Fast symplectic integrator for Nesterov-type acceleration method

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Abstract

In this paper, explicit stable integrators based on symplectic and contact geometries are proposed for a non-autonomous ordinarily differential equation (ODE) found in improving convergence rate of Nesterov’s accelerated gradient method. Symplectic geometry is known to be suitable for describing Hamiltonian mechanics, and contact geometry is known as an odd-dimensional counterpart of symplectic geometry. Moreover, a procedure, called symplectization, is a known way to construct a symplectic manifold from a contact manifold, yielding Hamiltonian systems from contact ones. It is found in this paper that a previously investigated non-autonomous ODE can be written as a contact Hamiltonian system. Then, by symplectization of a non-autonomous contact Hamiltonian vector field expressing the non-autonomous ODE, novel symplectic integrators are derived. Because the proposed symplectic integrators preserve hidden symplectic and contact structures in the ODE, they should be more stable than the Runge–Kutta method. Numerical experiments demonstrate that, as expected, the second-order symplectic integrator is stable and high convergence rates are achieved.

1 Introduction

Optimization plays a central role in solving various engineering problems such as machine learning for data analysis. To develop effective optimization methods, theoretical proposals that yield fast convergence rates and the design of stable numerical schemes for implementations are needed [Nocedal and Wright, 2006, Boyd and Vandenberghe, 2004, Sun et al., 2019].

For unconstrained smooth convex problems, several algorithms have been proposed, and Nesterov’s accelerated gradient descent (NAG) algorithm has been recognized as a major milestone [Nesterov, 1983]. Subsequently, a number of improvements have then been proposed [Defazio, 2019, O’donoghue and Candès, 2015, Fazlyab et al., 2018, Hu and Lessard, 2017, Scieur et al., 2016, Lessard et al., 2016, Attouch, Hedy et al., 2019]. One of them derives a non-autonomous second-order ordinary differential equation (ODE) corresponding to the NAG algorithm [Su et al., 2016]. Here, an autonomous ODE is synonymous with an ODE which does not explicitly depend on an independent
variable, where such a variable in this paper is time \( t \). This second-order ODE enables convergence rates and some related quantities to be estimated if the objectives are sufficiently smooth and the step sizes in the numerical schemes are sufficiently small. Determining such an appropriate step size is non-trivial in general. That is, there are nontrivial discrepancies between the continuous-time and discrete-time theories of finding an ideal scheme, and several approaches exist to address this issue.

For some discrete systems, discrete Lyapunov functions can be found so that the derivation of a convergence rate does not rely on the continuous-time limit. Unfortunately, finding such Lyapunov functions for discrete algorithms is highly nontrivial [Bof et al., 2018, Shi et al., 2019, Wilson et al., 2019]. In contrast, links between discrete systems and continuous ones have been studied in another context. Because a large number of physical phenomena are modeled as continuous-time dynamical systems, the construction of accurate numerical integrators that are suitable for continuous-time systems is of great importance. One sophisticated class of such integrators forms a class of geometric integrators, and these integrators preserve the mathematical or geometric structures of the continuous-time dynamical system under consideration [Hairer et al., 2006]. In particular symplectic integrators have been applied to various Hamiltonian systems including celestial ones because symplectic integrators preserve the symplectic property in Hamiltonian systems, and numerical errors do not significantly accumulate in long-time simulations [Kinoshita et al., 1990, Yoshida, 1993]. Symplectic integrators can be employed not only for problems in celestial mechanics, but also for engineering problems. In particular, if ODEs that are designed to achieve fast convergence rates are written as Hamiltonian systems, then the implementation of symplectic integrators is expected to realize more stable algorithms than Runge-Kutta integrators at a fixed order. To implement symplectic integrators to realize stable algorithms, a key mathematical tool should be a procedure for obtaining Hamiltonian systems from given ODEs. Note that there exists a systematic procedure yielding a class of autonomous Hamiltonian systems from a particular class of autonomous ODEs by introducing another degree of freedom. By contrast, for non-autonomous ODEs, such a procedure is unknown. This particular class, where autonomous Hamiltonian systems are obtained, is the so-called contact Hamiltonian systems, and the procedure to obtain Hamiltonian systems from contact ones is called symplectization.

In the recent literature the so-called contact integrators have been considered. The theoretical foundation of these integrators is based on contact geometry, which is often called an odd-dimensional analogue of symplectic geometry [da Silva, 2008]. The significance of the use of contact integrators has been shown in systems with Newtonian mechanics that have time-varying non-conserved forces [Bravetti et al., 2020]. In addition, contact integrators can be applied to accelerated algorithms [Bravetti et al., 2019], and their applicability in optimization should be further explored, as well as other related integrators [Vermeeren et al., 2019, França et al., 2020, Tao and Ohsawa, 2020].

1.1 Summary of this contribution

A non-autonomous ODE was proposed by Zhang et al. [2018] as a continuous-time limit of NAG so that a fast convergence rate was obtained. In this paper, using the theory of symplectic and contact geometries, the following are shown:

- It is shown that this ODE is described by a non-autonomous contact Hamiltonian system on an extended contact manifold. A symplectization of the contact Hamiltonian system is then
explicitly derived without any approximation. Thus, this ODE is shown to belong to both
non-autonomous contact Hamiltonian and Hamiltonian systems.

- A class of symplectic integrators is constructed from the obtained non-autonomous Hamil-
tonian system. Because the obtained Hamiltonian consists of the sum of integrable Hamilton-
ians, an explicit scheme is obtained for lower-order integrators. Higher-order integrators
can in principle be constructed with an existing method systematically if necessary. Such
higher-order integrators can be used if a higher rate is needed. The proposed integrators that
preserve the Hamiltonian nature should be stable. This stability was verified numerically.

This contribution is the first step toward the conceptualization of the symplectization of contact
manifolds as a tool for constructing high-performance algorithms in optimization problems. From a
broad perspective, because contact geometry is suitable for describing several algorithms for finding
minimizers of objectives [Bravetti et al., 2019] and symplectic geometry is suitable for construct-
ing integrators, the combination of these two geometries is expected to be a fruitful approach in
optimization problems.

In the following sections the ideas are emphasized, and the detailed calculations are shown in the
appendix. Related notions in differential geometry are also briefly summarized in the appendix.
In Section 2 basic tools for deriving symplectic integrators are summarized, and these are used
to describe Zhang’s equation. Using these tools, symplectic integrators for Zhang’s equation are
explicitly derived in Section 3. These theories are numerically verified in Section 4. Finally, Section 5
summarizes this work briefly.

2 Geometric description of non-autonomous ODEs

In this section, tools for describing Hamiltonian and contact Hamiltonian systems are briefly sum-
marized, and they are applied to the equation proposed by Zhang et al. [2018] and other ones Su et al.
[2016] Wibisono et al. [2016].

2.1 Systems of ODEs as contact and Hamiltonian systems

Symplectic and contact geometries are well-developed research areas in mathematics, and they
are closely related to each other. In this subsection a minimum description of these geometries
is summarized to argue properties of existing ODEs proposed as continuous-time optimization
methods.

Symplectic manifold is an even-dimensional manifold together with the so-called symplectic
structure. In Euclidean setting this is denoted \((\mathbb{R}^{2n},\omega)\) with \(n \geq 1\). For this manifold, coordinates
are \((q,p)\), where \(q = (q^1,\ldots,q^n) \in \mathbb{R}^n\), and \(p = (p_1,\ldots,p_n) \in \mathbb{R}^n\). The coordinates \(q\) express
generalized positions, and \(p\) their conjugate momenta. Symplectic structure \(\omega\) is defined as a 2-form,
and is then also called symplectic 2-form, written in a standard way as

\[
\omega = d\alpha, \quad \alpha = \sum_{a=1}^{n} p_a dq^a.
\]

where \(\alpha\) is a 1-form called a Liouville 1-form, \(d\) is the so-called exterior derivative. Symplectic
manifold is suitable for describing a class of energy conservative dynamical systems. Given a
function \( \mathcal{H} \) on \( \mathbb{R}^{2n} \), canonical equations of motion are

\[
\dot{q}^a = \frac{\partial \mathcal{H}}{\partial q^a}, \quad \dot{p}_a = -\frac{\partial \mathcal{H}}{\partial q^a}, \quad a = 1, \ldots, n.
\]

Here the function \( \mathcal{H} \) is called Hamiltonian that is physically identified with energy function, \( t \in \mathcal{I} \subseteq \mathbb{R} \), and \( \cdot \) differentiation with respect to \( t \). One of the roles of \( \omega \) is to provide the signs \( \pm \) appearing in the canonical equations. It is known that canonical equations of motion are written as a vector field on \( \mathbb{R}^{2n} \) in terms of \( \omega \). Moreover, the energy conservation law, \( d\mathcal{H}/dt = 0 \), can be verified.

In the Euclidean setting a contact manifold is an odd-dimensional manifold together with the so-called contact structure. This is denoted \((\mathbb{R}^{2n+1}, \ker \lambda)\) with \( n \geq 1 \). For this manifold, coordinates are \((q^0, q, \gamma)\), where \( q = (q^1, \ldots, q^n) \in \mathbb{R}^n \), \( \gamma = (\gamma_1, \ldots, \gamma_n) \in \mathbb{R}^n \), and \( q^0 \in \mathbb{R} \). In the case where a contact manifold is applied to describe a class of dissipative dynamical systems, \( q \) expresses generalized coordinates, \( \gamma \) momenta, and \( q^0 \) an action [Bravetti et al., 2019]. Contact structure \( \ker \lambda \) is defined by the kernel of a contact 1-form \( \lambda \), \( \ker \lambda = \{ X \in \mathbb{R}^{2n+1} | \lambda(X) = 0 \} \), and thus contact structure is a \( 2n \)-dimensional subspace of the ambient \((2n + 1)\)-dimensional vector space. Here a contact 1-form is written in a standard way as

\[
\lambda = dq^0 - \sum_{a=1}^{n} \gamma_a dq^a.
\]

Given a function \( \overline{K} \) on \( \mathbb{R}^{2n+1} \), equations of motion analogous to canonical equations in the symplectic case are

\[
\dot{q}^a = \frac{\partial \overline{K}}{\partial \gamma_a}, \quad \dot{\gamma}_a = -\frac{\partial \overline{K}}{\partial q^a} - \gamma_a \frac{\partial \overline{K}}{\partial q^0}, \quad a = 1, \ldots, n.
\]

\[
\dot{q}^0 = -\overline{K} + \sum_{a=1}^{n} \gamma_a \frac{\partial \overline{K}}{\partial \gamma_a}.
\]

Here the function \( \overline{K} \) is called contact Hamiltonian. Note that the energy conservation law does not hold in general, \( d\overline{K}/dt \neq 0 \).

Relations between symplectic manifolds and contact manifolds are often argued in autonomous systems [Libermann and Marle [1987], der Schaft and Maschke [2018]]. Symplectization (or symplectification) of a \((2n + 1)\)-dimensional contact manifold is a procedure giving \((2n + 2)\)-dimensional symplectic manifold. By contrast, such a procedure is unknown for non-autonomous systems, and then the existing symplectization for the autonomous systems will be extended for non-autonomous systems in this paper. This extended symplectization will be used to construct symplectic integrators from non-autonomous contact Hamiltonian systems in the later sections.

In the autonomous case, symplectization is summarized as follows. Given a prescribed contact manifold \((\mathbb{R}^{2n+1}, \ker \lambda)\), introduce the new variables \( p_0 \in \mathbb{R} \setminus \{0\} \) and

\[
\gamma_a = -\frac{p_a}{p_0}, \quad a = 1, \ldots, n.
\]

In addition, introduce a higher dimensional symplectic manifold \((\mathbb{R}^{2n+2}, \omega)\), where \( \omega \) is given by \( \omega = d\alpha \). This \( \alpha \) is called the Liouville 1-form, and can be constructed from the contact 1-form \( \lambda \).
with Eq. (1) as
\[ p_0 \lambda = p_0 d q^0 + \sum_{a=1}^{n} p_a d q^a = \alpha, \]
where \( \lambda \) has been treated as a 1-form on the symplectic manifold. Similar treatment is implicitly applied throughout. Then the system with the Hamiltonian on \( \mathbb{R}^{2n+2} \)
\[ \mathcal{H}(q^0, q^1, \ldots, q^n, p_0, p_1, \ldots, p_n) \]
induces the contact Hamiltonian system with \( \mathcal{K} \) on \( \mathbb{R}^{2n+1} \). The relation between \( \mathcal{H} \) and \( \mathcal{K} \) is given by
\[ \mathcal{H}(q^0, q^1, \ldots, q^n, p_0, p_1, \ldots, p_n) = -p_0 \mathcal{K}(q^0, q^1, \ldots, q^n, \gamma_1, \ldots, \gamma_n). \]
This is proven by comparing equations of motion associated with \( \mathcal{H} \) with those with \( \mathcal{K} \).

