

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 manifold-specific 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].

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 $\mathbb{T}_x\mathcal{M}$, one defines

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

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 $\mathbb{T}_x\mathcal{M}$, (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 \bar{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

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

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 $\mathbb{T}_x\mathcal{M}$, defined by

$$\mathcal{P}_x : \mathbb{T}_x\mathcal{E} \simeq \mathcal{E} \rightarrow \mathbb{T}_x\mathcal{M} : \xi \mapsto \mathcal{P}_x(\xi) \quad (2)$$

with $\langle \xi - \mathcal{P}_x(\xi), \zeta \rangle = 0$ for all $\zeta \in \mathbb{T}_x\mathcal{M}$. 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 $z \in \mathbb{T}_x\mathcal{M}$, we let

$$D_z F = \lim_{t \rightarrow 0} F(\gamma(t)),$$

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

We have

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

where $\text{grad } f(x)$ 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 $\text{Hess } f(x)$, the Riemannian Hessian of f at x , is the linear transformation of $\mathbb{T}_x\mathcal{M}$ defined, for all $z \in \mathbb{T}_x\mathcal{M}$, by

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

$$= \mathcal{P}_x D_z (\text{grad } f) \quad (5)$$

$$= \mathcal{P}_x D_z (\mathcal{P} \partial \bar{f}) \quad (6)$$

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

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 $z \in \mathbb{T}_x\mathcal{M}$. 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 $z \in \mathbb{T}_x\mathcal{M}$ and a normal vector $v \in \mathbb{T}_x^\perp\mathcal{M}$ and returns the tangent vector*

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

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

It is known [6, Prop. II.2.1] that $\mathcal{P}_x D_z V$ 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*

$$\mathfrak{A}_x(z, \mathcal{P}_x^\perp u) = \mathcal{P}_x D_z \mathcal{P} u = \mathcal{P}_x D_z \mathcal{P} \mathcal{P}_x^\perp u, \quad (8)$$

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

$$\mathcal{P}_x D_z \mathcal{P} = \mathcal{P}_x D_z \mathcal{P} \mathcal{P}_x^\perp, \quad (9)$$

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

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

$$-\mathcal{P}_x D_z (\mathcal{P}^\perp U) = -\mathcal{P}_x D_z \mathcal{P}^\perp U - \mathcal{P}_x \mathcal{P}_x^\perp D_z U = -\mathcal{P}_x D_z \mathcal{P}^\perp U = \mathcal{P}_x D_z \mathcal{P} U.$$

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 its normal component $\mathcal{P}_x^\perp \partial \bar{f}(x)$. In summary we have obtained the expression

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

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 $\text{St}(p, n)$, is the submanifold of the Euclidean space $\mathbb{R}^{n \times p}$ defined by

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

where I_p stands for the identity matrix of size p . We point out that the Riemannian metric obtained on $\text{St}(p, n)$ 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 $T_X \text{St}(p, n)$ is given by

$$\begin{aligned}\mathcal{P}_X U &= (I - XX^T)U + X \frac{1}{2}(X^T U - U^T X) \\ &= U - X \frac{1}{2}(X^T U + U^T X);\end{aligned}$$

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

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

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

$$\begin{aligned}\mathcal{P}_X D_Z \mathcal{P} V &= -\mathcal{P}_X ZS \\ &= -ZS + X \frac{1}{2}(X^T ZS + SZ^T X) \\ &= -ZS + \frac{1}{2}X\Omega S - \frac{1}{2}XS\Omega \\ &= -ZX^T V - \frac{1}{2}XZ^T V - \frac{1}{2}VX^T Z \\ &= -ZX^T V - X \frac{1}{2}(Z^T V + V^T Z).\end{aligned}$$

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

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

An equivalent formula can be found in [11, §4.1].

4.2 The sphere

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

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

and the Weingarten map reduces to

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

4.3 The orthogonal group

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

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

and the Weingarten map reduces to

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

4.4 The Grassmann manifold

Let $\text{Gr}_{m,n}$ 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.,

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

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

$$\begin{aligned} \mathcal{P}_X D_Z \mathcal{P} V &= \text{ad}_X^2 (\text{ad}_Z \text{ad}_X V + \text{ad}_X \text{ad}_Z V) \\ &= \text{ad}_X^2 \text{ad}_Z \text{ad}_X V + \text{ad}_X \text{ad}_Z V \\ &= \text{ad}_X \text{ad}_Z V \\ &= -\text{ad}_X \text{ad}_V Z, \end{aligned}$$

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

4.5 The fixed-rank manifold

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 $U \in \text{St}(p, m)$ and $V \in \text{St}(p, n)$. The projector \mathcal{P}_X onto $\text{T}_X \mathcal{M}_p(m \times n)$ is given by [20, §2.1]

$$\mathcal{P}_X W = P_U W P_V + P_U^\perp W P_V + P_U W P_V^\perp = W P_V + P_U W - P_U W P_V,$$

where $P_U := U U^T$ and $P_U^\perp := I - P_U$.

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

$$\begin{aligned} \mathcal{P}_X D_Z \mathcal{P} W &= \mathcal{P}_X \left(W \dot{P}_V + \dot{P}_U W - \dot{P}_U W P_V - P_U W \dot{P}_V \right) \\ &= \mathcal{P}_X \left(P_U^\perp W \dot{P}_V + \dot{P}_U W P_V^\perp \right) \\ &= P_U^\perp W \dot{P}_V P_V + P_U \dot{P}_U W P_V^\perp. \end{aligned}$$

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

$$P_U^\perp W \dot{P}_V P_V = W(\dot{V}V^\top + V\dot{V}^\top)P_V = W\dot{V}V^\top P_V = W\dot{V}V^\top.$$

Likewise, we obtain

$$P_U \dot{P}_U W P_V^\perp = U\dot{U}^\top W.$$

In summary, we have

$$\mathcal{P}_X D_Z \mathcal{P} W = W\dot{V}V^\top + U\dot{U}^\top W.$$

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 $X^+ = V\Sigma^{-1}U^\top$. Then, recalling that $WV = 0$, we find that

$$\begin{aligned} WZ^\top(X^+)^\top &= W(\dot{V}\Sigma U^\top + V(\dot{\Sigma}U^\top + \Sigma\dot{U}^\top))U\Sigma^{-1}V^\top \\ &= W\dot{V}\Sigma U^\top U\Sigma^{-1}V^\top \\ &= W\dot{V}V^\top. \end{aligned}$$

Similarly, we obtain that

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

In conclusion, we have

$$\mathcal{P}_X D_Z \mathcal{P} W = WZ^\top(X^+)^\top + (X^+)^\top Z^\top W.$$

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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