SOLVING MINIMAL-DISTANCE PROBLEMS OVER THE MANIFOLD OF REAL SYMPLECTIC MATRICES

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Abstract. The present paper discusses the question of formulating and solving minimal-distance problems over the group-manifold of real symplectic matrices. In order to tackle the related optimization problem, the real symplectic group is regarded as a pseudo-Riemannian manifold and a metric is chosen that affords the computation of geodesic arcs in closed forms. Then, the considered minimal-distance problem can be solved numerically via a gradient steepest descent algorithm implemented through a geodesic-stepping method. The minimal-distance problem investigated in this paper relies on a suitable notion of distance – induced by the Frobenius norm – as opposed to the natural pseudo-distance that corresponds to the pseudo-Riemannian metric that the real symplectic group is endowed with. Numerical tests about the computation of the empirical mean of a collection of symplectic matrices illustrate the discussed framework.

Key words. Group of real symplectic matrices. Pseudo-Riemannian geometry. Gradient-based optimization on manifolds. Geodesic stepping method.

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1. Introduction. Optimization problems over smooth manifolds have received considerable attention due to their broad application range (see, for instance, [2, 9, 10, 16] and references therein). In particular, the formulation of minimal-distance problems on compact Riemannian Lie groups relies on closed forms of geodesic curves and geodesic distances. Notwithstanding, on certain manifolds the problem of formulating a minimal-distance criterion function and of its optimization is substantially more involved, because it might be hard to compute geodesic distances in closed form. One of such manifolds is the real symplectic group.

Real symplectic matrices form an algebraic group denoted as $\mathrm{Sp}(2n,\mathbb{R})$, with $n \geq 1$. The real symplectic group is defined as follows:

$$\mathrm{Sp}(2n,\mathbb{R}) \stackrel{\mathrm{def}}{=} \{X \in \mathbb{R}^{2n\times 2n} | X^T Q_{2n} X = Q_{2n}\}, \text{ with } Q_{2n} \stackrel{\mathrm{def}}{=} \begin{bmatrix} 0_n & I_n \\ -I_n & 0_n \end{bmatrix}, \tag{1.1}$$

where symbol I_n denotes a $n \times n$ identity matrix and symbol 0_n denotes a whole-zero $n \times n$ matrix. A noticeable application of real symplectic matrices is to the control of beam systems in particle accelerators [12, 29], where Lie-group tools are applied to the characterization of beam dynamics in charged-particle optical systems. Such methods are applicable to accelerator design, charge-particle beam transport and electron microscopes. In the context of vibration analysis, real symplectic 'transfer matrices' are widely used for the dynamic analysis of engineering structures as well as for static analysis, and are particularly useful in the treatment of repetitive structures [38]. Other notable applications of real symplectic matrices are to coding theory [8], quantum computing [6, 22], time-series prediction [3], and automatic control [17]. A further list of applications of symplectic matrices is reported in [14].

The minimal-distance problem over the set of real symplectic matrices plays an important role in applied fields. A recent application which involves the solution

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of a minimal-distance problem in the real symplectic group of matrices is found in the study of optical systems in computational ophthalmology, where it is assumed that the optical nature of a centered optical system is completely described by a real symplectic matrix [23, 25] and involved symplectic matrices are of size 4×4 ($n = 2$). A notable application is found in the control of beam systems in particle accelerators [15], where the size of involved symplectic matrices is 6×6 ($n = 3$), and in the assessment of the fidelity of dynamical gates in quantum analog computation [41], where the integer n corresponds to the number of quantum observables and may be quite large (for example $n = 20$).

Although results are available about the real symplectic group [13, 14, 30], optimization on the manifold of real symplectic matrices appears to be far less studied than for other Lie groups. The present manuscript aims at discussing such problem and to present a solution based on the key idea of treating the space $\mathrm{Sp}(2n, \mathbb{R})$ as a manifold endowed with a pseudo-Riemannian metric that affords the computation of geodesic arcs in closed-forms. Then, the considered minimal-distance problem can be solved numerically via a gradient steepest descent algorithm implemented through a geodesic-stepping method. A proper minimal-distance objective function on the manifold $\mathrm{Sp}(2n, \mathbb{R})$ is constructed by building on a result available from the scientific literature about the Frobenius norm of the difference of two symplectic matrices. Given a collection $\{X_1, X_2, \ldots, X_N\}$ of real symplectic matrices of size $2n \times 2n$, the goal of this paper is the minimization of the function

$$f(X) \stackrel{\text{def}}{=} \frac{1}{2N} \sum_{k=1}^{N} \|X - X_k\|_{\mathrm{F}}^2 \tag{1.2}$$

over the manifold $\mathrm{Sp}(2n, \mathbb{R})$ to find the minimizing symplectic matrix.

The remainder of this paper is organized as follows. The §2 recalls those notions from differential geometry (with particular emphasis to pseudo-Riemannian geometry) that are instrumental in the development of an optimization algorithm on the manifold of symplectic matrices. Results about the computation of geodesic arcs and of the pseudo-Riemannian gradient of a regular function on the manifold of real symplectic matrices are presented. The §3 defines minimal-distance problems on manifolds and recalls the basic idea of the gradient-steepest-descent optimization method on pseudo-Riemannian manifolds. It deals explicitly with minimal-distance problems on the manifold of real symplectic matrices and recalls how to measure discrepancy between real symplectic matrices. The §4 presents results of numerical tests performed on an averaging problem over the manifold $\mathrm{Sp}(2n, \mathbb{R})$. The §5 concludes the paper.

2. The real symplectic matrix group and its geometry. The present section recalls notions of differential geometry that are instrumental in the development of the following topics, such as affine geodesic curves and the pseudo-Riemannian gradient. For a general-purpose reference on differential geometry, see [39], while for a specific reference on pseudo-Riemannian geometry and the calculus of variation on manifolds, see [32]. Throughout the present section and the rest of the paper, matrices are denoted by upper-case letters (e.g., X) while their entries are denoted by indexed lower-case letters (e.g., x_{ij}).

2.1. Notes on pseudo-Riemannian geometry. Let $\mathcal{M}$ denote a p-dimensional pseudo-Riemannian manifold. Associated with each point x in a p-dimensional differentiable manifold $\mathcal{M}$ is a tangent space, denoted by $T_x\mathcal{M}$. This is a p-dimensional vector space whose elements can be thought of as equivalence classes of curves passing through the point x. Symbol $T\mathcal{M} \stackrel{\text{def}}{=} \{(x,v) | x \in \mathcal{M}, v \in T_x\mathcal{M}\}$ denotes the tangent bundle associated to the manifold $\mathcal{M}$. Symbol $\Omega^1(\mathcal{M})$ denotes the set of analytic 1-forms on $\mathcal{M}$ and symbol $\mathfrak{X}(\mathcal{M})$ denotes the set of vector fields on $\mathcal{M}$. A vector field $\mathfrak{F} \in \mathfrak{X}(\mathcal{M})$ is a map $\mathfrak{F} : x \in \mathcal{M} \mapsto \mathfrak{F}(x) \in T_x\mathcal{M}$. Symbol $\langle\cdot,\cdot\rangle^{\mathrm{E}}$ denotes Euclidean inner product.

The pseudo-Riemannian manifold $\mathcal{M} \ni x$ is endowed with an indefinite inner product $\langle\cdot,\cdot\rangle_x : T_x\mathcal{M} \times T_x\mathcal{M} \to \mathbb{R}$. An indefinite inner product is a non-degenerate, smooth, symmetric, bilinear map which assigns a real number to pairs of tangent vectors at each tangent space of the manifold. That the metric is non-degenerate means that there are no non-zero $v \in T_x\mathcal{M}$ such that $\langle v, w\rangle_x = 0$ for all $w \in T_x\mathcal{M}$. Let $x = (x^1, x^2, \ldots, x^p)$ denote a local parametrization and $\{\partial_i\}$ denote the canonical basis of $T_x\mathcal{M}$. The metric tensor field $G : \mathcal{M} \to \mathbb{R}^{p\times p}$ of components $g_{ij}(x)$ associated to the indefinite inner product $\langle\cdot,\cdot\rangle_x$ is a covariant tensor field defined by:

$$g_{ij}(x) \stackrel{\text{def}}{=} \langle\partial_i, \partial_j\rangle_x, \tag{2.1}$$

which is smooth in x. Given tangent vectors $u, v \in T_x\mathcal{M}$ parameterized by $u = u^i\partial_i$ and $v = v^i\partial_i$ (Einstein summation convention used), their inner product expresses as:

$$\langle u, v\rangle_x = g_{ij}(x)u^i v^j. \tag{2.2}$$

In pseudo-Riemannian geometry, the metric tensor g_{ij} is symmetric and invertible (but not necessarily positive-definite, in fact, positive-definiteness is an additional property that characterizes Riemannian geometry). Therefore, it might hold $\langle u, u\rangle_x = 0$ even for nonzero tangent vectors u. The inverse G^{-1} of the metric tensor field is a contravariant tensor field whose components are denoted by $g^{ij}(x)$.

Given a regular function $f : \mathcal{M} \to \mathbb{R}$, the differential $df : T\mathcal{M} \to \Omega^1(\mathcal{M})$ is expressed by:

$$df_x(v) = \langle\nabla_x f, v\rangle_x,\ v \in T_x\mathcal{M}, \tag{2.3}$$

where $\nabla_x f : \mathcal{M} \to T_x\mathcal{M}$ denotes pseudo-Riemannian gradient. In local coordinates, it holds that:

$$df_x(v) = g_{ij}(x)(\nabla_x f)^i v^j. \tag{2.4}$$

As the differential does not depend on the choice of coordinates, it holds that $df_x(v) = (\partial_i f)_x v^i$. It follows that $g_{ij}(x)(\nabla_x f)^j = (\partial_i f)_x$. The sharp isomorphism $\sharp : \Omega^1(\mathcal{M}) \to \mathfrak{X}(\mathcal{M})$ takes a 1-form on $\mathcal{M}$ and returns a vector field on $\mathcal{M}$. It holds that:

$$(df_x)^\sharp = \nabla_x f. \tag{2.5}$$

The pseudo-Riemannian gradient may be computed by the metric compatibility condition:

$$\langle\partial_x f, v\rangle^{\mathrm{E}} = \langle\nabla_x f, v\rangle_x,\ \forall v \in T_x\mathcal{M}. \tag{2.6}$$

The notion of differential generalizes to the notion of *pushforward map*. Given differentiable manifolds $\mathcal{M}$ and $\mathcal{N}$ and a regular function $f : \mathcal{M} \to \mathcal{N}$, the pushforward map $df : T\mathcal{M} \to T\mathcal{N}$ is a linear map such that $df|_x : T_x\mathcal{M} \to T_{f(x)}\mathcal{N}$ for every $x \in \mathcal{M}$. Let $\gamma : [-a, a] \to \mathcal{M}$ be a smooth curve on the manifold $\mathcal{M}$ for some $a > 0$ and let $x \stackrel{\text{def}}{=} \gamma(0)$. The pushforward map $df|_x$ is defined by:

$$\left.\frac{d}{dt} f(\gamma(t))\right|_{t=0} = df|_x \left(\left.\frac{d\gamma}{dt}\right|_{t=0}\right). \tag{2.7}$$

The following result holds true.

LEMMA 2.1 (Adapted from [5]). *Let $\mathcal{M}$ denote a manifold of $n \times n$ real-valued matrices and let $f : \mathcal{M} \to \mathbb{R}^{n\times n}$ denote an analytic map about the point $X_0 \in \mathcal{M}$, namely:*

$$f(X) = a_0 I_n + \sum_{k=1}^{\infty} a_k (X - X_0)^k, \ a_k \in \mathbb{R}, \tag{2.8}$$

in a neighborhood of X_0. Then it holds that:

$$df|_X(V) = \sum_{k=1}^{\infty} a_k \sum_{r=1}^{k} (X - X_0)^{r-1} V (X - X_0)^{k-r}, \tag{2.9}$$

for any $V \in T_X\mathcal{M}$.

The covariant derivative (or *connection*) of a vector field $\mathfrak{F} \in \mathfrak{X}(\mathcal{M})$ in the direction of a vector $v \in T_x\mathcal{M}$ is denoted as $\nabla_v \mathfrak{F}$. The covariant derivative is defined axiomatically by the following properties:

$$\nabla_{fv+gw}\mathfrak{F} = f\nabla_v\mathfrak{F} + g\nabla_w\mathfrak{F}, \tag{2.10}$$
$$\nabla_v(\mathfrak{F} + \mathfrak{G}) = \nabla_v\mathfrak{F} + \nabla_v\mathfrak{G}, \tag{2.11}$$
$$\nabla_v(f\mathfrak{F}) = f\nabla_v\mathfrak{F} + \mathfrak{F} df_x(v), \tag{2.12}$$

for any vector fields $\mathfrak{F}, \mathfrak{G}$, tangent vectors v, w and scalar functions f, g. The covariant derivative of a vector field $\mathfrak{F} \in \mathfrak{X}(\mathcal{M})$ along a vector $v \in T_x\mathcal{M}$ may be extended to the covariant derivative of a vector field $\mathfrak{F}$ along a vector field $\mathfrak{G}$ by $\nabla_{\mathfrak{G}}\mathfrak{F}(x) \stackrel{\text{def}}{=} \nabla_{\mathfrak{G}(x)}\mathfrak{F}$. Such rule defines a connection $\nabla : \mathfrak{X}(\mathcal{M}) \times \mathfrak{X}(\mathcal{M}) \to \mathfrak{X}(\mathcal{M})$. The fundamental relationship for the connection is:

$$\nabla_{\partial_i}\partial_j = \Gamma_{ij}^k \partial_k, \tag{2.13}$$

where quantities $\Gamma_{ij}^k : \mathcal{M} \to \mathbb{R}$ are termed Christoffel symbols of the second kind and describe the structure of the connection. The derivative $\nabla_{\partial_i}\partial_j$ measures the change of the elementary vector field $\partial_j = \partial_j(x)$ in the direction ∂_i. By the properties (2.10)-(2.12), it is readily obtained that:

$$\nabla_{v^i\partial_i}(u^i\partial_i) = v^i \left(\Gamma_{ij}^k u^j + \frac{\partial u^k}{\partial x^i} \right) \partial_k, \tag{2.14}$$

where the functions $v^i = v^i(x)$ and the functions $u^i = u^i(x)$ are the components of vector fields in $\mathfrak{X}(\mathcal{M})$ in the basis $\{\partial_i\}$. The Christoffel symbols of the second kind may be specified arbitrarily and give rise to an arbitrary connection. In the *Levi-Civita geometry*, the Christoffel symbols of the second kind are associated to the metric tensor of components g_{ij} and are defined as:

$$\Gamma_{ij}^k \stackrel{\text{def}}{=} \frac{1}{2} g^{kh} \left(\frac{\partial g_{hj}}{\partial x^i} + \frac{\partial g_{ih}}{\partial x^j} - \frac{\partial g_{ij}}{\partial x^h} \right). \tag{2.15}$$

The Christoffel symbols of the second kind defined as in (2.14) are symmetric in the covariant indices, namely, $\Gamma_{ij}^k = \Gamma_{ji}^k$. The associated Christoffel form $\Gamma_x : T_x\mathcal{M} \times T_x\mathcal{M} \to \mathbb{R}^p$ is defined in local coordinates by $[\Gamma_x(v, w)]^k \stackrel{\text{def}}{=} \Gamma_{ij}^k v^i w^j$. In the present paper, the notion of connection refers to a Levi-Civita connection, unless otherwise stated.