To describe non-autonomous Hamiltonian systems and contact Hamiltonian systems, introduce additional space \( \mathcal{I}(\subset \mathbb{R}) \) whose coordinate expresses time \( t \) for each. The resultant phase spaces in Euclidean setting are \( \mathbb{R}^{2n+2} \times \mathcal{I} \) and \( \mathbb{R}^{2n+1} \times \mathcal{I} \), respectively. Given a (non-autonomous) Hamiltonian \( H \) on \( \mathbb{R}^{2n+2} \times \mathcal{I} \), the extended Liouville 1-form and extended symplectic 2-form on \( \mathbb{R}^{2n+2} \times \mathcal{I} \) can be defined as
\[ \alpha^E = \alpha - H dt, \]
and
\[ \omega^E = d \alpha^E. \]
This \( \omega^E \) is not the standard symplectic form, because it is defined on an odd-dimensional manifold. The canonical equations of motion are
\[ \dot{q}^a = \frac{\partial H}{\partial p_a}, \quad \dot{p}_a = -\frac{\partial H}{\partial q^a}, \quad i = 1, \]
where \( a = 0, \ldots, n \). Note that \( dH/dt = \partial H/\partial t \neq 0 \) in general.

In addition, given a (non-autonomous) contact Hamiltonian \( K \) on \( \mathbb{R}^{2n+1} \times \mathcal{I} \), the extended contact 1-form on \( \mathbb{R}^{2n+1} \times \mathcal{I} \) are defined by
\[ \lambda^E = \lambda + K dt. \]
The equations of motion are
\[ \dot{q}^a = \frac{\partial K}{\partial \gamma_a}, \quad \dot{\gamma}_a = -\frac{\partial K}{\partial q^a} - \gamma_a \frac{\partial K}{\partial q^0}, \quad i = 1, \]
\[ \dot{q}^0 = -K + \sum_{b=1}^{n} \gamma_b \frac{\partial K}{\partial \gamma_b}, \quad i = 1, \]
where \( a = 1, \ldots, n \).

In this paper \((\mathbb{R}^{2n+2} \times \mathcal{I}, \omega^E)\) is referred to as an extended symplectic manifold, and \((\mathbb{R}^{2n+1} \times \mathcal{I}, \ker \lambda^E)\) an extended contact manifold. They are specified after Hamiltonian and contact Hamiltonian are introduced, respectively. A link between non-autonomous Hamiltonian systems and non-autonomous contact Hamiltonian systems is as follows.
Proposition 2.1. A non-autonomous Hamiltonian system associated with $H$ on $\mathbb{R}^{2n+2} \times \mathcal{I}$ induces a non-autonomous contact Hamiltonian system associated with $K$ on $\mathbb{R}^{2n+1} \times \mathcal{I}$, where the relation between $H$ and $K$ is given by

$$H(q^0, q^1, \ldots, q^n, p_0, \ldots, p_n, t) = -p_0 K(q^0, q^1, \ldots, q^n, \gamma_1, \ldots, \gamma_n, t)$$

where $\gamma_a = -p_a / p_0$ for $p_0 \neq 0$. Moreover the relation $\alpha^E = p_0 \lambda^E$ hold.

Proof. The claim on equations of motion is verified by substituting the Hamiltonian $H$ into Eq. (4). The calculations are as follows. It immediately follows that

$$\dot{p}_0 = -\frac{\partial H}{\partial q_0} = p_0 \frac{\partial K}{\partial q_0}, \quad \dot{q}^0 = \frac{\partial H}{\partial p_0} = -K + \sum_{b=1}^{n} \gamma_b \frac{\partial K}{\partial \gamma_b},$$

and for $a = 1, \ldots, n$,

$$\dot{p}_a = -\frac{\partial H}{\partial q^a} = p_0 \frac{\partial K}{\partial q^a}, \quad \dot{q}^a = \frac{\partial H}{\partial p_a} = \frac{\partial K}{\partial \gamma_a}.$$

Combining these calculations, one has

$$\dot{\gamma}_a = \frac{d}{dt} \left( -\frac{p_a}{p_0} \right) = -\gamma a \frac{\partial K}{\partial q_0} - \frac{\partial K}{\partial q^a}.$$

Hence we have derived Eq. (5). The claim on 1-forms is verified as follows. First, it follows that

$$\alpha^E - p_0 \lambda^E = (\alpha - H dt) - p_0 (\lambda + K dt).$$

Then substituting $H = -p_0 K$ into the equation above, one has

$$\alpha^E - p_0 \lambda^E = \alpha - p_0 \lambda.$$

The right hand side of the equation above vanishes due to $\alpha = p_0 \lambda$ as in the case of the autonomous symplectization. Hence $\alpha^E = p_0 \lambda^E$.

The relation between a non-autonomous contact Hamiltonian system and its symplectization is summarized as follows:

$$(\mathbb{R}^{2n+2} \times \mathcal{I}, \omega^E) \quad (q, p, t)$$

$\uparrow$ Ext. Symplectization $\uparrow$

$$(\mathbb{R}^{2n+1} \times \mathcal{I}, \ker \lambda^E) \quad (q, \gamma, t)$$

2.2 Zhang’s equation as contact and Hamiltonian systems

To design a high performance solver, Zhang et al. [2018] proposed the autonomous ODE based on NAG,

$$\ddot{x} + \Gamma_1(t; \sigma) \dot{x} + \Gamma_0(t; \sigma) \nabla f(x) = 0, \quad \sigma \geq 2,$$

where $x \in \mathbb{R}^d$, $\nabla = (\partial / \partial x^1, \ldots, \partial / \partial x^d)$, $\dot{x} = dx / dt \in \mathbb{R}^d$, $t \in \mathcal{I} := \mathbb{R}_{>0}$, $f$ a prescribed function on $\mathbb{R}^d$ as an objective,

$$\Gamma_0(t; \sigma) := \sigma^2 t^{\sigma - 2}, \quad \text{and} \quad \Gamma_1(t; \sigma) := \frac{2\sigma + 1}{t}.$$

In what follows, this time-domain $\mathcal{I} := \mathbb{R}_{>0}$ is kept fixed so that there is no singularity in $\mathcal{I}$. In this paper Eq. (5) is called Zhang’s equation.
Proposition 2.2. Zhang’s equation (6) is expressed as a non-autonomous contact Hamiltonian system.

Proof. This proof is a generalization of that found in [Bravetti et al. 2019]. Identify \( n = d \), \( x = (q^1, \ldots, q^d) \) so that \( q = (q^0, x) \in \mathbb{R}^{d+1} \), and choose the contact Hamiltonian on \( \mathbb{R}^{2d+1} \times I \) as

\[
K^Z(q^0, q^1, \ldots, q^d, \gamma_1, \ldots, \gamma_d; t) = \frac{1}{2} \sum_{a=1}^{d} \dot{\gamma}_a^2 + \Gamma_0 (t; \sigma) f(q^1, \ldots, q^d) + \Gamma_1 (t; \sigma) q^0.
\]

Then Eq. (5) yields

\[
\dot{q}^a = \gamma_a, \quad \dot{\gamma}_a = -\gamma_a \frac{\partial f}{\partial q^a} - \Gamma_1 \gamma_a, \quad a = 1, \ldots, d,
\]

from which one has

\[
\ddot{q}^a + \Gamma_1 \dot{q}^a + \Gamma_0 \frac{\partial f}{\partial q^a} = 0, \quad a = 1, \ldots, d. \tag{7}
\]

The extended contact manifold is \( (\mathbb{R}^{2d+1} \times I, \ker \lambda^{E,Z}) \) with \( \lambda^{E,Z} = \lambda + K^Z dt \) and \( \lambda = dq^0 - \sum_{a=1}^{d} \gamma_a dq^a \).

Note that the equation \( \dot{q}^0 = \cdots \) does not contribute to the proof of Proposition 2.2.

Then one has the theorem that forms the theoretical foundation for constructing symplectic integrators.

Theorem 2.1. Zhang’s equation (6) is expressed as a non-autonomous Hamiltonian system.

Proof. By combining Propositions 2.1 and 2.2, the statement is proven. \( \square \)

Notice that the details of \( \Gamma_0 \) and \( \Gamma_1 \) are not necessary for this proof. This leads to the following:

Corollary 2.1. ODEs including the cases where (i) \( \Gamma_0 = 1, \Gamma_1 = 3/t, \) [Su et al. 2016], and (ii) \( \Gamma_0 = \sigma^2 t^\sigma - 2, \Gamma_1 = (\sigma + 1)/t, \) [Wibisono et al. 2016], can be expressed as non-autonomous Hamiltonian systems.

The explicit form of the Hamiltonian stated in Theorem 2.1 is obtained by applying Proposition 2.1 to Proposition 2.2 as

\[
H^{ZZ}(q^0, q^1, \ldots, q^d, p_0, p_1, \ldots, p_d, t) = -p_0 \left[ \frac{1}{2} \sum_{a=1}^{d} \frac{p_a^2}{p_0^2} + \Gamma_0 f(q^1, \ldots, q^d) + \Gamma_1 q^0 \right]. \tag{8}
\]

This \( H^{ZZ} \) induces \( (\mathbb{R}^{2d+2} \times I, \omega^{E,ZZ}) \) with \( \omega^{E,ZZ} = d(p_0 \lambda^{E,Z}) \). The explicit forms of equations of motion are obtained from Eq. (4) and Eq. (8) as

\[
\dot{q}^0 = \frac{1}{2} \sum_{b=1}^{d} \frac{p_b^2}{p_0^2} - \Gamma_0 f - \Gamma_1 q^0, \quad \dot{p}_0 = \Gamma_1 p_0, \\
\dot{q}^a = -\frac{p_a}{p_0}, \quad \dot{p}_a = p_0 \Gamma_0 \frac{\partial f}{\partial q^a}, \quad a = 1, \ldots, d.
\]

The last three equations above yield Eq. (7).
Features of the system with $H^{ZZ}$ deriving Eq. (9) are in order. The equation $\dot{q}^0 = \cdots$ does not contribute to Zhang’s equation, and a solution to the equation $\dot{p}_0 = \cdots$ with the explicit form of $\Gamma_1(t;\sigma)$ is given by

$$p_0(t;\sigma) = p_0(1) t^{2\sigma+1}, \quad t \in \mathcal{I}. \tag{9}$$

Because the pair of variables $(q^0, p_0)$ in $H^{ZZ}$ is redundant for deriving Eq. (9), a reduced Hamiltonian system is desired. Moreover, the use of the analytical expression (9) is expected to enhance accuracy of integrators.

To derive a reduced system that incorporates the analytical expression, the following will be applied to $H^{ZZ}$.

**Proposition 2.3.** Let $\bar{H}$ be a non-autonomous Hamiltonian on $\mathbb{R}^{2d} \times \mathcal{I}$, and $\Gamma$ a function of $t \in \mathcal{I}$. Moreover, let $H_1$ be a non-autonomous Hamiltonians defined on $\mathbb{R}^{2d+2} \times \mathcal{I}$, and $H_2$ a non-autonomous Hamiltonian on $\mathbb{R}^{2d} \times \mathcal{I}$ such that

$$H_1(q^0, \ldots, q^d, p_0, \ldots, p_d, t) = -p_0 \left[ \bar{H}(q_1, \ldots, q_d, p_1, \ldots, p_d, t) + \Gamma(t) q^0 \right],$$

$$H_2(q^1, \ldots, q^d, p_1, \ldots, p_d, t) = -p_0^{\text{sol}}(t) \bar{H}(q_1, \ldots, q_d, p_1, \ldots, p_d, t)$$

with $p_0^{\text{sol}}(t)$ an explicit solution to $p_0 = \Gamma(t) p_0$.

Then the equations of motion for $q^1, \ldots, q^d$ and $p_1, \ldots, p_d$ obtained by $H_1$ are also obtained by $H_2$. In addition, extended manifolds $(\mathbb{R}^{2d+2}, \omega^{E,1})$ and $(\mathbb{R}^{2d+1}, \omega^{E,2})$ are defined for the systems with $H_1$ and $H_2$.

**Proof.** The canonical equations of motion derived from $H_1$ are

$$\dot{q}^0 = -\bar{H} - \Gamma(t) q^0, \quad \dot{p}_0 = \Gamma(t) p_0,$$

$$\dot{q}^a = -p_0^{\text{sol}} \frac{\partial \bar{H}}{\partial p_a}, \quad \dot{p}_a = p_0^{\text{sol}} \frac{\partial \bar{H}}{\partial q^a}, \quad a = 1, \ldots, d.$$  

Similarly the equations of motion from $H_2$ are

$$\dot{q}^a = -p_0^{\text{sol}}(t) \frac{\partial \bar{H}}{\partial p_a}, \quad \dot{p}_a = p_0^{\text{sol}}(t) \frac{\partial \bar{H}}{\partial q^a}, \quad a = 1, \ldots, d.$$  

Comparing the derived equations from $H_1$ with those from $H_2$, one completes the first part of the proof. Then, the extended symplectic form for the system with $H_2$ is introduced by $\omega^{E,2} = d\alpha^{E,2}$, where $\alpha^{E,2} = \sum_{a=1}^{d} p_a dq^a - H_2 dt$. Similarly one can define $\omega^{E,1}$ for the system with $H_1$. \hfill \Box

With Proposition 2.3, a desired reduced Hamiltonian system for Zhang’s equation is explicitly obtained.

