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Variational Analysis of Spectral Functions Simplified

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Spectral functions of symmetric matrices – those depending on matrices only through their eigenvalues – appear often in optimization. A cornerstone variational analytic tool for studying such functions is a formula relating their subdifferentials to the subdifferentials of their diagonal restrictions. This paper presents a new, short, and revealing derivation of this result. The argument has a direct analogue for spectral functions of Hermitian matrices, and for singular value functions of rectangular matrices.

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1. Introduction.

This work revolves around *spectral functions.* These are functions on the space of $n \times n$ symmetric matrices $\mathbf{S}^n$ that depend on matrices only through their eigenvalues, that is, functions that are invariant under conjugation by orthogonal matrices. Spectral functions can always be written in a composite form $f \circ \lambda$, where f is a permutation-invariant function on $\mathbf{R}^n$ and λ is a mapping assigning to each matrix X the vector of eigenvalues $(\lambda_1(X), \ldots, \lambda_n(X))$ in nonincreasing order.

A pervasive theme in the study of such functions is that various variational properties of the permutation-invariant function f are inherited by the induced spectral function $f \circ \lambda$; see e.g. [3, 4, 5, 6, 8, 9, 20, 22]. Take convexity for example. Supposing that f is closed and convex, the main result of [11] shows

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that the Fenchel conjugate of $f \circ \lambda$ admits the elegant representation

$$(f \circ \lambda)^\star = f^\star \circ \lambda. \tag{1}$$

An immediate conclusion is that $f \circ \lambda$ agrees with its double conjugate and is therefore convex, that is, convexity of f is inherited by the spectral function $f \circ \lambda$. A convenient characterization of the subdifferential $\partial(f \circ \lambda)(X)$ in terms of $\partial f(\lambda(X))$ then readily follows [11, Theorem 3.1] — an important result for optimization specialists.

In a follow up paper [12], Lewis showed that even for nonconvex functions f, the following exact relationship holds:

$$\partial(f \circ \lambda)(X) = \{U(\operatorname{Diag} v)U^T : v \in \partial f(\lambda(X)),\, U \in \mathcal{O}^n_X\}, \tag{2}$$

where

$$\mathcal{O}^n_X := \{U \in \mathcal{O}^n : X = U(\operatorname{Diag} \lambda(X))U^T\}.$$

Here, the symbol $\mathcal{O}^n$ denotes the group of orthogonal matrices and the symbols $\partial(f \circ \lambda)$ and ∂f may refer to the Fréchet, limiting, or Clarke subdifferentials; see e.g. [18] for the relevant definitions. Thus calculating the subdifferential of the spectral function $f \circ \lambda$ on $\mathbf{S}^n$ reduces to computing the subdifferential of the usually much simpler function f on $\mathbf{R}^n$. For instance, subdifferential computation of the k'th largest eigenvalue function $X \mapsto \lambda_k(X)$ amounts to analyzing a piecewise polyhedral function, the k'th order statistic on $\mathbf{R}^n$ [12, Section 9]. Moreover, the subdifferential formula allows one to gauge the underlying geometry of spectral functions, via "active manifolds" [3], for example. A different proof of (2), based on cleverly constructed orbital projections, subsequently appeared in [2].

In striking contrast to the convex case [11], all known proofs of the general subdifferential formula (2), albeit elegant, require much finer tools. This paper presents a short, elementary, and revealing derivation of equation (2) that is no more involved than its convex counterpart. Here's the basic idea. Consider the *Moreau envelope*

$$f_\alpha(x) := \inf_y \left\{ f(y) + \tfrac{1}{2\alpha}|x-y|^2 \right\}.$$

Similar notation will be used for the envelope of $f \circ \lambda$. In direct analogy to equation (1), we will observe that the Moreau envelope satisfies the equation

$$(f \circ \lambda)_\alpha = f_\alpha \circ \lambda,$$

and derive a convenient formula for the corresponding proximal mapping. The case when f is an indicator function was treated in [4], and the argument presented here is a straightforward adaptation, depending solely on the Theobald–von Neumann inequality [23, 24]. The key observation now is independent of the eigenvalue setting: membership of a vector v in the proximal or in the

Fréchet subdifferential of any function g at a point x is completely determined by the local behavior of the univariate function $\alpha \mapsto g_\alpha(x+\alpha v)$ near zero. The proof of the subdifferential formula (2) quickly flows from there. It is interesting to note that the argument uses very little information about the properties of the eigenvalue map, with the exception of the Theobald–von Neumann inequality. Consequently, it applies equally well in a more general algebraic setting of certain isometric group actions, encompassing also an analogous subdifferential formula for functions of singular values derived in [15, 16, 19]; a discussion can be found in the appendix of the arXiv version of the paper. A different Lie theoretic approach in the convex case appears in [13].

We complete the paper by briefly revisiting the second-order theory of spectral functions. In [1, 14, 20, 21], the authors derived a formula for the second derivative of a C^2-smooth spectral function. In its simplest form, it reads

$$\nabla^2 F(\operatorname{Diag} a)[B] = \operatorname{Diag}\big(\nabla^2 f(a)\operatorname{diag}(B)\big) + \mathcal{A}\circ B,$$

where $\mathcal{A}\circ B$ is the Hadamard product and

$$\mathcal{A}_{ij} = \begin{cases} \frac{\nabla f(a)_i - \nabla f(a)_j}{a_i - a_j} & \text{if } a_i \neq a_j \\ \nabla^2 f(a)_{ii} - \nabla^2 f(a)_{ij} & \text{if } a_i = a_j \end{cases}.$$

This identity is quite mysterious at first sight. Seeking to illuminate the underlying geometry, we here provide a geometric interpretation of the proof of this result in [21], making clear the role of the invariance properties of the gradient graph.

