On Dissipative Symplectic Integration with Applications to Gradient-Based Optimization

Guilherme França, Michael I. Jordan and René Vidal

Mathematical Institute for Data Science, Johns Hopkins University, Baltimore, MD 21218, USA
Department of Electrical Engineering and Computer Sciences, University of California, Berkeley, CA 94720, USA
Department of Statistics, University of California, Berkeley, CA 94720, USA

Abstract

Continuous-time dynamical systems have proved useful in providing conceptual and quantitative insights into gradient-based optimization. An important question that arises in this line of work is how to discretize the continuous-time system in such a way that its stability and rates of convergence are preserved. In this paper we propose a geometric framework in which such discretizations can be realized systematically, enabling the derivation of rate-matching optimization algorithms without the need for a discrete-time convergence analysis. More specifically, we show that a generalization of symplectic integrators to dissipative Hamiltonian systems is able to preserve continuous-time rates of convergence up to a controlled error. Our arguments rely on a combination of backward-error analysis with fundamental results from symplectic geometry.
1 Introduction

A recent line of research at the interface of machine learning and optimization focuses on establishing connections between continuous-time dynamical systems and gradient-based optimization methods (see, e.g., Su et al. (2016); Krichene et al. (2015); Wibisono et al. (2016); Wilson et al. (2016); Scieur et al. (2017); Betancourt et al. (2018); Franca et al. (2018a); Zhang et al. (2018); Shi et al. (2019); Muehlebach and Jordan (2019); Diakonikolas and Jordan (2019); Franca et al. (2019) and references therein). From this perspective an optimization algorithm is a particular discretization of a differential equation. Moreover, accelerated methods such as Nesterov’s method (Nesterov, 1983) and Polyak’s heavy ball method (Polyak, 1963) are modeled as second-order differential equations (Su et al., 2016; Krichene et al., 2015; Wibisono et al., 2016; Franca et al., 2018a). There are advantages to working in the continuous-time formalism. In particular, the stability and convergence analysis of a continuous system tends to be simpler and more transparent, making use of general tools such as Lyapunov theory and variational formulations. Discrete-time analysis is often only applicable on a case-by-case basis and often requires painstaking algebra.

A particularly useful step has been the development of Lagrangian and Hamiltonian perspectives on acceleration methods (Wibisono et al., 2016). This framework, which involves the definition of a Bregman Lagrangian and a Bregman Hamiltonian, places momentum-based methods such as Nesterov acceleration into a larger class of dynamical systems and has accordingly helped to demystify the notion of “acceleration.” Two difficulties arise, however, when one attempts to further exploit and characterize this general class of dynamical systems. First, there are many different ways to discretize a continuous-time dynamical system. As pointed out by Wibisono et al. (2016), a naive discretization may be unable to preserve the continuous rate and may even lead to an unstable algorithm. Moreover, it is largely unknown if there is an underlying principle from which one can construct such “rate-matching” discretizations. Thus, a fundamental question arises:

Which classes of discretizations are capable of preserving the rates of convergence of the continuous dynamical systems of interest in optimization?

A second difficulty is that Hamiltonian concepts have traditionally been applied to conservative dynamical systems; in particular, systems characterized asymptotically by oscillations. Such dynamical behavior is incommensurate with the desire to converge to an optimum—a system that converges towards a limit cycle may have favorable stability properties, but the presence of limit cycles may preclude convergence to a point. Thus we have a second fundamental question:

Can we map discrete-time algorithms into dissipative continuous-time dynamical systems that provide analytical insight into the behavior of the original algorithm?

Clearly these two questions are related. Indeed, the ability to map between dynamical
systems while preserving rates is a form of invariance and Hamiltonian ideas have proved to be essential tools in the classical study of dynamical invariances.

In this paper, we attempt to provide answers to these two questions. Introducing a class of dissipative Hamiltonian systems, we combine fundamental results from symplectic geometry (Berndt, 2001; Aebischer et al., 1994) and backward-error analysis (Benettin and Giorigli, 1994; Reich, 1999; Hairer, 1994) to establish rates of convergence for discrete-time algorithms based on these continuous-time dynamics. In the next paragraphs we overview, at a high level, the main outlines of our analysis framework. We focus on optimization, although we note in passing that our results may be of interest to other fields where the simulation of dissipative systems is important, such as out-of-equilibrium statistical mechanics, complex systems, economics, and control theory.

Given an \( n \)-dimensional smooth manifold \( \mathcal{M} \) and a function \( f : \mathcal{M} \to \mathbb{R} \), consider the optimization problem

\[
\min_{x \in \mathcal{M}} f(x). \tag{1.1}
\]

An explicitly time-dependent Hamiltonian system is specified by a Hamiltonian function, \( H = H(t,q,p) \), where \( q = q(t) \) is a curve on \( \mathcal{M} \), parameterized by time \( t \) and with local coordinates \( q^1(t), \ldots, q^n(t) \) in \( \mathbb{R}^n \). The conjugate momentum \( p = p(t) \) is an element of the cotangent space and has coordinates \( p_1(t), \ldots, p_n(t) \). We often omit the time dependency of these variables for simplicity. Thus, points \( x \equiv (q,p) \) with coordinates \( (q^1, \ldots, q^n, p_1, \ldots, p_n) \) represent the state of the system and belong to the \( 2n \)-dimensional phase space.\(^1\) The time evolution of the system is required to obey Hamilton’s equations:

\[
\frac{dq_j}{dt} = \frac{\partial H}{\partial p_j}, \quad \frac{dp_j}{dt} = -\frac{\partial H}{\partial q_j} \quad (j = 1, \ldots, n). \tag{1.2}
\]

