

DEPARTMENT OF MATHEMATICAL SCIENCES

TMA4500 - Industrial Mathematics, Specialization Project

Optimization using second order information on the Symplectic Stiefel manifold

Author: Ole Gunnar Røsholt Hovland

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Introduction 1

2 Theory

Basic definitions 2.1

This section is designed to be a reference work to ensure that the reader has the necessary background to understand the optimization algorithms we will be studying.

The optimization algorithm we will be studying is defined on a Riemannian manifold. This is because the algorithms we will use are designed to utilize first and second order information, and we need to define what these concepts mean on a manifold.

Definition 1 (Tangent Space).

Definition 2 (Riemannian manifold). As defined in [3, def 2.6, p. 179]: a smooth manifold \mathcal{M} , as defined in [7, p. 13], is a Riemannian manifold if we can define a field of symmetric, positive definite, bilinear forms $g(\cdot,\cdot)$, called the Riemannian metric. By field we mean that g_p is defined on the tangent space $T_p\mathcal{M}$ at each point $p \in \mathcal{M}$ [3, def 2.1, p. 178]. We will assume that g is smooth, meaning that it is of class C^{∞} .

Definition 3 (Quotient manifold). We define the definition of quotient manifold as in ??p. 27]Ab- ref sil, Mahony, Sepulchre Let \mathcal{M} be a manifold equipped with the operation \sim called the equivalence relation. The equivalence relation has the following properties:

- 1. (reflexive) $p \sim p$ for all $p \in \mathcal{M}$,
- 2. (symmetric) $p \sim q$ if and only if $q \sim p$ for all $q, p \in \mathcal{M}$, and
- 3. (transitive) given $p \sim q$ and $q \sim r$ this implies that $p \sim r$ for all $p, q, r \in \mathcal{M}$.

Given the set $[p] := \{q \in \mathcal{M} : q \sim p\}$ called the equivalence class of all points equivalent to p, the

$$\mathcal{M}/\sim:=\{[p]:p\in\mathcal{M}\}$$

is called the quotient of \mathcal{M} by \sim . It is the set of all equivalence classes of \sim in \mathcal{M} . The mapping $\pi: \mathcal{M} \to \mathcal{M}/\sim called \ the \ natural -or \ canonical \ projection, \ defined \ by \ p \mapsto [p]$.

Definition 4 (Horizontal & Vertical Space). Given a Riemannian manifold $\overline{\mathcal{M}}$ with Riemannian metric \overline{g} , denote a quotient manifold of $\overline{\mathcal{M}}$ as $\mathcal{M} = \overline{\mathcal{M}}/\sim$. Following the definitions in Absil et al. [1, p. 43], for a point $p \in \mathcal{M}$, the equivalence class $[p] = \pi^{-1}(p)$ induces an embedded submanifold of $\overline{\mathcal{M}}$ (see Definition 3), hence it admits a tangent space,

$$\mathcal{V}_{\overline{p}} = T_{\overline{p}}(\pi^{-1}(p))$$

named the vertical space at \overline{p} . Canonically chosen as the orthogonal complement of $\mathcal{V}_{\overline{p}}$ in $T_{\overline{p}}\overline{\mathcal{M}}$, the horizontal space [1, p. 48] is defined as

$$\mathcal{H}_{\overline{p}} \coloneqq \mathcal{V}_{\overline{p}}^{\perp} = \{ Y_{\overline{p}} \in T_{\overline{p}} \overline{\mathcal{M}} : \overline{g}(Y_{\overline{p}}, Z_{\overline{p}}) = 0 \quad \forall \quad Z_{\overline{p}} \in \mathcal{V}_{\overline{p}} \}.$$

The horizontal lift at $\overline{p} \in \pi^{-1}(p)$ of a tangent vector $X_p \in T_p \mathcal{M}$ is the unique tangent vector $X_{\overline{p}} \in$ $\mathcal{H}_{\overline{p}} \ \ that \ \ satisfies \ \mathrm{D}\pi(\overline{p})[X_{\overline{p}}] = X_p. \ \ \ Note \ \ that \ \ given \ \ the \ \ horizontal \ \ space \ \ on \ \overline{\mathcal{M}}, \ \mathcal{H}_{\overline{p}} \oplus \overline{\mathcal{V}}_{\overline{p}} = T_{\overline{p}} \mathcal{M},$ where \oplus denotes the Whitney sum.

