b_{k_l}M_m^{i,j}|}{\|M_m\|} + o(1).$$

Using the fact that μ block refines vector $\nabla f(\mu)$, we can write the first summand in the absolute value as

$$\frac{1}{\|M_m\|}\Big(\sum_{s\neq l} f'_{k_s}(\mu)\sum_{p\in I_s} U_m^{i,p}U_m^{j,p} + f'_{k_l}(\mu)\sum_{p\in I_l} U_m^{i,p}U_m^{j,p}\Big).$$

We use parts (v) and (vi) of Lemma 2.4 to conclude that this expression converges to zero. We are left with

$$\frac{|U_m^i\big(\mathrm{Diag}\,(\nabla^2 f(\mu)h_m)\big)(U_m^j)^T - b_{k_l}M_m^{i,j}|}{\|M_m\|}.$$

Substituting above $\nabla^2 f(\mu) = B + \mathrm{Diag}\, b$ we get

$$\frac{|U_m^i\big(\mathrm{Diag}\,(Bh_m)\big)(U_m^j)^T + U_m^i\big(\mathrm{Diag}\,((\mathrm{Diag}\, b)h_m)\big)(U_m^j)^T - b_{k_l}M_m^{i,j}|}{\|M_m\|}.$$

Recall the notation from Lemma 2.1 used to denote the entries of the matrix B. Then the limit of the first summand above can be written as

$$\begin{aligned}\lim_{m\to\infty}\frac{|U_m^i\big(\mathrm{Diag}\,(Bh_m)\big)(U_m^j)^T|}{\|M_m\|} &= |U^i\big(\mathrm{Diag}\,(Bh)\big)(U^j)^T| \\ &= \sum_{s=1}^{r}\bigg(\Big(\sum_{l=1}^{r} a_{sl}\,\mathrm{tr}\,(X_l^T M X_l)\Big)\sum_{p\in I_s} U^{i,p}U^{j,p}\bigg) \\ &= 0,\end{aligned}$$

because clearly $\sum_{p\in I_s} U^{i,p}U^{j,p} = 0$ for all $s \in \{1, 2, ...r\}$. We are left with the following limit

$$\begin{aligned}\lim_{m\to\infty}&\frac{|U_m^i\big(\mathrm{Diag}\,((\mathrm{Diag}\, b)h_m)\big)(U_m^j)^T - b_{k_l}M_m^{i,j}|}{\|M_m\|} \\ &\qquad = |U^i\big(\mathrm{Diag}\,((\mathrm{Diag}\, b)h)\big)(U^j)^T - b_{k_l}M^{i,j}|.\end{aligned}$$

Using Lemma 2.4 part (vii) we observe that the last absolute value is zero.

Case III. If $i \in I_l$ and $j \in I_s$, where $l \neq s$, then using equation (12), the left hand side of inequality (11) becomes (up to $o(1)$)

$$\frac{|U_m^i\big(\mathrm{Diag}\,\nabla f(\mu)\big)(U_m^j)^T + U_m^i\big(\mathrm{Diag}\,\nabla^2 f(\mu)h_m\big)(U_m^j)^T - \frac{f'_{k_l}(\mu)-f'_{k_s}(\mu)}{\mu_{k_l}-\mu_{k_s}}M_m^{i,j}|}{\|M_m\|}.$$

We start with the second term above. Its limit is

$$\lim_{m\to\infty}\frac{U_m^i\big(\mathrm{Diag}\,(\nabla^2 f(\mu)h_m)\big)(U_m^j)^T}{\|M_m\|} = U^i\big(\mathrm{Diag}\,(\nabla^2 f(\mu)h)\big)(U^j)^T = 0,$$

because in our case, U^i has nonzero coordinates where the entries of U^j are zero. We are left with

$$\lim_{m\to\infty}\left|\frac{U^i_m\big(\mathrm{Diag}\,\nabla f(\mu)\big)(U^j_m)^T}{\|M_m\|}-\frac{f'_{k_l}(\mu)-f'_{k_s}(\mu)}{\mu_{k_l}-\mu_{k_s}}\frac{M^{i,j}_m}{\|M_m\|}\right|. \tag{14}$$

We expand the first term in this limit.