**Proposition 2.4.** Let $H_K^Z$, $H_V^Z$ and $H^Z$ be Hamiltonians on $\mathbb{R}^{2d} \times \mathcal{I}$ such that $H^Z = H_K^Z + H_V^Z$ with

$$H_K^Z(p_1, \ldots, p_d, t) = -\frac{1}{2p_0(t;\sigma)} \sum_{a=1}^{d} p_a^2,$$

$$H_V^Z(q^1, \ldots, q^d, t) = -p_0(t;\sigma) \Gamma_0(t;\sigma) f(q^1, \ldots, q^d).$$
Then the Hamiltonian $H^Z$ on $\mathbb{R}^{2d} \times \mathcal{I}$ yields Eq. (7), where $p_0(t; \sigma)$ has been given by Eq. (9). Moreover the corresponding extended symplectic manifold is $(\mathbb{R}^{2d} \times \mathcal{I}, \omega^{E,Z})$, where $\omega^{E,Z} = d\alpha^{E,Z}$ with $\alpha^{E,Z} = \sum_{a=1}^{d} p_a dq^a - H^Z dt$.

**Proof.** Applying Proposition 2.3 to Eq. (8), one completes the proof.

The relations among introduced systems are briefly summarized as

\[
\begin{array}{c}
K^Z \xrightarrow{\text{Prop. 2.1}} H^{ZZ} \\
\xrightarrow{\text{Prop. 2.2}} \xrightarrow{\text{Thm. 2.1}} \xrightarrow{\text{Prop. 2.3}} \\
\text{Zhang's Eq.} \xrightarrow{\text{Prop. 2.4}} H^Z \\
\end{array}
\]

where $A \xrightarrow{C} B$ indicates that $A$ induces $B$ with $C$.

Features of the system with $H^Z = H^Z_K + H^Z_V$ deriving Eq. (7) are in order. The redundant variable $q^0$ in $H^{ZZ}$ does not appear in $H^Z$, and the analytical solution $p_0(t)$ is incorporated in $H^Z$. In addition, although the whole system $H^Z$ could be non-integrable, an analytical solution can be derived for each system solely with $H^Z_K$ and that with $H^Z_V$ (see Sections D.1 and D.2 in the appendix). Unlike this case, there is no such a property for the system with $H^{ZZ}$. As will be discussed in the next section, these explicit solutions are beneficial in constructing integrators. Hence $H^Z$, rather than $H^{ZZ}$, is focused in the following sections.

### 3 Symplectic integrators for Zhang’s equation

In this section, the basic properties of symplectic integrators for the system with $H^Z$ are shown, and then corresponding integrators are constructed explicitly.

#### 3.1 Basic properties of integrators

A distinctive performance indicator of a numerical solver for optimization problems is the convergence rate for a given class of objectives. In [Zhang et al., 2018], the convergence rate for Eq. (6) with $\sigma \geq 2$ was derived as

\[
|f(x(t)) - f(x^*)| \leq O(t^{-\sigma}),
\]

where $x^*$ is the minimizer for a convex objective $f$. In addition a discretization error was taken into account for the $s$-th order Runge-Kutta integrator with a carefully chosen step size, so that the right hand side of Eq. (10) was replaced with $O(N^{-\sigma s/(s+1)})$, where $N$ is the total number of iterations. The rate (10) is realized with a higher-order integrator, and can also be applied to the system with $H^Z$ on $\mathbb{R}^{2d} \times \mathcal{I}$. This yields the following.

**Proposition 3.1.** The convergence rate for the non-autonomous Hamiltonian system in Proposition 2.4 is given by Eq. (10). Moreover this rate is obtained in the higher order limit of integrators.

Symplectic integrators are numerical integrators for Hamiltonian systems with the property that symplectic forms are preserved [Kinoshita et al., 1990]. These integrators are known to be stable, and error is not significantly accumulated. Although symplectic integrators are mostly...
Let an Euclidean setting be given. Symplectic integrators should be constructed for the system with Hamiltonian $H$. Unlike this, the system with $H$ solely is realized. Consider the case where explicit symplectic integrators are realized. Note that $H$ itself needs not be integrable.

The Hamiltonian $H^Z$ in Proposition 2.4 satisfies the condition that explicit symplectic integrators are realized. Unlike this, the system with $H^{ZZ}$ does not satisfy this condition, hence explicit symplectic integrators should be constructed for the system with $H^Z$.

Before closing this subsection, the definition of non-autonomous symplectic integrator in Euclidean setting is given.

**Definition 3.1.** Let $(\mathbb{R}^{2n+2}, \omega)$ be a symplectic manifold, $H$ a Hamiltonian on $\mathbb{R}^{2n+2} \times \mathcal{I}$, and $(\mathbb{R}^{2n+2} \times \mathcal{I}, \omega^E)$ the extended symplectic manifold with $\mathcal{I} \subseteq \mathbb{R}$ and $\omega^E$ being given by Eq. (3). In addition, let $z(t)$ be a point on $\mathbb{R}^{2n+2}$, and $z^E(t)$ a point on $\mathbb{R}^{2n+2} \times \mathcal{I}$ such that $z^E(t) = (z(t), t) = (q(t), p(t), t) \in \mathbb{R}^{2n+2} \times \mathcal{I}$ expresses an exact solution to the system with $H$ at $t \in \mathcal{I}$, and $z(s)(t)$ an approximate solution at $t$ labeled by some $s = 1, 2, \ldots$. If the two conditions, 1. an error between $z(t + \tau)$ and $z^s(t + \tau)$ appears in a $\sigma$-term in the Taylor expansion for $|\tau| \ll 1$ provided that $z(t) = z^s(t)$, and 2. $\omega|_{t+\tau} = \omega|_{t}$, are satisfied, then a discrete time-evolution algorithm is called an $s$-th order (non-autonomous) symplectic integrator.

### 3.2 Explicit representation of integrators

The Hamiltonian $H^Z$ can be split into the two pieces as stated in Proposition 2.4, and the solution to each piece can analytically be obtained (see Sections D.1 and D.2 in the appendix). This yields exact relations between 2 points on $\mathbb{R}^{2d} \times \mathcal{I}$ as follows.

**Lemma 3.1.** The non-autonomous Hamiltonian system solely with $H^Z_K$ and that solely by $H^Z_V$ satisfy the relations

\[
H^Z_K : \begin{cases} 
q^a(t + \tau) = q^a(t) + \frac{p_a(t)}{2\sigma p_0(1)} \left[ \left( \frac{1}{(t+\tau)^2} \right)^{2\sigma} - \frac{1}{t^{2\sigma}} \right], & p_a(t + \tau) = p_a(t), \\
\end{cases}
\]

and

\[
H^Z_V : \begin{cases} 
q^a(t + \tau) = q^a(t), \\
p_a(t + \tau) = p_a(t) + \frac{\sigma p_0(1)}{3} \left[ (t + \tau)^3 - t^3 \right] \frac{\partial f}{\partial q_a}(t), 
\end{cases}
\]

where $a = 1, \ldots, d$, and $\tau > 0$ is constant.

**Proof.** To verify the relations for $H^Z_K$, integrate

\[
\dot{q}^a = \frac{\partial H^Z_K}{\partial p_a} = -\frac{p_a}{p_0(t; \sigma)}, \quad \text{and} \quad \dot{p}_a = -\frac{\partial H^Z_K}{\partial q_a} = 0.
\]
where \( a = 1, \ldots, d \), over time from \( t \) to \( t + \tau \). This yields Eq. (11). Moreover, for \( H^Z \), integrate

\[
\dot{q}^a = \frac{\partial H^Z}{\partial p_a} = 0, \quad \text{and} \quad \dot{p}_a = -\frac{\partial H^Z}{\partial q_a} = p_0(t; \sigma) \Gamma_0(t; \sigma) \frac{\partial f}{\partial q^a},
\]

where \( a = 1, \ldots, d \). This yields Eq. (12). See D.1 and D.2 of the appendix for full derivations.

From Proposition 2.4 and an existing literature [Suzuki, 1993, Bravetti et al., 2020], one has the following:

**Theorem 3.1.** The concatenations \( \tilde{\Phi}_{H^Z,\tau}^1 \) and \( \tilde{\Phi}_{H^Z,\tau}^2 \) defined below are 1st and 2nd order symplectic integrators for Eq. (7):

\[
\tilde{\Phi}_{H^Z,\tau}^1 : z(t + \tau) = \Phi_{X_{t,\tau/2}} \circ \Phi_{H^Z_{\tau/2}} \circ \Phi_{H^Z_{\tau/2}} \circ \Phi_{X_{t,\tau/2}} z(t),
\]

\[
\tilde{\Phi}_{H^Z,\tau}^2 : z(t + \tau) = \Phi_{X_{t,\tau/2}} \circ \Phi_{H^Z_{\tau/2}} \circ \Phi_{H^Z_{\tau/2}} \circ \Phi_{X_{t,\tau/2}} z(t),
\]

where \( \Phi_{X_{t,\tau}} \) is the time-shift transform \( t \mapsto t + \tau \), \( \Phi_{H^Z_{\tau/2}} \) and \( \Phi_{H^Z_{\tau/2}} \) are the transforms \( z(t) \mapsto z(t + \tau) \) by Eqs. (12) and (11), respectively.

**Proof.** These integrators are obtained from Lemma 3.1 via the splitting method in [Suzuki, 1993].

A higher order integrator requires more gradient evaluations of \( f \), and its computational load is high in general. For \( \tilde{\Phi}_{H^Z,\tau}^2 \), it requires 1 for each iteration, and is focused below.

An explicit representation of the symplectic integrator for \( H^Z \) is as follows.

For the 2nd order integrator \( \tilde{\Phi}_{H^Z,\tau}^2 \), the following transforms are concatenated:

\[
\Phi_{X_{t,\tau/2}} \left( \begin{array}{c} q^a \\ p_a \\ t \end{array} \right) = \left( \begin{array}{c} q^a \\ p_a \\ t + \frac{\tau}{2} \end{array} \right),
\]

\[
\Phi_{H^Z_{\tau/2}} \left( \begin{array}{c} q^a \\ p_a \\ t \end{array} \right) = \left( \begin{array}{c} q^a \\ p_a \\ t \end{array} \right),
\]

\[
\Phi_{H^Z_{\tau/2}} \left( \begin{array}{c} q^a \\ p_a \\ t \end{array} \right) = \left( \begin{array}{c} q^a \\ p_a \\ t \end{array} \right),
\]

where \( a = 1, \ldots, d \), and

\[
q_*^a = q^a + \frac{p_a}{2 \sigma p_0(1)} \left[ (t + \tau/2)^{-2\sigma} - t^{-2\sigma} \right],
\]

\[
p_*^a = p_a + \frac{\sigma p_0(1)}{3} \left[ (t + \tau)^{3\sigma} - t^{3\sigma} \right] (\nabla f)_a.
\]
Table 1: Computational time (msec) of various methods, averages and SD of 10 trials from different random initialization.

| Data set     | RK2        | RK4        | SI2        | SI2(bt)     | NAG(bt)     |
|--------------|------------|------------|------------|-------------|-------------|
| BreastCancer | 14.51 ± 5.15 | 23.56 ± 7.89 | 10.85 ± 5.76 | 10.34 ± 22.658 | 20.41 ± 19.57 |
| Diabetes     | 5.96 ± 4.68  | 7.7 ± 4.2   | 6.17 ± 5.75 | 8.24 ± 27.33  | 14.77 ± 20.6  |
| HouseVotes   | 6.96 ± 4.67  | 6.9 ± 0.49  | 5.9 ± 4.96  | 11.49 ± 26.84 | 9.86 ± 20.369 |
| Sonar        | 22.9 ± 6.05  | 38.29 ± 7.21 | 15.97 ± 6.1 | 12.34 ± 25.77 | 37.05 ± 26.27 |
| MNIST        | 7430.42 ± 177.6 | 12886.94 ± 147.01 | 4717.85 ± 174.83 | 981.44 ± 248.15 | 6182.98 ± 89.43 |

Note that higher-order symplectic integrators for this system can systematically be obtained with the method in [Suzuki, 1993, Hatano and Suzuki, 2005].

As mentioned in [Zhang et al., 2018, Betancourt et al., 2018], symplectic integrators are known to be stable. In addition, as shown in Proposition 2.4, Zhang’s equation can be written as a non-autonomous Hamiltonian system. Hence, by combing these, the proposed symplectic integrators are expected to be stable.