The notion of covariant derivative is intimately tied to the notion of parallel translation (or transport) along a curve. Parallel translation allows, e.g., comparing vectors belonging to different tangent spaces. On a smooth pseudo-Riemannian manifold $\mathcal{M}$ with connection ∇, fix a smooth curve $\gamma : [-a,\, a] \to \mathcal{M}$ ($a > 0$). The parallel translation map $\Gamma_s^t(\gamma) : T_{\gamma(s)}\mathcal{M} \to T_{\gamma(t)}\mathcal{M}$ associated to the curve is a linear isomorphism for every $s, t \in [-a,\, a]$. The parallel translation map depends smoothly on its arguments and is such that $\Gamma_s^s(\gamma)$ is an identity map and $\Gamma_u^t(\gamma) \circ \Gamma_s^u(\gamma) = \Gamma_s^t(\gamma)$ for every $s, u, t \in [-a,\, a]$. Let $v = \dot\gamma(0)$. The covariant derivative of a vector field $\mathfrak{F} \in \mathfrak{X}(\mathcal{M})$ in the direction $v \in T_x\mathcal{M}$ is given by:

$$\nabla_v \mathfrak{F} = \lim_{\varepsilon \to 0} \frac{\Gamma_\epsilon^0(\gamma)\mathfrak{F}(\gamma(\varepsilon)) - \mathfrak{F}(\gamma(0))}{\varepsilon} = \left. \frac{d}{dt}\Gamma_t^0(\gamma)\mathfrak{F}(\gamma(t)) \right|_{t=0}. \tag{2.16}$$

The notion of *geodesic curve* generalizes the notion of straight line of Euclidean spaces. A distinguishing feature of a straight line of an Euclidean space is that it translates parallel to itself, namely, it is *self-parallel.* The notion of 'straight line' on a curved space inherits such distinguishing feature. An affine geodesic on a manifold $\mathcal{M}$ with connection ∇ and associated parallel translation map $\Gamma_\cdot^\cdot(\cdot)$, is a curve γ such that $\dot\gamma$ is parallel translated along γ itself, namely, for every $s, t \in [-a,\, a]$, it holds that:

$$\Gamma_s^t(\gamma)\dot\gamma(s) = \dot\gamma(t). \tag{2.17}$$

Setting $s = 0$, $\mathfrak{F}(\gamma(t)) \stackrel{\text{def}}{=} \dot\gamma(t)$, and invoking the relationship (2.16), it is seen that an affine geodesic curve must satisfy the condition:

$$\nabla_{\dot\gamma}\dot\gamma = 0. \tag{2.18}$$

A geodesic curve is denoted throughout the paper by $\rho(t)$. On a pseudo-Riemannian manifold $\mathcal{M}$, the parallel translation map about a curve $\gamma : [-a,\, a] \to \mathcal{M}$ preserves the angle between tangent vectors, namely:

$$\langle \Gamma_s^t(\gamma)v, \Gamma_s^t(\gamma)w \rangle_{\gamma(t)} = \langle v, w \rangle_{\gamma(s)}, \tag{2.19}$$

for every pair of tangent vectors $v, w \in T_{\gamma(s)}\mathcal{M}$ and for every $s, t \in [-a,\, a]$. For a geodesic curve $\rho : [0,\, 1] \to \mathcal{M}$, setting $v = w = \dot\rho(0)$, thanks to the self-translation property (2.17), it is immediate to verify that:

$$\frac{d}{dt}\langle \dot\rho(t), \dot\rho(t) \rangle_{\rho(t)} = 0, \tag{2.20}$$

for every $t \in [0,\, 1]$. (A regular re-parametrization does not modify the distinguishing properties of an affine geodesic curve.)

The 'total action' associated to a curve $\gamma : [0,\, 1] \to \mathcal{M}$ is defined as:

$$\mathcal{A}(\gamma) \stackrel{\text{def}}{=} \int_0^1 \langle \dot\gamma(t), \dot\gamma(t) \rangle_{\gamma(t)} dt. \tag{2.21}$$

On a geodesic arc $\rho : [0,\, 1] \to \mathcal{M}$, the integrand is constant, therefore the total action takes on the value $\mathcal{A}(\rho) = \langle \dot\rho(0), \dot\rho(0) \rangle_{\rho(0)}$. On a *Riemannian* manifold, the length of a curve $\gamma : [0,\, 1] \to \mathcal{M}$ is defined as:

$$\mathcal{L}(\gamma) \stackrel{\text{def}}{=} \int_0^1 \langle \dot\gamma(t), \dot\gamma(t) \rangle_{\gamma(t)}^{\frac{1}{2}} dt, \tag{2.22}$$

hence, the length of a geodesic arc ρ on a Riemannian manifold is computed by $\mathcal{L}(\rho) = \langle \dot\rho(0), \dot\rho(0)\rangle_{\rho(0)}^{\frac{1}{2}} = \mathcal{A}^{\frac{1}{2}}(\rho)$. On a Riemannian manifold, the total action is positive definite and the distance between two points may be calculated as the length of a geodesic arc which joins them (if it exists). On a pseudo-Riemannian manifold, however, such definition is no longer valid because the total action has indefinite sign.

2.2. An equivalence principle of pseudo-Riemannian geometry. The geodesic arc associated to a given metric on a pseudo-Riemannian manifold may be calculated through a variational stationary-action principle rather than via covariant derivation.

Lemma 2.2. *The equation (2.18) is equivalent to the equation:*

$$\delta \int_0^1 \langle \dot\gamma, \dot\gamma\rangle_\gamma dt = 0, \tag{2.23}$$

where symbol δ denotes the variation of the integral functional.

Proof. Substituting $u^k = v^k = \dot\gamma^k$ in the equation (2.14), leads to the expression $\nabla_{\dot\gamma}\dot\gamma = \dot\gamma^i\dot\gamma^j\Gamma^k_{ij}\partial_k + \ddot\gamma^k\partial_k$. Setting the above covariant derivative to zero leads to the geodesic equations for the components γ^k:

$$\ddot\gamma^k + \Gamma^k_{ij}\dot\gamma^i\dot\gamma^j = 0. \tag{2.24}$$

The integral functional in (2.23) represents the total action associated with the parameterized smooth curve $\gamma : [0,\, 1] \to \mathcal{M}$ of local coordinates $x^k = \gamma^k(t)$ and may be written explicitly as:

$$\int_0^1 \langle \dot\gamma, \dot\gamma\rangle_\gamma dt = \int_0^1 g_{ij}(\gamma(t))\dot\gamma^i(t)\dot\gamma^j(t)dt. \tag{2.25}$$

The variation δ in the expression (2.23) corresponds to a perturbation of the total action (2.25). Let $\eta : [0,\, 1] \to \mathcal{M}$ denote an arbitrary parameterized smooth curve of local coordinates $\eta^k(t)$ such that $\eta^k(0) = \eta^k(1) = 0$. Define the perturbed action:

$$\mathcal{I}_\eta(\varepsilon) \stackrel{\text{def}}{=} \int_0^1 g_{ij}(\gamma + \varepsilon\eta)(\dot\gamma^i + \varepsilon\dot\eta^i)(\dot\gamma^j + \varepsilon\dot\eta^j)dt, \tag{2.26}$$

with $\varepsilon \in [-a,\, a]$, $a > 0$. The condition (2.23) may be expressed explicitly in terms of the perturbed action as:

$$\lim_{\varepsilon\to 0} \frac{\mathcal{I}_\eta(\varepsilon) - \mathcal{I}_\eta(0)}{\varepsilon} = 0,\ \forall\eta. \tag{2.27}$$

The perturbed total action may be expanded around $\varepsilon = 0$ as follows:

$$\begin{aligned}
\mathcal{I}_\eta(\varepsilon) &= \int_0^1 \left[g_{ij}(x) + \varepsilon\frac{\partial g_{ij}}{\partial x^k}\eta^k + o(\varepsilon)\right][\dot\gamma^i\dot\gamma^j + \varepsilon(\dot\gamma^i\dot\eta^j + \dot\gamma^j\dot\eta^i) + o(\varepsilon)]dt \\
&= \int_0^1 g_{ij}(x)\dot\gamma^i\dot\gamma^j dt + \varepsilon\int_0^1 \left[g_{ij}(x)(\dot\gamma^i\dot\eta^j + \dot\gamma^j\dot\eta^i) + \eta^k\frac{\partial g_{ij}}{\partial x^k}\dot\gamma^i\dot\gamma^j\right]dt + o(\varepsilon) \\
&= \mathcal{I}_\eta(0) + \varepsilon\int_0^1 \left[g_{ik}(x)\dot\gamma^i\dot\eta^k + g_{kj}(x)\dot\gamma^j\dot\eta^k + \frac{\partial g_{ij}}{\partial x^k}\dot\gamma^i\dot\gamma^j\eta^k\right]dt + o(\varepsilon), \qquad (2.28)
\end{aligned}$$

where $o(\varepsilon)$ is such that $\lim_{\varepsilon\to 0} o(\varepsilon)/\varepsilon = 0$. The first term within the integral on the right-hand side of the expression (2.28) may be integrated by parts, namely:

$$\int_0^1 g_{ik}(x)\dot\gamma^i\dot\eta^k dt = g_{ik}(\gamma)\dot\gamma^i\eta^k\big|_0^1 - \int_0^1 \frac{d(g_{ik}(\gamma)\dot\gamma^i)}{dt}\eta^k dt. \tag{2.29}$$

The first term on the right-hand side vanishes to zero because $\eta^k(0) = \eta^k(1) = 0$, hence:

$$\int_0^1 g_{ik}(x)\dot\gamma^i\dot\eta^k dt = -\int_0^1 \left(\frac{\partial g_{ik}}{\partial x^j}\dot\gamma^i\dot\gamma^j + g_{ik}(x)\ddot\gamma^i\right)\eta^k dt. \tag{2.30}$$

A similar result holds true for the second term within the integral on the right-hand side of the expression (2.28). Therefore, it holds that:

$$\frac{\mathcal{I}_\eta(\varepsilon) - \mathcal{I}_\eta(0)}{\varepsilon} = \int_0^1 \left[\left(\frac{\partial g_{ij}}{\partial x^k} - \frac{\partial g_{ik}}{\partial x^j} - \frac{\partial g_{kj}}{\partial x^i}\right)\dot\gamma^i\dot\gamma^j - 2g_{ik}(x)\ddot\gamma^i\right]\eta^k dt + \frac{o(\varepsilon)}{\varepsilon}. \tag{2.31}$$

The condition (2.27), therefore, implies that:

$$g_{ik}\ddot\gamma^i + \frac{1}{2}\left(-\frac{\partial g_{ij}}{\partial x^k} + \frac{\partial g_{ik}}{\partial x^j} + \frac{\partial g_{kj}}{\partial x^i}\right)\dot\gamma^i\dot\gamma^j = 0. \tag{2.32}$$

As the metric tensor is invertible, the equation (2.32) is equivalent to the equation (2.24). □

The geodesic equation (2.24) may be written in compact form as:

$$\ddot\gamma(t) + \Gamma_{\gamma(t)}(\dot\gamma(t), \dot\gamma(t)) = 0. \tag{2.33}$$

In the above expressions, the over-dot and the double over-dot denote first-order and second-order derivation with respect to parameter t, respectively. The solution of the geodesic equation may be written in terms of two parameters, such as the initial values $\gamma(0) = x \in \mathcal{M}$ and $\dot\gamma(0) = v \in T_x\mathcal{M}$, in which case the solution of the geodesic equation (2.33) will be denoted as $\rho_{x,v}(t)$. A geodesic arc $\rho_{x,v} : [0, 1] \to \mathcal{M}$ is associated to a map $\exp_x : T_x\mathcal{M} \to \mathcal{M}$ defined as:

$$\exp_x(v) \stackrel{\text{def}}{=} \rho_{x,v}(1). \tag{2.34}$$

The function (2.34) is termed *exponential map* with pole $x \in \mathcal{M}$. The notion of exponential map is illustrated in the Figure 2.1.

The equivalency stated in the Lemma 2.2 proves useful when working in intrinsic coordinates. Intrinsic coordinates appear more appealing when it comes to implement an optimization method on a computation platform (for a detailed discussion, see, e.g., [11]). In order to make such equivalency profitable from a computational point of view, it pays to examine the variational method invoked in the Lemma 2.2 on smooth manifolds from an intrinsic-coordinate perspective.