Definition 5 (General Linear group). The real General Linear group is defined as the set of all invertible matrices in $\mathbb{R}^{n\times n}$, denoted by GL(n). [4, Example 9.11]

Definition 6 (Orthogonal group). The real Orthogonal group is defined as the set of all orthogonal matrices in $\mathbb{R}^{n \times n}$, denoted by O(n). [5, p. 3]

define w sum! i wrote it in obsidian in the H and V space file!

Definition 7 (Riemannian connection). The Riemanian connection, also known as the Levi-Civita connection, is the unique affine connection which is torsion free, and metric compatible [9, Def. 6.4]. In Appendix A of [6], denoting $\mathfrak{X}(\mathcal{M})$ as the space of smooth vector fiels on \mathcal{M} , it is defined as the unique \mathbb{R} -bilinear smooth map on \mathcal{M} with riemannian metric $\langle \cdot, \cdot \rangle_p$

$$\nabla : \mathfrak{X}(\mathcal{M}) \times \mathfrak{X}(\mathcal{M}) \to \mathfrak{X}(\mathcal{M}), \quad (X, Y) \mapsto \nabla_X Y,$$

such that the following properties hold. Given $X,Y,Z\in\mathfrak{X}(\mathcal{M}),$ and $f\in\mathcal{C}^{\infty}(M),$ $\nabla_X Y$ has the following properties:

- 1. (first argument linearity) $\nabla_{fX}Y = f\nabla_XY$,
- 2. (Leibnitz) $\nabla_X(fY) = (Xf)Y + f\nabla_XY$,
- 3. (torsion free) $\nabla_X Y \nabla_Y X = [X, Y]$, where $[\cdot, \cdot]$ is the Lie bracket, and
- 4. (metric compatibility) $Z\langle X, Y \rangle = \langle \nabla_Z X, Y \rangle + \langle X, \nabla_Z Y \rangle$.

Definition 8 (Christoffel symbols).

Definition 9.

Definition 10.

Definition 11.

For the rest of this paper we denote \mathcal{M} as being a Riemannian manifold.

After the basic definitions, talk about how the rest of the theory is a highlighted summary through BZ and JZ. The goal is to look at the findings in JZ, however it relies heavely on theory derived in BZ. It will be mentioned of some parts are from other works, or if they are original work.

2.2 The Symplectic group

The symplectic group is the space overarching the Symplectic Stiefel manifold, and we will look at this space first. To be able to define the symplectic group we first need some preliminary definitions. Define the *symplectic identity* as the following block matrix,

$$J_{2n} \coloneqq \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix},$$

where I_n denotes the $n \times n$ identity matrix. J_{2n} has som properties we will take advantage of frequently:

$$J_{2n}^{\mathrm{T}} = -J_{2n} = J_{2n}^{-1} \tag{2.1}$$

In addition, define the *Symplectic inverse* of a matrix $p \in \mathbb{R}^{2n \times 2l}$ as The symplectic group is a quotient space of the general linear group, where it is defined as the set of matrices which define the symplectic structure in the following sense. We define the real symplectic group as

$$\operatorname{Sp}(2n) := \{ p \in \mathbb{R}^{2n \times 2n} : p^+ p = I_{2n} \}, \tag{2.2}$$

where p^+ is the symplectic inverse of p, as defined in [symplectic inverse].

$$p^{+} \coloneqq J_{2k}^{\mathrm{T}} p^{\mathrm{T}} J_{2n} \tag{2.3}$$

The Lie algebra of Sp(2n) is the symplectic groups' tangent space at the identity. It is given by

$$\mathfrak{sp}(2n) := \{ \Omega \in \mathbb{R}^{2n \times 2n} : \Omega^+ = -\Omega \}, \tag{2.4}$$

where H is called the Hamiltonian matrix ref??. Now we can define the tangent space of Sp(2n) at a point p as

$$T_n \operatorname{Sp}(2n) = \{ p\Omega, \Omega p \in \mathbb{R}^{2n \times 2n} : \Omega \in \mathfrak{sp}(2n) \}.$$
 (2.5)

Define geodesics as in BZ, prop. 2.1. Maybe do the proof?