The outline of the manuscript is as follows. Section 2 records basic notation and an important preliminary result about the Moreau envelope (Lemma 2.1). Section 3 contains background material on orthogonally invariant functions. Section 4 describes the proof of the subdifferential formula and Section 5 focuses on the second-order theory.

2. Notation.

This section briefly records some basic notation, following closely the monograph [18]. The symbol $\mathbf{E}$ will always denote a Euclidean space (finite-dimensional real inner product space) with inner product $\langle\cdot,\cdot\rangle$ and induced norm $|\cdot|$. A closed ball of radius $\varepsilon > 0$ around a point x will be denoted by $\mathcal{B}_\varepsilon(x)$. The closure and the convex hull of a set Q in $\mathbf{E}$ will be denoted by $\operatorname{cl} Q$ and $\operatorname{conv} Q$, respectively.

Throughout, we will consider functions f on $\mathbf{E}$ taking values in the extended real line $\overline{\mathbf{R}} := \mathbf{R}\cup\{\pm\infty\}$. For such a function f and a point $\bar{x}$, with $f(\bar{x})$ finite, the *proximal subdifferential* $\partial_p f(\bar{x})$ consists of all vectors $v \in \mathbf{E}$ such that there exist constants $r > 0$ and $\varepsilon > 0$ satisfying

$$f(x) \geq f(\bar{x}) + \langle v, x-\bar{x}\rangle - \frac{r}{2}|x-\bar{x}|^2 \quad \text{for all } x \in \mathcal{B}_\varepsilon(\bar{x}).$$

When f is C^2-smooth near $\bar{x}$, the proximal subdifferential $\partial_p f(\bar{x})$ consists only of the gradient $\nabla f(\bar{x})$. A function f is said to be *prox-bounded* if it majorizes some quadratic function. In particular, all lower-bounded functions are prox-bounded. For prox-bounded functions, the inequality in the definition of the proximal subdifferential can be taken to hold globally at the cost of increasing r [18, Proposition 8.46]. The *Fréchet subdifferential* of f at $\bar{x}$, denoted $\hat{\partial} f(\bar{x})$, consists of all vectors $v \in \mathbf{E}$ satisfying

$$f(x) \geq f(\bar{x}) + \langle v, x - \bar{x} \rangle + o(|x - \bar{x}|).$$

Here, as usual, $o(|x - \bar{x}|)$ denotes any term satisfying $\frac{o(|x-\bar{x}|)}{|x-\bar{x}|} \to 0$. When f is C^1-smooth near $\bar{x}$, the set $\hat{\partial} f(\bar{x})$ consists only of the gradient $\nabla f(\bar{x})$. The subdifferentials $\partial_p f(\bar{x})$ and $\hat{\partial} f(\bar{x})$ are always convex, while $\hat{\partial} f(\bar{x})$ is also closed. The *limiting subdifferential* of f at $\bar{x}$, denoted $\partial f(\bar{x})$, consists of all vectors $v \in \mathbf{E}$ so that there exist sequences x_i and $v_i \in \hat{\partial} f(x_i)$ with $(x_i, f(x_i), v_i) \to (\bar{x}, f(\bar{x}), v)$. The same object arises if the vectors v_i are restricted instead to lie in $\partial_p f(x_i)$ for each index i; see [18, Corollary 8.47]. The *horizon subdifferential*, denoted $\partial^\infty f(\bar{x})$, consists of all limits of $\lambda_i v_i$ for some sequences $v_i \in \partial f(x_i)$ and $\lambda_i \geq 0$ satisfying $x_i \to \bar{x}$ and $\lambda_i \searrow 0$. This object records horizontal "normals" to the epigraph of the function. For example, f is locally Lipschitz continuous around $\bar{x}$ precisely when $\partial^\infty f(\bar{x})$ contains only the zero vector.

The two key constructions at the heart of the paper are defined as follows. Given a function $f \colon \mathbf{E} \to \overline{\mathbf{R}}$ and a parameter $\alpha > 0$, the *Moreau envelope* f_α and the *proximal mapping* $P_\alpha f$ are defined by

$$f_\alpha(x) := \inf_{y \in \mathbf{E}} \left\{ f(y) + \frac{1}{2\alpha}|y - x|^2 \right\},$$
$$P_\alpha f(x) := \operatorname*{argmin}_{y \in \mathbf{E}} \left\{ f(y) + \frac{1}{2\alpha}|y - x|^2 \right\}.$$

Extending the definition slightly, we will set $f_0(x) := f(x)$. It is easy to see that f is *prox-bounded* if and only if there exists some point $x \in \mathbf{E}$ and a real $\alpha > 0$ satisfying $f_\alpha(x) > -\infty$.

The proximal and Fréchet subdifferentials are conveniently characterized by a differential property of the function $\alpha \mapsto f_\alpha(x + \alpha v)$. This observation is recorded below. To this end, for any function $\varphi \colon [0, \infty) \to \overline{\mathbf{R}}$, the one-sided derivative will be denoted by

$$\varphi'_+(0) := \lim_{\alpha \searrow 0} \frac{\varphi(\alpha) - \varphi(0)}{\alpha}.$$

Lemma 2.1. (Subdifferential and the Moreau envelope)
Consider an lsc, prox-bounded function $f \colon \mathbf{E} \to \overline{\mathbf{R}}$, and a point x with $f(x)$ finite. Fix a vector $v \in \mathbf{E}$ and define the function $\varphi \colon [0, \infty) \to \overline{\mathbf{R}}$ by setting $\varphi(\alpha) := f_\alpha(x + \alpha v)$. Then the following are true.