Lemma 2.3. *The first variation of the integral functional*

$$\mathcal{F}(\gamma) \stackrel{\text{def}}{=} \int_0^1 F(\gamma, \dot\gamma)dt, \tag{2.35}$$

with $\gamma : [0, 1] \to \mathcal{M}$ denoting a curve on a pseudo-Riemannian manifold $\mathcal{M}$ and $F : T\mathcal{M} \to \mathbb{R}$ integrable, reads:

$$\delta\mathcal{F}(\gamma) = \int_0^1 \left\langle \frac{\partial F}{\partial \gamma} - \frac{d}{dt}\frac{\partial F}{\partial \dot\gamma}, \delta\gamma \right\rangle^{\mathrm{E}} dt. \tag{2.36}$$

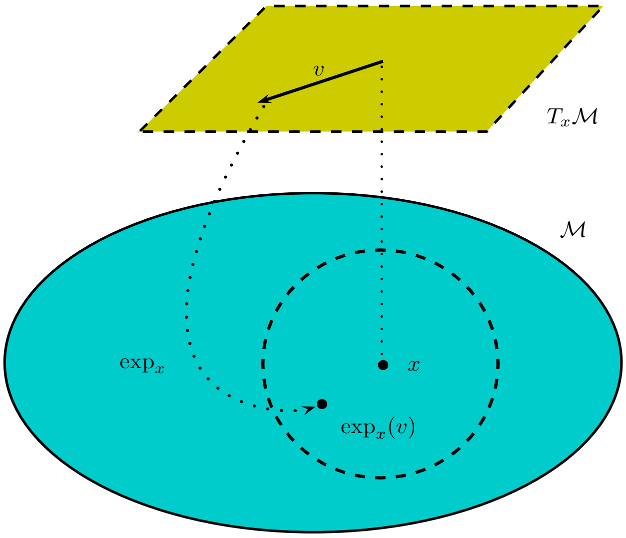

FIG. 2.1. *Notion of exponential mapping on a manifold* $\mathcal{M}$. *The point* $\exp_x(v)$ *lies on a neighborhood of the pole* x *denoted by the dashed circle.*

Proof. Define a smooth family of smooth curves $c : [0, 1] \times [-a, a]$, $a > 0$, such that:

$$c(t, 0) = \gamma(t), \;\; \forall t \in [0, 1], \tag{2.37}$$
$$c(0, \varepsilon) = \gamma(0), \;\; c(1, \varepsilon) = \gamma(1), \;\; \forall \varepsilon \in [-a, a], \tag{2.38}$$

for a fixed ε, $t \mapsto c(t, \varepsilon)$ is a smooth curve on the manifold $\mathcal{M}$, for a fixed t, $\varepsilon \mapsto c(t, \varepsilon)$ is a smooth curve on the manifold $\mathcal{M}$ for some $a > 0$ and $\frac{\partial^2 c}{\partial t \partial \varepsilon} = \frac{\partial^2 c}{\partial \varepsilon \partial t}$. Define:

$$\delta\gamma(t) \stackrel{\text{def}}{=} \frac{\partial}{\partial \varepsilon} c(t, \varepsilon)\bigg|_{\epsilon=0}. \tag{2.39}$$

Note that $\delta\gamma \in T_\gamma \mathcal{M}$ and $\delta\gamma(0) = \delta\gamma(1) = 0$. The variation $\delta\mathcal{F}(\gamma)$ may be written as:

$$\begin{aligned} \delta \int_0^1 F(\gamma, \dot{\gamma}) dt &\stackrel{\text{def}}{=} \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left[\int_0^1 F(c(t, \varepsilon), \dot{c}(t, \varepsilon)) dt - \int_0^1 F(c(t, 0), \dot{c}(t, 0)) dt \right] \\ &= \int_0^1 \lim_{\varepsilon \to 0} \frac{F(c(t, \varepsilon), \dot{c}(t, \varepsilon)) - F(c(t, 0), \dot{c}(t, 0))}{\varepsilon} dt \\ &= \int_0^1 \frac{\partial}{\partial \varepsilon} F(c(t, \varepsilon), \dot{c}(t, \varepsilon))\bigg|_{\varepsilon=0} dt. \end{aligned} \tag{2.40}$$

The partial derivative within the integral in equation (2.40) may be written as:

$$\frac{\partial F(c, \dot{c})}{\partial \varepsilon}\bigg|_{\varepsilon=0} = \left\langle \frac{\partial F(c, \dot{c})}{\partial c}, \frac{\partial c}{\partial \varepsilon} \right\rangle^{\mathrm{E}}\bigg|_{\varepsilon=0} + \left\langle \frac{\partial F(c, \dot{c})}{\partial \dot{c}}, \frac{\partial \dot{c}}{\partial \varepsilon} \right\rangle^{\mathrm{E}}\bigg|_{\varepsilon=0}. \tag{2.41}$$

The variation of the integral functional reads, therefore:

$$\delta \int_0^1 F(\gamma, \dot{\gamma}) dt = \int_0^1 \left\langle \frac{\partial F(\gamma, \dot{\gamma})}{\partial \gamma}, \delta\gamma \right\rangle^{\mathrm{E}} dt + \int_0^1 \left\langle \frac{\partial F(\gamma, \dot{\gamma})}{\partial \dot{\gamma}}, \frac{d\delta\gamma}{dt} \right\rangle^{\mathrm{E}} dt. \tag{2.42}$$

Integration by parts yields:

$$\int_0^1 \left\langle \frac{\partial F}{\partial \dot{\gamma}}, \frac{d}{dt}\delta\gamma \right\rangle^{\mathrm{E}} dt = \left\langle \frac{\partial F}{\partial \dot{\gamma}}, \delta\gamma \right\rangle^{\mathrm{E}} \Bigg|_0^1 - \int_0^1 \left\langle \frac{d}{dt}\frac{\partial F}{\partial \dot{\gamma}}, \delta\gamma \right\rangle^{\mathrm{E}} dt. \tag{2.43}$$

The first term in the right-hand side equals zero, hence, the variation of the integral functional assumes the final expression (2.36). □

A noticeable consequence of Lemma 2.3 is that the variation $\delta\mathcal{F}(\gamma)$ depends only on the tangential component $\delta\gamma \in T_\gamma\mathcal{M}$ of the perturbation.

It is worth noting the difference between Riemannian geodesics, that minimize the total action, and pseudo-Riemannian geodesics, that are only stationary points of the total action.

2.3. A pseudo-Riemannian geometric structure of the real symplectic group. The skew-symmetric matrix Q_{2n} defined in (1.1) enjoys the properties $Q_{2n}^2 = -I_{2n}$ and $Q_{2n}^{-1} = Q_{2n}^T = -Q_{2n}$. From now on, the subscript $2n$ on the symbol Q_{2n} will drop for a tidier notation. The dimension subscript of the zero-matrix 0_p will drop as well whenever its dimension is clear from the context.

The space $\mathrm{Sp}(2n,\mathbb{R})$ is a curved smooth manifold that may also be endowed with an algebraic-group structure (namely, group multiplication, group inverse and a unique identity element) in a manner that is compatible with the manifold structure. Therefore, the space $\mathrm{Sp}(2n,\mathbb{R})$ has the structure of a Lie group of dimension $(2n+1)n$. Standard matrix multiplication and inversion work as algebraic-group operations. (Any symplectic matrix $X \in \mathrm{Sp}(2n,\mathbb{R})$ is such that $\det^2(X) = 1$, where symbol $\det(\cdot)$ denotes determinant. Therefore, symplectic matrices are invertible.) The identity element of the group $\mathrm{Sp}(2n,\mathbb{R})$ is the matrix I_{2n}. The following identities hold: $\det(X) = 1$, $X^T = -QX^{-1}Q$, $X^{-T} = -QXQ$. It follows that the group $\mathrm{Sp}(2n,\mathbb{R})$ is a subgroup of $\mathrm{Sl}(2n,\mathbb{R})$ as well as of $\mathrm{Gl}(2n,\mathbb{R})$.

The tangent space $T_X\mathrm{Sp}(2n,\mathbb{R})$ has structure:

$$T_X\mathrm{Sp}(2n,\mathbb{R}) = \{V \in \mathbb{R}^{2n\times 2n} | V^TQX + X^TQV = 0\}. \tag{2.44}$$

The tangent space at the identity of the Lie group, namely the Lie algebra $\mathfrak{sp}(2n,\mathbb{R})$, has structure:

$$\mathfrak{sp}(2n,\mathbb{R}) = \{H \in \mathbb{R}^{2n\times 2n} | H^TQ + QH = 0\} \tag{2.45}$$

and the elements of the Lie algebra $\mathfrak{sp}(2n,\mathbb{R})$ are termed *Hamiltonian matrices.* By the embedding of the manifold $\mathrm{Sp}(2n,\mathbb{R})$ into the Euclidean space $\mathbb{R}^{2n\times 2n}$, at any point $X \in \mathrm{Sp}(2n,\mathbb{R})$ is associated the normal space:

$$N_X\mathrm{Sp}(2n,\mathbb{R}) \stackrel{\mathrm{def}}{=} \{P \in \mathbb{R}^{2n\times 2n} | \mathrm{tr}(P^TV) = 0, \forall V \in T_X\mathrm{Sp}(2n,\mathbb{R})\}, \tag{2.46}$$

where symbol $\mathrm{tr}(\cdot)$ denotes the trace operator. The tangent space and the Lie algebra associated to the real symplectic group may be characterized as follows:

$$\begin{cases} T_X\mathrm{Sp}(2n,\mathbb{R}) = \{XQS | S \in \mathbb{R}^{2n\times 2n},\ S^T = S\}, \\ \mathfrak{sp}(2n,\mathbb{R}) = \{QS | S \in \mathbb{R}^{2n\times 2n},\ S^T = S\}, \\ N_X\mathrm{Sp}(2n,\mathbb{R}) = \{QX\Omega | \Omega \in \mathfrak{so}(2n)\}, \end{cases} \tag{2.47}$$

where symbol $\mathfrak{so}(p)$ denotes the Lie algebra:

$$\mathfrak{so}(p) \stackrel{\mathrm{def}}{=} \{\Omega \in \mathbb{R}^{p\times p} | \Omega^T = -\Omega\}. \tag{2.48}$$

Consider the following indefinite inner product on the general linear group of matrices $\mathrm{Gl}(p,\mathbb{R})$:

$$\langle U,V\rangle_X \stackrel{\text{def}}{=} \mathrm{tr}(X^{-1}UX^{-1}V),\ X\in\mathrm{Gl}(p,\mathbb{R}),\ U,V\in T_X\mathrm{Gl}(p,\mathbb{R}), \tag{2.49}$$

referred to as Khvedelidze-Mladenov metric [26]. The above inner product gives rise to a metric which is not positive-definite on the space $\mathrm{Sp}(2n,\mathbb{R})\subset\mathrm{Gl}(2n,\mathbb{R})$. To verify such property, it is sufficient to evaluate the structure of the squared norm $\|V\|_X^2=\mathrm{tr}((X^{-1}V)^2)$ with $X\in\mathrm{Sp}(2n,\mathbb{R})$ and $V\in T_X\mathrm{Sp}(2n,\mathbb{R})$. By the structure of the tangent space $T_X\mathrm{Sp}(2n,\mathbb{R})$, it is known that $X^{-1}V=QS$ with $S\in\mathbb{R}^{2n\times 2n}$ symmetric. It holds that:

$$QS=\begin{bmatrix} 0_n & I_n\\ -I_n & 0_n\end{bmatrix}\begin{bmatrix} S_1 & S_2\\ S_2^T & S_3\end{bmatrix}=\begin{bmatrix} S_2^T & S_3\\ -S_1 & -S_2\end{bmatrix},$$

with $S_1,S_3\in\mathbb{R}^{n\times n}$ symmetric and $S_2\in\mathbb{R}^{n\times n}$ arbitrary. Hence, $\mathrm{tr}((QS)^2)=2\mathrm{tr}(S_2^2)-2\mathrm{tr}(S_1S_3)$ has indefinite sign.

Under the pseudo-Riemannian metric (2.49), it is indeed possible to solve the geodesic equation in closed form. The solution makes use of the exponential of a matrix $X\in\mathbb{R}^{p\times p}$, which is defined by the series:

$$\exp(X)\stackrel{\text{def}}{=} I_p+\sum_{r=1}^{\infty}\frac{X^r}{r!}. \tag{2.50}$$

THEOREM 2.4. *The geodesic curve $\rho_{X,V}:[0,\,1]\to\mathrm{Sp}(2n,\mathbb{R})$ with $X\in\mathrm{Sp}(2n,\mathbb{R})$, $V\in T_X\mathrm{Sp}(2n,\mathbb{R})$ corresponding to the indefinite Khvedelidze-Mladenov metric (2.49) has expression:*

$$\rho_{X,V}(t)=X\exp(tX^{-1}V). \tag{2.51}$$

Proof. By the equivalence principle stated in the Lemma 2.2, the geodesic equation in the variational form writes:

$$\delta\int_0^1 \mathrm{tr}(\gamma^{-1}\dot\gamma\gamma^{-1}\dot\gamma)dt=0, \tag{2.52}$$

where the natural parametrization is assumed. The above variation is computed on the basis of the variational method on manifolds recalled in the Lemma 2.3 and is facilitated by the following rules of calculus of variations:

$$\delta(X^{-1})=-X^{-1}(\delta X)X^{-1}, \tag{2.53}$$

$$\delta\left(\frac{dX}{dt}\right)=\frac{d}{dt}(\delta X), \tag{2.54}$$

$$\delta(XZ)=(\delta X)Z+X(\delta Z), \tag{2.55}$$

for curves $X,Z:[0,\,1]\to\mathrm{Sp}(2n,\mathbb{R})$. By computing the variations, integrating by parts and recalling that the variation vanishes at endpoints, it is found that the geodesic equation in variational form reads:

$$\int_0^1 \mathrm{tr}(\delta\gamma(\gamma^{-1}\ddot\gamma\gamma^{-1}-\gamma^{-1}\dot\gamma\gamma^{-1}\dot\gamma\gamma^{-1}))dt=0. \tag{2.56}$$

The variation $\delta\gamma \in T_\gamma\mathrm{Sp}(2n,\mathbb{R})$ is arbitrary. By the structure of the normal space $N_X\mathrm{Sp}(2n,\mathbb{R})$, the equation $\mathrm{tr}(P^T\delta\gamma)=0$, with $\delta\gamma \in T_\gamma\mathrm{Sp}(2n,\mathbb{R})$, implies that $P^T = \Omega Q\gamma^{-1}$ with $\Omega \in \mathfrak{so}(2n)$. Therefore, the equation (2.56) is satisfied if and only if:

$$\gamma^{-1}\ddot{\gamma}\gamma^{-1} - \gamma^{-1}\dot{\gamma}\gamma^{-1}\dot{\gamma}\gamma^{-1} = \Omega Q\gamma^{-1},\ \Omega \in \mathfrak{so}(2n), \tag{2.57}$$

or, equivalently,

$$\ddot{\gamma} - \dot{\gamma}\gamma^{-1}\dot{\gamma} = \gamma\Omega Q, \tag{2.58}$$

for some $\Omega \in \mathfrak{so}(2n)$. In order to determine the value of matrix Ω, note that:

$$\gamma^T Q\gamma - Q = 0 \Rightarrow \ddot{\gamma}^T Q\gamma + 2\dot{\gamma}^T q\dot{\gamma} + \gamma^T\ddot{\gamma} = 0.$$

Substituting the expression $\ddot{\gamma} = \dot{\gamma}\gamma^{-1}\dot{\gamma} + \gamma\Omega Q$ into the above equation yields the condition $Q\Omega Q = 0$. Hence, $\Omega = 0$ and the geodesic equation in Christoffel form reads:

$$\ddot{\gamma} - \dot{\gamma}\gamma^{-1}\dot{\gamma} = 0. \tag{2.59}$$

Its solution, with initial conditions $\gamma(0) = X \in \mathrm{Sp}(2n,\mathbb{R})$ and $\dot{\gamma}(0) = V \in T_X\mathrm{Sp}(2n,\mathbb{R})$, is found to be of the form (2.51). □

By definition of matrix exponential, it follows that $\dot{\rho}_{X,V}(t) = V\exp(tX^{-1}V)$. The Lemma 2.1 applies to the map $\exp : \mathfrak{sp}(2n,\mathbb{R}) \to \mathrm{Sp}(2n,\mathbb{R})$ around $0 \in \mathfrak{sp}(2n,\mathbb{R})$ and implies, in particular, that $d\exp|_0(H) = H$ for every $H \in \mathfrak{sp}(2n,\mathbb{R})$.