In JZ this was stated wrongly

citation

Why do we need sp? We will use quotient properties to map stuff to Spst

2.3 The Symplectic Stiefel manifold

Now that we have defined thy symplectic group, we introduce the manifold of interest, the real symplectic Stiefel manifold. It is defined as

$$SpSt(2n, 2k) := \{ p \in \mathbb{R}^{2n \times 2k} : p^{T} J_{2n} p = J_{2k} \}.$$

Following [2, Prop. 3.1], it is explicitly connected to the symplectic group in the sense that SpSt(2n, 2k) is diffeomorphic to the following quotient manifold of sp(2n):

$$\operatorname{SpSt}(2n, 2k) \cong \operatorname{Sp}(2n)/\operatorname{Sp}(2(n-k)),$$

where the notion of quotient manifold is as in Definition 3. It has dimension $\dim(\operatorname{SpSt}(2n,2k)) = (2n-2k+1)k$.

The following piece of insight can give some further intuition on what the Symplectic Stiefel manifold is. We note that the Stiefel manifold is a quotient space, as defined in Definition 3, of the orthogonal group as defined in Definition 6 such that St(2n, 2k) = O(n)/O(n-k).

This is probably unnecessary

Derive tangent space. See obsidian

2.4 Right-invariant framework

Intro for this section. now that sp and spst are defined, define right inv. framework in sp, then guide the framework through to spst.

The goal for this section is to use the right-invariant metric defined on the symplectic group to define an appropriate metric on the symplectic Stiefel manifold.

many of the usual SpSt metrics do not have geodesics, therefore... We need a proper metric for SpSt(2n, 2k) in the sense that we need a metric that allows us to perform optimization on this manifold. To this end we need a metric that makes it possible to derive geodesics, as opposed to (BZ sources). The following metric defined in BZ fulfils our criteria.

Define the point-wise right-invariant metric on $\operatorname{Sp}(2n,\mathbb{R})$ as the mapping $g_p^{\operatorname{Sp}}: T_p\operatorname{Sp}(2n,\mathbb{R}) \times T_p\operatorname{Sp}(2n,\mathbb{R}) \to \mathbb{R}$,

$$g_p^{\mathrm{Sp}}(X_1, X_2) := \frac{1}{2} \operatorname{tr}((X_1 p^+)^T X_2 p^+), \quad X_1, X_2 \in T_p \operatorname{Sp}(2n, \mathbb{R}).$$
 (2.6)

It is right-invariant in the sense that $g_{pq}^{\mathrm{Sp}}(X_1q,X_2q)=\frac{1}{2}\mathrm{tr}((X_1qq^+p^+)^TX_2qq^+p^+)=g_p^{\mathrm{Sp}}(X_1,X_2)$ for all $p\in\mathrm{Sp}(2n,\mathbb{R})$.

Now that we have defined $g_p^{\rm Sp}$, we want to, in a sense, transport it to ${\rm SpSt}(2n,2k)$ in a way that preserves the right-invariance. To achieve this we will use a *horizontal lift* to define a metric on ${\rm SpSt}(2n,2k)$ through 2.6. Split $T_p{\rm Sp}(2n,\mathbb{R})$ into to parts: the horizontal- and vertical part, with respect to $g_p^{\rm Sp}$ and π :

$$T_p \operatorname{Sp}(2n) = \operatorname{Ver}_n^{\pi} \operatorname{Sp}(2n) \oplus \operatorname{Hor}_n^{\pi} \operatorname{Sp}(2n).$$
 (2.7)

Define $\operatorname{Ver}_p^{\pi} \operatorname{Sp}(2n)$ and $\operatorname{Hor}_p^{\pi} \operatorname{Sp}(2n)$ in a smart way. Maybe just a reference if I do not have the space.