4 Numerical experiments

In this section the performance of the proposed 2nd order symplectic integrator (SI2) is compared with that of the following existing methods

1. the s-th order Runge-Kutta (RK) methods for Zhang’s equation, where \( s = 2, 4 \) [Griffiths and Higham, 2010];
2. the NAG method, described by

\[
\begin{align*}
x^{(k)} &= y^{(k-1)} - s_N \nabla f(y^{(k-1)}), \\
y^{(k)} &= x^{(k)} + \frac{k-1}{k+2}(x^{(k)} - x^{(k-1)}),
\end{align*}
\]

where \( s_N > 0 \) is a step size parameter, \( x^{(k)} \) and \( y^{(k)} \) denote \( x \in \mathbb{R}^d \) and \( y \in \mathbb{R}^d \) at discrete step \( k \geq 0 \), respectively.

We consider two-class classification problems by the regularized logistic regression of the form

\[
f(x) = \frac{1}{|D|} \sum_{i \in D} \ell_i(x) + \lambda_{\text{reg}} \|x\|_2^2,
\]

where \( D \) is the training dataset, \( \ell_i(x) \) is a logistic loss function for parameter \( x \) given the i-th datum in \( D \) (pair of observed input and output), \( \|x\|_2^2 := x_1^2 + \cdots + x_d^2 \), and \( \lambda_{\text{reg}} \) is kept fixed with \( 10^{-8} \) throughout for simplicity. To this end, the four popular datasets (breastcancer, diabetes, housevotes, sonar) are chosen from UCI machine learning repository, and MNIST dataset where the problem is discriminating even and odd numbers. Because SI2, RK2 and RK4 are derived from the same ODE, the convergence behavior and computational cost are focused and classification accuracy is not discussed. Accuracies of the classifier obtained by SI2 and NAG were almost the same.

\(^1\text{All of the experiments are conducted with MacBook Pro with 2.4Ghz 8-core Intel Core i9 and 64GB RAM. Source code to reproduce the experimental results is available from https://github.com/hideitsu/Contact_SymplecticIntegrator}\)
4.1 Comparison to Runge-Kutta methods

We first compare the performance of RK2/4 and SI2 with different parameter values $\sigma$ in the original ODE (6), which controls the convergence speed. Theoretically, by increasing the value of $\sigma$ in the continuous-time limit, faster convergence rates should be achieved. In reality, partly due to discretization errors, too large $\sigma$ may cause numerical instability. We fixed the learning rate $\tau = 0.01$ for all of the three methods, and report the convergence behaviors of objective functions for MNIST dataset in Fig. 1. Figures for other datasets are shown in the appendix. From Fig. 1, it is verified that in general, with larger $\sigma$, the convergence speed is high. However, RK2 often exhibits instability, particularly for MNIST dataset, while SI2 and RK4 are relatively stable. This instability is partly due to the fact that RK2 is derived based on the lower order Taylor expansion and it is more deviated from the continuous-time system compared to RK4.

Now we compare the computational speed of the three methods. Table 1 shows the average of the computational time to reach the stopping criterion (relative difference of the objective function value is less than $10^{-6}$) for RK2, RK4, SI2, and SI2 with backtracking and NAG with backtracking for adjusting step size (see next subsection). It is seen that the speed with SI2 is slightly faster than that with RK2 or on par for the first four datasets, and faster than that with RK4. For MNIST, which is the largest size dataset among five datasets, the speed with SI2 is significantly faster than those with the other two methods. This faster computational time of SI2 is due to the fact that one step computation of SI2 requires only one gradient evaluation, while RK2 and RK4 require two and four-times gradient evaluations, respectively.

4.2 Comparison to NAG method

We then compare SI2 to NAG. From the results of the previous experiment, we see that for SI2, $\sigma$ less than 8.0 offers stable results. In this section, the convergence rate parameter $\sigma$ is fixed to 6.0. For both SI2 and NAG, step size remains to be a tuning parameter. We adopt the backtracking method for automatically adjusting the step size in each iteration. In addition, we implemented the momentum restarting mechanism to NAG for stabilizing the performance.

From Table 1, column SI2(BT) and NAG(BT), it is seen that computational time of SI2 with backtracking is significantly faster than NAG, particularly for MNIST dataset.

The results of these experiments show that the SI2 is a stable integrator with a high convergence rate.
5 Conclusion

This paper has shown that the symplectization of a contact manifold can be used for constructing non-autonomous symplectic integrators when ODEs are written as non-autonomous contact Hamiltonian systems. In particular, for Zhang’s equation [Zhang et al., 2018], which belongs to a class of continuous-time accelerated gradient methods, explicit non-autonomous symplectic integrators have been constructed. Because the proposed symplectic integrators preserve hidden geometric structures in Zhang’s equation, this should improve performance. The resultant 2nd order integrator for Zhang’s equation was then shown to be as stable as the 4-th order Runge-Kutta method, while the convergence rate was unchanged. The reason why such explicit integrators can successfully be obtained is that the split Hamiltonians yield integrable systems. However, a profound connection between this integrability and Zhang’s equation is not yet apparent. Because Zhang’s equation is not only a Hamiltonian system but also a contact Hamiltonian system, the benefits obtained from its contact integrators should also be explored. By addressing these questions, we believe that faster and more stable algorithms will be realized. In a practical aspect, in experiments on logistic regression using real-world datasets, the convergence speed of the proposed SI2 with larger $\sigma$ has been shown to be faster than that of NAG. It would be important to automatically determine an appropriate value of the convergence rate parameter $\sigma$ for the objective function and the given dataset, which is left to future research. In addition, the estimate of the existing theoretical convergence rate without the backtracking method should be extended for the case where the backtracking method is applied.

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A Geometric description of non-autonomous ODEs

To describe the geometric nature of continuous-time dynamical systems expressed as ODEs, some known facts about contact and symplectic geometries are summarized [Libermann and Marle, 1987, der Schaft and Maschke, 2018, Bravetti et al., 2017]. These descriptions are used to reveal the nature of ODEs. Every geometric object is assumed smooth and real throughout.

A.1 Autonomous systems

A symplectic manifold is a pair consisting of an even dimensional manifold and a closed non-degenerate 2-form. Roughly speaking, this manifold is a generalization of a phase space for an autonomous Hamiltonian system. Then contact manifolds are roughly speaking odd-dimensional counterparts of symplectic manifolds. Let $n$ be an integer with $n \geq 1$. A $(2n + 1)$-dimensional contact manifold is a pair consisting of a $(2n + 1)$-dimensional manifold $C$ and a contact structure $A$ defined below. First, a 1-form $\lambda$ on $C$ is called a contact form if the $(2n + 1)$-form $\lambda \wedge d\lambda \wedge \cdots \wedge d\lambda$ does not vanish, where $d$ denotes the exterior derivative, and $\wedge$ the exterior or wedge product. Then a contact structure on $C$ is a $2n$-dimensional subspace $A \subset T C$ such that $A = \ker \lambda := \{X \in$
TC\mid \lambda(X) = 0\}, where TC denotes the tangent bundle of C, \lambda(X) the (duality) pairing between \lambda and X, giving a real number. As shown bellow, typical symplectic and contact manifolds are constructed from bundles.

Let Q be an (n + 1)-dimensional manifold, q its coordinates with \( q = (q^0, \ldots, q^n) \), and \( T^*Q \) its cotangent bundle. A point on \( T^*Q \) is expressed as \((q, p)\) in coordinates with \( p = (p^0, \ldots, p_n) \). Let \( \mathbb{P}(T^*Q) \) be the projective cotangent bundle, which is briefly outlined below. The manifold \( \mathbb{P}(T^*Q) \) is the fiber bundle whose base space is \( Q \), and whose fiber at \( q \in Q \) is the projective space, \( \mathbb{P}(T^*_q Q) := (T^*_q Q \setminus \{0\})/\sim \). Here this \( \sim \) is an equivalence relation, and is given as follows. If two points \( p \) and \( p' \) on \( T^*_q Q \) are related by \( p' = \zeta p \) with some \( \zeta \in \mathbb{R} \setminus \{0\} \), then we write \( p' \sim p \). In a neighborhood where \( p_0 \neq 0 \), the set \( \gamma = (\gamma_1, \ldots, \gamma_n) \) with

\[
\gamma_a = -\frac{p_a}{p_0}, \quad a = 1, \ldots, n,
\]

(13)
can be used as a coordinate set. In other neighborhoods similar coordinates can be found. Then a \((2n+1)\)-dimensional manifold \( \mathbb{P}(T^*Q) \) is expressed as \((q, \gamma)\) in coordinates, and \( \pi : T^*Q \to \mathbb{P}(T^*Q) \) denotes a projection, \((q, p) \mapsto (q, \gamma)\).

It is known that \( T^*Q \) induces a \((2n + 2)\)-dimensional symplectic manifold \((T^*Q, \omega)\), where \( \omega = dq \) is a symplectic 2-form with \( \alpha \) being a Liouville 1-form. In addition, \( \mathbb{P}(T^*Q) \) induces a \((2n + 1)\)-dimensional contact manifold \((\mathbb{P}(T^*Q), \ker \lambda)\). According to Darboux’s theorem [Arnold 1989], there exist coordinates \( p = (p_0, \ldots, p_n) \) for \( T^*_q Q \) and \( \gamma = (\gamma_1, \ldots, \gamma_n) \) for \( \mathbb{P}(T^*_q Q) \) such that

\[
\alpha = p_0 dq^0 + \sum_{a=1}^n p_a dq^a, \quad \text{and} \quad \lambda = dq^0 - \sum_{a=1}^n \gamma_a dq^a,
\]
in a neighborhood where \( p_0 \neq 0 \) in \( T^*_q Q \). Then, it follows immediately from \( \omega = d\alpha \) that

\[
\omega = \sum_{a=0}^{n} dp_a \wedge dq^a,
\]

and it is verified that

\[
\ker \lambda = \text{span} \left( \Gamma_1, \ldots, \Gamma_n, \Gamma^1, \ldots, \Gamma^n \right),
\]

\[
\Gamma_a := \gamma_a \frac{\partial}{\partial q^0} + \frac{\partial}{\partial q^a}, \quad \Gamma^a := \frac{\partial}{\partial \gamma_a}
\]

and \( \alpha = p_0(\pi^*\lambda) \), where \( \pi^* \) is the pull-back induced by \( \pi \) (pull-backs and push-forwards are explained in Section B.2). A symplectic vector field is a vector field if it preserves a symplectic 2-form. Then, the Hamiltonian vector field \( X_H \) associated with a Hamiltonian \( H \) is a unique vector field satisfying \( \iota_{X_H} \omega = -dH \), where \( \iota_X \) denotes the interior product with a vector field \( X \) acting on forms. In contrast, contact vector field is a vector field if it preserves contact structure, \( \ker \lambda \). Then, the contact Hamiltonian vector field associated with a function \( K \) called contact Hamiltonian, denoted by \( X_K \), is a unique vector field satisfying both

\[
\mathcal{L}_{X_K} \lambda = g \lambda, \quad \text{and} \quad K = -\iota_{X_K} \lambda,
\]

where \( g \) is some function and \( \mathcal{L}_X \) denotes the Lie derivative along a vector field \( X \). Note that there are several conventions of signs in the literature.
The following diagram shows how the introduced manifolds and their vector fields are related:

\[ T(T^*Q) \xrightarrow{\pi^*} T(P(T^*Q)), \]

\[ T^*Q \xrightarrow{\pi} P(T^*Q), \]

where \( \pi^* \) is the push-forward induced by \( \pi \) sending \( X_H \in T(T^*Q) \) to \( X_K \in T(P(T^*Q)) \). Although the relation between \( X_H \) and \( X_K \) via \( \pi^* \) is not used in this paper, its non-autonomous analogue is used.

A.2 Non-autonomous systems

To describe time-dependent Hamiltonian and contact Hamiltonian vector fields, define first \( S^E = T^*Q \times I \) and \( C^E = P(T^*Q) \times I \), where the coordinate for \( I \subseteq \mathbb{R} \) expresses time \( t \). The manifold \( S^E \) is referred to as an extended phase space in the context of analytical mechanics [Hand and Finch 1998], and \( S^E \) together with a symplectic form is referred to as an extended symplectic manifold in this paper. Then \( C^E \) together with a contact structure is referred to as an extended contact manifold in this paper. Similar to the case of analytical mechanics, the so-called (time-dependent) Hamiltonian \( H \) can be defined as a function on \( S^E \). Likewise, (time-dependent) contact Hamiltonian \( K \) can be defined on \( C^E \). Next, given \( H \) and \( K \), 1-forms on \( S^E \) and \( C^E \) are defined as

\[ \alpha^E = \alpha - H dt, \quad \text{and} \quad \lambda^E = \lambda + K dt, \]

where \( \alpha^E \) is known as the Poincaré-Cartan form. It is known that non-autonomous Hamiltonian vector field \( X_H^E \) is defined as the one satisfying the condition

\[ \iota_{X_H^E} d\alpha^E = 0, \]

so that \( \mathcal{L}_{X_H^E} \omega^E = 0 \) with \( \omega^E := d\alpha^E \). This condition and the choice \( X_H^E = X_H + \partial / \partial t \) with \( dt(X_H) = 0 \) give

\[ \iota_{X_H^E} \omega = -d_{T^*Q} H, \quad \text{and} \quad X_H H = 0, \]

where

\[ d_{T^*Q} H := dH - \frac{\partial H}{\partial t} dt. \]

In Darboux coordinates, \( X_H^E \) is expressed as

\[ X_H^E = \sum_{a=0}^{n} \left[ \dot{q}^a \frac{\partial}{\partial q^a} + \dot{p}_a \frac{\partial}{\partial p_a} \right] + \frac{\partial}{\partial t}, \quad (14) \]

where \( \dot{q}^a \) and \( \dot{p}_a \) are given by

\[ \dot{q}^a = \frac{\partial H}{\partial p_a}, \quad \text{and} \quad \dot{p}_a = -\frac{\partial H}{\partial p_a}, \quad a = 0, 1, \ldots, n. \quad (15) \]

A full derivation of Eq. [15] is given in Section C.1. By identifying \( \dot{} = d/dt \), these equations are well-known canonical equations of motion. One way to define a vector field extended from an
autonomous contact vector field is as follows [Bravetti et al., 2017]. The non-autonomous contact vector field, denoted by $X^E_K$, is defined as the one satisfying both

$$\mathcal{L}_{X^E_K} \lambda^E = g^E \lambda^E,$$

and

$$K = -i_{X^E_K} \lambda,$$

where $g^E$ is some function. Notice that although the pair $(\mathcal{C}^E, d\lambda^E)$ becomes a symplectic manifold, the vector field $X^E_K$ does not preserve the symplectic structure $d\lambda^E$, in the sense that $\mathcal{L}_{X^E_K} d\lambda^E \neq 0$.