We will design time-dependent Hamiltonian systems whose trajectories tend to a low-energy level set that is consistent with a minimum \( f^* \) of \( f \).\(^2\)

Specifically, we consider dissipative systems arising from the following general family of Hamiltonians:

\[
H \equiv e^{-\eta_1(t)}T(t,q,p) + e^{\eta_2(t)}f(q), \tag{1.3}
\]

where the functions \( \eta_1 \) and \( \eta_2 \) are positive and monotone increasing, and are responsible for introducing dissipation in the system. The kinetic energy \( T \) is assumed to be Lipschitz continuous. Note that this Hamiltonian is of a general form that includes many dissipative systems that are relevant to optimization, including the Bregman dynamics of Wibisono et al. (2016) and the conformal Hamiltonian systems used in França et al. (2019) (see Appendix B). One can obtain continuous-time rates of convergence for these systems through a Lyapunov

\(^1\)The phase space is the cotangent bundle \( T^*\mathcal{M} \) associated to the manifold \( \mathcal{M} \) (see Appendix A). It suffices to assume \( \mathcal{M} = \mathbb{R}^n \) and \( (q,p) \in \mathbb{R}^{2n} \) for this discussion.

\(^2\)By way of contrast, a classical conservative system has a time-independent Hamiltonian, \( H = H(q,p) \), such that \( \frac{dH}{dt} = 0 \), implying that trajectories oscillate around a minimum instead of converging.
analysis (Su et al., 2016; Wibisono et al., 2016; Wilson et al., 2016; França et al., 2018b), leading to upper bounds of the form:

\[ f(q(t)) - f^* = \mathcal{O}(\mathcal{R}(t)), \tag{1.4} \]

for some decreasing function \( \mathcal{R}(t) \). Our goal is to construct rate-matching discretizations; i.e., integration methods that are able to reproduce such continuous-time rates in discrete time.

We will propose a class of discretizations that we refer to as \textit{presymplectic integrators} that are designed to preserve a fundamental geometric structure associated with dissipative Hamiltonian systems.\footnote{We will provide a formal presentation later, but briefly the idea is that the phase space of a dissipative Hamiltonian system is a \textit{presymplectic manifold} that is endowed with a closed degenerate symplectic 2-form. Presymplectic integrators preserve this 2-form exactly. Presymplectic integrators generalize symplectic integrators, which are widely used for conservative Hamiltonian systems (Leimkuhler and Reich, 2004; Hairer et al., 2006; Sanz-Serna, 1992; McLachlan and Quispel, 2006; Iserles and Quispel, 2018).}

A numerical integrator is a map \( \phi_h : \mathbb{R}^{2n} \to \mathbb{R}^{2n} \), with step size \( h > 0 \), such that iterations

\[ x_\ell = \phi_h(x_{\ell-1}), \quad x_0 = x(0), \tag{1.5} \]

approximate the true state of the system, \( x(t_\ell) \equiv (q(t_\ell), p(t_\ell)) \), at discrete instants \( t_\ell = h\ell \), for \( \ell = 1, 2, \ldots \). Let \( \varphi_t \) denote the true flow of the Hamiltonian system (1.2). A numerical integrator \( \phi_h \) is said to be of order \( r \geq 1 \) if

\[ \|\phi_h(x) - \varphi_t(x)\| = \mathcal{O}(h^{r+1}), \tag{1.6} \]

for any \( x \in T^*M \). We also introduce a Lipschitz assumption for the integrator:

\[ \|\phi_h(y) - \phi_h(x)\| \leq (1 + hL_\phi)\|y - x\|, \tag{1.7} \]

for some constant \( L_\phi > 0 \), and for all \( x, y \in T^*M \). This Lipschitz condition is satisfied by a large class of numerical methods, even including simple discretizations such as the explicit Euler method which do not preserve dynamical invariances (Hairer et al., 2006; Leimkuhler and Reich, 2004). We now state our main result, which we will further explicate and establish formally in the remainder of the paper.

**Theorem 1.1.** Consider a dissipative Hamiltonian system (1.2) obtained from (1.3). Let \( \phi_h \) be a presymplectic integrator of order \( r \), assumed to obey the Lipschitz condition (1.7). Then \( \phi_h \) preserves the continuous rates of convergence up to a small error given by

\[ \underbrace{f(q_\ell) - f^*}_{\text{discrete rate}} = \underbrace{f(q(t_\ell)) - f^*}_{\text{continuous rate}} + \underbrace{\mathcal{O}\left(h^r e^{-\eta(t_\ell)}\right)}_{\text{small error}}, \tag{1.8} \]

provided \( e^{L_\phi t_\ell - \eta(t_\ell)} < \infty \) for sufficiently large \( t_\ell \). This holds for exponentially large times \( t_\ell \equiv h\ell = \mathcal{O}(h^r e^r e^{h_0/h}) \), where the constant \( h_0 > 0 \) is independent of \( h \).
This theorem shows that presymplectic integration can provide answers to the questions posed earlier regarding the possibility of rate-preserving discretization of dissipative dynamical systems. The assumptions of the theorem are mild. The restriction on $t_\ell$ may be irrelevant in practice; to give an idea of orders of magnitude, with $r = 1$, $h_0 = 1$, and $h = 0.1$ we have a maximum iteration number $\ell \sim 10^5$, and if we further reduce $h = 0.01$ we get $\ell \sim 10^{43}$. More importantly, the error in (1.8) is small and improves with $r$, though it is dominated by $\eta_2$ which suggests that, in this context, higher-order integrators are not likely to be needed. Note that choosing a suitable $\eta_2$ is essential since it can make the error negligible; e.g., with $\eta_2 \sim t$ the error is exponentially small.