Rework the following paragraph. see obsidian

The point-wise right-invariant Riemannian metric on $\operatorname{SpSt}(2n,2k)$ is defined as the mapping $g_p: T_p\operatorname{SpSt}(2n,2k) \times T_p\operatorname{SpSt}(2n,2k) \to \mathbb{R}, \ g_p(X_1,X_2) \coloneqq g_p^{\operatorname{Sp}}((X_1)_p^{\operatorname{hor}},(X_2)_p^{\operatorname{hor}}).$ More explicitly

Look at 20, Theorem 2.28 in BZ to maybe skip the derivation up to gp

$$g_p(X_1, X_2) = \operatorname{tr}\left(X_1^T \left(I_{2n} - \frac{1}{2}J_{2n}^T p(p^T p)^{-1} p^T J_{2n}\right) X_2(p^T p)^{-1}\right), \tag{2.8}$$

for $X_1, X_2 \in T_p \operatorname{SpSt}(2n, 2k)$. For this metric, π denotes a Riemannian submersion.

Define geodesics as in BZ

pi here is weird, change this so it is more clear what it does

$$p^{\mathrm{T}}J\nabla f(p)p^{\mathrm{T}}p + p^{\mathrm{T}}JJp(\nabla f(p))^{\mathrm{T}}Jp + p^{\mathrm{T}}p(\nabla f(p))^{\mathrm{T}}Jp + p^{\mathrm{T}}J^{\mathrm{T}}\nabla f(p)p^{\mathrm{T}}J^{\mathrm{T}}Jp$$

$$= -p^{\mathrm{T}}J^{\mathrm{T}}\nabla f(p)p^{\mathrm{T}}J^{\mathrm{T}}Jp$$

$$(2.9)$$

2.5 Riemannian gradient of the Symplectic Stiefel manifold

Now that we have chosen a metric, we can justify a choice for a Riemannian gradient.

Proposition 1. Given a function $f : \operatorname{SpSt}(2n, 2k) \to \mathbb{R}$, the Riemannian gradient with respect to g_p is given by

$$\operatorname{grad} f(p) = \nabla f(p) p^{T} p + J_{2n} p (\nabla f(p))^{T} J_{2n} p, \tag{2.11}$$

where $\nabla f(p)$ is the Euclidean gradient of a smooth extension around $p \in \operatorname{SpSt}(2n, 2k)$ in $\mathbb{R}^{2n \times 2k}$ at p.

Proof. We can see that this is the Riemannian gradient by the following two observations stated in $[\mathbf{BZ}]$, which we verify ourselves below.

Firstly, gradient must be in $T_p \operatorname{SpSt}(2n, 2k)$, which means by ref?? that $0 = p^+ \operatorname{grad} f(p) + (\operatorname{grad} f(p))^+ p$. Computing this we get

$$p^{T}J\nabla f(p)p^{T}p + p^{T}JJp(\nabla f(p))^{T}Jp + p^{T}p(\nabla f(p))^{T}Jp + p^{T}J^{T}\nabla f(p)p^{T}J^{T}Jp = 0$$
 (2.12)

where we have used $JJ = -J^{T}J = -I_{2n}$ and (2.1).

Secondly, the gradient also has to satisfy $g_p(\operatorname{grad} f(p), X) = \operatorname{d} f_p(X) = \operatorname{tr}((\nabla f(p))^T X)$ for all $X \in T_p\operatorname{SpSt}(2n, 2k)$:

$$g_p(\operatorname{grad} f(p), X) = \operatorname{tr}\left((p^{\mathrm{T}} p(\nabla f(p))^{\mathrm{T}} + p^{\mathrm{T}} J^{\mathrm{T}} \nabla f(p) p^{\mathrm{T}} J^{\mathrm{T}})(I_{2n} - \frac{1}{2}G)X(p^{\mathrm{T}} p)^{-1}\right),$$

where $G := J^{\mathrm{T}} p(p^{\mathrm{T}} p)^{-1} p^{\mathrm{T}} J$. Expanding this expression we obtain