(i) *Vector v lies in $\hat{\partial} f(x)$ if and only if*

$$\varphi'_+(0) = \frac{|v|^2}{2}. \tag{3}$$

(ii) *Vector v lies in $\partial_p f(x)$ if and only if there exists $\alpha > 0$ satisfying $x \in P_\alpha f(x + \alpha v)$, or equivalently*

$$\varphi(\alpha) = f(x) + \frac{|v|^2}{2}\alpha.$$

In this case, the equation above continues to hold for all $\tilde{\alpha} \in [0, \alpha]$.

Proof. Claim (ii) is immediate from definitions; see for example [18, Proposition 8.46]. Hence we focus on claim (i). To this end, note that the inequality

$$\frac{f_\alpha(x + \alpha v) - f(x)}{\alpha} \leq \frac{|v|^2}{2} \qquad \text{holds for any } v \in \mathbf{E}. \tag{4}$$

Consider now a vector $v \in \hat{\partial} f(x)$ and any sequence $\alpha_i \searrow 0$. Appealing to [18, Theorem 1.25], we deduce that the sets $P_{\alpha_i}(x + \alpha_i v)$ are nonempty for all small α_i. Choose now any points $x_i \in P_{\alpha_i}(x + \alpha_i v)$. We may assume $x_i \neq x$ for all large i, since otherwise there's nothing to prove. We claim that the sequence x_i converges to x. To see this, note that since f is prox-bounded, there exists some real $r > 0$ satisfying $f(z) \geq -\frac{r}{2}|z|^2$ for all $z \in \mathbf{E}$. In particular, we have $f(x_i) \geq -r(|x_i - x|^2 + |x|^2)$ for all indices i. We therefore deduce

$$\begin{aligned} f_{\alpha_i}(x + \alpha_i v) &= f(x_i) + \frac{1}{2\alpha_i}|(x_i - x) - \alpha_i v)|^2 \\ &\geq -r(|x_i - x|^2 + |x|^2) + \frac{1}{2\alpha_i}|x_i - x|^2 - \langle v, x_i - x\rangle + \frac{\alpha_i}{2}|v|^2 \\ &\geq \left(\frac{1}{2\alpha_i} - r - \frac{|v|}{|x_i - x|}\right)|x_i - x|^2 + \frac{\alpha_i}{2}|v|^2 - r|x|^2. \end{aligned}$$

Inequality (4) shows that the left-hand-side is bounded, and therefore we conclude $x_i \to x$, as claimed. Observe now

$$f_{\alpha_i}(x + \alpha_i v) - f(x) = f(x_i) - f(x) - \langle v, x_i - x\rangle + \frac{1}{2\alpha_i}|x_i - x|^2 + \frac{\alpha_i}{2}|v|^2.$$

Dividing through by α_i, while taking into account statement (4) and the inclusion $v \in \hat{\partial} f(x)$, yields the inequality

$$\frac{|v|^2}{2} \geq \frac{f_{\alpha_i}(x + \alpha_i v) - f(x)}{\alpha_i} \geq \frac{|x_i - x|}{\alpha_i} \cdot \frac{o(|x_i - x|)}{|x_i - x|} + \frac{1}{2}\left|\frac{x_i - x}{\alpha_i}\right|^2 + \frac{|v|^2}{2}. \tag{5}$$

Rearranging, we obtain

$$0 \geq \frac{|x_i - x|}{\alpha_i} \cdot \left(\frac{o(|x_i - x|)}{|x_i - x|} + \frac{1}{2}\left|\frac{x_i - x}{\alpha_i}\right| \right).$$

In particular, we conclude $\frac{x_i - x}{\alpha_i} \to 0$. Finally appealing to (5), we obtain equation (3), as claimed.

Conversely suppose that equation (3) holds, and for the sake of contradiction that v does not lie in $\hat{\partial} f(x)$. Then there exists $\kappa > 0$ and a sequence $y_i \to x$ satisfying

$$f(y_i) - f(x) - \langle v, y_i - x \rangle \leq -\kappa |y_i - x|.$$

Then for any $\alpha > 0$, we deduce

$$\begin{aligned} \frac{f_\alpha(x + \alpha v) - f(x)}{\alpha} &\leq \frac{1}{\alpha}\Big(f(y_i) - f(x) + \frac{1}{2\alpha}|(y_i - x) - \alpha v|^2 \Big) \\ &\leq -\kappa \frac{|y_i - x|}{\alpha} + \frac{1}{2}\left|\frac{y_i - x}{\alpha}\right|^2 + \frac{|v|^2}{2}. \end{aligned}$$

Setting $\alpha_i := \frac{|y_i - x|}{\kappa}$ and letting i tend to ∞ yields a contradiction. $\square$

3. Symmetry and orthogonal invariance

Next we recall a basic correspondence between symmetric functions and spectral functions of symmetric matrices. The discussion follows that of [12]. Henceforth $\mathbf{R}^n$ will denote an n-dimensional real Euclidean space with a specified basis. Hence one can associate $\mathbf{R}^n$ with a collection of n-tuples $(x_1, \ldots, x_n)$, in which case the inner product $\langle \cdot, \cdot \rangle$ is the usual dot product. The finite group of coordinate permutations of $\mathbf{R}^n$ will be denoted by Π^n. A function $f \colon \mathbf{R}^n \to \overline{\mathbf{R}}$ is *symmetric* whenever it is Π^n-invariant, meaning

$$f(\pi x) = f(x) \quad \text{for all } x \in \mathbf{R}^n \text{ and } \pi \in \Pi^n.$$

It is immediate to verify that if f is symmetric, then so is the Moreau envelope f_α for any $\alpha \geq 0$. This elementary observation will be important later.