$$\frac{U^i_m\big(\mathrm{Diag}\,\nabla f(\mu)\big)(U^j_m)^T}{\|M_m\|}=f'_{k_l}(\mu)\frac{\sum_{p\in I_l}U^{i,p}_mU^{j,p}_m}{\|M_m\|}+$$

$$f'_{k_s}(\mu)\frac{\sum_{p\in I_s}U^{i,p}_mU^{j,p}_m}{\|M_m\|}+\sum_{t\neq l,s}f'_{k_t}(\mu)\frac{\sum_{p\in I_t}U^{i,p}_mU^{j,p}_m}{\|M_m\|}.$$

Using Lemma 2.4 part (viii) we see that the third summand above converges to zero as m goes to infinity. Part (ix) of the same lemma tells us that

$$\lim_{m\to\infty}\frac{M^{i,j}_m}{\|M_m\|}=\lim_{m\to\infty}\left(\mu_{k_l}\frac{\sum_{p\in I_l}U^{i,p}_mU^{j,p}_m}{\|M_m\|}+\mu_{k_s}\frac{\sum_{p\in I_s}U^{i,p}_mU^{j,p}_m}{\|M_m\|}\right).$$

In order to abbreviate the formulae we introduce the following notation

$$\beta^l_m:=\frac{\sum_{p\in I_l}U^{i,p}_mU^{j,p}_m}{\|M_m\|},\qquad \text{for all}\quad l=1,2,...,r.$$

Substituting everything in (14) we get the following equivalent limit:

$$\lim_{m\to\infty}\left|\Big(f'_{k_l}(\mu)\beta^l_m+f'_{k_s}(\mu)\beta^s_m\Big)-\frac{f'_{k_l}(\mu)-f'_{k_s}(\mu)}{\mu_{k_l}-\mu_{k_s}}\big(\mu_{k_l}\beta^l_m+\mu_{k_s}\beta^s_m\big)\right|.$$

Simplifying we get

$$\lim_{m\to\infty}(\beta^l_m+\beta^s_m)\frac{f'_{k_s}(\mu)\mu_{k_l}-f'_{k_l}(\mu)\mu_{k_s}}{\mu_{k_l}-\mu_{k_s}}.$$

Notice now that

$$\sum_{l=1}^r\beta^l_m=0,\quad \text{for all}\ \ m,$$

because U_m is an orthogonal matrix and the numerator of the above sum is the product of its i-th and the j-th row. Next, Lemma 2.4, part (viii) says that

$$\lim_{m\to\infty}\sum_{t\neq l,s}\beta^t_m=0,$$

so

$$\lim_{m\to\infty}(\beta_m^l+\beta_m^s)=0,$$

which completes the proof. ■

We are finally ready to give and prove the full version of our main result.

Theorem 3.3 *Let A be an $n\times n$ symmetric matrix. The symmetric function $f:\mathbb{R}^n\to\mathbb{R}$ is twice differentiable at the point $\lambda(A)$ if and only if the spectral function $f\circ\lambda$ is twice differentiable at the matrix A. Moreover in this case the Hessian of the spectral function at the matrix A is*

$$\nabla^2(f\circ\lambda)(A)[H]=W\big(\mathrm{Diag}\,\big(\nabla^2 f(\lambda(A))\mathrm{diag}\,\tilde{H}\big)+\mathcal{A}\circ\tilde{H}\big)W^T,$$

where W is any orthogonal matrix such that $A=W\big(\mathrm{Diag}\,\lambda(A)\big)W^T$, $\tilde{H}=W^THW$, and $\mathcal{A}=\mathcal{A}(\lambda(A))$ is defined by equation (9). Hence

$$\nabla^2(f\circ\lambda)(A)[H,H]=\nabla^2 f(\lambda(A))[\mathrm{diag}\,\tilde{H},\mathrm{diag}\,\tilde{H}]+\langle\mathcal{A},\tilde{H}\circ\tilde{H}\rangle.$$

Proof. Let W be an orthogonal matrix which diagonalizes A in an ordered fashion, that is

$$A=W\big(\mathrm{Diag}\,\lambda(A)\big)W^T.$$

Let M_m be a sequence of symmetric matrices converging to zero, and let U_m be a sequence of orthogonal matrices such that

$$\mathrm{Diag}\,\lambda(A)+W^TM_mW=U_m\big(\mathrm{Diag}\,\lambda(\mathrm{Diag}\,\lambda(A)+W^TM_mW)\big)U_m^T.$$