The structure of the pseudo-Riemannian gradient associated to the Khvedelidze-Mladenov metric (2.49) applied to the case of the real symplectic group $\mathrm{Sp}(2n,\mathbb{R})$ is given by the following result.

THEOREM 2.5. *The pseudo-Riemannian gradient of a sufficiently regular function $f : \mathrm{Sp}(2n,\mathbb{R}) \to \mathbb{R}$ associated to the Khvedelidze-Mladenov metric (2.49) reads:*

$$\nabla_X f = \frac{1}{2}XQ\left(X^T\partial_X fQ - Q\partial_X^T fX\right). \tag{2.60}$$

Proof. The pseudo-Riemannian gradient of a regular function $f : \mathrm{Sp}(2n,\mathbb{R}) \to \mathbb{R}$ associated to the metric (2.49) is computed as the solution of the following system of equations:

$$\begin{cases} \mathrm{tr}(X^{-1}\nabla_X fX^{-1}V) = \mathrm{tr}(\partial_X^T fV),\ \forall V \in T_X\mathrm{Sp}(2n,\mathbb{R}), \\ \nabla_X^T fQX + X^TQ\nabla_X f = 0. \end{cases} \tag{2.61}$$

The first equation expresses the compatibility of the pseudo-Riemannian gradient with the metric, while the second equation expresses the requirement that the pseudo-Riemannian gradient be a tangent vector. The metric compatibility condition may be rewritten as:

$$\mathrm{tr}(V^T(\partial_X f - X^{-T}\nabla_X^T fX^{-T})) = 0, \tag{2.62}$$

where superscript $^{-T}$ denotes the inverse of the transposed matrix. The above condition implies that $\partial_X f - X^{-T}\nabla_X^T fX^{-T} \in N_X\mathrm{Sp}(2n,\mathbb{R})$, hence that $\partial_X f - X^{-T}\nabla_X^T fX^{-T} = QX\Omega$ with $\Omega \in \mathfrak{so}(2n)$. Therefore, the pseudo-Riemannian gradient of the criterion function f has the expression:

$$\nabla_X f = X\partial_X^T fX - X\Omega Q. \tag{2.63}$$

In order to determine the value of the matrix Ω, it is sufficient to substitute the expression (2.63) of the gradient within the tangency condition, which becomes:

$$\left(X\partial_X^T fX - X\Omega Q\right)^T QX + X^T Q\left(X\partial_X^T fX - X\Omega Q\right) = 0. \tag{2.64}$$

Solving for Ω gives:

$$\Omega = -\frac{1}{2}\left(QX^T\partial_X f + \partial_X^T fXQ\right). \tag{2.65}$$

Substituting the above expression of the variable Ω into the expression (2.63) of the pseudo-Riemannian gradient gives the result (2.60). ☐

2.4. A Riemannian structure of the real symplectic group. For completeness of exposition, it is instructive to recall an advanced result about a Riemannian structure of the real symplectic group of matrices.

THEOREM 2.6 ([7]). *Let $\sigma : \mathfrak{sp}(2n,\mathbb{R}) \to \mathfrak{sp}(2n,\mathbb{R})$ be a symmetric positive-definite operator with respect to the Euclidean inner product on the space $\mathfrak{sp}(2n,\mathbb{R})$. The minimizing curve of the integral*

$$\int_0^1 \langle H(t), \sigma(H(t))\rangle^{\mathrm{E}} dt$$

over all curves $\gamma : [0,\,1] \to \mathrm{Sp}(2n,\mathbb{R})$ with fixed endpoints $\gamma(0)$, $\gamma(1)$, having defined $H(t) \stackrel{\text{def}}{=} \gamma^{-1}(t)\dot\gamma(t)$, is the solution of the system:

$$\begin{cases} \dot\gamma(t) = \gamma(t)H(t),\\ \dot M(t) = \sigma^T(H(t))M(t) - H(t)\sigma^T(H(t)),\\ H(t) = \sigma^{-1}(M(t)), \end{cases} \tag{2.66}$$

where symbol σ^{-1} denotes the inverse of the operator σ.

The simplest choice for the symmetric positive-definite operator σ is the identity map of the space $\mathfrak{sp}(2n,\mathbb{R})$, which corresponds to a Riemannian metric for the real symplectic group $\mathrm{Sp}(2n,\mathbb{R})$ given by the inner product:

$$\langle U, V\rangle_X = \mathrm{tr}((X^{-1}U)^T(X^{-1}V)),\ X \in \mathrm{Sp}(2n,\mathbb{R}),\ U, V \in T_X\mathrm{Sp}(2n,\mathbb{R}). \tag{2.67}$$

Such a metric leads to the 'natural gradient' on the space of real invertible matrices $\mathrm{Gl}(p,\mathbb{R})$ studied in [1]. The above choice for the operator σ implies that $M = H$ and that the corresponding curve on the real symplectic group satisfies the equations:

$$\begin{cases} \dot H(t) = H^T(t)H(t) - H(t)H^T(t),\\ H(t) = \gamma^{-1}(t)\dot\gamma(t), \end{cases} \tag{2.68}$$

or, in Christoffel form:

$$\ddot\gamma - \dot\gamma\gamma^{-1}\dot\gamma + \gamma\dot\gamma^T Q\gamma Q\gamma^{-1}\dot\gamma - \dot\gamma\dot\gamma^T Q\gamma Q = 0. \tag{2.69}$$

The above equations describe geodesic arcs on the real symplectic group corresponding to the metric (2.67). Closed form solutions of the above equations are unknown to the authors of [7] and to the present author.

The structure of the Riemannian gradient is given by the following result.

THEOREM 2.7. *The Riemannian gradient $\nabla_X f$ of a sufficiently regular function $f : \mathrm{Sp}(2n, \mathbb{R}) \to \mathbb{R}$ corresponding to the metric (2.67) reads:*

$$\nabla_X f = \frac{1}{2} XQ \left(\partial_X^T f XQ - QX^T \partial_X f \right). \tag{2.70}$$

Proof. The Riemannian gradient $\nabla_X f$ of a regular function $f : \mathrm{Sp}(2n, \mathbb{R}) \to \mathbb{R}$ must satisfy condition:

$$\nabla_X f = XQ(\Omega - X^{-1} Q \partial_X f), \text{ with } \Omega = \frac{1}{2}(X^{-1} Q \partial_X f + \partial_X^T f XQ), \tag{2.71}$$

from which the expression of the Riemannian gradient associated to the metric (2.67) follows. □

Clearly, the expressions of the gradients (2.60) and (2.70) differ from each other because the metrics that they correspond to are different.

3. Minimal-distance optimization on pseudo-Riemannian manifolds. Several numerical applications require the solution of a least-squares problem on a pseudo-Riemannian manifold. As an example, given a 'cloud' of points $x_k \in \mathcal{M}$ on a manifold $\mathcal{M}$ endowed with a distance function $d(\cdot, \cdot)$, its empirical mean $\mu \in \mathcal{M}$ is defined as:

$$\mu \stackrel{\text{def}}{=} \arg \min_{x \in \mathcal{M}} \sum_k d^2(x, x_k). \tag{3.1}$$

For a recent review, see, e.g., [19]. The empirical mean value μ of a distribution of points on a manifold is instrumental in several applications. The mean value μ is, by definition, close to all points in the distribution. Therefore, the tangent space $T_\mu \mathcal{M}$ associated to a cloud of data-points may serve as reference tangent space in the development of algorithms to process those data (see, for example, the discussion in [37] about 'principal geodesic analysis' of data). The notion of averaging over a curved manifold is depicted in the Figure 3.1. In addition, given a cloud of N points $x_k \in \mathcal{M}$ on a manifold $\mathcal{M}$ endowed with a distance function $d(\cdot, \cdot)$, its empirical m^{th}-order (centered) moment is defined as:

$$\mu_m \stackrel{\text{def}}{=} \frac{1}{N} \sum_k d^m(\mu, x_k), \ m \geq 2, \tag{3.2}$$

where $\mu \in \mathcal{M}$ denotes the empirical mean of the cloud. In particular, the moment μ_2 denotes the empirical variance of the manifold-valued samples, which measures the width of the cloud around its center. The definition of empirical moments μ_m is paired with the definition of empirical mean as in applied statistics on manifold they provide a characterization of the distribution of a data-cloud.

3.1. Optimization on manifolds. Optimization on manifold is a modern formulation of some classical constrained optimization problems. In particular, given a differentiable manifold $\mathcal{M}$ and a sufficiently regular function $f : \mathcal{M} \to \mathbb{R}$, minimization on manifold is expressed as:

$$\min_{x \in \mathcal{M}} \{f(x)\}. \tag{3.3}$$

The main tool for building algorithms to solve the optimization problem (3.3) was Riemannian geometry. Two seminal contributions in this area are the geodesic-stepping

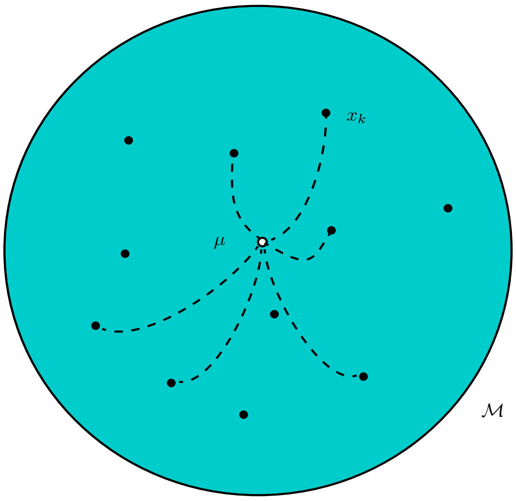

FIG. 3.1. *Notion of averaging over a manifold $\mathcal{M}$. Dots represent the samples $x_k \in \mathcal{M}$ to average while the open circle represents the empirical mean $\mu \in \mathcal{M}$. The dashed lines represent the distances among the sample-points and the midpoint.*

Riemannian-gradient-steepest-descent method of Luenberger [28] and its extension to Riemannian-Newtonian and quasi-Newtonian methods by Gabay [21], that have been inspiring further research in the area of optimization on curved spaces since their inception.

In particular, the Riemannian-gradient-steepest-descent numerical optimization method is based on the knowledge of the explicit form of the geodesic arc emanating from a given point along a given direction and of the Riemannian gradient of the (sufficiently regular) criterion function to optimize. The geodesic-based Riemannian-gradient-steepest-descent optimization method may be expressed as:

$$x_{(\ell+1)} = \exp_{x_{(\ell)}}(-t_{(\ell)}\nabla_{x_{(\ell)}} f), \text{ with} \tag{3.4}$$

$$t_{(\ell)} = \arg\min_{t>0}\{f(\exp_{x_{(\ell)}}(-t\nabla_{x_{(\ell)}} f))\}, \tag{3.5}$$

with $\ell \geq 0$ and with the initial guess $x_{(0)} \in \mathcal{M}$ being arbitrarily chosen. The rule (3.5) to compute a stepsize schedule is well defined for any integer ℓ such that $x_{(\ell)}$ is not a critical point. In fact, it holds:

$$\begin{aligned} &\frac{d}{dt} f(\exp_{x_{(\ell)}}(-t\nabla_{x_{(\ell)}} f)) = \\ &\langle \nabla_{\exp_{x_{(\ell)}}(-t\nabla_{x_{(\ell)}} f)} f, d\exp_{x_{(\ell)}}|_{-t\nabla_{x_{(\ell)}} f}(-\nabla_{x_{(\ell)}} f)\rangle_{\exp_{x_{(\ell)}}(-t\nabla_{x_{(\ell)}} f)}, \end{aligned} \tag{3.6}$$

hence, it holds that:

$$\left.\frac{d}{dt} f(\exp_{x_{(\ell)}}(-t\nabla_{x_{(\ell)}} f))\right|_{t=0} = \langle \nabla_{x_{(\ell)}} f, -\nabla_{x_{(\ell)}} f\rangle_{x_{(\ell)}} = -\|\nabla_{x_{(\ell)}} f\|^2_{x_{(\ell)}} < 0, \tag{3.7}$$

provided $x_{(\ell)}$ is not a critical point of the function f. The convergence of the geodesic-based Riemannian-gradient-steepest-descent optimization method (3.4) endowed with the stepsize selection rule (3.5) is ensured by the following result.

THEOREM 3.1 ([21]). *Assume that the function f is continuously differentiable, that its critical values are distinct and that the connected subset of the level-set $\{x \in$*

$\mathcal{M}|f(x) < f(x_{(0)})\}$ *containing* $x_{(0)}$ *is compact. Then the sequence* $x_{(\ell)}$ *constructed by the method (3.4) and (3.5) converges to a critical point of the function* f.