There is another important aspect of presymplectic integrators worth noting. Since they exactly preserve the phase-space geometry, they reproduce the qualitative features of the phase portrait, and in particular the stability of critical points. This is not the case for typical discretizations, which in general introduce spurious damping or excitation and may change the stability around critical points.

Let us now comment on some related works. Although there have been numerous papers exploring connections between continuous dynamical systems and optimization, there are relatively few that consider “structure-preserving” discretizations for optimization. The first paper proposing the use of symplectic integrators in this context is Betancourt et al. (2018). More recently, conformal symplectic integrators have been studied França et al. (2019). Muehlebach and Jordan (2020) have presented arguments indicating why preserving the symplectic structure is useful for optimization. On the other hand, although the literature on structure-preserving methods for conservative systems is vast, there are relatively few papers in the literature that consider structure-preserving methods for dissipative systems. Such methods include conformal symplectic integrators (Bhatt et al., 2016; Moore, 2017; Bhatt and Moore, 2019) and methods for systems with a reversible-irreversible coupling (Shang and Öttinger, 2020). These approaches tend to split the system into conservative and linear dissipative parts, so that a standard symplectic integrator can be applied to the former while the latter is simple enough to be integrated exactly. In our approach, we treat the system in its entirety, without any decomposition, allowing our framework to embrace a richer family of dissipative structures. Not surprisingly, conformal symplectic integrators correspond to a particular case of our formalism (see Appendix B).

An important property of symplectic integrators is that they not only conserve the Hamiltonian but also have long-term stability; this is the theoretical result that underlies the empirical success of symplectic integration (Benettin and Giorgilli, 1994). It is unknown if a similar property holds for dissipative Hamiltonian systems. One of our main contributions is to show that presymplectic integrators preserve the time-varying Hamiltonian and exhibit long-term stability, despite the absence of a conservation law.

Our work is organized as follows. In Appendix A, we introduce notation and recall some basic concepts from differential geometry which are needed throughout the paper. In Section 2, we introduce some ideas from backward-error analysis and symplectic integration, presenting geometric proofs of earlier results (see, e.g., Benettin and Giorgilli, 1994; Hairer,
1994; Reich, 1999) so as to anticipate our generalizations to dissipative systems. In Section 3, we introduce dissipative Hamiltonian systems from the point of view of symplectic geometry. We show how the phase space of such systems can be embedded in the phase space of a higher-dimensional and conservative Hamiltonian system; this is known as symplectification and is the fundamental mathematical tool used in this paper. We then define presymplectic integrators and argue that they extend the useful properties of symplectic integrators into a dissipative setting. We consider the implications for solving optimization problems and we prove Theorem 1.1. In Section 4, we construct explicit presymplectic integrators for the Bregman Hamiltonian in full generality. Section 5 contains our final remarks.

2 Hamiltonian Systems and Symplectic Integrators

We start with a brief review of pertinent concepts from dynamical systems and numerical integration, focusing on the notion of modified or perturbed equations. These concepts will be necessary in order to understand how one can draw conclusions about structure-preserving methods without a discrete-time analysis. We refer the reader to Appendix A for basic background material on differential geometry.

2.1 Numerical integrators and modified equations

Let $\mathcal{M}$ be an $n$-dimensional smooth manifold, and let $(\mathcal{U}, x)$ be a chart such that every point $p \in \mathcal{U} \subset \mathcal{M}$ has local coordinates $x^1, \ldots, x^n$ in $\mathbb{R}^n$. From now on we refer to a point $p$ by its coordinates $x$. Given a vector field $X \in T\mathcal{M}$, where $T\mathcal{M}$ denotes the tangent bundle, one has the system of differential equations

$$ \frac{dx^j}{dt} = X^j(x), \quad x^j(0) = x^j_0 \quad (j = 1, \ldots, n),$$

where $t \in \mathbb{R}$ is the time. This vector field can be represented by the differential operator

$$ X(x) = X^j(x) \partial_j, \quad (2.2) $$

where $\partial_1, \ldots, \partial_n$ is the induced coordinate basis in $T\mathcal{M}$. An integral curve of (2.1) defines a flow $\varphi_t : \mathcal{M} \rightarrow \mathcal{M}$. Notice that (2.1) has unique solutions, at least locally, since $X$ is locally Lipschitz because $\mathcal{M}$ is smooth. The flow can be represented by the exponential map

$$ \varphi_t = e^{tx} = I + tx + \frac{1}{2}t^2X^2 + \cdots . $$

(2.3)

Through its pullback, denoted by $\varphi_t^*$, the Lie derivative of a tensor $\alpha$ of rank $(0, q)$ along $X$ is defined by

$$ (\mathcal{L}_X \alpha)(x) = \left. \frac{d}{dt} \right|_{t=0} \varphi_t^* \alpha(x) = \lim_{t \rightarrow 0} \frac{\varphi_t^* \alpha(\varphi_t(x)) - \alpha(x)}{t}. $$

(2.4)

4We use the well-known Einstein summation convention throughout the paper, where upper and lower indices are summed over; e.g., $A^j B_j \equiv \sum_{i,j=1}^n A^j B_j$, and so on. See Appendix A for more discussion.
The dynamical system is said to preserve $\alpha$ if and only if $L_X \alpha = 0$.