In Darboux coordinates, $X^E_K$ is expressed as

$$X^E_K = \dot{q}^0 \frac{\partial}{\partial q^0} + \sum_{a=1}^n \left( \dot{q}^a \frac{\partial}{\partial q^a} + \dot{\gamma}_a \frac{\partial}{\partial \gamma_a} \right) + \frac{\partial}{\partial t},$$

where we have chosen the scale factor for $t$ to be unity and

$$\dot{q}^0 = -K + \sum_{a=1}^n \gamma_a \frac{\partial K}{\partial \gamma_a}, \quad \dot{q}^a = \frac{\partial K}{\partial q^a}, \quad (16a)$$

$$\dot{\gamma}_a = -\frac{\partial K}{\partial q^a} - \gamma_a \frac{\partial K}{\partial q^0}, \quad a = 1, \ldots, n. \quad (16b)$$

A full derivation of Eq. $(16)$ is given in Section C.2.

A way to bridge a contact Hamiltonian vector field on $\mathbb{P}(T^*Q)$ and a Hamiltonian vector field on $T^*Q$ is known [Libermann and Marle, 1987, der Schaft and Maschke, 2018]. By extending this existing method, the following holds.

**Proposition A.1.** A non-autonomous contact Hamiltonian vector field $X^E_K$ associated with $K$ on $\mathbb{P}(T^*Q) \times \mathcal{I}$ is lifted to $X^E_H$ associated with an appropriate $H$ on $T^*Q \times \mathcal{I}$, that is, $\pi^E_* X^E_K = X^E_H$, with $\pi^E_*$ being the push-forward induced by $\pi^E : T^*Q \times \mathcal{I} \rightarrow \mathbb{P}(T^*Q) \times \mathcal{I}$.

**Proof.** In a neighborhood where $p_0 \neq 0$, choose $H$ to be

$$H(q^0, q^1, \ldots, q^n, p_0, p_1, \ldots, p_n, t) = -p_0 K(q^0, q^1, \ldots, q^n, \gamma_1, \ldots, \gamma_n, t), \quad \gamma_a = -\frac{p_a}{p_0},$$

where $p$ is determined by Eq. $(13)$. Then Eq. $(14)$ and Eq. $(15)$ yield Eq. $(16)$. This is verified as

$$\dot{p}_0 = -\frac{\partial H}{\partial q^0} = p_0 \frac{\partial K}{\partial q^0}, \quad \dot{q}^0 = \frac{\partial H}{\partial p_0} = -K + \sum_{a=1}^n \gamma_a \frac{\partial K}{\partial \gamma_a},$$

and

$$\dot{p}_a = -\frac{\partial H}{\partial q^a} = p_0 \frac{\partial K}{\partial q^a}, \quad \dot{q}^a = \frac{\partial H}{\partial p_a} = \frac{\partial K}{\partial q^a}, \quad a = 1, \ldots, n$$

from which

$$\dot{\gamma}_a = \frac{d}{dt} \left( -\frac{p_a}{p_0} \right) = -\gamma_a \frac{\partial K}{\partial q^0} - \frac{\partial K}{\partial q^a}, \quad a = 1, \ldots, n.$$

It can also be proven for other neighborhoods.
In this paper a resultant (non-autonomous) Hamiltonian vector field obtained by the procedure in Proposition A.1 is called a symplectization of a (non-autonomous) contact Hamiltonian vector field. Here, roughly speaking, symplectization is a procedure for obtaining a symplectic manifold from a lower-dimensional contact manifold. In this paper, extended symplectization is the procedure for obtaining an extended symplectic manifold from a lower-dimensional extended contact manifold, which is accomplished by $\omega^E = d\alpha^E$ with $\alpha^E = p_0(\pi^E \ast \lambda^E)$. The following diagrams show the relations among the introduced manifolds:

\[
\begin{array}{c}
T(T^*Q \times I) \xrightarrow{\pi^E} T(P(T^*Q) \times I), \\
T^*Q \times I \xrightarrow{\pi^E} P(T^*Q) \times I
\end{array}
\]

which in coordinates,

\[
(q, p, t, \dot{q}, \dot{p}, \dot{t}) \mapsto (q, \gamma, t, \dot{q}, \dot{\gamma}, 1).
\]

The symplectization for autonomous systems and extended symplectizations for non-autonomous systems are summarized as

\[
\begin{array}{c}
(T^*Q, \omega) \xrightarrow{\text{Symplectization}} (T^*Q \times I, \omega^E), \\
(P(T^*Q), \ker \lambda) \xrightarrow{\text{Ext. symplectization}} (P(T^*Q) \times I, \ker \lambda^E).
\end{array}
\]

**B Brief summary of tools in differential geometry**

The natural mathematical language for discussing objects on manifolds is in terms of differential forms and their associated objects, because these terms reveal properties that do not depend on any particular coordinate system. This language is suitable for describing Hamiltonian systems and contact Hamiltonian systems, and is hence used in this paper. In this section some of tools used in this paper are summarized.

**B.1 Vector fields and differential forms**

At a point $p$ of a differentiable $m$-dimensional manifold $\mathcal{M}$, a vector space is denoted $T_p\mathcal{M}$. It follows that $\dim(T_p\mathcal{M}) = m$. Let $x = (x^1, \ldots, x^m)$ be a coordinate set for $\mathcal{M}$, then the natural basis

\[
\left\{ \frac{\partial}{\partial x^1}, \ldots, \frac{\partial}{\partial x^m} \right\}
\]

spans $T_p\mathcal{M}$. At a point $p \in \mathcal{M}$, the sum $X = \sum_{a=1}^m X^a(p)\partial/\partial x^a$ is an element of $T_p\mathcal{M}$, where $\{X^a\}_{a=1}^m$ is a set of functions. Points on $\mathcal{M}$ are often denoted in terms of their coordinates, so that

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2We refer the reader to related textbooks, for example, (i) Mikio Nakahara. *Geometry, Topology and Physics; 2nd ed.* CRC Press 2003, (ii) Shoshichi Kobayashi and Katsumi Nomizu. *Foundations of Differential Geometry; Vol. 1* Interscience Publishers, 1963, for further details.
\[ X = \sum_{a=1}^{m} X^a(x) \partial/\partial x^a. \] The set \( T\mathcal{M} := \bigcup_{p \in \mathcal{M}} T_p\mathcal{M} \) is called a tangent bundle, and it follows that \( \dim T\mathcal{M} = 2m \).

Next, the dual of \( T_p\mathcal{M} \) defined at \( p \in \mathcal{M} \) is denoted \( T^*_p\mathcal{M} \). By definition, an element \( \alpha \in T^*_p\mathcal{M} \) sends a vector \( X \in T_p\mathcal{M} \) to a real number \( \mathbb{R} \):

\[ T^*_p\mathcal{M} : T_p\mathcal{M} \to \mathbb{R}, \quad \alpha : X \mapsto \alpha(X), \]

where \( \alpha(X) \in \mathbb{R} \) is called a pairing between \( \alpha \) and \( X \). Pairing is written in some textbooks as

\[ \langle \alpha, X \rangle : T^*_p\mathcal{M} \times T_p\mathcal{M} \ni (\alpha, X) \mapsto \langle \alpha, X \rangle := \alpha(X) \in \mathbb{R}. \]

By the definition of dual space, the sum of two elements \( \alpha, \beta \in T^*_p\mathcal{M} \), denoted by \( \alpha + \beta \), and scalar multiplication \( c\alpha \) are equipped on \( T^*_p\mathcal{M} \) so that

\[ (\alpha + \beta)(X) = \alpha(X) + \beta(X), \quad (c\alpha)(X) = c[\alpha(X)], \]

where \( X \in T_p\mathcal{M} \), \( c \in \mathbb{R} \). Then the set \( T^*\mathcal{M} := \bigcup_{p \in \mathcal{M}} T^*_p\mathcal{M} \) is called a cotangent bundle. An element of \( T^*\mathcal{M} \) is called a 1-form, and one typical example is \( df \in T^*_p\mathcal{M} \) where \( f \) is a function on \( \mathcal{M} \). This \( d \) is a map that sends a function to a 1-form so that

\[ (df)(X) = Xf, \quad (Xf)(p) = X_p f, \quad p \in \mathcal{M}. \]

where a vector field \( X \) can act on a function \( f \) and \( Xf \) is another function. This operator \( d \) will be extended to the one acting on wider spaces. A function on a manifold is also called a 0-form.

Let \( \Lambda^0\mathcal{M} \) be a space of 0-forms on \( \mathcal{M} \), and \( \Lambda^1\mathcal{M} \) a space of 1-forms. Then, one can write

\[ d : \Lambda^0\mathcal{M} \to \Lambda^1\mathcal{M}. \]

There are various bases for \( T^*_p\mathcal{M} \), and one of them is

\[ \{ dx^1, \ldots, dx^m \}, \]

so that the pairing between \( dx^a \) and \( \partial/\partial x^b \) is

\[ dx^a \left( \frac{\partial}{\partial x^b} \right) = \delta^a_b := \begin{cases} 1 & a = b \\ 0 & a \neq b \end{cases}. \]

In terms of the basis \( \{dx^a\}_{a=1}^m \) and a set of functions \( \{X_a\}_{a=1}^m \), a 1-form at \( p \in \mathcal{M} \) can be written as the sum \( \sum_{a=1}^m X_a(p)dx^a \). For a given function \( f \), the 1-form \( df \) is calculated from the definition as

\[ df = \sum_{a=1}^m \frac{\partial f}{\partial x^a} dx^a. \]

This expression is derived below. Because \( df \) is a 1-form, it can be written as a sum with the basis \( \{dx^a\}_{a=1}^m \) as

\[ df = \sum_{a=1}^m g_a dx^a, \]
with \( \{g_a\}_{a=1}^m \) being a set of functions to be determined below. Let \( X \) be a vector written in terms of basis \( \{\partial/\partial x^a\}_{a=1}^m \), that is,

\[
X = \sum_{a=1}^m X^a \frac{\partial}{\partial x^a},
\]

where \( \{X^a\}_{a=1}^m \) is a set of functions. Then it immediately follows that

\[
Xf = \sum_{a=1}^m X^a \frac{\partial f}{\partial x^a},
\]

and

\[
(df)(X) = \sum_{b=1}^m g_b \, dx^b \left( \sum_{a=1}^m X^a \frac{\partial}{\partial x^a} \right) = \sum_{a=1}^m g_a X^a.
\]

Comparing these two equations, one has

\[
\begin{align*}
g_a &= \frac{\partial f}{\partial x^a}, \quad a = 1, \ldots, m. \\
\end{align*}
\]

Given \( \alpha = \sum_{a=1}^m f_a \, dx^a \in T^*_pM \) and \( X = \sum_{b=1}^m g_b \, \partial/\partial x^b \in T_pM \), the paring between them is calculated as

\[
\alpha(X) = \sum_{a=1}^m f_a \, dx^a \left( \sum_{b=1}^m g_b \frac{\partial}{\partial x^b} \right)
= \sum_{a=1}^m \sum_{b=1}^m f_a g_b \left[ dx^a \left( \frac{\partial}{\partial x^b} \right) \right]
= \sum_{a=1}^m \sum_{b=1}^m f_a g_b \delta^a_b
= \sum_{a=1}^m f_a g^a.
\]

A (differential) \( k \)-form (field) \( \alpha \in \Lambda^k \mathcal{M} \) with \( 0 \leq k \leq m \) defines a map at \( p \in \mathcal{M} \)

\[
\alpha_p : \underbrace{T_pM \times \cdots \times T_pM}_{k} \to \mathbb{R}
\]

equipped with the properties

\[
\begin{align*}
\text{(i)} \quad & \alpha(X_1, \ldots, fX_r + f'X'_r, \ldots, X_k) \\
& = f \alpha(X_1, \ldots, X_r, \ldots, X_k) \\
& \quad + f' \alpha(X_1, \ldots, X'_r, \ldots, X_k), \\
\text{(ii)} \quad & \alpha(X_1, \ldots, X'_r, \ldots, X_r, \ldots, X_k) \\
& = - \alpha(X_1, \ldots, X_r, \ldots, X'_r, \ldots, X_k), \\
\text{(iii)} \quad & \alpha(X_1, \ldots, X_k) \\
& \quad \text{is a differentiable function on } \mathcal{M}.
\end{align*}
\]
Here \( f, f' \in \Lambda^0 M, \ X_1, \ldots, X_k \in T_p M \). Any \( k \)-forms with \( k > m \) are defined such that \( \alpha(X) = 0 \) for all \( X \). Then the abbreviation \( \alpha = 0 \) can be used for \( \alpha \in \Lambda^k M \) with \( k > \dim M \).