Moreover, under appropriate conditions (see, e.g., Thorem 4.4 in [21]), the gradient-based optimization method converges linearly.

The application of such optimization method to the computation of the intrinsic mean of a set of points on a manifold is based on the knowledge of the explicit form of the geodesic distance between two given points on a manifold. The short discussion presented in the §2.4 shows that the Riemannian setting is not always suitable to such purpose as some quantities needed to set-up an optimization procedure may be unavailable.

For such a reason, it is of interest to devise optimization algorithms that abstract from the Riemannian context. A notable contribution in this regard is given by the work [34] that suggests how to tackle optimization on affine manifolds. The ideas conveyed by paper [34] are summarized in the following.

Let $\mathcal{M}$ be a p-dimensional differentiable manifold and ∇ a connection on $\mathcal{M}$. According to what has been recalled in §2.1, a connection is completely specified by Christoffel symbols, which, in turn, completely specify parallel translation. Parallel translation defines geodesic arcs which, in turn, define exponential maps. Denote by $\exp_x^{\nabla} : T_x\mathcal{M} \to \mathcal{M}$ the exponential map determined by the connection ∇ that carries vectors from tangent spaces $T_x\mathcal{M}$ to ∇-self-parallel curves through the pole $x \in \mathcal{M}$. The descent method on an affine manifold proposed in [34] to numerically solve the optimization problem (3.3) is summarized in the Algorithm 1. The method applies

Algorithm 1 Descent method on an affine manifold proposed in [34] to numerically solve the optimization problem (3.3). The method is expressed in a completely coordinate-free fashion.

Set $x_{(0)}$ to an initial guess in $\mathcal{M}$
Set $\ell = 0$
repeat
  Choose a tangent vector $v_{(\ell)} \in T_{x_{(\ell)}}\mathcal{M}$ such that $df_{x_{(\ell)}}(v_{(\ell)}) < 0$
  Choose a connection $\nabla_{(\ell)}$
  Determine a value $t_{(\ell)} \in \mathbb{R}$ such that $f(\exp_{x_{(\ell)}}^{\nabla_{(\ell)}}(t_{(\ell)}v_{(\ell)})) < f(x_{(\ell)})$
  Set $x_{(\ell+1)} = \exp_{x_{(\ell)}}^{\nabla_{(\ell)}}(t_{(\ell)}v_{(\ell)})$
  Set $\ell = \ell + 1$
until $x_{(\ell)}$ is close enough to a critical point of f

to the case that the initial guess $x_{(0)}$ is not a critical point of the criterion function f already (a preventive check of this situation was omitted from the Algorithm 1). At any optimization step, a different connection $\nabla_{(\ell)}$ may be chosen (not necessarily a Levi-Civita connection), implying that no metrics are selected *a priori* and that the method depends on local affine structures. The paper [34] does not comment on how to choose the move-along direction $v_{(\ell)}$ nor a stepsize schedule $t_{(\ell)}$ but suggests a stopping criterion to halt the iteration. Let Γ^{∇} denote the parallel translation operation defined by the connection ∇ and $t \mapsto \exp_x^{\nabla}(tv)$ the curve associated to the exponential map $\exp_x^{\nabla}$ emanating from the point x along the direction $v \in T_x\mathcal{M}$ of an extent t. At $x_{(0)}$, select a basis $\{e_1^{(0)}, \ldots, e_p^{(0)}\}$ of the tangent space $T_{x_{(0)}}\mathcal{M}$ and a precision constant $\varepsilon > 0$. A basis $\{e_1^{(\ell)}, \ldots, e_p^{(\ell)}\}$ of the tangent space $T_{x_{(\ell)}}\mathcal{M}$ may be parallel translated along the curve $\gamma_{x_{(\ell)},v_{(\ell)}}(t) \stackrel{\text{def}}{=} \exp_{x_{(\ell)}}^{\nabla_{(\ell)}}(tv_{(\ell)})$ to give a basis

$\{e_1^{(\ell+1)}, \dots, e_p^{(\ell+1)}\}$ of the tangent space $T_{x_{(\ell+1)}}\mathcal{M}$, namely, by

$$e_i^{(\ell+1)} = \Gamma^{\nabla_{(\ell)}}(\gamma_{x_{(\ell)},v_{(\ell)}})_0^{t_{(\ell)}} e_i^{(\ell)}. \tag{3.8}$$

The proposed stopping criterion is to halt the iteration at step ℓ if it holds that:

$$|df_{x_{(\ell)}}(e_i^{(\ell)})| < \varepsilon \text{ for every } i \in \{1, \dots, p\}. \tag{3.9}$$

The analysis of convergence of the method in the Algorithm 1 with stopping criterion (3.9) is summarized as follows.

THEOREM 3.2 ([34]). *Let $\mathcal{M}$ be a p-dimensional differentiable manifold, f be a sufficiently regular function and $\{x_{(\ell)}\}$ be the sequence generated by the method of Figure 1. Suppose that the function f is bounded from below and that the connected component of the level set $\{x \in \mathcal{M} | f(x) < f(x_{(0)})\}$ containing $x_{(0)}$ is compact. Denote by γ the piecewise differentiable curve constructed by joining together all the $\nabla_{(\ell)}$-self-parallel curves properly re-parameterized. Let $(\mathfrak{E}_1, \dots, \mathfrak{E}_p)$ denote a piecewise continuous frame along the curve γ, where each vector field $\mathfrak{E}_j \in \mathfrak{X}(\mathcal{M})$ is obtained by the prolongation of the tangent vectors $e_j^{(\ell)}$ along the curve γ in the intervals $(t_{(\ell)}, t_{(\ell+1)})$.*

(i) If there exists a frame $(\mathfrak{E}_1, \dots, \mathfrak{E}_p)$ along the curve γ such that for every $\varepsilon > 0$ the method halts according to the stopping criterion (3.9), then there exists a subsequence of $\{x_{(\ell)}\}$ converging to a critical point of f.

(ii) If the function f is convex along γ, then the sequence $\{x_{(\ell)}\}$ converges to a unique minimum point of the function f.

It is to be underlined that such a method relies on parallel translation to propagate a basis of the tangent spaces, which is not surely available or efficiently computable for manifolds of interest.

3.2. Gradient-based optimization on pseudo-Riemannian manifolds. Let $\mathcal{M}$ denote a p-dimensional pseudo-Riemannian manifold. A key step in pseudo-Riemannian geometry is to decompose each tangent space $T_x\mathcal{M}$ as follows:

$$\begin{cases} T_x^+\mathcal{M} \stackrel{\text{def}}{=} \{v \in T_x\mathcal{M} | \langle v, v\rangle_x > 0\}, \\ T_x^0\mathcal{M} \stackrel{\text{def}}{=} \{v \in T_x\mathcal{M} | \langle v, v\rangle_x = 0\}, \\ T_x^-\mathcal{M} \stackrel{\text{def}}{=} \{v \in T_x\mathcal{M} | \langle v, v\rangle_x < 0\}. \end{cases} \tag{3.10}$$

The above three components may be characterized by defining $Q_x^\alpha \stackrel{\text{def}}{=} \{v \in T_x\mathcal{M} | \langle v, v\rangle_x = \alpha\}$. If the set Q_x^α with $\alpha \neq 0$ is nonempty, it is a submanifold of the space $T_x\mathcal{M}$ of dimension $p-1$. The set $Q_x^0 = T_x^0\mathcal{M}$ is nonempty as $0 \in Q_x^0$ and is a set of null measure in $T_x\mathcal{M}$.

EXAMPLE 1. *The space* $\mathrm{Sp}(2,\mathbb{R})$ *is a* 3*-dimensional manifold (in fact,* $\mathrm{Sp}(2,\mathbb{R}) = \mathrm{Sl}(2,\mathbb{R})$*, the special linear group), therefore the following parametrization may be taken advantage of:*

$$\begin{cases} (x_{11}, x_{12}, x_{21}) \leftrightarrow \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & \frac{1+x_{12}x_{21}}{x_{11}} \end{bmatrix} \in \mathrm{Sp}_{\mathrm{I}}(2,\mathbb{R}), \ \textit{for } x_{11} \neq 0, \\ (0, x_{12}, x_{22}) \leftrightarrow \begin{bmatrix} 0 & x_{12} \\ -\frac{1}{x_{12}} & x_{22} \end{bmatrix} \in \mathrm{Sp}_{\mathrm{II}}(2,\mathbb{R}), \ \textit{for } x_{12} \neq 0, \end{cases} \tag{3.11}$$

where $(\mathrm{Sp_I}(2,\mathbb{R}), \mathrm{Sp_{II}}(2,\mathbb{R}))$ *is a partition of the space* $\mathrm{Sp}(2,\mathbb{R})$*. For* $X \in \mathrm{Sp_{II}}(2,\mathbb{R})$*, it holds that:*

$$X^{-1} = \begin{bmatrix} 0 & x_{12} \\ -\frac{1}{x_{12}} & x_{22} \end{bmatrix}^{-1} = \begin{bmatrix} x_{22} & -x_{12} \\ \frac{1}{x_{12}} & 0 \end{bmatrix}, \tag{3.12}$$

$$T_X \mathrm{Sp_{II}}(2,\mathbb{R}) \ni V = \begin{bmatrix} v_{11} & v_{12} \\ v_{11}\frac{x_{22}}{x_{12}} + v_{12}\frac{1}{x_{12}^2} & v_{22} \end{bmatrix}. \tag{3.13}$$

Hence, straightforward calculations lead to:

$$\langle V, V\rangle_X = 2\left(\frac{v_{12}^2}{x_{12}^2} + \frac{v_{11}x_{22}v_{12}}{x_{12}} - v_{11}v_{22}\right). \tag{3.14}$$

As a consequence, it holds that:

$$T_X^0 \mathrm{Sp_{II}}(2,\mathbb{R}) = \left\{ \begin{bmatrix} v_{11} & v_{12} \\ v_{11}\frac{x_{22}}{x_{12}} + v_{12}\frac{1}{x_{12}^2} & v_{22} \end{bmatrix} \middle| v_{12}^2 + v_{11}v_{12}x_{22}x_{12} - v_{11}v_{22}x_{12}^2 = 0 \right\}. \tag{3.15}$$

When a pseudo-Riemannian manifold of interest $\mathcal{M}$ and a regular criterion function $f : \mathcal{M} \to \mathbb{R}$ are specified, an optimization rule is 'gradient steepest descent', expressed by [20]:

$$\dot{x} = \begin{cases} -\nabla_x f \text{ if } \nabla_x f \in T_x^+\mathcal{M} \cup T_x^0\mathcal{M}, \\ \nabla_x f \text{ if } \nabla_x f \in T_x^-\mathcal{M}, \end{cases} \tag{3.16}$$

whose solution induces the dynamics:

$$\dot{f} = \left\{ \begin{array}{l} -\|\nabla_x f\|_x^2 \text{ if } \nabla_x f \in T_x^+\mathcal{M} \cup T_x^0\mathcal{M} \\ \|\nabla_x f\|_x^2 \text{ if } \nabla_x f \in T_x^-\mathcal{M} \end{array} \right\} \leq 0. \tag{3.17}$$

The differential equation (3.16) on the manifold $\mathcal{M}$ may be solved numerically by a geodesic-based stepping method. It generalizes the forward Euler method, which moves a point along a straight line in the direction of the Euclidean gradient. In the Euler method, the extension of each step is controlled by a parameter termed stepsize. In the same manner, a geodesic-based stepping method moves a point along a short arc in the direction of the pseudo-Riemannian gradient.

The optimization method based on geodesic stepping reads:

$$x_{(\ell+1)} = \begin{cases} \exp_{x_{(\ell)}}(-t_{(\ell)}\nabla_{x_{(\ell)}} f) \text{ if } \nabla_{x_{(\ell)}} f \in T_{x_{(\ell)}}^+\mathcal{M} \cup T_{x_{(\ell)}}^0\mathcal{M}, \\ \exp_{x_{(\ell)}}(t_{(\ell)}\nabla_{x_{(\ell)}} f) \text{ if } \nabla_{x_{(\ell)}} f \in T_{x_{(\ell)}}^-\mathcal{M}, \end{cases} \tag{3.18}$$

where $\ell \geq 0$ denotes iteration step-counter, symbol $\exp_x(v)$ denotes an exponential map on $\mathcal{M}$ at a point $x \in \mathcal{M}$ applied to the tangent vector $v \in T_x\mathcal{M}$, while the succession $t_{(\ell)} > 0$ denotes an optimization stepsize schedule and the succession $x_{(\ell)} \in \mathcal{M}$ denotes an approximation of the actual solution of the differential equation (3.16) at time $\sum_{i=1}^{\ell-1} t_{(i)}$. The initial guess to start iteration is denoted by $x_{(0)} \in \mathcal{M}$.

The stepsize $t_{(\ell)}$ at any step may be defined by the counterpart of the 'line search' method of the geodesic-based gradient-steepest-descent optimization on Riemannian manifolds (3.5) adapted to the present geometrical setting. Such a method may be expressed as:

$$t_{(\ell)} \stackrel{\text{def}}{=} \begin{cases} \arg\min_{t>0}\{f(\exp_{x_{(\ell)}}(-t\nabla_{x_{(\ell)}}f))\} & \text{if} \quad \nabla_{x_{(\ell)}}f \in T^+_{x_{(\ell)}}\mathcal{M}, \\ 1 & \text{if} \quad \nabla_{x_{(\ell)}}f \in T^0_{x_{(\ell)}}\mathcal{M}, \\ \arg\min_{t>0}\{f(\exp_{x_{(\ell)}}(t\nabla_{x_{(\ell)}}f))\} & \text{if} \quad \nabla_{x_{(\ell)}}f \in T^-_{x_{(\ell)}}\mathcal{M}, \end{cases} \tag{3.19}$$

provided $x_{(\ell)}$ is not a critical point. The method (3.19) involves a nonlinear optimization sub-problem in the parameter t that does not admit any closed-form solution, in general. Moreover, the definition (3.19) is given in a way that takes into account that the function $f(\exp_{x_{(\ell)}}(\mp t\nabla_{x_{(\ell)}}f))$ is locally decreasing for $\nabla_{x_{(\ell)}}f \in T^{\pm}_{x_{(\ell)}}\mathcal{M}$ while it is locally flat for $\nabla_{x_{(\ell)}}f \in T^0_{x_{(\ell)}}\mathcal{M}$. A consequence of such phenomenon is that the line-search method (3.5) cannot be extended directly, otherwise the resulting stepsize would not be well-defined. The obstruction just encountered is due to the presence of the tangent-space part $T^0_x\mathcal{M}$, as moving along a direction $v \in T^0_x\mathcal{M}$ might *increase* the value of the criterion function for any value of the stepsize t, unless $t = 0$. The case $t = 0$ would clearly imply that the optimization method has reached an *impasse point*, namely, the method cannot proceed any further in the optimization of the criterion function f.

