An Extrinsic Look at the Riemannian Hessian

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Abstract. Let f be a real-valued function on a Riemannian submanifold of a Euclidean space, and let \bar{f} be a local extension of f. We show that the Riemannian Hessian of f can be conveniently obtained from the Euclidean gradient and Hessian of \bar{f} by means of two manifoldspecific objects: the orthogonal projector onto the tangent space and the Weingarten map. Expressions for the Weingarten map are provided on various specific submanifolds.

Keywords: Riemannian Hessian, Euclidean Hessian, Weingarten map, shape operator.

1 Introduction

This paper concerns optimization methods on Riemannian manifolds that make explicit use of second-order information. This research area is motivated by various problems in the sciences and engineering that can be formulated as optimizing a real-valued function defined on a Riemannian manifold (see, e.g., [20,16,17,12,7] for some recently considered applications), and by the well-known fact that second-order methods tend to have the edge over first-order methods in situations where an accurate solution is sought or when the Hessian gets ill conditioned (see [1] for a recent example).

The archetypical second-order optimization method is Newton's method, of which several generalizations have been proposed on manifolds. Most of them fit in the framework given in [19,5] and [2, Alg. 5]. Besides a smooth real-valued function f defined on a Riemannian manifold \mathcal{M} , the ingredients of the Riemannian Newton method [2, Alg. 5] are an affine connection ∇ on \mathcal{M} and a retraction R on \mathcal{M} . Turning the Riemannian Newton method into a successful numerical algorithm relies much on choosing ∇ and R and on computing them efficiently.

A retraction R on \mathcal{M} can be viewed as a tool that turns a tangent update vector into a new iterate on \mathcal{M} . Retractions have been given particular attention in the recent literature, in general [3] and also specifically for the important cases where \mathcal{M} is the Stiefel manifold of orthonormal matrices [15,21,13] or the manifold of fixed-rank matrices [20,18].

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As for the affine connection ∇ , it is instrumental in the definition of the Hessian operator of f on \mathcal{M} . Namely, for all $x \in \mathcal{M}$ and all z in the tangent space $T_x \mathcal{M}$, one defines

$$\operatorname{Hess} f(x)[z] := \nabla_z \operatorname{grad} f \quad \in \operatorname{T}_x \mathcal{M}. \tag{1}$$

While the convergence analysis of the Riemannian Newton method in [2, §6.3] provides for using any affine connection, a natural choice for ∇ is the uniquely defined Riemannian connection, also termed Levi-Civita connection or canonical connection.

In this paper, for the case where \mathcal{M} is a Riemannian submanifold of a Euclidean space \mathcal{E} (examples can be found in Section 4) and where ∇ is chosen to be the Riemannian connection, we give a formula for the Hessian (1) that relies solely on four objects: (i) the classical gradient $\partial \bar{f}(x)$ of a smooth extension \bar{f} of f in a neighborhood of \mathcal{M} in \mathcal{E} , (ii) the classical Hessian $\partial^2 \bar{f}(x)$ of \bar{f} , (iii) the orthogonal projector \mathcal{P}_x onto $T_x \mathcal{M}$, (iv) the Weingarten map \mathfrak{A}_x , also called shape operator. (The symbol \mathfrak{A} is "A" in Fraktur font.) We provide expressions for \mathcal{P}_x and \mathfrak{A}_x on some important Riemannian submanifolds. These expressions yield a formula for the Riemannian Hessian where f is involved only through the classical gradient and Hessian, $\partial \bar{f}(x)$ and $\partial^2 \bar{f}(x)$. These results can be exploited in various Riemannian optimization schemes, such as Newton's method or trust-region methods, where the knowledge of the Hessian is either mandatory or potentially beneficial.

The paper is organized as follows. Section 2 recalls in more details the definition of the Riemannian Hessian on submanifolds of Euclidean spaces. Section 3 lays out the relation between the Riemannian Hessian and the Weingarten map. Finally, section 4 provides formulas for the Weingarten map on several specific manifolds.

An early version of Sections 2 and 3 of this paper can be found in section 6 of the technical report [4].