Let $\phi_h : \mathbb{R}^n \to \mathbb{R}^n$ be a numerical integrator of order $r \geq 1$ for the system (2.1), as defined in (1.5) and (1.6). Since $X$ is locally Lipschitz, we have $\|X(y) - X(x)\| \leq L_X \|y - x\|$ for a constant $L_X > 0$ and for all $x, y \in \mathcal{M}$ in some region of interest. It follows from classical results (see, e.g., Hairer et al., 2006; Leimkuhler and Reich, 2004) that there exists $L_{\phi} > L_X$ such that we have control on a global error:

$$\|\phi_h^t(x_0) - \varphi_{t^e}(x_0)\| \leq C(e^{L_{\phi} t^e} - 1)h^r$$  \hspace{1cm} (2.5)

for some constant $C > 0$ and initial state $x_0 \in \mathcal{M}$. We have denoted $\phi_h^t \equiv \phi_h \circ \cdots \circ \phi_h$. Thus, for a fixed $t^e$ the numerical method is accurate up to order $O(h^r)$. However, if $t^e$ is free the error grows exponentially. For this reason, although typical higher-order methods may provide accurate solutions in a short span of time, they can be inaccurate and unstable for large times.

Formally, every numerical integrator $\phi_h$ can be seen as the exact flow of a modified or perturbed system (Benettin and Giorgilli, 1994; Hairer, 1994; Hairer and Lubich, 1997; Reich, 1999; Hairer et al., 2006; Leimkuhler and Reich, 2004)

$$\frac{dx^j}{dt} = \tilde{X}^j(x), \quad \tilde{X} \equiv X + \Delta X_1 h + \Delta X_2 h^2 + \cdots$$  \hspace{1cm} (2.6)

where the $\Delta X$’s are expressed in terms of $X$ and its derivatives. We refer to $\tilde{X}$ as the shadow vector field. In general, the series in (2.6) is divergent, and it is necessary to consider a truncation (Hairer and Lubich, 1997). Following Reich (1999), suppose we have found a truncation

$$\tilde{X}_k = X + \Delta X_1 h + \cdots + \Delta X_k h^k \quad (k \geq r),$$  \hspace{1cm} (2.7)

such that $\phi_h$ is an integrator of order $k$, namely $\|\phi_h(x) - \varphi_{h,\tilde{X}_k}(x)\| = O(h^{k+1})$, where $\varphi_{h,\tilde{X}_k}$ denotes the exact flow of (2.6) with $\tilde{X}$ replaced by $\tilde{X}_k$. Define

$$\Delta X_{k+1}(x) \equiv \lim_{h \to 0} \frac{\phi_h(x) - \varphi_{h,\tilde{X}_k}(x)}{h^{k+1}}.$$  \hspace{1cm} (2.8)

Then one can show (Reich, 1999) that:

$$\tilde{X}_{k+1} = \tilde{X}_k + \Delta X_{k+1} h^{k+1}$$  \hspace{1cm} (2.9)

yields a flow for which $\phi_h$ is an integrator of order $k+1$. Proceeding inductively, one can find higher-order vector fields $\tilde{X}_k$, with increasing $k$, such that $\varphi_{h,\tilde{X}_k}$ becomes closer and closer to $\phi_h$. However, since the series (2.6) eventually diverges, there exists a truncation point $k^*$ such that $\|\phi_h(x) - \varphi_{h,\tilde{X}_{k^*}}(x)\|$ is as small as possible. Finding $k^*$ and estimating the size of the $\Delta X$’s terms is quite technical, but it has been carried out in seminal work (Benettin and Giorgilli, 1994), and the approach has been further improved in subsequent literature (Hairer and Lubich, 1997; Reich, 1999).

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5Which exists for $k = r$ by assumption.
Theorem 2.1 (see Reich (1999)). Assume that \( X \) is real analytic and bounded on a compact subset of its domain. Assume that the numerical method \( \phi_h \) is real analytic. Then, there exists a family of shadow vector fields \( \tilde{X} \) such that

\[
\|X(x) - \tilde{X}(x)\| = O(h^r), \quad \|\phi_h(x) - \varphi_{h,\tilde{X}}(x)\| \leq C h e^{-r_0/h},
\]

where the constants \( C, h_0 > 0 \) do not depend on the step size \( h \).

This result holds in full generality, for any autonomous dynamical system and any numerical integrator. Next we will discuss how it becomes particularly useful in the case of conservative Hamiltonian systems.

2.2 Conservative Hamiltonian systems

Before talking about symplectic integrators, we need to introduce conservative Hamiltonian systems. Hamiltonian systems are ubiquitous because they are naturally attached to the geometry of the cotangent bundle \( T^*M \) of any differentiable manifold \( M \) (Berndt, 2001; Aebischer et al., 1994). We provide a concise introduction to key results that will be necessary later on.

Definition 2.2. Let \( M \) be an even-dimensional smooth manifold supplied with a closed nondegenerate 2-form \( \omega \). More precisely:

1. \( d\omega = 0 \);
2. On any tangent space \( T_xM \), if \( \omega(X, Y) = 0 \) for all \( Y \neq 0 \in T_xM \), then \( X = 0 \).