Then using Lemma 3.1 we get

$$\begin{aligned}
&\nabla(f\circ\lambda)(A+M_m)\\
&\quad=\ \nabla(f\circ\lambda)\big(W(\mathrm{Diag}\,\lambda(A)+W^TM_mW)W^T\big)\\
&\quad=\ \nabla(f\circ\lambda)\big(WU_m(\mathrm{Diag}\,\lambda(\mathrm{Diag}\,\lambda(A)+W^TM_mW))U_m^TW^T\big)\\
&\quad=\ WU_m\big(\mathrm{Diag}\,\nabla f(\lambda(\mathrm{Diag}\,\lambda(A)+W^TM_mW))\big)U_m^TW^T.
\end{aligned}$$

We also have that

$$\nabla(f\circ\lambda)(A)=W\big(\mathrm{Diag}\,\nabla f(\lambda(A))\big)W^T,$$

and $W^TM_mW\to 0$, as m goes to infinity. Because W is an orthogonal matrix we have $\|WXW^T\|=\|X\|$ for any matrix X. It is now easy to check the result by Theorem 3.2. ■

4 Continuity of the Hessian

Suppose now the symmetric function $f : \mathbb{R}^n \to \mathbb{R}$ is twice differentiable in a neighbourhood of the point $\lambda(A)$ and its Hessian is continuous at the point $\lambda(A)$. Then $f \circ \lambda$ as we saw above will be twice differentiable in a neighbourhood of the point A, and in this section we are going to show that $\nabla^2(f \circ \lambda)$ is also continuous at the point A.

We define a basis, $\{H_{ij}\}$, on the space of symmetric matrices. If $i \neq j$ all the entries of the matrix H_{ij} are zeros, except the (i,j)-th and (j,i)-th, which are one. If $i = j$ we have one only on the (i,i)-th position. It suffices to prove that the Hessian is continuous when applied to any matrix of the basis. We begin with a lemma treating in some sense all special cases at once.

Lemma 4.1 *Let $\mu \in \mathbb{R}^n_\downarrow$ be such that*

$$\mu_1 = \cdots = \mu_{k_1} > \mu_{k_1+1} = \cdots = \mu_{k_2} > \mu_{k_2+1} \cdots \mu_{k_r}, \qquad (k_0 = 0,\ k_r = n).$$

and let the symmetric function $f : \mathbb{R}^n \to \mathbb{R}$ be twice continuously differentiable at the point μ. Let $\{\mu^m\}_{m=1}^\infty$ be a sequence of vectors in $\mathbb{R}^n$ converging to μ. Then

$$\lim_{m\to\infty} \nabla^2(f \circ \lambda)(\mathrm{Diag}\,\mu^m) = \nabla^2(f \circ \lambda)(\mathrm{Diag}\,\mu).$$

Proof. For every m there is a permutation matrix P_m such that $P_m^T \mu^m = \overline{\mu^m}$. (See the beginning of Section 2 for the meaning of the bar above a vector.) But there are finitely many permutation matrices (namely $n!$) so we can form $n!$ subsequences of $\{\mu^m\}$ such that any two vectors in a particular subsequence can be ordered in descending order by the same permutation matrix. If we prove the lemma for every such subsequence we will be done. So without loss of generality we may assume that $P^T \mu^m = \overline{\mu^m}$ for every m, and some fixed permutation matrix P. Clearly for all large enough m, we are going to have

$$\mu^m_{k_1} > \mu^m_{k_1+1}, \quad \mu^m_{k_2} > \mu^m_{k_2+1}, \cdots, \mu^m_{k_{r-1}} > \mu^m_{k_{r-1}+1},$$