The exterior product or wedge product \( \alpha \wedge \alpha' \) of the two forms \( \alpha \in \Lambda^k M \) and \( \alpha' \in \Lambda^l M \) is such that

\[
(\alpha \wedge \alpha')(X_1, \ldots, X_k, X_{k+1}, \ldots, X_{k+l}) = \frac{1}{k!l!} \sum_{\sigma} (\text{sign } \sigma) \alpha(X_{\sigma(1)}, \ldots, X_{\sigma(k)}) \cdot \alpha'(X_{\sigma(k+1)}, \ldots, X_{\sigma(k+l)}),
\]

where the numerical factor \( k!l! \) is replaced with \((k+l)!\) in another convention. Moreover, for the \( \sigma \) permutation of \((1, \ldots, k + l)\), \( \text{sign } \sigma = 1 \) for even permutations and \( \text{sign } \sigma = -1 \) for odd permutations. The following hold:

(i) \( \alpha \wedge \alpha = 0 \), \( \alpha \in \Lambda^k M \), where \( k \) is odd,
(ii) \( \alpha' \wedge \alpha = (-1)^{kl} \alpha \wedge \alpha' \), where \( \alpha \in \Lambda^k M, \alpha' \in \Lambda^l M \),
(iii) \( (\alpha \wedge \alpha')(X, X') = \alpha(X) \alpha'(X') - \alpha(X') \alpha'(X) \), where \( \alpha, \alpha' \in \Lambda^1 M \).

The definition of the exterior derivative is then extended to the operator

\[
d : \Lambda^k M \to \Lambda^{k+1} M, \quad 0 \leq k \leq m,
\]
equipped with the properties

(i) \( d(\ c \alpha + c' \alpha') = c d\alpha + c' d\alpha' \), \( c, c' \in \mathbb{R} \),
(ii) \( d(\alpha \wedge \alpha') = (d\alpha) \wedge \alpha' + (-1)^k \alpha \wedge (d\alpha') \), where \( \alpha \in \Lambda^k M, \alpha' \in \Lambda^l M \),
(iii) \( d^2 \alpha = 0 \), where \( \alpha \in \Lambda^k M, d^2 \alpha := d(d\alpha) \),
(iv) \( (df)(X) = Xf, \quad X \in T_p M, \quad f \in \Lambda^0 M \).

Interior product \( \iota_X : \Lambda^k M \to \Lambda^{k-1} M \) with \( X \in T_p M \) is

\[
(\iota_X \alpha)(X_1, \ldots, X_{k-1}) = \alpha(X, X_1, \ldots, X_{k-1}),
\]

and

\[
\iota_X f = 0, \quad f \in \Lambda^0 M.
\]

Then it follows that

(i) \( \iota_X (f \alpha + f' \alpha') = f \iota_X \alpha + f' \iota_X \alpha' \), where \( f, f' \in \Lambda^0 M, \ \alpha, \alpha' \in \Lambda^k M \),
(ii) \( \iota_X (\alpha \wedge \alpha') = (\iota_X \alpha) \wedge \alpha' + (-1)^k \alpha \wedge (\iota_X \alpha') \), where \( \alpha \in \Lambda^k M, \ \alpha' \in \Lambda^l M \),
(iii) \( \iota_X^2 \alpha = 0 \), where \( \alpha \in \Lambda^k M, \ \iota_X^2 \alpha := \iota_X (\iota_X \alpha) \).

Combining \( \iota_X \) and \( d \), one has that \( \iota_X df = df(X) = Xf \) for a function \( f \).
B.2 Push-forward and pull-back

Let $M$ and $M'$ be manifolds whose dimensions need not be the same, and let $\varphi : M \to M'$ be an invertible map. This map induces the map

$$\varphi_* : T_pM \to T_{\varphi(p)}M', \quad p \in M$$

which is called the push-forward induced by $\varphi$. Let $x = (x^1, \ldots, x^m)$ be a set of coordinates for $M$ with $\dim M = m$, and $y = (y^1, \ldots, y^n)$ with $\dim M' = n$. For $X \in T_pM$ given by

$$X = \sum_{a=1}^{m} f_a(x) \frac{\partial}{\partial x^a},$$

its push-forward $\varphi_*$ is calculated to be

$$\varphi_* X = \sum_{a=1}^{m} \sum_{b=1}^{n} f_a(x(y)) \frac{\partial y^b}{\partial x^a}(y) \frac{\partial}{\partial y^b}, \quad \in T_{\varphi(p)}M'.$$

The map $\varphi : M \to M'$ induces another map

$$\varphi^* : T_{\varphi(p)}^*M' \to T_p^*M, \quad p \in M,$n

which is called the pull-back induced by $\varphi$. This is also defined for $k$-forms such that

$$(\varphi^* \alpha)(X_1, \ldots, X_k) = \alpha(\varphi_* X_1, \ldots, \varphi_* X_k),$$

$$X_1, \ldots, X_k \in T_pM, \quad \alpha \in \Lambda^k M'.$$

More precisely,

$$(\varphi^* \alpha)_p(X_1, \ldots, X_k) = \alpha_{\varphi(p)}(\varphi_* X_1, \ldots, \varphi_* X_k),$$

$$X_1, \ldots, X_k \in T_pM, \quad \alpha \in \Lambda^k M'.$$

For functions, the pull-back is defined as

$$\varphi^* f = f \circ \varphi, \quad f \in \Lambda^0 M.$$

It follows that

$$(i) \quad \varphi^*(\alpha \wedge \alpha') = (\varphi^* \alpha) \wedge (\varphi^* \alpha'),$$

$$\alpha \in \Lambda^k M, \quad \alpha' \in \Lambda^l M,$$

$$(ii) \quad \varphi^*(d\alpha) = d(\varphi^* \alpha), \quad \alpha \in \Lambda^k M.$$

B.3 One-parameter group of transforms and the Lie derivative

The Lie derivative is a tool for evaluating changes in various objects in differential geometry, and it is used in Section A. This is briefly explained here.

Suppose that a diffeomorphism $\varphi_t : M \to M$ is given for each $t \in \mathbb{R}$. If the map

$$\varphi : \mathbb{R} \times M \to M, \quad \varphi(t, x) = \varphi_t(x), \quad t \in \mathbb{R}, \quad x \in M,$$
is differentiable and satisfies
\[ \varphi_t \circ \varphi_{t'} = \varphi_{t+t'}, \]
then \{ \varphi_t; t \in \mathbb{R} \} is called a 1-parameter group of transforms. If a domain for \( t \) is a bounded domain of \( \mathbb{R} \), \{ \varphi_t \} is called 1-parameter group of local transforms.

Given a \( \varphi_t \), there is a vector field \( X \) satisfying
\[ X_p f = \frac{df}{dt} \bigg|_{t=0} f(\varphi_t p), \quad p \in \mathcal{M}, \]
for any function \( f \). This vector field \( X \) is called an infinitesimal transform. In contrast, given a vector field \( X \), there is a 1-parameter group of local transforms \( \{ \Phi_{X,t} \} \) such that \( X \) is the infinitesimal transform. This induced \( \{ \Phi_{X,t} \} \) is called the 1-parameter group of (local) transforms induced by \( X \). The word “local” is often omitted.

Let \( X \) be a vector field, and \( \{ \Phi_{X,t} \} \) the 1-parameter group of (local) transform. Given \( \alpha \in \Lambda^k \mathcal{M} \), the \( k \)-form
\[ \mathcal{L}_X \alpha := \lim_{t \to 0} \frac{1}{t} (\Phi_{X,t}^* \alpha - \alpha), \]
is called the Lie derivative of \( \alpha \) along \( X \). Although Lie derivative can be defined for other objects, including vector fields, such details are not discussed here. For forms, it follows that
\[ \begin{align*}
(\text{i}) \quad & \mathcal{L}_X (\alpha \wedge \alpha') = (\mathcal{L}_X \alpha) \wedge \alpha' + \alpha \wedge (\mathcal{L}_X \alpha'), \\
& \alpha \in \Lambda^k \mathcal{M}, \quad \alpha' \in \Lambda^l \mathcal{M}, \\
(\text{ii}) \quad & \mathcal{L}_X \alpha = (i_X d + d i_X) \alpha, \quad \alpha \in \Lambda^k \mathcal{M}, \\
& \text{(this is known as the Cartan formula)}, \\
(\text{iii}) \quad & d \mathcal{L}_X \alpha = \mathcal{L}_X d \alpha, \quad \alpha \in \Lambda^k \mathcal{M}, \\
(\text{iv}) \quad & \mathcal{L}_X f = X f, \quad f \in \Lambda^0 \mathcal{M}.
\end{align*} \]

C Detailed derivations of equations

C.1 Equation (15)

Suppose that a Hamiltonian \( H \) is given on the manifold \( S^E = T^*Q \times I \) with \( \dim Q = n + 1 \). Then the Poincaré-Cartan form \( \alpha^E = \alpha - H dt \) is obtained, which is written in coordinates as
\[ \alpha^E = \sum_{a=0}^{n} p_a dq^a - H dt, \]
so that
\[ \omega^E = d \alpha^E = \omega - dH \wedge dt, \quad \text{where} \quad \omega = \sum_{a=0}^{n} dp_a \wedge dq^a. \]

Let \( \dot{q}, \dot{p}, \dot{t} \) be some functions on \( S^E \). Then a non-autonomous Hamiltonian vector field with
\[ X^E_H = \sum_{a=0}^{n} \left[ \dot{q}_a \frac{\partial}{\partial q^a} + \dot{p}_a \frac{\partial}{\partial p_a} \right] + \dot{t} \frac{\partial}{\partial t} \]

is differentiable and satisfies
\[ \varphi_t \circ \varphi_{t'} = \varphi_{t+t'}, \]
then \( \{ \varphi_t; t \in \mathbb{R} \} \) is called a 1-parameter group of transforms. If a domain for \( t \) is a bounded domain of \( \mathbb{R} \), \( \{ \varphi_t \} \) is called 1-parameter group of local transforms.

Given a \( \varphi_t \), there is a vector field \( X \) satisfying
\[ X_p f = \frac{df}{dt} \bigg|_{t=0} f(\varphi_t p), \quad p \in \mathcal{M}, \]
for any function \( f \). This vector field \( X \) is called an infinitesimal transform. In contrast, given a vector field \( X \), there is a 1-parameter group of local transforms \( \{ \Phi_{X,t} \} \) such that \( X \) is the infinitesimal transform. This induced \( \{ \Phi_{X,t} \} \) is called the 1-parameter group of (local) transforms induced by \( X \). The word “local” is often omitted.

Let \( X \) be a vector field, and \( \{ \Phi_{X,t} \} \) the 1-parameter group of (local) transform. Given \( \alpha \in \Lambda^k \mathcal{M} \), the \( k \)-form
\[ \mathcal{L}_X \alpha := \lim_{t \to 0} \frac{1}{t} (\Phi_{X,t}^* \alpha - \alpha), \]
is called the Lie derivative of \( \alpha \) along \( X \). Although Lie derivative can be defined for other objects, including vector fields, such details are not discussed here. For forms, it follows that
\[ \begin{align*}
(\text{i}) \quad & \mathcal{L}_X (\alpha \wedge \alpha') = (\mathcal{L}_X \alpha) \wedge \alpha' + \alpha \wedge (\mathcal{L}_X \alpha'), \\
& \alpha \in \Lambda^k \mathcal{M}, \quad \alpha' \in \Lambda^l \mathcal{M}, \\
(\text{ii}) \quad & \mathcal{L}_X \alpha = (i_X d + d i_X) \alpha, \quad \alpha \in \Lambda^k \mathcal{M}, \\
& \text{(this is known as the Cartan formula)}, \\
(\text{iii}) \quad & d \mathcal{L}_X \alpha = \mathcal{L}_X d \alpha, \quad \alpha \in \Lambda^k \mathcal{M}, \\
(\text{iv}) \quad & \mathcal{L}_X f = X f, \quad f \in \Lambda^0 \mathcal{M}.
\end{align*} \]

C Detailed derivations of equations

C.1 Equation (15)

Suppose that a Hamiltonian \( H \) is given on the manifold \( S^E = T^*Q \times I \) with \( \dim Q = n + 1 \). Then the Poincaré-Cartan form \( \alpha^E = \alpha - H dt \) is obtained, which is written in coordinates as
\[ \alpha^E = \sum_{a=0}^{n} p_a dq^a - H dt, \]
so that
\[ \omega^E = d \alpha^E = \omega - dH \wedge dt, \quad \text{where} \quad \omega = \sum_{a=0}^{n} dp_a \wedge dq^a. \]

Let \( \dot{q}, \dot{p}, \dot{t} \) be some functions on \( S^E \). Then a non-autonomous Hamiltonian vector field with
\[ X^E_H = \sum_{a=0}^{n} \left[ \dot{q}_a \frac{\partial}{\partial q^a} + \dot{p}_a \frac{\partial}{\partial p_a} \right] + \dot{t} \frac{\partial}{\partial t} \]
reduces to Eq. (14) when the condition $\dot{t} = 1$ is imposed.