The vector space of real $n \times n$ symmetric matrices will be denoted by $\mathbf{S}^n$ and will be endowed with the trace inner product $\langle X, Y \rangle = \operatorname{tr} XY$, and the induced Frobenius norm $|X| = \sqrt{\operatorname{tr} X^2}$. For any $x \in \mathbf{R}^n$, the symbol $\operatorname{Diag} x$ will denote the $n \times n$ matrix with x on its diagonal and with zeros off the diagonal, while for a matrix $X \in \mathbf{S}^n$, the symbol $\operatorname{diag} X$ will denote the n-vector of its diagonal entries.

The group of real $n \times n$ orthogonal matrices will be written as $\mathcal{O}^n$. The eigenvalue map $\lambda \colon \mathbf{S}^n \to \mathbf{R}^n$ assigns to each matrix X in $\mathbf{S}^n$ the vector of its eigenvalues $(\lambda_1(X), \ldots, \lambda_n(X))$ in a nonincreasing order. A function $F \colon \mathbf{S}^n \to \overline{\mathbf{R}}$ is *spectral* if it is $\mathcal{O}^n$-invariant under the conjugation action, meaning

$$F(UXU^T) = F(X) \quad \text{for all } X \in \mathbf{S}^n \text{ and } U \in \mathcal{O}^n.$$

In other words, spectral functions are those that depend on matrices only through their eigenvalues. A basic fact is that any spectral function F on $\mathbf{S}^n$ can be written as a composition $F = f \circ \lambda$ for some symmetric function f on $\mathbf{R}^n$. Indeed, f can be realized as the restriction of F to diagonal matrices $f(x) = F(\operatorname{Diag} x)$.

Two matrices X and Y in $\mathbf{S}^n$ are said to admit a *simultaneous spectral decomposition* if there exists an orthogonal matrix $U \in \mathcal{O}^n$ such that UXU^T and UYU^T are both diagonal matrices. It is well-known that this condition holds if and only if X and Y commute. The matrices X and Y are said to admit a *simultaneous ordered spectral decomposition* if there exists an orthogonal matrix $U \in \mathcal{O}^n$ satisfying $UXU^T = \operatorname{Diag} \lambda(X)$ and $UYU^T = \operatorname{Diag} \lambda(Y)$. The following result characterizing this property, essentially due to Theobald [23] and von Neumann [24], plays a central role in spectral variation analysis.

Theorem 3.1. (Von Neumann-Theobald) *Any two matrices X and Y in $\mathbf{S}^n$ satisfy the inequality*

$$|\lambda(X) - \lambda(Y)| \leq |X - Y|.$$

Equality holds if and only if X and Y admit a simultaneous ordered spectral decomposition.

This result is often called a trace inequality. The reason is that the eigenvalue mapping being 1-Lipschitz (as in the statement above) is equivalent to the inequality

$$\langle \lambda(X), \lambda(Y) \rangle \geq \langle X, Y \rangle \quad \text{for all } X, Y \in \mathbf{S}^n.$$

4. Derivation of the subdifferential formula

In this section, we derive the subdifferential formula (2) for spectral functions, first established in [12]. In what follows, for any matrix $X \in \mathbf{S}^n$ define the diagonalizing matrix set

$$\mathcal{O}_X := \{U \in \mathcal{O}^n : U(\operatorname{Diag} \lambda(X))U^T = X\}.$$

The spectral subdifferential formula will readily follow from Lemma 2.1 and the following intuitive proposition, a proof of which can essentially be seen in [4, Proposition 8].

Theorem 4.1. (Proximal analysis of spectral functions)
Consider a symmetric function $f \colon \mathbf{R}^n \to \overline{\mathbf{R}}$. Then the equation

$$(f \circ \lambda)_\alpha = f_\alpha \circ \lambda \tag{6}$$

holds. In addition, the proximal mapping admits the representation:

$$P_\alpha(f \circ \lambda)(X) = \big\{U\big(\mathit{Diag}\ y\big)U^T : y \in P_\alpha f(\lambda(X)),\ U \in \mathcal{O}_X\big\}. \tag{7}$$

Moreover, for any $Y \in P_\alpha(f \circ \lambda)(X)$ the matrices X and Y admit a simultaneous ordered spectral decomposition.

Proof. For any X and Y, applying the trace inequality (Theorem 3.1), we deduce

$$f(\lambda(Y)) + \frac{1}{2\alpha}|Y - X|^2 \geq f(\lambda(Y)) + \frac{1}{2\alpha}|\lambda(Y) - \lambda(X)|^2 \geq f_\alpha(\lambda(X)). \qquad (8)$$

Taking the infimum over Y, we deduce $(f \circ \lambda)_\alpha(X) \geq f_\alpha(\lambda(X))$. On the other hand, for any $U \in \mathcal{O}_X$, the inequalities hold:

$$\begin{aligned}
(f \circ \lambda)_\alpha(X) &= \inf_Y \left\{ f(\lambda(Y)) + \frac{1}{2\alpha}|Y - X|^2 \right\} \\
&= \inf_Y \left\{ f(\lambda(Y)) + \frac{1}{2\alpha}|U^T Y U - \operatorname{Diag}\lambda(X)|^2 \right\} \\
&\leq \inf_{y \in \mathbf{R}^n} \left\{ f(\lambda(U(\operatorname{Diag} y)U^T)) + \frac{1}{2\alpha}|U^T(U(\operatorname{Diag} y)U^T)U - \operatorname{Diag}\lambda(X)|^2 \right\} \\
&= \inf_{y \in \mathbf{R}^n} \left\{ f(y) + \frac{1}{2\alpha}|y - \lambda(X)|^2 \right\} = f_\alpha(\lambda(X)).
\end{aligned}$$

This establishes (6).