Consequently the matrix P is block-diagonal with permutation matrices on the main diagonal, and dimensions matching the block structure of μ, so $P\mu = \mu$. Consider now the block structure of the vectors $\{\overline{\mu^m}\}$. Because there are finitely many different block structures, we can divide this sequence into subsequences such that the vectors in a particular subsequence have the same block structure. If we prove the lemma for each subsequence we will be done. So without loss of generality we may assume that the vectors $\{\overline{\mu^m}\}$ have the same block structure for every m. Next, using the formula for the Hessian in Theorem 3.3 we have

$$\begin{aligned}&\nabla^2(f\circ\lambda)(\operatorname{Diag}\mu^m)[H_{ij}] = \\ &\quad P\Big(\operatorname{Diag}\big(\nabla^2 f(\overline{\mu^m})\operatorname{diag}(P^T H_{ij}P)\big) + \mathcal{A}(\overline{\mu^m})\circ(P^T H_{ij}P)\Big)P^T,\end{aligned}$$

and Lemma 2.1 together with Theorem 3.2 give us

$$\begin{aligned}\nabla^2(f\circ\lambda)(\operatorname{Diag}\mu)[H_{ij}] &= \operatorname{Diag}\big(\nabla^2 f(\mu)\operatorname{diag}H_{ij}\big) + \mathcal{A}(\mu)\circ H_{ij} \\ &= P\Big(\operatorname{Diag}\big(\nabla^2 f(\mu)\operatorname{diag}(P^T H_{ij}P)\big) + \\ &\qquad\qquad \mathcal{A}(\mu)\circ(P^T H_{ij}P)\Big)P^T.\end{aligned}$$

These equations show that without loss of generality it suffices to prove the lemma only in the case when all vectors $\{\mu^m\}$ are ordered in descending order, that is, the vectors μ^m all block refine the vector μ. In that case we have

$$\nabla^2(f\circ\lambda)(\operatorname{Diag}\mu^m)[H_{ij}] = \operatorname{Diag}\big(\nabla^2 f(\mu^m)\operatorname{diag}H_{ij}\big) + \mathcal{A}(\mu^m)\circ H_{ij},$$

and

$$\nabla^2(f\circ\lambda)(\operatorname{Diag}\mu)[H_{ij}] = \operatorname{Diag}\big(\nabla^2 f(\mu)\operatorname{diag}H_{ij}\big) + \mathcal{A}(\mu)\circ H_{ij}.$$

We consider four cases.

Case I. If $i = j$ then

$$\begin{aligned}\lim_{m\to\infty}\nabla^2(f\circ\lambda)(\operatorname{Diag}\mu^m)[H_{ij}] &= \lim_{m\to\infty}\operatorname{Diag}\big(\nabla^2 f(\mu^m)e^i\big) \\ &= \operatorname{Diag}\big(\nabla^2 f(\mu)e^i\big) \\ &= \nabla^2(f\circ\lambda)(\operatorname{Diag}\mu)[H_{ij}],\end{aligned}$$

just because $\nabla^2 f(\cdot)$ is continuous at μ.

Case II. If $i \neq j$, but belong to the same block for μ^m, then i, j will be in the same block of μ as well and we have

$$\begin{aligned}
\lim_{m\to\infty} \nabla^2(f\circ\lambda)(\operatorname{Diag}\mu^m)[H_{ij}] &= \lim_{m\to\infty} b_i(\mu^m)H_{ij} \\
&= b_i(\mu)H_{ij} \\
&= \nabla^2(f\circ\lambda)(\operatorname{Diag}\mu)[H_{ij}],
\end{aligned}$$

again because $\nabla^2 f(\cdot)$ is continuous at μ.

Case III. If i and j belong to different blocks of μ^m but to the same block of μ, then

$$\lim_{m\to\infty} \nabla^2(f\circ\lambda)(\operatorname{Diag}\mu^m)[H_{ij}] = \lim_{m\to\infty} \frac{f_i'(\mu^m) - f_j'(\mu^m)}{\mu_i^m - \mu_j^m} H_{ij},$$

and

$$\nabla^2(f\circ\lambda)(\operatorname{Diag}\mu)[H_{ij}] = b_i(\mu)H_{ij}.$$

So we have to prove that

$$\lim_{m\to\infty} \frac{f_i'(\mu^m) - f_j'(\mu^m)}{\mu_i^m - \mu_j^m} = f_{ii}''(\mu) - f_{ij}''(\mu).$$