A vector field $X_H^E \in TSE$ satisfying

$$\iota_{X_H^E} \omega^E = 0$$

expresses non-autonomous Hamiltonian equations of motion, that is, Eq. (15). This statement, and the decomposed form

$$\iota_{X_H^E} \omega = -d_{\ast} Q H, \quad \text{and} \quad X_H H = 0,$$

where

$$d_{\ast} Q H := dH - \frac{\partial H}{\partial t} dt,$$

are verified below.

First the decomposed form is obtained. Substituting

$$\iota_{X_H^E} \omega = \iota_{X_H^E} (dH \wedge dt)$$

$$= \iota_{X_H^E} \omega - (\iota_{X_H^E} dH) dt + (\iota_{X_H^E} dt) dH$$

$$= \iota_{X_H^E} \omega - (X_H^E H) dt + (X_H^E t) dH$$

$$= \iota_{X_H^E} \omega - \left[(X_H H) + \frac{\partial H}{\partial t}\right] dt + dH$$

$$= \iota_{X_H^E} \omega - (X_H H) dt + d_{\ast} Q H,$$

into the condition $\iota_{X_H^E} \omega^E = 0$, and noticing that the 1-form

$$\iota_{X_H^E} \omega + d_{\ast} Q H$$

does not contain $dt$, one has the decomposed form.

Second, Eq. (15) is derived below. Because

$$\iota_{X_H^E} \omega = \sum_{a=0}^{n} \left[ (\iota_{X_H^E} dp_a) dq^a - (\iota_{X_H^E} dq^a) dp_a \right]$$

$$= \sum_{a=0}^{n} \left[ (X_H^E p_a) dq^a - (X_H^E q^a) dp_a \right]$$

$$= \sum_{a=0}^{n} \left[ \dot{p}_a dq^a - \dot{q}^a dp_a \right],$$

$$-d_{\ast} Q H = -dH + \frac{\partial H}{\partial t} dt$$

$$= -\sum_{a=0}^{n} \left[ \frac{\partial H}{\partial q^a} dq^a + \frac{\partial H}{\partial p_a} dp_a \right],$$

and $dq^a, dp_a, dt$ form a basis on $T^*S^E$, one has the desired equations

$$dq^a : \dot{p}_a = -\frac{\partial H}{\partial q^a}, \quad dp_a : \dot{q}^a = \frac{\partial H}{\partial p_a}, \quad a = 1, \ldots, n.$$
C.2 Equation (16)

Suppose that a contact Hamiltonian $K$ is given on the manifold $\mathcal{C}^E = \mathbb{P}(T^*Q) \times \mathcal{I}$ with $\dim Q = n + 1$. Then

$$\lambda^E = \lambda + Kdt$$

is obtained, where $\lambda$ is a contact 1-form on $\mathcal{C} = \mathbb{P}(T^*Q)$. In a neighborhood it is expressed as

$$\lambda = dq^0 - \sum_{a=1}^{n} \gamma_a dq^a.$$

The non-autonomous contact vector field, denoted by $X^E_K$, is defined as the one satisfying both

$$\mathcal{L}_{X^E_K} \lambda^E = g^E \lambda^E \quad \text{and} \quad K = -\iota_{X^E_K} \lambda,$$

where $g^E$ is some function. In Darboux coordinates, $X^E_K$ is expressed as

$$X^E_K = q^0 \frac{\partial}{\partial q^0} + \sum_{a=1}^{n} \left[ \dot{q}^a \frac{\partial}{\partial q^a} + \dot{\gamma}_a \frac{\partial}{\partial \gamma_a} \right] + \frac{\partial}{\partial t},$$

and $\dot{q}^0$, $\dot{q}^a$, and $\dot{\gamma}_a$ obey Eq. (16).

This statement is verified below. First, the 2nd condition is equivalent to

$$\lambda^E(X^E_K) = 0,$$

because

$$0 = \iota_{X^E_K} \lambda + K = \iota_{X^E_K} (\lambda + Kdt) = \iota_{X^E_K} \lambda^E = \lambda^E(X^E_K).$$

From this 2nd condition and the Cartan formula, one has that

$$\mathcal{L}_{X^E_K} \lambda^E = (\iota_{X^E_K} d + d\iota_{X^E_K}) \lambda^E = \iota_{X^E_K} d\lambda^E,$$

from which the 1st condition can be written as

$$\iota_{X^E_K} d\lambda^E = g^E \lambda^E.$$

The right hand side of the equation above is

$$g^E \lambda^E = g^E \left( dq^0 - \sum_{a=1}^{n} \gamma_a dq^a + K dt \right).$$

The left hand side reduces from

$$d\lambda^E = \left( dq^0 - \sum_{a=1}^{n} \gamma_a dq^a + K dt \right)$$

$$= dK \land dt - \sum_{a=1}^{n} d\gamma_a \land dq^a.$$

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to
\[ \tau_{X^E_K} \, d\lambda^E \]
\[ = \tau_{X^E_K} (dK \wedge dt) - \tau_{X^E_K} \left( \sum_{a=1}^{n} d\gamma_a \wedge dq^a \right) \]
\[ = (\tau_{X^E_K} dK) \, dt - (\tau_{X^E_K} dt) \, dK - \sum_{a=1}^{n} \left[ (\tau_{X^E_K} d\gamma_a) \, dq^a - (\tau_{X^E_K} dq^a) \, d\gamma_a \right] \]
\[ = (X^E_K) \, dt - dK - \sum_{a=1}^{n} \left[ (X^E_K \gamma_a) \, dq^a - (X^E_K q^a) \, d\gamma_a \right] \]
\[ = (X^E_K) \, dt - dK - \sum_{a=1}^{n} \left[ \dot{\gamma}_a \, dq^a - \dot{q}^a \, d\gamma_a \right]. \]

To reduce the equation further, substituting
\[ (X^E_K) \, dt - dK \]
\[ = (X^E_K) \, dt - \left[ \frac{\partial K}{\partial t} \, dt + \frac{\partial K}{\partial q^0} dq^0 + \sum_{a=1}^{n} \left( \frac{\partial K}{\partial q^a} dq^a + \frac{\partial K}{\partial \gamma_a} d\gamma_a \right) \right] \]
\[ = \left[ (X^E_K) - \frac{\partial K}{\partial t} \right] \, dt - \frac{\partial K}{\partial q^0} dq^0 - \sum_{a=1}^{n} \left( \frac{\partial K}{\partial q^a} dq^a + \frac{\partial K}{\partial \gamma_a} d\gamma_a \right) \]

into the equation above, one has
\[ \tau_{X^E_K} \, d\lambda^E = \left[ (X^E_K) - \frac{\partial K}{\partial t} \right] \, dt - \frac{\partial K}{\partial q^0} dq^0 \]
\[ - \sum_{a=1}^{n} \left[ \left( \dot{\gamma}_a + \frac{\partial K}{\partial q^0} \right) dq^a + \left( -\dot{q}^a + \frac{\partial K}{\partial \gamma_a} \right) d\gamma_a \right]. \]

Because \( dq^0 \), \( dq^a \), \( d\gamma_a \), \( dt \) form a basis for \( T^* C^E \), the 1st condition yields
\[ dt : (X^E_K) - \frac{\partial K}{\partial t} = g^E K, \]
\[ dq^0 : - \frac{\partial K}{\partial q^0} = g^E, \]
\[ dq^a : \dot{\gamma}_a + \frac{\partial K}{\partial q^a} = \gamma a g^E, \]
\[ d\gamma_a : -\dot{q}^a + \frac{\partial K}{\partial \gamma_a} = 0. \]

From these equations, one has
\[ \dot{q}^a = \frac{\partial K}{\partial \gamma_a}, \quad \dot{\gamma}_a = - \frac{\partial K}{\partial q^a} - \gamma_a \frac{\partial K}{\partial q^0}, \quad a = 1, \ldots, n. \]

Observe that
\[ \frac{d}{dt} K = X^E_K K = \frac{\partial K}{\partial t} - \frac{\partial K}{\partial q^0} K. \]
The 2nd condition is equivalent to

\[ 0 = \lambda^E(X^E_K) \]

\[ = \left( dq^0 - \sum_{b=1}^{n} \gamma_b dq^b + K dt \right) (X^E_K) \]

\[ = X^E_K q^0 - \sum_{b=1}^{n} \gamma_b X^E_K q^b + K X^E_K t \]

\[ = \dot{q}^0 - \sum_{a=1}^{n} \gamma_a \dot{q}^a + K. \]

Then one has

\[ \dot{q}^0 = \sum_{a=1}^{n} \gamma_a \frac{\partial K}{\partial \gamma_a} - K. \]

### D Derivations of equations in the main text

#### D.1 Equation (11) in the main text

Given the Hamiltonian

\[ H^Z_K(q, p, t) = -\frac{1}{2p_0(t; \sigma)} \sum_{b=1}^{d} p^2_b, \]

with

\[ p_0(t; \sigma) = p_0(1) t^{2\sigma+1}, \]

the canonical equations of motion Eq. (15) are

\[ \dot{q}^a = \frac{\partial H^Z_K}{\partial p_a} = -\frac{p_a}{p_0(t; \sigma)}, \]

\[ \dot{p}_a = -\frac{\partial H^Z_K}{\partial q_a} = 0, \]

for \( a = 1, \ldots, d \). The solution to this set of equations is then obtained by integration. With

\[ -\int_t^{t+\tau} \frac{dt'}{p_0(t'; \sigma)} = -\frac{1}{p_0(1)} \int_t^{t+\tau} \frac{dt'}{(t')^{2\sigma+1}} = \frac{1}{2\sigma p_0(1)} \left[ \frac{1}{(t+\tau)^{2\sigma}} - \frac{1}{t^{2\sigma}} \right], \]

one has

\[ q^a(t + \tau) = q^a(t) + \frac{1}{2\sigma p_0(1)} \left[ \frac{1}{(t+\tau)^{2\sigma}} - \frac{1}{t^{2\sigma}} \right], \]

\[ p_a(t + \tau) = p_a(t), \]

for \( a = 1, \ldots, d \). For the sake of completeness, the solution to the system with \( H^Z_K \) is obtained as

\[ q^a(t) = q^a(1) + \frac{1}{2\sigma p_0(1)} \left[ \frac{1}{t^{2\sigma}} - 1 \right], \]

\[ p_a(t) = p_a(1), \]

for \( a = 1, \ldots, d \).
D.2 Equation (12) in the main text

Given the Hamiltonian

\[ H_Z(q, p, t) = -p_0(t; \sigma) \Gamma_0(t; \sigma) f(q), \]

with

\[ p_0(t; \sigma) = p_0(1) t^{2\sigma+1}, \quad \Gamma_0(t; \sigma) = \sigma^2 t^{\sigma-2}, \]

the canonical equations of motion Eq. (15) are

\[
\dot{q}^a = \frac{\partial H_Z}{\partial p_a} = 0,
\]

\[
\dot{p}_a = -\frac{\partial H_Z}{\partial q_a} = p_0(t; \sigma) \Gamma_0(t; \sigma) \frac{\partial f}{\partial q^a},
\]

for \( a = 1, \ldots, d \). Then the solution to this set of equations is obtained by integration. With

\[
\int_t^{t+\tau} p_0(t'; \sigma) \Gamma_0(t'; \sigma) \, dt' = \sigma^2 p_0(1) \int_t^{t+\tau} (t')^{3\sigma-1} \, dt' = \frac{\sigma^2 p_0(1)}{3\sigma} \left[ (t + \tau)^{3\sigma} - t^{3\sigma} \right],
\]

one has

\[
q^a(t + \tau) = q^a(t),
\]

\[
p_a(t + \tau) = p_a(t) + \frac{\sigma p_0(1)}{3} \left[ (t + \tau)^{3\sigma} - t^{3\sigma} \right] \frac{\partial f}{\partial q^a},
\]

for \( a = 1, \ldots, d \). For the sake of completeness, the solution to the system with \( H_Z \) is obtained as

\[
q^a(t) = q^a(1),
\]

\[
p_a(t) = p_a(1) + \frac{\sigma p_0(1)}{3} \left[ t^{3\sigma} - 1 \right] \frac{\partial f}{\partial q^a},
\]

for \( a = 1, \ldots, d \).