2 The Riemannian Hessian on Submanifolds

Let \mathcal{M} be a *d*-dimensional Riemannian submanifold of an *n*-dimensional Euclidean space \mathcal{E} ; see, e.g., [2, §3.6.1] or [9, §2.A.3] for details. Let x_0 be a point of \mathcal{M} , let f be a smooth real-valued function on \mathcal{M} around x_0 , and let \overline{f} be a smooth extension of f to a neighborhood \mathcal{U} of x_0 in \mathcal{E} .

For all $x \in \mathcal{M}$, we let $\partial \bar{f}(x)$ and $\partial^2 \bar{f}(x)$ denote the (Euclidean) gradient and (Euclidean) Hessian of \bar{f} at x. In coordinates, we have

$$\partial \bar{f}(x) = \left[\partial_1 \bar{f}(x) \dots \partial_n \bar{f}(x)\right]^{\mathrm{T}}$$

and

$$[\partial^2 \bar{f}(x)]_{ij} = \partial_{ij} \bar{f}(x), \quad i, j = 1, \dots, n.$$

We also let \mathcal{P}_x denote the orthogonal projector onto $T_x\mathcal{M}$, defined by

$$\mathcal{P}_x : \mathrm{T}_x \mathcal{E} \simeq \mathcal{E} \to \mathrm{T}_x \mathcal{M} : \xi \mapsto \mathcal{P}_x(\xi)$$
 (2)

with $\langle \xi - \mathcal{P}_x(\xi), \zeta \rangle = 0$ for all $\zeta \in T_x \mathcal{M}$. Examples will be given in Section 4. Once an orthonormal basis is chosen for \mathcal{E} , \mathcal{P}_x is represented as a (symmetric) matrix; hence \mathcal{P} can be viewed as a matrix-valued function on \mathcal{M} . For any function F on \mathcal{M} into a vector space, and for any $z \in T_x \mathcal{M}$, we let

$$\mathbf{D}_z F = \lim_{t \to 0} F(\gamma(t)),$$

where γ is any curve on \mathcal{M} with $\gamma(0) = x$ and $\gamma'(0) = z$.

We have

$$\operatorname{grad} f(x) = \mathcal{P}_x \partial \bar{f}(x),$$
(3)

where grad f(x) denotes the (Riemannian) gradient of f at x; see [2, §3.6.1] for details. Moreover, letting ∇ denote the Riemannian connection on \mathcal{M} , we have that Hess f(x), the Riemannian Hessian of f at x, is the linear transformation of $T_x \mathcal{M}$ defined, for all $z \in T_x \mathcal{M}$, by

$$\operatorname{Hess} f(x)[z] = \nabla_z \operatorname{grad} f \tag{4}$$

$$= \mathcal{P}_x \mathcal{D}_z \,(\operatorname{grad} f) \tag{5}$$

$$= \mathcal{P}_x \mathcal{D}_z \left(\mathcal{P} \partial \bar{f} \right) \tag{6}$$

$$= \mathcal{P}_x \partial^2 \bar{f}(x) z + \mathcal{P}_x \mathcal{D}_z \mathcal{P} \partial \bar{f}(x).$$
(7)

Equation (4) is the definition (1). Equation (5) comes from the classical expression of the Riemannian connection on a Riemannian submanifold of a Euclidean space; see, e.g., [2, §5.3.3] or [9, §2.B.2]. Equation (6) follows from (3). Finally, (7) is an application of the product rule, observing that \mathcal{P} is a matrix-valued function, $\partial \bar{f}$ a vector-valued function, and $\mathcal{P}_x \mathcal{P}_x = \mathcal{P}_x$ since \mathcal{P}_x is a projector.

Expression (7) features the four ingredients alluded to in the introduction, namely $\partial \bar{f}(x)$, $\partial^2 \bar{f}(x)$, \mathcal{P}_x , $\mathcal{P}_x D_z \mathcal{P}$. The rest of this paper is devoted to establishing the relation of $\mathcal{P}_x D_z \mathcal{P}$ with the Weingarten map and to working out formulas for $\mathcal{P}_x D_z \mathcal{P}$ on various specific Riemannian submanifolds.