(See the definition of $b_i(\mu)$ in the beginning of Section 3.) For every m we define the vectors $\dot{\mu}^m$ and $\ddot{\mu}^m$ coordinatewise as follows

$$\dot{\mu}_p^m = \begin{cases} \mu_p^m, & p \neq i \\ \mu_j^m, & p = i \end{cases}, \qquad \ddot{\mu}_p^m = \begin{cases} \mu_p^m, & p \neq i, j \\ \mu_j^m, & p = i \\ \mu_i^m, & p = j. \end{cases}$$

Because $\mu_i = \mu_j$ we conclude that both sequences $\{\dot{\mu}^m\}_{m=1}^\infty$ and $\{\ddot{\mu}^m\}_{m=1}^\infty$ converge to μ, because $\{\mu^m\}_{m=1}^\infty$ does so. Below we are applying the mean value theorem twice:

$$\begin{aligned}
\frac{f_i'(\mu^m) - f_j'(\mu^m)}{\mu_i^m - \mu_j^m} &= \frac{f_i'(\mu^m) - f_i'(\dot{\mu}^m) + f_i'(\dot{\mu}^m) - f_j'(\mu^m)}{\mu_i^m - \mu_j^m} \\
&= \frac{(\mu_i^m - \mu_j^m) f_{ii}''(\xi^m) + f_i'(\dot{\mu}^m) - f_j'(\mu^m)}{\mu_i^m - \mu_j^m} \\
&= f_{ii}''(\xi^m) + \frac{f_i'(\dot{\mu}^m) - f_i'(\ddot{\mu}^m) + f_i'(\ddot{\mu}^m) - f_j'(\mu^m)}{\mu_i^m - \mu_j^m} \\
&= f_{ii}''(\xi^m) + \frac{(\mu_j^m - \mu_i^m) f_{ij}''(\eta^m) + f_i'(\ddot{\mu}^m) - f_j'(\mu^m)}{\mu_i^m - \mu_j^m} \\
&= f_{ii}''(\xi^m) - f_{ij}''(\eta^m),
\end{aligned}$$

where ξ^m is a vector between μ^m and $\dot{\mu}^m$, and η^m is a vector between $\dot{\mu}^m$ and $\ddot{\mu}^m$. Consequently $\xi^m \to \mu$, and $\eta^m \to \mu$. Notice that vector $\ddot{\mu}^m$ is obtained from μ^m by swapping the i-th and the j-th coordinate. Then using the first part of Lemma 2.1 we see that $f_i'(\ddot{\mu}^m) = f_j'(\mu^m)$. Finally we just have to take the limit above and use again the continuity of the Hessian of f at the point μ.

Case IV. If i and j belong to different blocks of μ^m and to different blocks of μ, then

$$\begin{aligned}
\lim_{m\to\infty} \nabla^2 (f \circ \lambda)(\operatorname{Diag} \mu^m)[H_{ij}] &= \lim_{m\to\infty} \frac{f_i'(\mu^m) - f_j'(\mu^m)}{\mu_i^m - \mu_j^m} H_{ij} \\
&= \frac{f_i'(\mu) - f_j'(\mu)}{\mu_i - \mu_j} H_{ij} \\
&= \nabla^2 (f \circ \lambda)(\operatorname{Diag} \mu)[H_{ij}],
\end{aligned}$$

because $\nabla f(\cdot)$ is continuous at μ and the denominator is never zero. ■

Now we are ready to prove the main result of this section.

Theorem 4.2 *Let A be an $n \times n$ symmetric matrix. The symmetric function $f : \mathbb{R}^n \to \mathbb{R}$ is twice continuously differentiable at the point $\lambda(A)$ if and only if the spectral function $f \circ \lambda$ is twice continuously differentiable at the matrix A.*

Proof. We know that $f \circ \lambda$ is twice differentiable at A if and only if f is twice differentiable at $\lambda(A)$, so what is left to prove is the continuity of the Hessian. Suppose that f is twice continuously differentiable at $\lambda(A)$ and that $f \circ \lambda$ is not twice continuously differentiable at A. That is, the Hessian $\nabla^2(f \circ \lambda)$ is not continuous at A. Take a sequence, $\{A_m\}_{m=1}^{\infty}$, of symmetric matrices converging to A such that for some $\epsilon > 0$ we have

$$\|\nabla^2(f \circ \lambda)(A_m) - \nabla^2(f \circ \lambda)(A)\| > \epsilon,$$

for all m. Let $\{U_m\}_{m=1}^{\infty}$ be a sequence of orthogonal matrices such that