To establish equation (7), consider first a matrix $U \in \mathcal{O}_X$ and a vector $y \in P_\alpha f(\lambda(X))$, and define $Y := U(\operatorname{Diag} y)U^T$. Then we have

$$(f \circ \lambda)(Y) + \frac{1}{2\alpha}|Y - X|^2 = f(y) + \frac{1}{2\alpha}|y - \lambda(X)|^2 = f_\alpha(\lambda(X)) = (f \circ \lambda)_\alpha(X).$$

Hence the inclusion $Y \in P_\alpha(f \circ \lambda)(X)$ is valid, as claimed. Conversely, fix any matrix $Y \in P_\alpha(f \circ \lambda)(X)$. Then plugging in Y into (8), the left-hand-side equals $(f \circ \lambda)_\alpha(X)$ and hence the two inequalities in (8) hold as equalities. The second equality immediately yields the inclusion $\lambda(Y) \in P_\alpha f(\lambda(X))$, while the first along with Theorem 3.1 implies that X and Y admit a simultaneous ordered spectral decomposition, as claimed. □

Combining Lemma 2.1 and Theorem 4.1, the main result of the paper readily follows.

Theorem 4.2. (Subdifferentials of spectral functions)
Consider an lsc symmetric function $f \colon \mathbf{R}^n \to \overline{\mathbf{R}}$. Then the equation holds:

$$\partial(f \circ \lambda)(X) = \left\{ U\big(\operatorname{Diag} v\big)U^T : v \in \partial f(\lambda(X)),\, U \in \mathcal{O}_X \right\}. \qquad (9)$$

Analogous formulas hold for proximal, Fréchet, and horizon subdifferentials.

Proof. Fix a matrix X in the domain of $f \circ \lambda$ and define $x := \lambda(X)$. Without loss of generality, suppose that f is lower-bounded. Indeed if this were not the case, then since f is lsc there exists $\varepsilon > 0$ so that f is lower-bounded on the ball $\mathcal{B}_\epsilon(x)$. Consequently adding to f the indicator function of the symmetric set $\cup_{\pi \in \Pi} \mathcal{B}_\epsilon(\pi x)$ assures that the function is lower-bounded.

We first dispense with the easy inclusion $\subseteq$ for all the subdifferentials. To this end, recall that if V is a proximal subgradient of $f \circ \lambda$ at X, then there exists $\alpha > 0$ satisfying $X \in P_\alpha(f \circ \lambda)(X + \alpha V)$. Theorem 4.1 then implies that X and V commute. Taking limits, we deduce that all Fréchet, limiting, and horizon subgradients of $f \circ \lambda$ at X also commute with X. Recalling that commuting matrices admit simultaneous spectral decomposition, basic definitions immediately yield the inclusion $\subseteq$ in equation (9) for the proximal and for the Fréchet subdifferentials. Taking limits, we deduce the inclusion $\subseteq$ in (9) for the limiting and for the horizon subdifferentials, as well.

Next, we argue the reverse inclusion. To this end, define $V := U(\mathrm{Diag}\, v)U^T$ for an arbitrary matrix $U \in \mathcal{O}_X$ and any vector $v \in \mathbf{R}^n$. Then Theorem 4.1, along with the symmetry of the envelope f_α, yields the equation

$$\frac{(f \circ \lambda)_\alpha(X + \alpha V) - f(\lambda(X))}{\alpha} = \frac{f_\alpha(x + \alpha v) - f(x)}{\alpha}.$$

Consequently if v lies in $\partial_p f(x)$, then Lemma 2.1 shows that for some $\alpha > 0$ the right-hand-side equals $\frac{|v|^2}{2}$, or equivalently $\frac{|V|^2}{2}$. Lemma 2.1 then yields the inclusion $V \in \partial_p(f \circ \lambda)(X)$. Similarly if v lies in $\hat{\partial} f(x)$, then the same argument but with α tending to 0 shows that V lies in $\hat{\partial}(f \circ \lambda)(X)$. Thus the inclusion $\supseteq$ in equation (9) holds for the proximal and for the Fréchet subdifferentials. Taking limits, the same inclusion holds for the limiting and for the horizon subdifferentials. This completes the proof. $\square$

Remark 4.3. It easily follows from Theorem 4.2 that the inclusion $\supseteq$ holds for the Clarke subdifferential. The reverse inclusion, on the other hand, requires a separate argument given in [12, Sections 7-8]. $\square$

In conclusion, we should mention that all the arguments in the section apply equally well for functions of singular values of rectangular matrices, thereby recovering the main results of [15]. Namely, consider the space of $m \times n$ matrices endowed with the trace product $\langle X, Y \rangle = \mathrm{tr}\, X^T Y$, and the induced Frobenius norm. Assume without loss of generality $m \leq n$ and let $\sigma \colon \mathbf{R}^{m \times n} \to \mathbf{R}^m$ be the map assigning to each matrix X the vector of its singular values $\sigma(X) = (\sigma_1(X), \ldots, \sigma_m(X))$ in a nonincreasing order. Then entirely analogous arguments to ones given in this section show that for any lsc function $f \colon \mathbf{R}^m \to \overline{\mathbf{R}}$ that is invariant under signed permutations, we have

$$\partial(f \circ \sigma)(X) = \big\{U\big(\mathrm{Diag}\, v\big)W^T : v \in \partial f(\sigma(X)),\, (U, W) \in \mathcal{O}_X^{m,n}\big\}, \tag{10}$$

where

$$\mathcal{O}_X^{m,n} := \{(U, W) \in \mathcal{O}^m \times \mathcal{O}^n : \; U(\mathrm{Diag}\, \sigma(X))W^T = X\}.$$

This formula is the main result of [15]. For more details on the generality of the argument, see the appendix in the arXiv version of the paper.