In the hypothesis that over an optimization trajectory it holds that $\nabla_x f \notin T^0_x\mathcal{M}$, a stepsize schedule $\hat{t}_{(\ell)}$ that approximates the result of the line-search method (3.19) may be chosen on the basis of the following argument. Define the function:

$$\tilde{f}_{(\ell)} \stackrel{\text{def}}{=} f \circ \rho_{x_{(\ell)},v_{(\ell)}} : [0,\,1] \to \mathbb{R}, \tag{3.20}$$

where $v_{(\ell)} = -\nabla_{x_{(\ell)}}f$ if $\nabla_{x_{(\ell)}}f \in T^+_{x_{(\ell)}}\mathcal{M}$ while $v_{(\ell)} = \nabla_{x_{(\ell)}}f$ if $\nabla_{x_{(\ell)}}f \in T^-_{x_{(\ell)}}\mathcal{M}$. The value $\tilde{f}_{(\ell)}(0) - \tilde{f}_{(\ell)}(t) \geq 0$ denotes the decrease of the criterion function f subjected to a pseudo-geodesic step of stepsize t. If the value of the geodesic stepsize t is small enough, such decrease may be expanded in Taylor series truncated to the second order:

$$\tilde{f}_{(\ell)}(0) - \tilde{f}_{(\ell)}(t) = -\tilde{f}_{1(\ell)}t - \frac{1}{2}\tilde{f}_{2(\ell)}t^2 + o(t^2), \tag{3.21}$$

where, by definition of Taylor series expansion:

$$\tilde{f}_{1(\ell)} \stackrel{\text{def}}{=} \left.\frac{d\tilde{f}_{(\ell)}}{dt}\right|_{t=0}, \quad \tilde{f}_{2(\ell)} \stackrel{\text{def}}{=} \left.\frac{d^2\tilde{f}_{(\ell)}}{dt^2}\right|_{t=0}. \tag{3.22}$$

Under such second-order Taylor approximation, the stepsize value that maximizes the decrease rate is:

$$\hat{t}_{(\ell)} \stackrel{\text{def}}{=} \arg\max_t \left(-\tilde{f}_{1(\ell)}t - \frac{1}{2}\tilde{f}_{2(\ell)}t^2\right) = -\tilde{f}_{1(\ell)}\tilde{f}^{-1}_{2(\ell)}. \tag{3.23}$$

(The above choice of optimization stepsize is sound only if $\tilde{f}_{1(\ell)} \leq 0$ and $\tilde{f}_{2(\ell)} > 0$, hence $\hat{t}_{(\ell)} \geq 0$.) The above procedure may increase significantly the computational complexity of the optimization algorithm as the repeated computation of the coefficient $\tilde{f}_{2(\ell)}$ at every iteration may be computationally cumbersome. Therefore, as far as the computational complexity of the optimization algorithm is of concern, the above procedure should be limited to cases where the computation of second derivatives is simple.

A stopping criterion for the iteration (3.18) may be adapted from criterion (3.9). Denote by $\{e_i^{(\ell)}\}$ a frame of the tangent space $T_{x_{(\ell)}}\mathcal{M}$ of the pseudo-Riemannian manifold $\mathcal{M}$. Given a precision value $\varepsilon > 0$, the stopping criterion (3.9) halts iteration at step ℓ if:

$$|\langle \nabla_{x_{(\ell)}} f, e_i^{(\ell)} \rangle_{x_{(\ell)}}| < \varepsilon \text{ for every } i \in \{1, \ldots, p\}, \tag{3.24}$$

where the initial frame $\{e_i^{(0)}\}$ is propagated via the rule (3.8).

Another stopping criterion, given a precision value $\varepsilon > 0$ and under the hypothesis that over an optimization trajectory it holds that $\nabla_x f \notin T_x^0\mathcal{M}$, halts iteration at step ℓ if:

$$-\tilde{f}_{1(\ell)} < \varepsilon. \tag{3.25}$$

Such stopping criterion is simpler to implement than (3.24) and will be actually used in the following sections.

Unlike the method (3.4)-(3.5), that converges under appropriate conditions, the method (3.18) is not necessarily convergent, in general, due to the presence of the tangent-space component $T_x^0\mathcal{M}$. However, numerical experiments suggest that optimization trajectories $\ell \mapsto x_{(\ell)}$ are such that $\nabla_{x_{(\ell)}} f \notin T^0_{x_{(\ell)}}\mathcal{M}$ and that, as a consequence, the optimization method (3.18) endowed with the stepsize selection method (3.19) enjoys the convergence properties expressed by Theorem 3.1 and, provided that it generates a sequence converging to a critical point of the criterion function, its convergence is linear.

3.3. A distance function on the real symplectic group. In the present paper, the real symplectic group is treated as a pseudo-Riemannian manifold with a bi-invariant pseudo-Riemannian metric. Although it is possible to introduce a pseudo-distance function that is compatible with the pseudo-Riemannian metric (see, e.g., [33]), such function is not positive definite and cannot be interpreted as a distance function.

The research work [42] is concerned with the distance function on the manifold of real symplectic matrices defined by:

$$d^2(X, Y) \stackrel{\text{def}}{=} \|X - Y\|_{\mathrm{F}}^2 = \mathrm{tr}((X - Y)^T (X - Y)),\ X, Y \in \mathrm{Sp}(2n, \mathbb{R}). \tag{3.26}$$

The paper [42] investigated on the nature of the critical points of the function $d^2(X, \bar{Y})$ with $\bar{Y} \in \mathrm{Sp}(2n, \mathbb{R})$ fixed, namely, of the points that satisfy the equation $\nabla_X d^2(X, \bar{Y}) = 0$. Generally, there exist multiple solutions for the critical points, which form a submanifold of the space $\mathrm{Sp}(2n, \mathbb{R})$. A topological study of the critical submanifold based on Hessian analysis reveals that it is formed by a number of separate submanifolds, each of which is characterized by a dimension and a local optimality status (local maximum, minimum or saddle). The result of such non-trivial analysis is summarized by the following theorem.

Theorem 3.3 ([42]). *The least-squares distance function $X \mapsto d^2(X, \bar{Y})$ with fixed $\bar{Y} \in \mathrm{Sp}(2n, \mathbb{R})$ has a unique minimum $X = \bar{Y}$ in $\mathrm{Sp}(2n, \mathbb{R})$ and the rest of critical submanifolds are all saddles.*

On the manifold $\mathrm{Sp}(2n, \mathbb{R})$, the empirical mean $\mu \in \mathrm{Sp}(2n, \mathbb{R})$ of a data-set $\{X_k\} \subset \mathrm{Sp}(2n, \mathbb{R})$ of cardinality N may be defined as in equation (3.1) with distance function chosen as in definition (3.26). Likewise, the empirical variance of the data-set may be defined as in equation (3.2) with $m = 2$. The criterion function $f : \mathrm{Sp}(2n, \mathbb{R}) \to \mathbb{R}$ to minimize is:

$$f(X) \stackrel{\text{def}}{=} \frac{1}{2N} \sum_k \|X - X_k\|_{\mathrm{F}}^2. \tag{3.27}$$

For the sake of notational convenience, set:

$$C \stackrel{\text{def}}{=} \frac{1}{N} \sum_k X_k \in \mathbb{R}^{2n\times 2n}. \tag{3.28}$$

The criterion function (3.27) may be recast as $f(X) = \frac{1}{2}\|X - C\|_{\mathrm{F}}^2 + \text{constant}$. The analytical study of the critical landscape topology of such function is nontrivial and the present author is not aware of any result about the critical points of the function $\|X - C\|_{\mathrm{F}}^2$ over $X \in \mathrm{Sp}(2n, \mathbb{R})$. Hence, the problem of its minimization is treated numerically in the present paper. It holds that $\partial_X f = X - C$, hence, according to the Theorem 2.5, the pseudo-Riemannian gradient of the criterion function (3.27) on the real symplectic group endowed with the Khvedelidze-Mladenov metric reads:

$$\nabla_X f = \frac{1}{2} Q(X - C)Q + \frac{1}{2} X(X - C)^T X. \tag{3.29}$$

In order to compute the partition (3.10), it is worth noting that:

$$2\mathrm{tr}\left(\left(X^{-1}\nabla_X f\right)^2\right) = \mathrm{tr}\left((X - C)^T X(X - C)^T X + (X - C)^T Q(X - C)Q\right). \tag{3.30}$$

The computation of the stepsize at each iteration of the algorithm (3.18) to optimize the criterion function (3.27) according to the rule (3.23), is based on the following results:

$$\frac{1}{2}\frac{d}{dt}\|X \exp(tX^{-1}V) - Y\|_{\mathrm{F}}^2 = \mathrm{tr}\left(\left(X \exp(tX^{-1}V) - Y\right)^T V \exp(tX^{-1}V)\right) \tag{3.31}$$

$$\frac{1}{2}\frac{d^2}{dt^2}\|X \exp(tX^{-1}V) - Y\|_{\mathrm{F}}^2 = \|V \exp(tX^{-1}V)\|_{\mathrm{F}}^2 + \mathrm{tr}\left(\left(X \exp(tX^{-1}V) - Y\right)^T V X^{-1} V \exp(tX^{-1}V)\right). \tag{3.32}$$

The coefficients $\tilde{f}_1$ and $\tilde{f}_2$ of the function $\tilde{f} = f \circ \rho_{X,V}$, with f as in definition (3.27), read:

$$\tilde{f}_1 = \mathrm{tr}\left((X - C)^T V\right), \tag{3.33}$$

$$\tilde{f}_2 = \mathrm{tr}\left(V^T V + (X - C)^T V X^{-1} V\right). \tag{3.34}$$

The sign of the coefficients $\tilde{f}_1$ and $\tilde{f}_2$ may be evaluated as follows. In the case that $\nabla_X f \in T_X^+\mathrm{Sp}(2n, \mathbb{R}) \cup T_X^0\mathrm{Sp}(2n, \mathbb{R})$, the algorithm (3.18) takes $V = -\nabla_X f$, hence $\tilde{f}_1 = -\mathrm{tr}((X - C)^T \nabla_X f) = \frac{1}{2}\mathrm{tr}((X - C)^T X(X - C)^T X + (X - C)^T Q(X - C)Q)$, therefore, by equation (3.30), it holds that $\tilde{f}_1 = -\mathrm{tr}((X^{-1}\nabla_X f)^2) \leq 0$. Conversely, when $\nabla_X f \in T_X^-\mathrm{Sp}(2n, \mathbb{R})$, the algorithm (3.18) takes the search direction $V = \nabla_X f$, hence $\tilde{f}_1 = \mathrm{tr}((X^{-1}\nabla_X f)^2) \leq 0$. The coefficient $\tilde{f}_2$ has a quadratic dependence on matrix V, hence it has the same value for $V = \pm\nabla_X f$. The coefficient $\tilde{f}_2$ is computed as the sum of two terms, $\|V\|_{\mathrm{F}}^2$ and $\mathrm{tr}((X-C)^T V X^{-1} V)$. The first term is non-negative for every $V \in T_X\mathrm{Sp}(2n,\mathbb{R})$, while the second term is indefinite. To evaluate the magnitude of the second term, note that:

$$|\mathrm{tr}((X-C)^T V X^{-1} V)| \leq \|X-C\|_{\mathrm{F}} \|V X^{-1} V\|_{\mathrm{F}} \leq \|X-C\|_{\mathrm{F}} \|V\|_{\mathrm{F}}^2 \|X^{-1}\|_{\mathrm{F}}. \quad (3.35)$$

By the identity $X^{-1} = -QX^TQ$, it follows that $\|X^{-1}\|_{\mathrm{F}} = \|X\|_{\mathrm{F}}$. Moreover, by the triangle inequality it follows that $\|X\|_{\mathrm{F}} \leq \|X-C\|_{\mathrm{F}} + \|C\|_{\mathrm{F}}$. Hence:

$$|\mathrm{tr}((X-C)^T V X^{-1} V)| \leq (\|X-C\|_{\mathrm{F}}^2 + \|X-C\|_{\mathrm{F}} \|C\|_{\mathrm{F}}) \|V\|_{\mathrm{F}}^2. \quad (3.36)$$

Fixed $\|C\|_{\mathrm{F}}$, for $\|X-C\|_{\mathrm{F}}$ sufficiently small, the term $\|V\|_{\mathrm{F}}^2$ dominates the sum in the expression (3.34), hence $\tilde{f}_2$ may be non-negative as well.

The initial guess $X_{(0)}$ may be chosen or randomly generated in $\mathrm{Sp}(2n,\mathbb{R})$, provided it meets the condition

$$\mathrm{tr}\left(\nabla_{X_{(0)}}^T f \nabla_{X_{(0)}} f + (X_{(0)} - C)^T \nabla_{X_{(0)}} f X_{(0)}^{-1} \nabla_{X_{(0)}} f\right) > 0. \quad (3.37)$$

The proposed procedure to optimize the criterion function (3.27) may be summarized by the pseudocode listed in the Algorithm 2, where it is assumed that the optimization sequence $\ell \mapsto X_{(\ell)}$ is such that $\nabla_{X_{(\ell)}} f \notin T^0_{X_{(\ell)}}\mathcal{M}$. In the Algorithm 2, the quantity ℓ denotes a step counter, the matrix $J_{(\ell)}$ represents the Euclidean gradient of the criterion function (3.27), the matrix $U_{(\ell)}$ represents its Riemannian gradient and the sign of the scalar quantity $s_{(\ell)}$ determines whether the matrix $U_{(\ell)}$ belongs to the space $T^+_{X_{(\ell)}}\mathrm{Sp}(2n,\mathbb{R})$ or to the space $T^-_{X_{(\ell)}}\mathrm{Sp}(2n,\mathbb{R})$.