Then \( \omega \) is called a symplectic structure and \((M, \omega)\) a symplectic manifold.

Theorem 2.3. Let \( q^1, \ldots, q^n \) be local coordinates of \( M \) and \( q^1, \ldots, q^n, p_1, \ldots, p_n \) the corresponding induced coordinates of the cotangent bundle \( T^*M \). Then \( T^*M \) admits a closed nondegenerate symplectic structure,

\[
\omega = dp_j \wedge dq^j,
\]

and is therefore a symplectic manifold.

Proof. There always exists a globally defined Liouville-Poincaré 1-form, \( \lambda \equiv p_j dq^j \in T^*M \) (Berndt, 2001). Applying the exterior derivative induces the Poincaré 2-form \( \omega \equiv d\lambda = dp_j \wedge dq^j \). Since \( d^2 = 0 \) (see A.9) we trivially have \( d\omega = 0 \). It is also easy to see that \( \omega \) is nondegenerate; e.g., in a matrix representation \( \omega = (0 \quad -I \quad +I \quad 0) \). Thus \( \det(\omega) = 1 \neq 0 \). \( \square \)

Theorem 2.4. A dynamical system with the phase space \( T^*M \) preserves the symplectic structure \((2.11)\) if and only if it is a conservative Hamiltonian system, namely has the form in \((1.2)\) with a time-independent Hamiltonian \( H = H(q,p) \).
Proof. Let $\gamma : \mathbb{R} \to \mathcal{M}$ be a curve parametrized by $t$, so that $q_j^i(t) \equiv (q^i \circ \gamma)(t)$ and $p_j^i(t) \equiv (p^i \circ \gamma)(t)$ are time-dependent coordinates over $T^*\mathcal{M}$. Consider the tangent vector $\dot{X} \equiv \frac{d}{dt}$ to this curve, which in a coordinate basis is given by

$$X = \frac{dq_j^i}{dt} \frac{\partial}{\partial q^i} + \frac{dp_j^i}{dt} \frac{\partial}{\partial p^i}. \tag{2.12}$$

Note that $X$ lives in the tangent bundle of the phase space $T^*\mathcal{M}$. The vector field $X$ preserves $(2.11)$ if and only if $\mathcal{L}_X \omega = 0$. Recalling Cartan’s magic formula

$$\mathcal{L}_X = d \circ i_X + i_X \circ d, \tag{2.13}$$

we conclude that $(d \circ i_X)(\omega) = 0$. The Poincaré lemma thus implies the existence of a Hamiltonian function $H : T^*\mathcal{M} \to \mathbb{R}$, such that

$$i_X(\omega) = -dH. \tag{2.14}$$

This is actually Hamilton’s equations (1.2) in disguise; indeed, in component form we have $i_X(\omega) = p_j dq^i - \dot{q}^i dp_j$ which by comparison with (2.14) yields (1.2). We have just shown that a vector field that preserves the symplectic form (2.11) generates Hamiltonian dynamics. It is now easy to show the converse, namely that the flow of a Hamiltonian system preserves the 2-form (2.11). Given a Hamiltonian $H$, we have the equations of motion (1.2) with an associated vector field $\dot{X}_H$. These equations can equivalently be written in the form (2.14), as already shown. Using the identities $d^2 H = 0$ and $d\omega = 0$ in (2.13) implies $\mathcal{L}_{X_H} \omega = 0$.

Finally, another fundamental property of Hamiltonian systems is the conservation of energy. From the equations of motion (1.2) one immediately concludes that

$$\frac{dH}{dt} = 0. \tag{2.15}$$

In summary, any conservative Hamiltonian system have two fundamental properties:

- Its flow preserve the symplectic structure (2.11);
- The energy, or in this case the Hamiltonian $H$, is a constant of motion (2.15).

Next, we introduce an important class of discretizations that are desirable for simulating Hamiltonian systems since they preserve the symplectic structure (2.11) exactly, and at the same time “almost” conserve the Hamiltonian; see Theorem 2.6 below.

### 2.3 Symplectic integrators

Consider the following class of numerical methods.
Definition 2.5. A numerical integrator \( \phi_h \) for a conservative Hamiltonian system is called a symplectic integrator if it preserves the symplectic structure (2.11); i.e., \( \phi_h^* \omega \circ \phi_h = \omega \), where \( \phi_h^* \) is the pullback.

It is now easy to see that the flow of the perturbed system (2.6) associated to a symplectic integrator also preserves \( \omega \) exactly. As a consequence, Theorem 2.4 implies that the perturbed system must be Hamiltonian; i.e., there exists a shadow Hamiltonian \( \tilde{H} \) which is a perturbed version of \( H \). Indeed, since \( \phi_h \) preserves \( \omega \) by assumption, and the flow of the perturbed system (2.6) is an exact description of \( \phi_h \), the shadow vector field \( \tilde{X} \) obeys \( \mathcal{L}_{\tilde{X}} \omega = 0 \). Replacing the expansion (2.6) and using the linearity of the Lie derivative in the vector field implies \( \mathcal{L}_{\Delta X_j} \omega = 0 \) for each \( j = 1, 2, \ldots \). Hence, Theorem 2.4 implies that not only \( \tilde{X} \) but all \( \Delta X_j \)'s are Hamiltonian vector fields. That is, by the same argument leading to (2.14), there exists a function \( \tilde{H} \) and functions \( H_j \)'s such that

\[
\begin{align*}
  i_{\tilde{X}}(\omega) &= -d\tilde{H}, \\
  i_{\Delta X_j}(\omega) &= -dH_j.
\end{align*}
\]