$$A_m = U_m\big(\operatorname{Diag}\lambda(A_m)\big)U_m^T.$$

Without loss of generality we may assume that $U_m \to U$, where U is orthogonal and then

$$A = U\big(\operatorname{Diag}\lambda(A)\big)U^T.$$

(Otherwise we take subsequences of $\{A_m\}$ and $\{U_m\}$.) Using the formula for the Hessian given in Theorem 3.3 and Lemma 4.1 we can easily see that

$$\lim_{m\to\infty} \nabla^2(f \circ \lambda)(A_m)[H] = \nabla^2(f \circ \lambda)(A)[H],$$

for every symmetric H. This is a contradiction.

The other direction follows from the chain rule after observing

$$f(x) = (f \circ \lambda)(\operatorname{Diag} x).$$

This completes the proof. ■

5 Example and Conjecture

As an example, suppose we require the second directional derivative of the function $f \circ \lambda$ at the point A in the direction B. That is, we want to find the second derivative of the function

$$g(t) = (f \circ \lambda)(A + tB),$$

at $t = 0$. Let W be an orthogonal matrix such that $A = W(\operatorname{Diag}\lambda(A))W^T$. Let $\tilde{B} = W^T BW$. We differentiate twice:

$$g''(t) \;=\; \nabla^2(f \circ \lambda)(A + tB)[B, B].$$

Using Lemma 3.1 and Theorem 3.3 at $t = 0$ we get

$$\begin{aligned}
g(0) &= f(\lambda(A)) \\
g'(0) &= \operatorname{tr}\left(\tilde{B}\operatorname{Diag}\nabla f(\lambda(A))\right) \\
g''(0) &= \nabla^2(f\circ\lambda)(\lambda(A))[\operatorname{diag}\tilde{B},\operatorname{diag}\tilde{B}] + \langle \mathcal{A}, \tilde{B}\circ\tilde{B}\rangle \\
&= \sum_{i,j=1}^{n} f''_{ij}(\lambda(A))(\tilde{B}^{i,i})(\tilde{B}^{j,j}) + \sum_{\substack{i\neq j\\ \lambda_i=\lambda_j}} b_i(\tilde{B}^{i,j})^2 \\
&\quad + \sum_{\substack{i,j\\ \lambda_i\neq\lambda_j}} \frac{f'_i(\lambda(A)) - f'_j(\lambda(A))}{\lambda_i(A)-\lambda_j(A)}(\tilde{B}^{i,j})^2,
\end{aligned}$$

In principle, if the function f is analytic, this second directional derivative can also be computed using the implicit formulae from [17]. Some work shows that the answers agree.

As a final illustration, consider the classical example of the power series expansion of a simple eigenvalue. In this case we consider the function f given by

$$f(x) = \bar{x}_k := \text{the } k\text{-th largest entry in } x,$$

and the matrix

$$A = \operatorname{Diag}\mu,$$

where $\mu \in \mathbb{R}^n_{\downarrow}$ and

$$\mu_{k-1} > \mu_k > \mu_{k+1}.$$

Then we have

$$f'(\mu) = e^k, \quad \text{and} \quad f''(\mu) = 0,$$

so for the function $g(t) = \lambda_k(\operatorname{Diag}\mu + tB)$ our results show the following formulae (familiar in perturbation theory and quantum mechanics):

$$\begin{aligned}
g(0) &= \mu_k \\
g'(0) &= B^{k,k} \\
g''(0) &= \sum_{j\neq k}\frac{1}{\mu_k-\mu_j}(B^{k,j})^2 + \sum_{i\neq k}\frac{-1}{\mu_i-\mu_k}(B^{i,k})^2 \\
&= 2\sum_{j\neq k}\frac{1}{\mu_k-\mu_j}(B^{k,j})^2.
\end{aligned}$$

This agrees with the result in [4, p. 92].

We conclude with the following natural conjecture.

Conjecture 5.1 *A spectral function $f \circ \lambda$ is k-times differentiable at the matrix A if and only if its corresponding symmetric function f is k-times differentiable at the point $\lambda(A)$. Moreover, $f \circ \lambda$ is $\mathcal{C}^k$ if and only if f is $\mathcal{C}^k$.*

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