Remark 4.4. (Comparison of the argument with that in [12] and [2]) It is instructive to compare the approach taken here with that of Lewis [12] and Ciligot-Travain, Traore [2]. Lewis' approach for establishing the subdifferential formula (2) is based on sophisticated properties of the directional derivative of the eigenvalue map $\lambda(\cdot)$, culminating in the key description [12, Theorem 4]. The paper [2] of Ciligot-Travain and Traore takes a very different approach. The authors proceed by relating variational properties of the spectral function at X and those of its restriction to the normal space of the orbit of X under the orthogonal group action by conjugation. In particular, they view the spectral function F on a neighborhood of a matrix X as a composition of the restriction of F to the aforementioned normal space and a cleverly constructed smooth "orbital projection" map π_X. The two key properties of the map π_X are the equality $\pi_X(X) = X$ and that π_X is orbit preserving, meaning that for all Y near X, the matrices $\pi_X(Y)$ and Y lie in the same orbit. $\square$

5. Hessians of C^2-smooth spectral functions.

In this section, we revisit the second-order theory of spectral functions. To this end, fix for the entire section an lsc symmetric function $f\colon \mathbf{R}^n \to \overline{\mathbf{R}}$ and define the spectral function $F := f \circ \lambda$ on $\mathbf{S}^n$. It is well known that f is C^2-smooth around a matrix X if and only if F is C^2-smooth around $\lambda(X)$; see [14, 20, 21, 22]. Moreover, a formula for the Hessian of F is available:

$$\nabla^2 F(\operatorname{Diag} a)[B] = \operatorname{Diag}\big(\nabla^2 f(a)\operatorname{diag}(B)\big) + \mathcal{A} \circ B,$$

where $\mathcal{A} \circ B$ is the Hadamard product and

$$\mathcal{A}_{ij} = \begin{cases} \frac{\nabla f(a)_i - \nabla f(a)_j}{a_i - a_j} & \text{if } a_i \neq a_j \\ \nabla^2 f(a)_{ii} - \nabla^2 f(a)_{ij} & \text{if } a_i = a_j \end{cases}.$$

The assumption that the Hessian $\nabla^2 F$ is evaluated at a diagonal matrix $\operatorname{Diag} a$ is made without loss of generality, as will be apparent shortly. In this section, we seek a transparent geometric explanation for the Hessian formula. We do so through a geometric interpretation of the proof of this result in [21], focusing on the invariance properties of $\operatorname{gph} \nabla F$. Throughout, given a smooth manifold Q in some ambient space and a point $x \in Q$, we let $N_Q(x)$ denote the normal space to Q at x.

Remark 5.1. (Hessian and the gradient graph) Throughout the section we will appeal to the following basic property of the Hessian. For any C^2-smooth function g on a Euclidean space $\mathbf{E}$ and points $a, b \in \mathbf{E}$, there is a unique vector z satisfying $(z, -b) \in N_{\operatorname{gph} \nabla g}(a, \nabla g(a))$, namely $z := \nabla^2 g(a)[b]$. $\square$

Consider now the action of the orthogonal group $\mathcal{O}^n$ on $\mathbf{S}^n$ by conjugation $U.X = UXU^T$. Recall that F is *invariant* under this action, meaning $F(U.X) = F(X)$ for all orthogonal matrices U. This action naturally extends to the product space $\mathbf{S}^n \times \mathbf{S}^n$ by setting $U.(X,Y) = (U.X, U.Y)$. As we have seen, the graph $\operatorname{gph} \nabla F$ is then *invariant* with respect to this action:

$$U.\operatorname{gph} \nabla F = \operatorname{gph} \nabla F \quad \text{ for all } U \in \mathcal{O}^n.$$

One immediate observation is that $N_{\operatorname{gph} \nabla F}(U.X, U.Y) = U.N_{\operatorname{gph} \nabla F}(X,Y)$. Consequently we deduce

$$(Z, -B) \in N_{\operatorname{gph} \nabla F}(X,Y) \quad \Longleftrightarrow \quad (U.Z, -U.B) \in N_{\operatorname{gph} \nabla F}(U.X, U.Y).$$

The formula

$$\nabla^2 F(X)[B] = U^T.\nabla^2 F(U.X)[U.B] \tag{11}$$

now follows directly from Remark 5.1, whenever F is C^2-smooth around X. As a result, when speaking about the operator $\nabla^2 F(X)$, we may assume without loss of generality that X and $\nabla F(X)$ are both diagonal matrices.

Next we briefly recall a few rudimentary properties of the conjugation action. The text [10, Sections 4, 8, 9] is a good reference. A matrix $W \in \mathbf{R}^{n\times n}$ is *skew-symmetric* if $W^T = -W$. It is well-known that $\mathcal{O}^n$ is a smooth manifold and the tangent space to $\mathcal{O}^n$ at the identity matrix consists of skew-symmetric matrices:

$$T_{\mathcal{O}^n}(I) = \{W \in \mathbf{R}^{n\times n} : W \text{ is skew-symmetric}\}.$$