Using the series (2.6), combining these two equations, and using (2.14), we have:

\[
-d\tilde{H} = i_X(\omega) + \sum_j h^j i_{\Delta X_j}(\omega) = -dH - \sum_j h^j dH_j,
\]

or equivalently

\[
\tilde{H} = H + hH_1 + h^2H_2 + \cdots.
\]

Moreover, the shadow Hamiltonian \( \tilde{H} \) is exactly conserved by the perturbed system, or equivalently by the symplectic integrator \( \phi_h \): \( \tilde{H} \circ \phi_h = \tilde{H} \). If we now consider a truncation (2.9), or equivalently if we truncate (2.18), then the flow \( \varphi_{h,\tilde{X}_k} \) exactly conserves the truncated shadow Hamiltonian \( \tilde{H}_k \):

\[
\tilde{H}_k \circ \varphi_{h,\tilde{X}_k} = \tilde{H}_k.
\]

We are now ready to state the most important property of symplectic integrators. Adapting ideas from Benettin and Giorgilli (1994) we can prove the following.

Theorem 2.6. Let \( \phi_h \) be a symplectic integrator of order \( r \). Assume that the Hamiltonian \( H \) is Lipschitz. Then \( \phi_h \) conserves \( H \) up to

\[
H \circ \phi_h^\ell = H \circ \varphi_{\ell h} + \mathcal{O}(h^r),
\]

for exponentially large times \( t_\ell = \mathcal{O}(h^r e^{h_0/h}) \). We recall that \( \varphi_{\ell h} \) is the exact flow of (1.2), at time \( t_\ell = h\ell \), and \( H = H \circ \varphi_{\ell h} \) is conserved.

Proof. Let \( \tilde{X} \equiv \tilde{X}_k \) be a truncated shadow vector field associated to \( \phi_h \)—in what follows we omit \( k \) for simplicity. We already know that (2.19) holds true, hence

\[
\tilde{H} \circ \phi_h^\ell - \tilde{H} = \sum_{i=0}^{\ell-1} \left( \tilde{H} \circ \phi_h^{i+1} - \tilde{H} \circ \phi_h^i \right) = \sum_{i=0}^{\ell-1} \left( \tilde{H} \circ \phi_h - \tilde{H} \circ \varphi_{h,\tilde{X}} \right) \circ \phi_h^i,
\]

(2.21)
where the first equality is an identity. Let $\tilde{L}$ be the Lipschitz constant of $\tilde{H}$. Using the second relation of (2.10) we have:

$$\left| (\tilde{H} \circ \phi_h^\ell - \tilde{H})(x_0) \right| \leq \tilde{L} \sum_{i=0}^{\ell-1} \| \phi_h(x_i) - \varphi_{h,X}(x_i) \| \leq \tilde{L} \ell h e^{-r} e^{-h_0/h}, \quad (2.22)$$

so $\phi_h$ preserves $\tilde{H}$ up to an exponentially small error in $h^{-1}$. In order to approximate $H$, write (2.18) in the form $\tilde{H} = H + O(h^r)$—since $\phi_h$ is order $r$—to obtain (2.20). Note that to ensure that the contribution of (2.22) remains smaller than $O(h^r)$ we have to choose $t_\ell = h \ell$ such that $t_\ell e^{-r} e^{-h_0/h} \sim h^r$.

Theorem 2.6 explains the benefits of symplectic integrators. Besides preserving the symplectic structure of the system, such methods generate solutions that remain within $O(h^r)$ of the true energy surface of the system, and thus exhibit long-term stability. It is well known that symplectic integrators tend to outperform alternative approaches when simulating conservative Hamiltonian systems (see, e.g., Sanz-Serna, 1992; McLachlan and Quispel, 2006; Iserles and Quispel, 2018).

The dissipative setting The situation is quite different in the case of dissipative, or more generally time-dependent, Hamiltonian systems. Even if one applies a symplectic integrator to the system written in the extended phase space—so as to transform the nonautonomous system into an autonomous one—the Hamiltonian is no longer conserved. The conservation of the Hamiltonian is the most basic assumption underneath Theorem 2.6; if (2.15) is no longer true, then (2.19) is no longer true, and the argument leading to (2.21) and (2.22) breaks down. It is not guaranteed that applying a symplectic integrator to a dissipative Hamiltonian system will closely reproduce the Hamiltonian, which is varying over time, nor is it guaranteed that the method will exhibit long-term stability. One of the main contributions of the current paper is to show that Theorem 2.6 can be extended to a dissipative setting, despite the nonexistence of a conservation law.