3 The Riemannian Hessian and the Weingarten Map

We are thus concerned with $\mathcal{P}_x D_z \mathcal{P}$, where $z \in T_x \mathcal{M}$. In this section, we establish a relation (8) between $\mathcal{P}_x D_z \mathcal{P}$ and the Weingarten map, defined next. This relation does not seem to have been previously pointed out in the literature, but it is present in the technical report [4].

Definition 1 (Weingarten map). The Weingarten map of the submanifold \mathcal{M} at x is the operator \mathfrak{A}_x that takes as arguments a tangent vector $z \in T_x \mathcal{M}$ and a normal vector $v \in T_x^{\perp} \mathcal{M}$ and returns the tangent vector

$$\mathfrak{A}_x(z,v) = -\mathcal{P}_x \mathcal{D}_z V,$$

where V is any local extention of v to a normal vector field on \mathcal{M} .

It is known [6, Prop. II.2.1] that $\mathcal{P}_x \mathbf{D}_z V$ does not depend on the choice of the extension V, and this makes the above definition valid. The next result confirms this fact and gives an alternate expression of $\mathfrak{A}_x(z, v)$. Let

$$\mathcal{P}_x^{\perp} = I - \mathcal{P}_x$$

denote the orthogonal projector onto the normal space to \mathcal{M} at x. It is useful to keep in mind that, in our convention, D applies only to the expression that directly follows: $D_z FG = (D_z F)G \neq D_z(FG)$.

Theorem 1. The Weingarten map \mathfrak{A}_x satisfies

$$\mathfrak{A}_x(z, \mathcal{P}_x^{\perp} u) = \mathcal{P}_x \mathcal{D}_z \mathcal{P} u = \mathcal{P}_x \mathcal{D}_z \mathcal{P} \mathcal{P}_x^{\perp} u, \tag{8}$$

for all $x \in \mathcal{M}$, $z \in T_x \mathcal{M}$, and $u \in T_x \mathcal{E} \simeq \mathcal{E}$.

Proof. We first show that

$$\mathcal{P}_x \mathcal{D}_z \mathcal{P} = \mathcal{P}_x \mathcal{D}_z \mathcal{P} \mathcal{P}_x^{\perp},\tag{9}$$

which takes care of the second equality in (8). Since $\mathcal{PP}^{\perp} = 0$, we have $0 = D_z \mathcal{PP}_x^{\perp} + \mathcal{P}_x D_z \mathcal{P}^{\perp} = D_z \mathcal{PP}_x^{\perp} - \mathcal{P}_x D_z \mathcal{P}$. It follows that $\mathcal{P}_x D_z \mathcal{PP}_x = 0$. Hence, since $\mathcal{P}_x + \mathcal{P}_x^{\perp} = I$, we have $\mathcal{P}_x D_z \mathcal{P} = \mathcal{P}_x D_z \mathcal{P}(\mathcal{P}_x + \mathcal{P}_x^{\perp}) = \mathcal{P}_x D_z \mathcal{PP}_x + \mathcal{P}_x D_z \mathcal{PP}_x^{\perp} = \mathcal{P}_x D_z \mathcal{PP}_x^{\perp}$, and the claim (9) is proven.

For the first equality in (9), we have, for all extension U of u,

$$-\mathcal{P}_x \mathbf{D}_z (\mathcal{P}^{\perp} U) = -\mathcal{P}_x \mathbf{D}_z \mathcal{P}^{\perp} U - \mathcal{P}_x \mathcal{P}_x^{\perp} \mathbf{D}_z U = -\mathcal{P}_x \mathbf{D}_z \mathcal{P}^{\perp} U = \mathcal{P}_x \mathbf{D}_z \mathcal{P} U.$$

This concludes the proof.