$$= \operatorname{tr} \left(p^{\mathsf{T}} p(\nabla f(p))^{\mathsf{T}} X(p^{\mathsf{T}} p)^{-1} \right) - \frac{1}{2} \operatorname{tr} \left(p^{\mathsf{T}} p(\nabla f(p))^{\mathsf{T}} G X(p^{\mathsf{T}} p)^{-1} \right) \\ + \operatorname{tr} \left(p^{\mathsf{T}} J^{\mathsf{T}} \nabla f(p) p^{\mathsf{T}} J^{\mathsf{T}} X(p^{\mathsf{T}} p)^{-1} \right) - \frac{1}{2} \operatorname{tr} \left(p^{\mathsf{T}} J^{\mathsf{T}} \nabla f(p) p^{\mathsf{T}} J^{\mathsf{T}} G X(p^{\mathsf{T}} p)^{-1} \right),$$

where the cancellations used the fact that the trace is invariant under circular shifts. Noting that the first term is by definition $d f_p(X)$, and inserting the definition of G, the expression becomes

$$\begin{split} &=\mathrm{d}\,f_p(X) - \tfrac{1}{2}\mathrm{tr}\big((\nabla f(p))^\mathrm{T}J^\mathrm{T}p(p^\mathrm{T}p)^{-1}p^\mathrm{T}JX\big) \\ &+ \mathrm{tr}\big(p^\mathrm{T}J^\mathrm{T}\nabla f(p)p^\mathrm{T}J^\mathrm{T}X(p^\mathrm{T}p)^{-1}\big) \\ &- \tfrac{1}{2}\mathrm{tr}\big(p^\mathrm{T}J^\mathrm{T}\nabla f(p)p^\mathrm{T}J^\mathrm{T}J^\mathrm{T}p(p^\mathrm{T}p)^{-1}p^\mathrm{T}JX(p^\mathrm{T}p)^{-1}\big). \end{split}$$

After using $J^{\mathrm{T}}J^{\mathrm{T}} = -I_{2n}$ and (2.1) on the last term, we notice that we can cancel $p^{\mathrm{T}}p(p^{\mathrm{T}})p^{-1}$, making it equal to the second to last term. Now focusing on the second term: for the first equality we use the fact that for any matrix, A, $\operatorname{tr}(A) = \operatorname{tr}(A^{\mathrm{T}})$, and for the second equality we utilize the cyclic property of the trace, and (2.1),

$$\frac{1}{2}\operatorname{tr}\left((\nabla f(p))^{\mathrm{T}}J^{\mathrm{T}}p(p^{\mathrm{T}}p)^{-1}p^{\mathrm{T}}JX\right) = \frac{1}{2}\operatorname{tr}\left(X^{\mathrm{T}}J^{\mathrm{T}}p(p^{\mathrm{T}}p)^{-1}p^{\mathrm{T}}J\nabla f(p)\right)
= -\frac{1}{2}\operatorname{tr}\left(p^{\mathrm{T}}J^{\mathrm{T}}\nabla f(p)X^{\mathrm{T}}J^{\mathrm{T}}p(p^{\mathrm{T}}p)^{-1}\right)$$
(2.13)

Inserting 2.13 into our expression we end up with:

$$d f_p(X) = d f_p(X) + \frac{1}{2} tr(p^T J \nabla f(p) X^T J^T p(p^T p)^{-1}) + \frac{1}{2} tr(p^T J^T \nabla f(p) p^T J^T X (p^T p)^{-1}),$$

where the last two terms cancel after applying (2.1), and the tangent space condition ref ??, add ref to $p^{T}JX = -X^{T}Jp$.

2.6 Riemannian Hessian

(Christoffel symbols)

With our metric 2.8 the Hessian at p of a smooth function $f: \operatorname{SpSt}(2n, 2k) \to \mathbb{R}$ is the endomorphism $\operatorname{Hess} f(p): T_p \operatorname{SpSt}(2n, 2k) \to T_p \operatorname{SpSt}(2n, 2k)$. It is defined as

$$\operatorname{Hess} f(p)[X] = \left. \frac{d}{dt} \operatorname{grad} f(c(t)) \right|_{t=0} + \Gamma(\operatorname{grad} f(p), X),$$

where grad $f(\cdot)$ is as in 2.11. Define an arbitrary curve $c(t) \in \operatorname{SpSt}(2n, 2k)$ such that c(0) = p and c'(0) = X

Note: If I've only written ISBN, It's because I couldn't find the DOI.

Question: Is BZ not published?

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