The *commutator* of two matrices $A, B \in \mathbf{R}^{n\times n}$, denoted by $[A,B]$ is the matrix $[A,B] := AB - BA$. An easy computation shows that the commutator of a skew-symmetric matrix with a symmetric matrix is itself symmetric. Moreover, the identity

$$\langle X, [W,Z]\rangle = \langle [X,W], Z\rangle$$

holds for any matrices $X, Z \in \mathbf{S}^n$ and skew-symmetric W. For any matrix $A \in \mathbf{S}^n$, the *orbit of* A, denoted by $\mathcal{O}^n.A$ is the set

$$\mathcal{O}^n.A = \{U.A \,:\, U \in \mathcal{O}^n\}.$$

Similarly, the orbit of a pair $(A,B) \in \mathbf{S}^n \times \mathbf{S}^n$ is the set

$$\mathcal{O}^n.(A,B) = \{(U.A, U.B) \,:\, U \in \mathcal{O}^n\}.$$

A standard computation[1] now shows that orbits are smooth manifolds with tangent spaces

$$T_{\mathcal{O}^n.A}(A) = \{[W,A] : W \text{ is skew-symmetric}\},$$
$$T_{\mathcal{O}^n.(A,B)}(A,B) = \{([W,A],[W,B]) : W \text{ is skew-symmetric}\}.$$

Now supposing that F is twice differentiable at a matrix $A \in \mathbf{S}^{n\times n}$, the graph $\operatorname{gph} \nabla F$ certainly contains the orbit $\mathcal{O}^n.(A, \nabla F(A))$. In particular, this implies

[1]Compute the differential of the mapping $\mathcal{O}^n \ni U \mapsto U.A$

that the tangent space to $\operatorname{gph} \nabla F$ at $(A, \nabla F(A))$ contains the tangent space to the orbit:

$$\{([W, A], [W, \nabla F(A)]) : W \text{ skew-symmetric}\}.$$

Thus, for any $B \in \mathbf{S}^n$, the tuple $(\nabla^2 F(A)[B], -B)$ is orthogonal to the tuple $([W, A], [W, \nabla F(A)])$ for any skew-symmetric matrix W. We record this observation in the following lemma; this also appears as [21, Lemma 3.2].

Lemma 5.2. (Orthogonality to orbits) *Suppose F is C^2-smooth around $A \in \mathbf{S}^n$. Then for any skew-symmetric matrix W and any $B \in \mathbf{S}^n$, we have*

$$\left\langle \nabla^2 F(A)[B], [W, A] \right\rangle = \langle B, [W, \nabla F(A)] \rangle .$$

Proof. This is immediate from the preceding discussion. □

Next recall that the *stabilizer* of a matrix $A \in \mathbf{S}^n$ is the set:

$$\operatorname{Stab}(A) = \{U \in \mathcal{O}^n \ : \ U.A = A\}.$$

Similarly we may define $\operatorname{Stab}(A, B)$.

Lemma 5.3. (Tangent space to the stabilizer) *For any matrices $A, B \in \mathbf{S}^n$, the tangent spaces to Stab(A) and to Stab(A, B) at the identity matrix are the sets*

$$\{W \in \mathbf{R}^{n\times n} \ : \ W \text{ skew-symmetric, } [W, A] = 0\},$$

$$\left\{W \in \mathbf{R}^{n\times n} \ : \ W \text{ skew-symmetric}, [W, A] = [W, B] = 0\right\},$$

respectively.

Proof. Define the orbit map $\theta^{(A)} \colon \mathcal{O}^n \to \mathcal{O}^n.A$ by setting $\theta^{(A)}(U) := U.A$. A quick computation shows that $\theta^{(A)}$ is equivariant with respect to left-multiplication action of $\mathcal{O}^n$ on itself and the conjugation action of $\mathcal{O}^n$ on $\mathcal{O}^n.A$. Hence the equivariant rank theorem [10, Theorem 7.25] implies that $\theta^{(A)}$ has constant rank. In fact, since $\theta^{(A)}$ is surjective, it is a submersion. It follows that the stabilizer

$$\operatorname{Stab}(A) = (\theta^{(A)})^{-1}(A)$$

is a smooth manifold with tangent space at the identity equal to the kernel of the differential $d\,\theta^{(A)}\big|_{U=I}(W) = [W, A]$. The expression for the tangent space to $\operatorname{Stab}(A)$ immediately follows. The analogous expression for $\operatorname{Stab}(A, B)$ follows along similar lines. □

With this geometric preliminaries at hand, we are able to prove the Hessian formula.

Theorem 5.4. (Hessian of C^2-smooth spectral functions)
Consider a symmetric function $f\colon \mathbf{R}^n \to \mathbf{R}$ and the spectral function $F = f \circ \lambda$. Suppose that F is C^2-smooth around a matrix $A := \mathrm{Diag}\,(a)$ and for any matrix matrix $B \in \mathbf{S}^n$ define $Z := \nabla^2 F(A)[B]$. Then equality

$$\mathrm{diag}\,(Z) = \nabla^2 f(a)[\mathrm{diag}\,(B)],$$

holds, while for indices $i \neq j$, we have

$$Z_{ij} = \begin{cases} B_{ij}\left(\frac{\nabla f(a)_i - \nabla f(a)_j}{a_i - a_j}\right) & \text{if } a_i \neq a_j \\ B_{ij}\big(\nabla^2 f(a)_{ii} - \nabla^2 f(a)_{ij}\big) & \text{if } a_i = a_j. \end{cases}$$

Proof. First observe that clearly f must be C^2 smooth at a. Now, since A is diagonal, so is the gradient $\nabla F(A)$. So, without loss of generality, we can assume $\nabla F(A) = \mathrm{Diag}(\nabla f(a))$.