3.4. Computational issues. From a computational viewpoint, the evaluation of the geodesic function (2.51) is the most expensive operation required in the implementation of the optimization algorithm (3.18).

By definition, the exponential of a Hamiltonian matrix $H \in \mathfrak{sp}(2n,\mathbb{R})$ is given by the infinite series (2.50). A fundamental result to ease such computation is the Cayley-Hamilton theorem. The characteristic polynomial of $H \in \mathfrak{sp}(2n,\mathbb{R})$ is defined as $q(\lambda) \stackrel{\mathrm{def}}{=} \det(\lambda I_{2n} - H)$, where $\lambda \in \mathbb{C}$. According to the Cayley-Hamilton theorem applied to the present case, the matrix H satisfies the equation $q(H) = 0$. A direct consequence of such result is that the power H^{2n} may be expressed as a liner combination of the powers H^r with $r = 0, 1, \ldots, 2n-1$. Hence, the geodesic equation (2.51) may be expressed as the *finite* sum:

$$\rho_{X,V}(t) = X[\rho_0(t, X^{-1}V) I_{2n} + \rho_1(t, X^{-1}V) X^{-1}V + \cdots + \rho_{2n-1}(t, X^{-1}V)(X^{-1}V)^{2n-1}], \quad (3.38)$$

with $\rho_i : [0,\, 1] \times \mathfrak{sp}(2n,\mathbb{R}) \to \mathbb{R}$. The advantages of the expression (3.38) of the matrix-exponential are that the expression is exact and that its computational complexity is very reasonable, as the coefficients ρ_i are scalar functions of the entries of the matrix $X^{-1}V$ and a careful implementation of the matrix-powers in the expression (3.38) costs as much as the computation of the highest-order term $(X^{-1}V)^{2n-1}$. The problem of the computation of the coefficients ρ_i has been studied and expressions of such coefficients are available from the literature [35, 36]. The computation of the scalar coefficients ρ_i is facilitated by the highly-structured form of the Hamiltonian matrices.

EXAMPLE 2. *From the expression of the tangent space $T_X\mathrm{Sp}_{\mathrm{I}}(2,\mathbb{R})$ evaluated at the identity ($X = I_2$), it follows that the Lie algebra $\mathfrak{sp}(2,\mathbb{R})$ coincides with the*

Algorithm 2 Pseudocode to implement averaging over the real symplectic group according to the optimization rule (3.18) endowed with stepsize-selection rule (3.23) and stopping criterion (3.25).

Set $Q = \begin{bmatrix} 0_n & I_n \\ -I_n & 0_n \end{bmatrix}$
Set $\ell = 0$
Set $C = \frac{1}{N}\sum_k X_k$
Set $X_{(0)}$ to an initial guess in $\mathrm{Sp}(2n, \mathbb{R})$
Set ε to desired precision
repeat
  Compute $J_{(\ell)} = X_{(\ell)} - C$
  Compute $U_{(\ell)} = \frac{1}{2}(QJ_{(\ell)}Q + X_{(\ell)}J_{(\ell)}^T X_{(\ell)})$
  Compute $s_{(\ell)} = \mathrm{tr}((X_{(\ell)}^{-1}U_{(\ell)})^2)$
  if $s_{(\ell)} > 0$ **then**
    Set $V_{(\ell)} = -U_{(\ell)}$
  else
    Set $V_{(\ell)} = U_{(\ell)}$
  end if
  Compute $\tilde{f}_{1(\ell)} = \mathrm{tr}(J_{(\ell)}^T V_{(\ell)})$
  Compute $\tilde{f}_{2(\ell)} = \mathrm{tr}(V_{(\ell)}^T V_{(\ell)}) + \mathrm{tr}(J_{(\ell)}^T V_{(\ell)} X_{(\ell)}^{-1} V_{(\ell)})$
  Set $\hat{t}_{(\ell)} = -\tilde{f}_{1(\ell)}/\tilde{f}_{2(\ell)}$
  Set $X_{(\ell+1)} = X_{(\ell)} \exp(\hat{t}_{(\ell)} X_{(\ell)}^{-1} V_{(\ell)})$
  Set $\ell = \ell + 1$
until $-\tilde{f}_{1(\ell)} < \varepsilon$

set of real 2×2 matrices with zero trace. Namely, any matrix $H \in \mathfrak{sp}(2, \mathbb{R})$ may be represented as:

$$H = \begin{bmatrix} h_{11} & h_{12} \\ h_{21} & -h_{11} \end{bmatrix}. \tag{3.39}$$

It follows that $H^2 = (h_{11}^2 + h_{12}h_{21})I_2$, $H^3 = (h_{11}^2 + h_{12}h_{21})H$, $H^4 = (h_{11}^2 + h_{12}h_{21})^2 I_2$, and so forth. Hence, by the definition of matrix exponential, it follows that:

$$\begin{aligned} \exp(H) = {} & \left[1 + \frac{1}{2!}(h_{11}^2 + h_{12}h_{21}) + \frac{1}{4!}(h_{11}^2 + h_{12}h_{21})^2 + \dots\right] I_2 \\ & + \left[1 + \frac{1}{3!}(h_{11}^2 + h_{12}h_{21}) + \frac{1}{5!}(h_{11}^2 + h_{12}h_{21})^2 + \dots\right] H, \end{aligned} \tag{3.40}$$

namely:

$$\exp(H) = \begin{cases} I_2 \cosh\sqrt{-\det(H)} + H\frac{\sinh\sqrt{-\det(H)}}{\sqrt{-\det(H)}} & \textit{if } \det(H) < 0, \\ I_2 + H & \textit{if } \det(H) = 0, \\ I_2 \cos\sqrt{\det(H)} + H\frac{\sin\sqrt{\det(H)}}{\sqrt{\det(H)}} & \textit{if } \det(H) > 0. \end{cases} \tag{3.41}$$

Another exact method applies when the matrix to be exponentiated is diagonalizable. As a reference on the eigen-structure of a Hamiltonian matrix see, e.g.,

[40]. Assume that there exist matrices $U, D \in \mathbb{R}^{2n\times 2n}$ with D diagonal such that $X^{-1}V = UDU^{-1}$. Then, it holds that:

$$\rho_{X,V}(t) = XU \exp(tD)U^{-1}. \tag{3.42}$$

In addition, in numerical linear algebra, there is a large body of numerical recipes to compute the exponential of a matrix (see, for example, [24]). An interesting example is based on the following approximation:

$$\exp(H) = \exp\left(\frac{H}{2}\right)\left(\exp\left(-\frac{H}{2}\right)\right)^{-1} \approx \left(I_{2n} + \frac{H}{2}\right)\left(I_{2n} - \frac{H}{2}\right)^{-1}, \tag{3.43}$$

for $H \in \mathfrak{sp}(2n, \mathbb{R})$ and $H - 2I_{2n} \in \mathrm{Gl}(2n, \mathbb{R})$. The map on the rightmost side is known as *Cayley map*, which is defined as $\mathrm{cay}(X) \stackrel{\mathrm{def}}{=} (I_p + X)(I_p - X)^{-1}$ for $X \in \mathbb{R}^{p\times p}$ and $X - I_p$ nonsingular. Note that $\mathrm{cay}(\frac{1}{2}H)$ is an approximation of $\exp(H)$, yet the Cayley function maps a Hamiltonian matrix into a real symplectic matrix[1] [4].

The computation burden associated to the operations listed in the Algorithm 2, besides of the exponential function, may be evaluated in terms of the size $2n$ of the involved matrices. Few preliminary observations are in order:

- The implementation of the Algorithm 2 requires the evaluation of the inverse X^{-1} of a symplectic matrix $X \in \mathrm{Sp}(2n, \mathbb{R})$. By the definition of symplectic matrices, it is inferred that $X^{-1} = -QX^TQ$, which essentially corresponds to block swapping and sign-switching. Namely, upon the $n \times n$ 4-block partition $X = \left[\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right]$, it results that $X^{-1} = \left[\begin{smallmatrix} D^T & -B^T \\ -C^T & A^T \end{smallmatrix}\right]$. Hence, in the present evaluation of computation burden, the inversion of a symplectic matrix is considered as costless.
- Some terms repeat across the lines of the pseudocode of Algorithm 2, hence a careful implementation is assumed, which does not perform the same computation more than once.
- Except for matrix exponentiation and one scalar division, the rest of the operations are multiplications and additions. The latter are grouped into MAC (Multiply & ACcumulate) operations.

On the basis of the above observations, the computational complexity of the terms involved in the Algorithm 2 have been estimated as shown in the Table 3.1. The total computation burden of the algorithm has been estimated in $64n^3$ MACs, 1 scalar division and 1 matrix exponential evaluation.

4. Numerical tests. The numerical behavior of the developed minimal-distance algorithm will be illustrated via different tests. A numerical test concerns the computation of the empirical mean out of a set of real symplectic matrices of size 2×2. The space $\mathrm{Sp}(2, \mathbb{R})$ is 3-dimensional, therefore graphical representations of the quantities of interest is allowed. A further numerical test concerns the computation of the empirical mean of a set of given real symplectic matrices in $\mathrm{Sp}(2n, \mathbb{R})$ with $n > 1$. The optimization algorithm was coded in MATLAB® 6.0.

The numerical experiments presented in the following sections rely on the availability of a way to generate pseudo-random samples on the the real symplectic group $\mathrm{Sp}(2n, \mathbb{R})$. Given a point $X \in \mathrm{Sp}(2n, \mathbb{R})$, that will be referred to in the following as

[1] Indeed, the Cayley map may be applied in the numerical integration of ordinary differential equations on quadratic matrix group-manifolds [27] that generalize the notion of symplectic group.

Term	**MACs**	**div**	**exp**
$U_{(\ell)}$	$16n^3$	–	–
$s_{(\ell)}$	$16n^3$	–	–
$\tilde{f}_{1(\ell)}$	$8n^3$	–	–
$\tilde{f}_{2(\ell)}$	$16n^3$	–	–
$\hat{t}_{(\ell)}$	–	1	–
$X_{(\ell+1)}$	$8n^3$	–	1

TABLE 3.1

*Estimate of the computational complexity of the terms involved in the Algorithm 2. (The symbol '**div**' denotes scalar division while the term '**exp**' denotes matrix exponential.)*

'center of mass' or simply center of the random distribution, it is possible to generate a random sample $Y \in \mathrm{Sp}(2n, \mathbb{R})$ in a neighbor of matrix X by the rule:

$$Y = X \exp(X^{-1}V), \tag{4.1}$$

where the direction $V \in T_X\mathrm{Sp}(2n, \mathbb{R})$ is randomly generated around $0 \in T_X\mathrm{Sp}(2n, \mathbb{R})$. That the points Y generated by the exponential rule (4.1) distribute around the point X is confirmed by the following result.

LEMMA 4.1. *Let $(X, V) \in T\mathrm{Sp}(2n, \mathbb{R})$ and $Y = X \exp(X^{-1}V)$. Then it holds that:*

$$\|Y - X\|_{\mathrm{F}} \leq \|X\|_{\mathrm{F}}[\exp(\|X^{-1}V\|_{\mathrm{F}}) - 1]. \tag{4.2}$$

Proof. As $\|Y - X\|_{\mathrm{F}} = \|X(\exp(X^{-1}V) - I_{2n})\|_{\mathrm{F}}$, it follows that:

$$\|Y - X\|_{\mathrm{F}} \leq \|X\|_{\mathrm{F}} \left\| \sum_{k=1}^{\infty} \frac{(X^{-1}V)^k}{k!} \right\|_{\mathrm{F}} \leq \|X\|_{\mathrm{F}} \sum_{k=1}^{\infty} \frac{\|X^{-1}V\|_{\mathrm{F}}^k}{k!}. \tag{4.3}$$

The series on the rightmost term converges to $\exp(\|X^{-1}V\|_{\mathrm{F}}) - 1$. ◻

Recall that, given a point $X \in \mathrm{Sp}(2n, \mathbb{R})$ and a matrix $S \in \mathbb{R}^{2n \times 2n}$ symmetric, because of the structure of the tangent space $T_X\mathrm{Sp}(2n, \mathbb{R})$, the matrix $V = XQS$ belongs to the space $T_X\mathrm{Sp}(2n, \mathbb{R})$. Hence, it is sufficient to generate a random symmetric matrix $S \in \mathbb{R}^{2n \times 2n}$ to get a random point $X \exp(QS)$ in $\mathrm{Sp}(2n, \mathbb{R})$. In turn, a symmetric $2n \times 2n$ matrix may be generated by the rule $S = A^T + A$, with $A \in \mathbb{R}^{2n \times 2n}$ having zero-mean randomly-generated entries. All in one:

$$Y = X \exp(Q(A^T + A)). \tag{4.4}$$

Note that $\|Q(A^T + A)\|_{\mathrm{F}}^2 = 2(\mathrm{tr}(A^2) + \|A\|_{\mathrm{F}}^2)$, hence, by the Lemma 4.1, it holds that $\|Y - X\|_{\mathrm{F}} \leq \sqrt{2}\|X\|_{\mathrm{F}}\sqrt{\mathrm{tr}(A^2) + \|A\|_{\mathrm{F}}^2}$, namely, the variance of the entries a_{ij} controls the spread of the random real-symplectic sample-matrices Y around the center of mass X.

4.1. Averaging over the manifold $\mathrm{Sp}(2, \mathbb{R})$**.** A close-up of the numerical behavior of the minimal-distance optimization algorithm (3.18) stems from the examination of the case of averaging over the manifold $\mathrm{Sp}(2n, \mathbb{R})$ for $n = 1$ and $N = 100$. The elements of the group $\mathrm{Sp}(2, \mathbb{R})$ may be rendered on a 3-dimensional drawing.