A consequence of Theorem 1 for the Riemannian Hessian expression (7) is that $\mathcal{P}_x D_z \mathcal{P} \partial \bar{f}(x) = \mathcal{P}_x D_z \mathcal{P} \mathcal{P}_x^{\perp} \partial \bar{f}(x) = \mathfrak{A}_x(z, \mathcal{P}_x^{\perp} \partial \bar{f}(x))$. Observe in particular that $\mathcal{P}_x D_z \mathcal{P} \partial \bar{f}(x)$ depends on $\partial \bar{f}(x)$ only through is normal component $\mathcal{P}_x^{\perp} \partial \bar{f}(x)$. In summary we have obtained the expression

$$\operatorname{Hess} f(x)[z] = \mathcal{P}_x \partial^2 \bar{f}(x) z + \mathfrak{A}_x(z, \mathcal{P}_x^{\perp} \partial \bar{f}).$$
(10)

4 Projector and Weingarten Map on Specific Manifolds

We now present formulas for the projector \mathcal{P} and the Weingarten map \mathfrak{A} on various specific manifolds. All the formulas provided for \mathcal{P} and most—but apparently not all—of those provided for \mathfrak{A} can be found in the literature.

4.1 The Stiefel Manifold

The *Stiefel manifold* of orthonormal *p*-frames in \mathbb{R}^n , denoted by $\operatorname{St}(p, n)$, is the submanifold of the Euclidean space $\mathbb{R}^{n \times p}$ defined by

$$\operatorname{St}(p,n) = \{ X \in \mathbb{R}^{n \times p} : X^{\mathrm{T}} X = I_p \},\$$

where I_p stands for the identity matrix of size p. We point out that the Riemannian metric obtained on $\operatorname{St}(p, n)$ by making it a Riemannian submanifold of $\mathbb{R}^{n \times p}$ is different from the canonical metric mentioned in [8, §2.3.1]. The orthogonal projector \mathcal{P}_X onto $\operatorname{T}_X\operatorname{St}(p, n)$ is given by

$$\mathcal{P}_{X}U = (I - XX^{\mathrm{T}})U + X\frac{1}{2}(X^{\mathrm{T}}U - U^{\mathrm{T}}X)$$
$$= U - X\frac{1}{2}(X^{\mathrm{T}}U + U^{\mathrm{T}}X);$$

see, e.g., [2, §3.6.1].

Let $Z \in T_X \mathcal{M}$ and $V \in T_X^{\perp} \mathcal{M}$. Hence V = XS with $S = S^T$ and $Z = X_{\perp}K + X\Omega$ where $\Omega = -\Omega^T$, K is an arbitrary $(n-p) \times p$ matrix, and X_{\perp} is an orthonormal $n \times (n-p)$ matrix such that $X^T X_{\perp} = 0$; see [2, §3.6.1] for details. We have

$$\mathcal{P}_X \mathcal{D}_Z \mathcal{P} V = \mathcal{P}_X \left(V - Z \frac{1}{2} (X^{\mathrm{T}} V + V^{\mathrm{T}} X) - X \frac{1}{2} (Z^{\mathrm{T}} V + V^{\mathrm{T}} Z) \right).$$

Since V and $X\frac{1}{2}(Z^{\mathrm{T}}V + V^{\mathrm{T}}Z)$ belong to the normal space $T_X^{\perp}\mathrm{St}(p, n)$, and since $\frac{1}{2}(X^{\mathrm{T}}V + V^{\mathrm{T}}X) = S$, we are left with

$$\begin{aligned} \mathcal{P}_X \mathbf{D}_Z \mathcal{P} V &= -\mathcal{P}_X Z S \\ &= -ZS + X \frac{1}{2} (X^{\mathrm{T}} Z S + S Z^{\mathrm{T}} X) \\ &= -ZS + \frac{1}{2} X \Omega S - \frac{1}{2} X S \Omega \\ &= -ZX^{\mathrm{T}} V - \frac{1}{2} X Z^{\mathrm{T}} V - \frac{1}{2} V X^{\mathrm{T}} Z \\ &= -ZX^{\mathrm{T}} V - X \frac{1}{2} (Z^{\mathrm{T}} V + V^{\mathrm{T}} Z). \end{aligned}$$

In summary, for all $Z \in T_X \mathcal{M}$ and $V \in T_X^{\perp} \mathcal{M}$, we have

$$\mathfrak{A}_X(Z,V) = -ZX^{\mathrm{T}}V - X\frac{1}{2}(Z^{\mathrm{T}}V + V^{\mathrm{T}}Z).$$

An equivalent formula can be found in $[11, \S4.1]$.