Observe now that $(Z, -B)$ is orthogonal to the tangent space of $\mathrm{gph}\,\nabla F$ at $(A, \nabla F(A))$. On the other hand, for any vector $a' \in \mathbf{R}^n$, we have the equality

$$\left\langle \begin{pmatrix} Z \\ -B \end{pmatrix}, \begin{pmatrix} \mathrm{Diag}(a') - \mathrm{Diag}(a) \\ \mathrm{Diag}(\nabla f(a')) - \mathrm{Diag}(\nabla f(a)) \end{pmatrix} \right\rangle =$$

$$= \left\langle \begin{pmatrix} \mathrm{diag}(Z) \\ -\mathrm{diag}(B) \end{pmatrix}, \begin{pmatrix} a' - a \\ \nabla f(a') - \nabla f(a) \end{pmatrix} \right\rangle.$$

It follows immediately that the tuple $(\mathrm{diag}(Z), -\mathrm{diag}(B))$ is orthogonal to the tangent space of $\mathrm{gph}\,\nabla f$ at $(a, \nabla f(a))$. Hence we deduce the equality $\mathrm{diag}(Z) = \nabla^2 f(a)[\mathrm{diag}(B)]$ as claimed.

Next fix indices i and j with $a_i \neq a_j$, and define the skew-symmetric matrix $W^{(i,j)} := e_i e_j^T - e_j e_i^T$, where e_k denotes the k'th coordinate vector. Applying Lemma 5.2 with the skew-symmetric matrix $W = \frac{1}{a_i - a_j} W^{(i,j)}$, we obtain

$$\begin{aligned} -2Z_{ij} &= \left\langle Z, \left[\tfrac{1}{a_i - a_j} W^{(i,j)}, A\right] \right\rangle = -\left\langle \left[\tfrac{1}{a_i - a_j} W^{i,j}, B\right], \nabla F(A) \right\rangle \\ &= -\left\langle \mathrm{diag}\left[\tfrac{1}{a_i - a_j} W^{i,j}, B\right], \nabla f(a) \right\rangle = -2B_{ij}\left(\frac{\nabla f(a)_i - \nabla f(a)_j}{a_i - a_j}\right). \end{aligned}$$

The claimed formula $Z_{ij} = B_{ij}\left(\frac{\nabla f(a)_i - \nabla f(a)_j}{a_i - a_j}\right)$ follows.

Finally, fix indices i and j, with $a_i = a_j$. Observe now the inclusion

$$\mathrm{Stab}(A) \subset \mathrm{Stab}(\nabla F(A)).$$

Indeed for any matrix $U \in \mathrm{Stab}(A)$, we have

$$\nabla F(A) = \nabla F(UAU^T) = U \nabla F(A) U^T.$$

This immediately implies that the tangent space $T_{\mathrm{gph}\,\nabla F}(A, \nabla F(A))$ is invariant under the action of $\mathrm{Stab}(A)$, that is

$$U.T_{\mathrm{gph}\,\nabla F}(A, \nabla F(A)) = T_{\mathrm{gph}\,\nabla F}(A, \nabla F(A))$$

for any $U \in \mathrm{Stab}(A)$. Hence the entire orbit $\mathrm{Stab}(A).(X, Y)$ of any tangent vector $(X, Y) \in T_{\mathrm{gph}\,\nabla F}(A, \nabla F(A))$ is contained in the tangent space $T_{\mathrm{gph}\,\nabla F}(A, \nabla F(A))$. We conclude that the tangent space to such an orbit $\mathrm{Stab}(A).(X, Y)$ at (X, Y) is contained in $T_{\mathrm{gph}\,\nabla F}(A, \nabla F(A))$ as well.

Define now the matrices $E_i := \mathrm{Diag}(e_i)$ and $\hat{Z} := \mathrm{Diag}(\nabla^2 f(a)[e_i])$. Because F is C^2-smooth, clearly the inclusion $(E_i, \hat{Z}) \in T_{\mathrm{gph}\nabla F}(A, \nabla F(A)$ holds. The above argument, along with Lemma 5.3, immediately implies the inclusion

$$\{([W, E_i], [W, \hat{Z}]) : W \text{ skew-symmetric}, [W, A] = 0\} \quad \subseteq \quad T_{\mathrm{gph}\nabla F}(A, \nabla F(A))$$

and in particular, $([W, E_i], [W, \hat{Z}])$ is orthogonal to $(Z, -B)$ for any skew-symmetric W satisfying $[W, A] = 0$. To finish the proof, simply set $W = W^{(i,j)}$. Then since $a_i = a_j$, we have $[W, A] = 0$ and therefore

$$\begin{aligned} -2Z_{ij} = \left\langle Z, [W^{(i,j)}, E_i]\right\rangle = \langle B, [W^{(i,j)}, \hat{Z}]\rangle = -\left\langle [W^{(i,j)}, B], \hat{Z}\right\rangle \\ = -2B_{ij}\big(\nabla^2 f(a)_{ii} - \nabla^2 f(a)_{ij}\big), \end{aligned}$$

as claimed. This completes the proof. $\square$

Remark 5.5. The appealing geometric techniques presented in this section seem promising for obtaining at least necessary conditions for the generalized Hessian, in the sense of [17], of spectral functions that are not necessarily C^2-smooth. For example, exact formulas are available for special cases such as the indicator function to the positive semi-definite cone [7]. Indeed, the arguments presented here deal entirely with the graph $\mathrm{gph}\,\nabla f$, a setting perfectly adapted to generalized Hessian computations. This is not immediate, however. To illustrate, consider a matrix $Z \in \partial^2 F(A|V)$. Then one can easily establish properties of $\mathrm{Diag}\,Z$ analogous to those presented in Theorem 5.4, as well as properties of Z_{ij} for indices i and j satisfying $a_i \neq a_j$. The difficulty occurs for indices i and j with $a_i = a_j$. In this case, our argument used explicitly the fact that tangent cones to $\mathrm{gph}\,\partial f$ are linear subspaces, a property that is decisively false in the general setting. $\square$

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