E Numerical evaluation in more detail

This section is intended to provide more information about the performance of the 2nd symplectic integrator (SI2) that has been discussed in Section 4, that is, the performance of the SI2 is compared with those of the existing methods RK2, RK4, and NAG in detail.

To this end, recall that one of the significant characteristics in numerical simulations for a method is how many times demanding or heavy calculations is needed. For a given dynamical system \( \dot{x} = F(x, t) \) with some differentiable function \( F : \mathbb{R}^d \times I \to \mathbb{R}^d \), suppose that we numerically solve for \( x(t) \in \mathbb{R}^d \) with some integrator. One significant computational load is to evaluate \( F \) numerically, and the number of evaluations depends on the algorithm. For SI2, it is the total
Table 2: Profile of datasets.

| Data set     | BreastCancer | Diabetis | HouseVote | Sonar | MNIST |
|--------------|--------------|----------|-----------|-------|-------|
| Dimension    | 9            | 8        | 16        | 60    | 784   |
| Sample size  | 615          | 353      | 209       | 187   | 60000 |

iteration number. For RK2, it is twice the total iteration number. For RK4, it is 4 times the total iteration number. This means that the computation cost of SI2 is the lowest among these ODE based algorithms.

In this section, as a realistic problem with convex objective function, we consider two-class classification by regularized logistic regression.

E.1 Objective function

We adopt a standard logistic loss function with regularization to prevent complete separation:

\[
f(w) = -\frac{1}{|D|} \sum_{i \in D} \{y_i \log(h(x_i; w)) + (1 - y_i) \log(1 - h(x_i; w))\} + \lambda_{\text{reg}} \|w\|^2_2,\]

where \(D\) is the training dataset, and the regularization parameter \(\lambda_{\text{reg}}\) is fixed to \(10^{-8}\) and \(h(x; w) = \frac{1}{1 + e^{-w^\top x}}\). Our aim is to develop a novel optimization algorithm based on geometric notion and not to develop a good classifier, hence the regularization parameter is commonly used for all of the algorithms and not tuned. We also note that in the main text of the paper, \(x\) is used for parameter while in the above objective function of logistic regression, we follow convention that \(w\) is the parameter of the model and \((x_i, y_i)\) are the observation where \(x_i \in \mathbb{R}^d\) and \(y_i \in \{+1, -1\}\).

E.2 Datasets

We use four popular datasets for classification from UCI machine learning repository, and the famous MNIST dataset. Profile of these datasets are summarized in table 2.

E.3 Comparison to Runge-Kutta methods

We first consider comparison to 2nd and 4th order Runge-Kutta methods (RK2 and RK4) [Griffiths and Higham, 2010] with different parameter \(\sigma\) in the original ODE defined in Eq. (6) in the main text, which controls the convergence speed. Theoretically, by increasing the value of \(\sigma\), we can achieve faster convergence rate. In reality, partly due to discretization errors, too large \(\sigma\) may cause numerical instability. We fixed the learning rate \(\tau = 0.01\) for our SI2, RK2 and RK4, and report the convergence behaviors of objective functions for five datasets in Fig. 2.

From Fig. 2, it is seen that in general, with larger \(\sigma\), the convergence speed is high. However, too large \(\sigma\) cause instability, particularly for MNIST dataset. SI2 and RK4 are relatively stabler than RK2. This behavior is partly contributed to the fact that RK2 is based on the lower degree of Taylor expansion and it is deviated from the original ODE compared to RK4.
Figure 2: Objective values along with the iteration of optimization with varying convergence parameter values of $\sigma$.

Now we compare the computational speed of the three methods. Table I shows average of the computational time to reach the stopping criterion (relative difference of the objective function value is less than $10^{-6}$) for RK2, RK4, SI2, and SI2 with backtracking and NAG with backtracking for adjusting step size (see next subsection). It is seen that SI2 is slightly faster than RK2 or on par for the first four datasets, and faster than RK4. For MNIST, which is the largest size among five datasets, SI2 is significantly faster than other two methods.

We note that SI2, RK2 and RK4 is derived from the same ODE, hence we focus on the conver-
gence behavior and computational cost.

E.4 Comparison to NAG method

We then compare SI2 to NAG described by

\[
\begin{align*}
  x^{(k)} &= y^{(k-1)} - s_N \nabla f(y^{(k-1)}), \\
  y^{(k)} &= x^{(k)} + \frac{k-1}{k+2} (x^{(k)} - x^{(k-1)}),
\end{align*}
\]

where \( s_N > 0 \) is a step size parameter, \( x^{(k)} \) and \( y^{(k)} \) denote \( x \in \mathbb{R}^d \) and \( y \in \mathbb{R}^d \) at discrete step \( k \geq 0 \), respectively.

From the results of the previous experiment, we see that for SI2, \( \sigma \) less than 8.0 offers stable results. In this section, the convergence rate parameter \( \sigma \) is fixed to 6.0. For both SI2 and NAG, step size remains to be a tuning parameter. For fair comparison, we adopt the backtracking method for automatically adjust the step size in each iteration. We implemented the momentum restarting mechanism to NAG for stabilizing the performance.

From Fig. 3, it is seen that in general, SI2 requires less iteration for convergence of the objective function value compared to NAG.

From Table 1, column SI2(BT) and NAG(BT), it is seen that computational time of SI2 with backtracking is significantly faster than NAG, particularly for MNIST dataset.

References

Jorge Nocedal and Stephen J. Wright. Numerical optimization. Springer, 2006. doi: https://doi.org/10.1007/978-0-387-40065-5.

Stephen Boyd and Lieven Vandenberghe. Convex Optimization. Cambridge University Press, USA, 2004. ISBN 0521833787.
Shiliang Sun, Zehui Cao, Han Zhu, and Jing Zhao. A survey of optimization methods from a machine learning perspective. *IEEE Transactions on Cybernetics*, pages 1–14, 2019.

Yurii Nesterov. A method for unconstrained convex minimization problem with the rate of convergence $o(1/k^2)$. *Soviet Mathematics Doklady*, 27:372–376, 1983.

Aaron Defazio. On the curved geometry of accelerated optimization. In *Advances in Neural Information Processing Systems 32*, pages 1766–1775. Curran Associates, Inc., 2019.

Brendan O’donoghue and Emmanuel Candès. Adaptive restart for accelerated gradient schemes. *Foundation of Computational Mathematics*, 15(3):715–732, June 2015. ISSN 1615-3375. doi: 10.1007/s10208-013-9150-3.

Mahyar Fazlyab, Alejandro Ribeiro, Manfred Morari, and Victor M. Preciado. Analysis of optimization algorithms via integral quadratic constraints: Nonstrongly convex problems. *SIAM Journal on Optimization*, 28(3):2654–2689, 2018. doi: 10.1137/17M1136845.

Bin Hu and Laurent Lessard. Dissipativity theory for Nesterov’s accelerated method. In Doina Precup and Yee Whye Teh, editors, *Proceedings of the 34th International Conference on Machine Learning*, volume 70 of *Proceedings of Machine Learning Research*, pages 1549–1557, International Convention Centre, Sydney, Australia, 8 2017. PMLR.

Damien Scieur, Alexandre de Aspremont, and Francis Bach. Regularized nonlinear acceleration. In D. D. Lee, M. Sugiyama, U. V. Luxburg, I. Guyon, and R. Garnett, editors, *Advances in Neural Information Processing Systems 29*, pages 712–720. Curran Associates, Inc., 2016.

Laurent Lessard, Benjamin Recht, and Andrew Packard. Analysis and design of optimization algorithms via integral quadratic constraints. *SIAM Journal on Optimization*, 26(1):57–95, 2016. doi: 10.1137/15M1009597.

Attouch, Hedy, Chbani, Zaki, and Riahi, Hassan. Rate of convergence of the nesterov accelerated gradient method in the subcritical case 3. *ESAIM: COCV*, 25:2, 2019. doi: 10.1051/cocv/2017083. URL https://doi.org/10.1051/cocv/2017083.

Weijie Su, Stephen Boyd, and Emmanuel J. Candès. A differential equation for modeling nesterov’s accelerated gradient method: Theory and insights. *Journal of Machine Learning Research*, 17 (153):1–43, 2016.

Nicoletta Bof, Ruggero Carli, and Luca Schenato. Lyapunov theory for discrete time systems, 2018.

Bin Shi, Simon S Du, Weijie Su, and Michael I Jordan. Acceleration via symplectic discretization of high-resolution differential equations. In *Advances in Neural Information Processing Systems 32*, pages 5744–5752. Curran Associates, Inc., 2019.

Ashia C Wilson, Lester Mackey, and Andre Wibisono. Accelerating rescaled gradient descent: Fast optimization of smooth functions. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d Alché-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems 32*, pages 13555–13565. Curran Associates, Inc., 2019.
Ernst Hairer, Christian Lubich, and Gerhard Wanner. *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations; 2nd ed.* Springer, Dordrecht, 2006. doi: 10.1007/3-540-30666-8.

Hiroshi Kinoshita, Haruo Yoshida, and Hiroshi Nakai. Symplectic integrators and their application to dynamical astronomy. *Celestial Mechanics and Dynamical Astronomy, 50:*59–71, 1990. doi: 10.1007/BF00048986.

Haruo Yoshida. Recent progress in the theory and application of symplectic integrators. *Celestial Mechanics and Dynamical Astronomy, 56:*27–43, 1993. doi: https://doi.org/10.1007/BF00699717.

Ana Cannas da Silva. *Lectures on Symplectic Geometry.* Springer, Berlin, Heidelberg, 2008. doi: https://doi.org/10.1007/978-3-540-45330-7.

Alessandro Bravetti, Marcello Seri, Mats Vermeeren, and Federico Zadra. Numerical integration in celestial mechanics: a case for contact geometry. *Celestial Mechanics and Dynamical Astronomy, 132,* 2020. doi: https://doi.org/10.1007/s10569-019-9946-9.

Alessandro Bravetti, Maria L. Daza-Torres, Hugo Flores-Arguedas, and Michael Betancourt. Optimization algorithms inspired by the geometry of dissipative systems, 2019.

Mats Vermeeren, Alessandro Bravetti, and Marcello Seri. Contact variational integrators. *Journal of Physics A: Mathematical and Theoretical,* 52(44):445206, 10 2019. doi: 10.1088/1751-8121/ab4767.

Guilherme França, Michael I. Jordan, and René Vidal. On dissipative symplectic integration with applications to gradient-based optimization, 2020.

Molei Tao and Tomoki Ohsawa. Variational optimization on lie groups, with examples of leading (generalized) eigenvalue problems. In *Artificial Intelligence and Statistics 2021,* pages –. AISTATS, 2020.

Jingzhao Zhang, Aryan Mokhtari, Suvrit Sra, and Ali Jadbabaie. Direct runge-kutta discretization achieves acceleration. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, *Advances in Neural Information Processing Systems 31,* pages 3900–3909. Curran Associates, Inc., 2018.

Andre Wibisono, Ashia C. Wilson, and Michael I. Jordan. A variational perspective on accelerated methods in optimization. *Proceedings of the National Academy of Sciences,* 113(47):E7351–E7358, 2016. ISSN 0027-8424. doi: 10.1073/pnas.1614734113.

P. Libermann and C.M. Marle. *Symplectic Geometry and Analytical Mechanics.* Mathematics and Its Applications. Springer Netherlands, 1987. ISBN 9789027724380.

Arjan Van der Schaft and Bernhard Maschke. Geometry of thermodynamic processes. *Entropy,* 20(12)(925), 2018. doi: https://doi.org/10.3390/e20120925.

Masuo Suzuki. General decomposition theory of ordered exponentials. *Proceedings of the Japan Academy, Series B,* 69(7):161–166, 1993. doi: 10.2183/pjab.69.161.
Naomichi Hatano and Masuo Suzuki. *Finding Exponential Product Formulas of Higher Orders*, pages 37–68. Springer Berlin Heidelberg, Berlin, Heidelberg, 2005. ISBN 978-3-540-31515-5.

Michael Betancourt, Michael I. Jordan, and Ashia C. Wilson. On symplectic optimization, 2018.

David Griffiths and Desmond J. Higham. *Numerical Methods for Ordinary Differential Equations*. Springer, 2010. doi: 10.1007/978-0-85729-148-6.

Alessandro Bravetti, Hans Cruz, and Diego Tapias. Contact hamiltonian mechanics. *Annals of Physics*, 376:17 – 39, 2017. ISSN 0003-4916. doi: https://doi.org/10.1016/j.aop.2016.11.003.

Vladimir I. Arnold. *Mathematical methods of classical mechanics*, volume 60. Springer, 1989.

Louis N. Hand and Janet D. Finch. *Analytical Mechanics*. Cambridge University Press, 1998. doi: 10.1017/CBO9780511801662.