The Figure 4.1 shows a result obtained with the iterative algorithm (3.18) and the 100 samples X_k generated randomly around a randomly-selected center of mass. The Figure 4.1 shows the location of the target matrices X_k (circles), the location of the center-of-mass (cross), the trajectory of the optimization algorithm over the search space (solid-dotted line) and the location of the final point computed by the algorithm (diamond). In order to emphasize the behavior of the optimization method (3.18), in this experiment a constant stepsize schedule $t_{(\ell)} = \frac{1}{2}$ was used and no stopping criterion was used, in order to evidence the numerical stability of the method. The

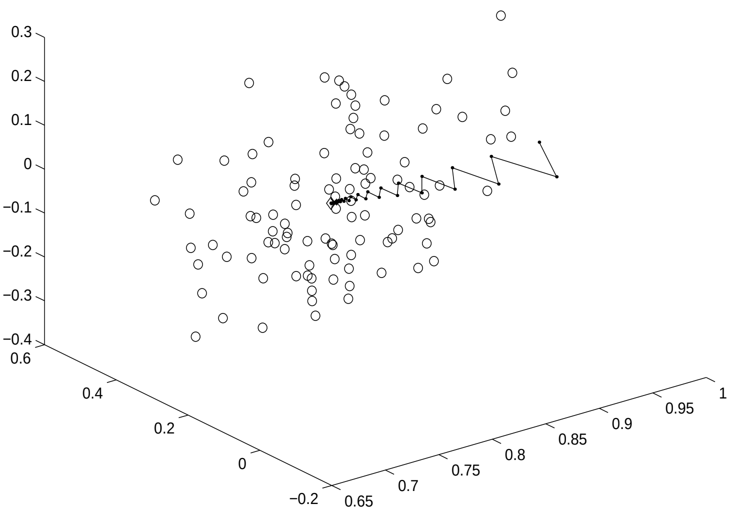

FIG. 4.1. *Averaging over the real symplectic group* $\mathrm{Sp}(2, \mathbb{R})$. *Target matrices* X_k *are denoted by circles. The center-of-mass is denoted by a cross mark. The trajectory of the optimization algorithm is denoted by a solid-dotted line, where any dot corresponds to an approximate solution* $X_{(\ell)}$. *The last point of the trajectory is denoted by a diamond mark and represents the computed empirical mean* μ.

Figure 4.1 shows that the algorithm is convergent toward the center of mass. The Figure 4.2 shows the value of the criterion function $\frac{1}{2N} \sum_k d^2(X, X_k)$ during iteration, the value of the Frobenius norm of its pseudo-Riemannian gradient during iteration, the distances $d(X, X_k)$ before iteration (with initial guess chosen as $X_{(0)} = I_2$) and after iteration.

4.2. Averaging over the manifold $\mathrm{Sp}(2n, \mathbb{R})$ **with** $n > 1$**.** The Figure 4.3 shows a result obtained with the iterative algorithm (3.18) for $n = 5$ and $N = 50$. The Figure 4.3 shows the value of the criterion function $\frac{1}{2N} \sum_k d^2(X, X_k)$ as well as the value of the Frobenius norm of its pseudo-Riemannian gradient during iteration. In the shown example, the squared pseudo-norm of the pseudo-Riemannian gradient of the criterion function to optimize may assume negative, zero, as well as positive values during optimization, therefore, the Frobenius norm was selected for displaying in order not to miss the link with the zero-gradient condition at convergence. The Figure 4.3 also shows the distances $d(X, X_k)$ before iteration (with initial guess chosen as $X_{(0)} = I_{10}$) and after the iteration. Such numerical results were obtained by the

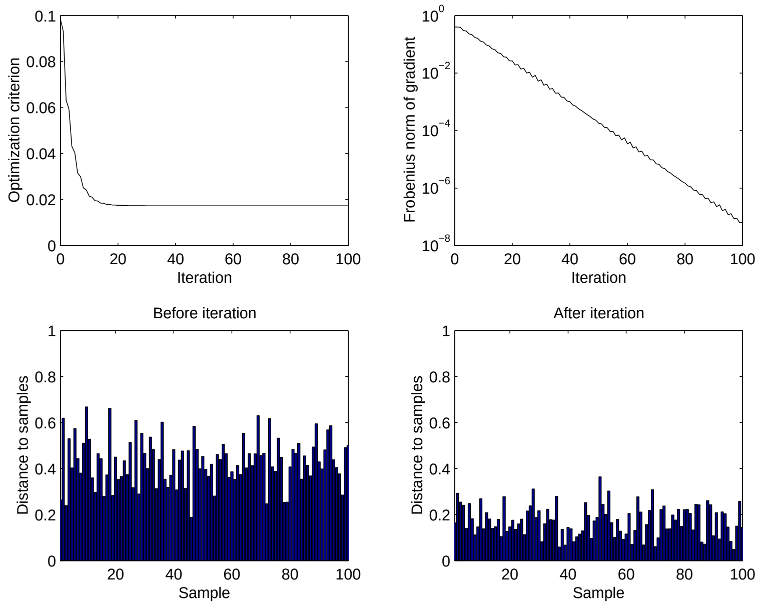

FIG. 4.2. *Averaging over the real symplectic group* $\mathrm{Sp}(2,\mathbb{R})$*. Criterion function (3.27) during iteration, value of the Frobenius norm of the pseudo-Riemannian gradient of the criterion function during iteration, distances* $d(X, X_k)$ *before iteration (*$X = X_{(0)}$*) and after iteration (*$X = \mu$*).*

adaptive optimization stepsize schedule explained in subsection 3.2 and by employing the stopping condition (3.25) with precision $\varepsilon = 10^{-6}$. The Figure 4.3 shows that the algorithm converges steadily toward the minimal distance configuration (in fact, the distances from the found empirical mean are much smaller than the distances from the initial guess). The Figure 4.4 shows the value of the 'symplecticity' index $\|X^T QX - Q\|_{\mathrm{F}}$ during iteration as well as the value of the optimization stepsize schedule. The value of the coefficients $\tilde{f}_1$ and $\tilde{f}_2$ during iteration is displayed as well. The panels show that the matrix sequence $X_{(\ell)}$ remains on the manifold $\mathrm{Sp}(10,\mathbb{R})$ at each iteration (up to machine precision).

The Figure 4.5 shows the result of an empirical statistical analysis about the behavior of the optimization algorithm over 500 independent trials. In each trial, the algorithm starts from a randomly generated initial guess $X_{(0)}$. In particular, the Figure 4.5 shows the distribution of the number of iterations that optimization takes to reach the desired precision on each trial. The convergence speed varies with the initial guess while the algorithm converges in every trial to the same value of the criterion function (namely, to $\frac{1}{2}\mu_2 \approx 0.9827$, in this test) and takes no more than 10^{-3} seconds to run on an average computation platform (4GB RAM, 2.17 GHz clock).

5. Conclusion. Gradient-based optimization methods can be used to solve applied mathematics problems and are relatively easy to implement on a computer. The present paper discusses a minimal-distance problem formulated over the manifold of real symplectic matrices. The present research takes its moves from the following observations:

- Minimal-distance problems may be extended from flat spaces to curved smooth metrizable manifolds by the choice of an appropriate distance function.
- The resulting minimization problem on manifold may be tackled via a gradient-

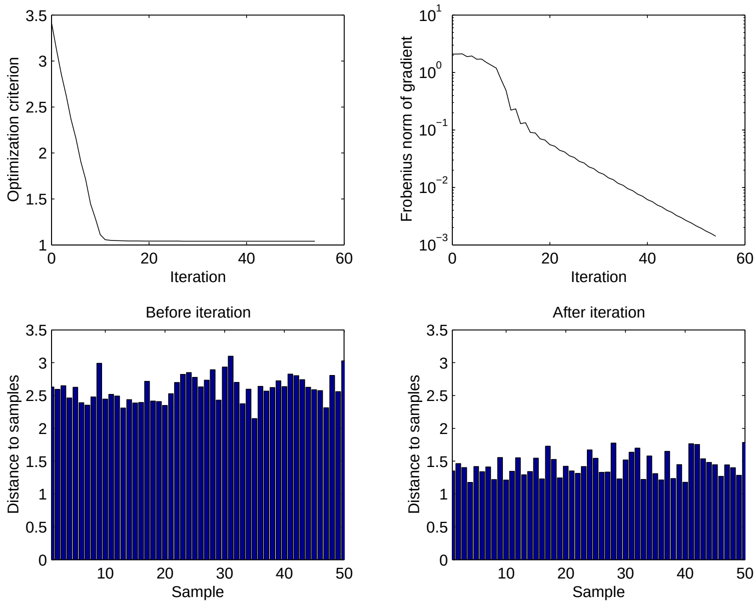

FIG. 4.3. *Optimization over the symplectic group* $\mathrm{Sp}(10,\mathbb{R})$*. Criterion function (3.27) during iteration, value of the Frobenius norm of the pseudo-Riemannian gradient of the criterion function during iteration, distances* $d(X, X_k)$ *before iteration* ($X = X_{(0)}$) *and after iteration* ($X = \mu$)*.*

descent algorithm tailored to the geometry of parameter manifold through a geodesic-stepping method.

The real symplectic group is regarded as a pseudo-Riemannian manifold and a metric is chosen that affords the computation of closed-forms of geodesic arcs. Within such geometric setting, the considered minimal-distance problem may be set up and the geodesic-based numerical stepping method may be implemented. The paper also presents a way of selecting an appropriate stepsize schedule based on local quadratic approximation of the criterion function restricted on a geodesic arc.

The present manuscript is related to the previous manuscript [18]. The present manuscript is entirely dedicated to the optimization over the manifold of real symplectic matrices. The mathematical instruments needed within the present paper are expressed in the §2 in a fully differential-geometrical fashion, while paper [18] was based on different concepts (for example, the Lagrange multipliers method). The optimization problem to tackle differs from the problem considered in the previous paper [18] and is fully supported by the study conducted in [42]. The §3 presents a discussion about the difficulties encountered when trying to extend the Riemannian optimization setting to a pseudo-Riemannian optimization setting and, more in general, to a general manifold, along with a discussion on the selection of a stepsize schedule as well as of stopping criteria, on the convergence and on the computational issues related to the discussed optimization method. In particular, the §3 evidences how the computational complexity of the discussed optimization algorithm on the space $\mathrm{Sp}(2n,\mathbb{R})$ is of order $(2n)^3$ (without any specifically-optimized linear-algebra tool).

Although the present paper focuses on the study of minimal-distance problems on the manifold of real symplectic matrices, the main results of the paper and the

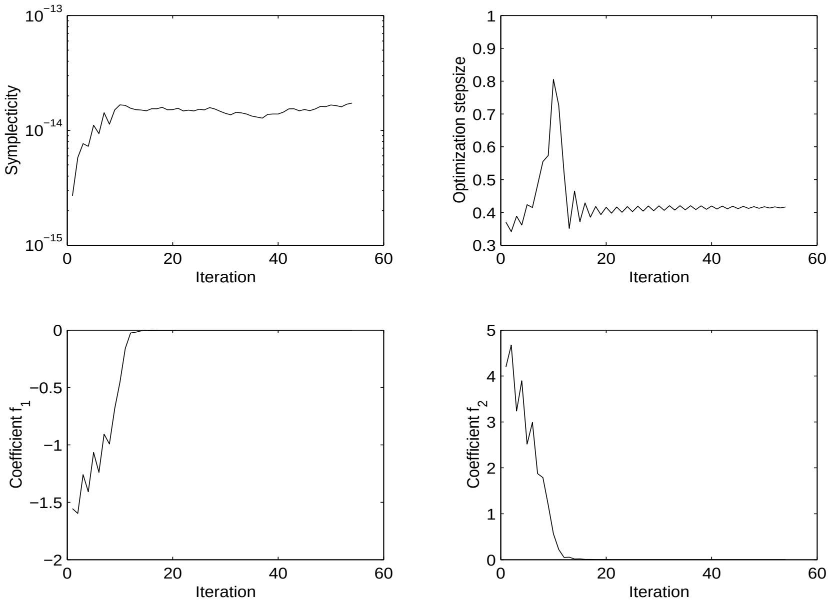

FIG. 4.4. *Optimization over the symplectic group* $\mathrm{Sp}(10,\mathbb{R})$. *Value of the symplecticity index* $\|X^T_{(\ell)}QX_{(\ell)} - Q\|_\mathrm{F}$*, of the coefficient* $\tilde{f}_{1(\ell)}$ *and of the coefficient* $\tilde{f}_{2(\ell)}$ *during iteration and value of the optimization stepsize schedule* $\hat{t}_{(\ell)}$ *(the index* ℓ *is denoted as 'Iteration').*

relevant calculations were presented in a rather general fashion, so that they could be applied to other manifolds of interest to the readers.

Numerical tests have been performed with reference to the computation of the empirical mean of a collection of symplectic matrices. The obtained numerical results show that the pseudo-Riemannian-gradient-based algorithm, along with a pseudo-geodesic-based stepping method, is suitable to the numerical solution of the posed minimal-distance problem.

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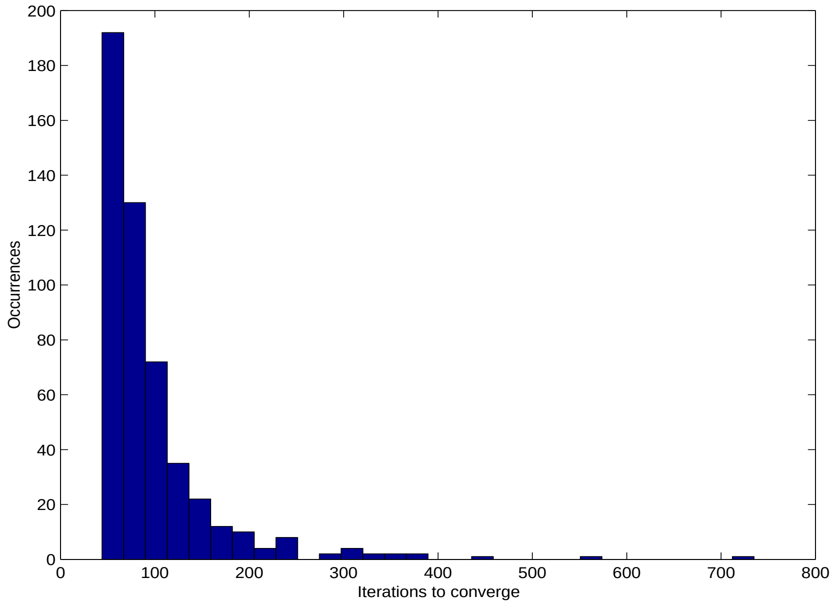

FIG. 4.5. *Optimization over the symplectic group* Sp$(10, \mathbb{R})$. *Distribution of the number of iterations to converge on each trial on a total of* 500 *independent trials.*

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