3 Dissipative Hamiltonian Systems

We consider a time-dependent Hamiltonian $H = H(t, q, p)$.\footnote{We often refer to “dissipative Hamiltonian systems,” though the reader should keep in mind that everything we say actually holds for any explicitly time-dependent Hamiltonian system.} The evolution of the system is still governed by Hamilton’s equations (3.3); however, the energy conservation law (2.15) no longer holds and is replaced by

$$\frac{dH}{dt} = \frac{\partial H}{\partial t}.$$ (3.1)
We begin by introducing an \((2n + 1)\)-dimensional extended phase space \(T^*\bar{\mathcal{M}}\) in which time becomes a new coordinate, so that \(q^0 = t, q^1, \ldots, q^n, p_1, \ldots, p_n\) are local coordinates of \(T^*\bar{\mathcal{M}}\). The evolution of the system is now generated by the vector field

\[
X \equiv X^\mu \partial_\mu = \frac{\partial}{\partial q^0} + \frac{dq^j}{ds} \frac{\partial}{\partial q^j} + \frac{dp_j}{ds} \frac{\partial}{\partial p_j},
\]

where \(\mu = 0, 1, \ldots, n\), \(X^0 = 1\), and \(s\) denotes the “new time parameter.” Thus, the nonautonomous Hamiltonian system (1.2) is equivalent to the autonomous system

\[
\frac{dq^0}{ds} = 1, \quad \frac{dq^j}{ds} = \frac{\partial H}{\partial p_j}, \quad \frac{dp_j}{ds} = -\frac{\partial H}{\partial q^j},
\]

over \(T^*\bar{\mathcal{M}}\), where \(H = H(q^0, \ldots, q^n, p_1, \ldots, p_n)\) is independent of \(s\). Importantly, \(T^*\bar{\mathcal{M}}\) is odd-dimensional so this phase space is no longer a symplectic manifold.

We thus introduce another dimension by adding a conjugate momentum \(p_0\) that pairs with \(q^0 = t\). To make the distinction clear, we denote the \((n + 1)\)-dimensional configuration manifold by \(\bar{\mathcal{M}} \equiv \mathbb{R} \times \mathcal{M}\), which has local coordinates \(q^0, \ldots, q^n\). The associated cotangent bundle \(T^*\bar{\mathcal{M}}\) is now of even dimensionality \(2n + 2\), with coordinates \(q^0, \ldots, q^n, p_0, \ldots, p_n\). Therefore, \(T^*\bar{\mathcal{M}}\) has a natural Liouville-Poincaré 1-form \(\Lambda = p_\mu dq^\mu\) which, as in the proof of Theorem 2.3, induces the closed nondegenerate Poincaré 2-form:

\[
\Omega \equiv d\Lambda = dp_\mu \wedge dq^\mu.
\]

This makes \(T^*\bar{\mathcal{M}}\) a proper symplectic manifold. Requiring that the vector field

\[
Y \equiv Y^\mu \partial_\mu = \frac{dq^\mu}{ds} \frac{\partial}{\partial q^\mu} + \frac{dp_\mu}{ds} \frac{\partial}{\partial p_\mu}
\]

preserves the symplectic structure (3.4) implies, by the argument leading to (2.14), that

\[
i_Y \Omega = -d\mathcal{H},
\]

for some Hamiltonian \(\mathcal{H} : T^*\bar{\mathcal{M}} \rightarrow \mathbb{R}\). In components, we have Hamilton’s equations:

\[
\frac{dq^0}{ds} = \frac{\partial \mathcal{H}}{\partial p_0}, \quad \frac{dp_0}{ds} = -\frac{\partial \mathcal{H}}{\partial q^0}, \quad \frac{dq^j}{ds} = \frac{\partial \mathcal{H}}{\partial p_j}, \quad \frac{dp_j}{ds} = -\frac{\partial \mathcal{H}}{\partial q^j},
\]

where \(j = 1, \ldots, n\) ranges over the spatial components. Moreover, since now \(\mathcal{H}\) does not depend explicitly on time \(s\), this system is actually conservative:

\[
\frac{d\mathcal{H}}{ds} = 0.
\]

At this stage, the higher-dimensional system (3.7) is not equivalent to (3.3). In order to create this equivalence we need to impose constraints, which means fixing a gauge. Note
that the symplectic form (3.4) is \( \Omega = dp_0 \wedge dq^0 + \omega \), where \( \omega \) is the symplectic form (2.11) for the original phase space \( T^*\mathcal{M} \). Requiring the vector fields (3.5) and (3.2) to be the same, and using (3.6) together with (2.14), yields:

\[
0 = iy\Omega + d\mathcal{H} = i_X dp_0 \wedge dq^0 + i_X \omega + d\mathcal{H} = d(-p_0 - H + \mathcal{H}).
\]

(3.9)

Thus, up to an irrelevant constant, we must have

\[
\mathcal{H}(q^0, \ldots, q^n, p_0, \ldots, p_n) = p_0(s) + H(q^0, \ldots, q^n, p_1, \ldots, p_n).
\]

(3.10)

Note that we carefully made the variable dependencies of each term explicit. This equation defines an embedded submanifold in the symplectic manifold \( T^*\hat{\mathcal{M}} \). Hence, the dynamics of the dissipative Hamiltonian system (3.2) lies on a hypersurface of constant energy \( \mathcal{H} \). More precisely, from (3.10) the first equation in (3.7) gives

\[
\frac{dq^0}{ds} = 1,
\]

(3.11)

which together with the two last equations of (3.7) becomes precisely the original dissipative system (3.3) over the extended phase space \( T^*\mathcal{M} \). The second equation of (3.7) reproduces the dissipation given by (3.1):

\[
\frac{dp_0}{ds} = -\frac{\partial H}{\partial q^0} = -\frac{dH}{ds},
\]

(3.12)

where the second equality follows from (3.8) together with (3.10). Hence, up to another irrelevant constant, we have

\[
p_0(s) = -H(s),
\]

(3.13)

with \( H(s) = H(q(s), p(s)) \). Note that in (3.13) the Hamiltonian is solely a function of time; the actual trajectories have been replaced. Therefore, \( p_0 \) is completely fixed.