4.2 The Sphere

The unit sphere S^{n-1} is the Stiefel manifold St(p, n) with p = 1. The orthogonal projector \mathcal{P}_x onto the tangent space reduces to

$$\mathcal{P}_x u = (I - xx^{\mathrm{T}})u = u - xx^{\mathrm{T}}u,$$

and the Weingarten map reduces to

$$\mathfrak{A}_x(z,v) = -zx^{\mathrm{T}}v.$$

4.3 The Orthogonal Group

The orthogonal group O(n) is the Stiefel manifold St(p,n) with p = n. The orthogonal projector \mathcal{P}_X onto the tangent space reduces to

$$\mathcal{P}_X U = X \frac{1}{2} (X^{\mathrm{T}} U - U^{\mathrm{T}} X),$$

and the Weingarten map reduces to

$$\mathfrak{A}_X(Z,V) = -X\frac{1}{2}(V^{\mathrm{T}}Z - Z^{\mathrm{T}}V).$$

4.4 The Grassmann Manifold

Let $\operatorname{Gr}_{m,n}$ denote the Grassmann manifold of *m*-dimensional subspaces of \mathbb{R}^n , viewed as the set of rank-*m* orthogonal projectors in \mathbb{R}^n , i.e.,

$$\operatorname{Gr}_{m,n} = \{ X \in \mathbb{R}^{n \times n} : X^{\mathrm{T}} = X, X^{2} = X, \operatorname{tr} X = n \}.$$

Then, from [10, Prop. 2.1], we have that $\mathcal{P}_X = \operatorname{ad}_X^2$ with $\operatorname{ad}_X A := [X, A] := XA - AX$ and $\operatorname{ad}_X^2 := \operatorname{ad}_X \circ \operatorname{ad}_X$. It follows that, for all $Z \in \operatorname{T}_X \operatorname{Gr}_{m,n}$ and all $V \in \operatorname{T}_X^{\perp} \operatorname{Gr}_{m,n}$, it holds that

$$\mathcal{P}_X \operatorname{D}_Z \mathcal{P} V = \operatorname{ad}_X^2 (\operatorname{ad}_Z \operatorname{ad}_X V + \operatorname{ad}_X \operatorname{ad}_Z V)$$

= $\operatorname{ad}_X^2 \operatorname{ad}_Z \operatorname{ad}_X V + \operatorname{ad}_X \operatorname{ad}_Z V$
= $\operatorname{ad}_X \operatorname{ad}_Z V$
= $-\operatorname{ad}_X \operatorname{ad}_V Z$,

where $\operatorname{ad}_A B := [A, B] := AB - BA$. One recovers from (10) the Hessian formula of [10, (2.109)].

4.5 The Fixed-Rank Manifol

Let $\mathcal{M}_p(m \times n)$ denote the set of all $m \times n$ matrices of rank p. This is a submanifold of $\mathbb{R}^{m \times n}$ of dimension (m + n - p)p; see [14, Example 8.14]. Let $X \in \mathcal{M}_p(m \times n)$ and, without loss of generality, let $X = U\Sigma V^T$ with $U \in \operatorname{St}(p,m)$ and $V \in \operatorname{St}(p,n)$. The projector \mathcal{P}_X onto $\operatorname{T}_X \mathcal{M}_p(m \times n)$ is given by [20, §2.1]

$$\mathcal{P}_X W = \mathcal{P}_U W \mathcal{P}_V + \mathcal{P}_U^{\perp} W \mathcal{P}_V + \mathcal{P}_U W \mathcal{P}_V^{\perp} = W \mathcal{P}_V + \mathcal{P}_U W - \mathcal{P}_U W \mathcal{P}_V,$$

where $\mathbf{P}_U := UU^{\mathrm{T}}$ and $\mathbf{P}_U^{\perp} := I - \mathbf{P}_U$.

We now turn to the Weingarten map. Let $Z \in T_X \mathcal{M}_p(m \times n)$. Let $\dot{U} \in T_U \mathrm{St}(p,m)$, $\dot{\Sigma}$ diagonal, and $\dot{V} \in T_V \mathrm{St}(p,n)$ be such that $Z = D_{\dot{U},\dot{\Sigma},\dot{V}}(U\Sigma V^{\mathrm{T}}) = \dot{U}\Sigma V^{\mathrm{T}} + U\dot{\Sigma}V^{\mathrm{T}} + U\Sigma\dot{V}^{\mathrm{T}}$. We also let $\dot{P}_U = D_{\dot{U}}P_U = \dot{U}U^{\mathrm{T}} + U\dot{U}^{\mathrm{T}}$, and likewise with \dot{P}_V . Let $W \in T_X^{\mathrm{T}} \mathcal{M}_p(m \times n)$. We have

$$\mathcal{P}_X D_Z \mathcal{P} W = \mathcal{P}_X \left(W \dot{\mathbf{P}}_V + \dot{\mathbf{P}}_U W - \dot{\mathbf{P}}_U W \mathbf{P}_V - \mathbf{P}_U W \dot{\mathbf{P}}_V \right)$$
$$= \mathcal{P}_X \left(\mathbf{P}_U^{\perp} W \dot{\mathbf{P}}_V + \dot{P}_U W \mathbf{P}_V^{\perp} \right)$$
$$= \mathbf{P}_U^{\perp} W \dot{\mathbf{P}}_V \mathbf{P}_V + \mathbf{P}_U \dot{\mathbf{P}}_U W \mathbf{P}_V^{\perp}.$$

Since $W \in T_X^{\perp} \mathcal{M}_p(m \times n)$, we have $W = U_{\perp} L_W V_{\perp}^T$ with L_W arbitrary; this follows from the expression of $T_X \mathcal{M}_p(m \times n)$ in [20, §2.1]. Hence $U^T W = 0$, $P_U^{\perp} W = W$, WV = 0, $WP_V^{\perp} = W$. Using these equations, one obtains

$$\mathbf{P}_U^{\perp} W \dot{\mathbf{P}}_V \mathbf{P}_V = W (\dot{V} V^{\mathrm{T}} + V \dot{V}^{\mathrm{T}}) \mathbf{P}_V = W \dot{V}^{\mathrm{T}} V^{\mathrm{T}} \mathbf{P}_V = W \dot{V}^{\mathrm{T}} V.$$

Likewise, we obtain

$$\mathbf{P}_U \dot{\mathbf{P}}_U W \mathbf{P}_V^{\perp} = U \dot{U}^{\mathrm{T}} W.$$

In summary, we have

$$\mathcal{P}_X \operatorname{D}_Z \mathcal{P} W = W \dot{V}^{\mathrm{T}} V + U \dot{U}^{\mathrm{T}} W.$$

We now seek an alternate expression where only X, Z, and W appear. To this end, observe that the pseudo-inverse of X is given by $X^+ = V \Sigma^{-1} U^{\mathrm{T}}$. Then, recalling that WV = 0, we find that

$$WZ^{\mathrm{T}}(X^{+})^{\mathrm{T}} = W(\dot{V}\Sigma U^{\mathrm{T}} + V(\dot{\Sigma}U^{\mathrm{T}} + \Sigma\dot{U}^{\mathrm{T}}))U\Sigma^{-1}V^{\mathrm{T}}$$
$$= W\dot{V}\Sigma U^{\mathrm{T}}U\Sigma^{-1}V^{\mathrm{T}}$$
$$= W\dot{V}V^{\mathrm{T}}.$$

Similarly, we obtain that

$$(X^+)^{\mathrm{T}} Z^{\mathrm{T}} W = U \dot{U}^{\mathrm{T}} W.$$

In conclusion, we have

$$\mathcal{P}_X \operatorname{D}_Z \mathcal{P} W = W Z^{\mathrm{T}} (X^+)^{\mathrm{T}} + (X^+)^{\mathrm{T}} Z^{\mathrm{T}} W.$$

It is interesting to note that this expression, combined with (10), provides an expression that allows to recover the Hessian formula found in [20, §2.3].

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