We remark that (3.11) and (3.13) are specific choices of coordinates on \( T^*\hat{\mathcal{M}} \) which remove the spurious degrees of freedom that are not present in the original system. This procedure of embedding the phase space of the dissipative Hamiltonian system (3.3) over a higher-dimensional symplectic manifold is called symplectification (Berndt, 2001; Aebischer et al., 1994). We provide an illustration in Fig. 1.

Let us comment on another point behind the gauge choice (3.11) and (3.13). On the extended phase space \( T^*\mathcal{M} \) it is still possible to distinguish between position \( q^0 \) and momentum \( p_0 \). The flow \( \varphi_s = e^{sX} \) defines orbits \( s \mapsto q^\mu(s) \) on \( \mathcal{M} \). Such orbits are considered equivalent by time reparametrization, \( s \mapsto s'(s) \). However, to match the original orbits of the time-dependent Hamiltonian system over \( \mathcal{M} \), one must fix \( s = q^0 = t \). This means fixing a reference frame on \( T^*\mathcal{M} \). For this reason, time-dependent Hamiltonian systems are not covariant and one is not free to reparametrize the original time \( t \). In other words, since the Hamiltonian system is explicitly time-dependent, time transformations are not canonical.
Figure 1: The symplectification consists of the embeddings $T^*\mathcal{M} \hookrightarrow T^*\hat{\mathcal{M}} \hookrightarrow T^*\hat{\mathcal{M}}$, each of dimension $2n$, $2n+1$, and $2n+2$, respectively. The original dissipative Hamiltonian system has phase space $T^*\mathcal{M}$. When the system is written in autonomous form it has phase space $T^*\bar{\mathcal{M}}$, which is a presymplectic manifold that can naturally be embedded as a submanifold of constant energy $\mathcal{H} = 0$ in the symplectic manifold $T^*\hat{\mathcal{M}}$, which can be associated to the phase space of a conservative Hamiltonian system.

3.1 Presymplectic manifolds

We are now in a position to delineate the specific geometry underlying dissipative Hamiltonian systems. First, we introduce a useful generalization of symplectic manifolds (Berndt, 2001).

**Definition 3.1.** Let $\mathcal{M}$ be a differentiable manifold of dimension $(2n + \bar{n})$, $\bar{n} \geq 0$, supplied with a 2-form $\omega$ of rank $2n$ everywhere. Then $\omega$ is called a presymplectic form and $(\mathcal{M}, \omega)$ a presymplectic manifold.

When $\bar{n} = 0$ this definition reduces to that of a symplectic manifold, and when $\bar{n} = 1$ it reduces to the definition of a weak contact manifold. A weak contact manifold supplied with a 1-form $\vartheta$ obeying $\vartheta \wedge (d\vartheta)^n \neq 0$ is a contact manifold (Berndt, 2001; Aebischer et al., 1994). There is an alternative theory of contact manifolds, but they are intimately related to symplectic manifolds. They correspond to a particular case of presymplectic manifolds and therefore can naturally be embedded as hypersurfaces in their symplectification, which is a symplectic manifold in $2n + 2$ dimensions that is associated to $\mathcal{M}$. Furthermore, in Appendix B we show that a generalization of the so-called conformal Hamiltonian systems (McLachlan and Perlmutter, 2001) also corresponds to a particular case of the time-dependent Hamiltonian formalism discussed above.

In order to project the symplectic form (3.4) into the hypersurface defined by (3.10) we can simply replace the gauge choice $q^0 = t$ and $p_0 = -H$ to obtain

$$\Omega = -dH \wedge dt + \omega,$$

(3.14)
where we recall that $\omega$ is the original symplectic form of $T^*\mathcal{M}$. Moreover, the equations of motion (3.6) reduce to
\[ i_X\Omega = 0, \quad i_X dt = 1. \tag{3.15} \]

The vector field $X$, whose flow $\varphi_s = e^{sX}$ generates the dynamical evolution on $\dot{\mathcal{M}}$, is thus a zero mode of $\Omega$. Note that, from Cartan’s formula (2.13), if we require that a vector field $X$ obeys (3.15), then it immediately implies $\mathcal{L}_X\Omega = 0$ so that $\Omega$ is preserved. The symplectic form $\Omega$ is closed, however when projected into $T^*\mathcal{M}$ it becomes degenerate. One can see this through the matrix representation (Sternberg, 1964, Thm. 6.1):
\[ \Omega = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -I \\ 0 & I & 0 \end{pmatrix}, \tag{3.16} \]

which has a vanishing determinant. Therefore, the phase space of the dissipative Hamiltonian system written in the autonomous form (3.3) is a presymplectic manifold (see again Fig. 1).

### 3.2 Presymplectic integrators

Since a dissipative Hamiltonian system (3.3) admits a symplectification, we can construct structure-preserving discretizations by imposing constraints on a symplectic integrator. More precisely, we can apply any standard symplectic integrator to the higher-dimensional, conservative system (3.7). Then by the gauge choice in (3.11) and (3.13) we obtain an integrator for the dissipative system (3.3). Such a method will preserve a presymplectic structure. Accordingly, we refer to such integrators as presymplectic integrators.

**Definition 3.2.** A numerical map $\phi_h$ is a presymplectic integrator for a time-dependent Hamiltonian system if it is obtained from a symplectic integrator for its symplectification under the gauge fixing (3.13) and (3.11).

Since the Hamiltonian $\mathcal{H}$ of the higher-dimensional system (3.7) is conserved, we can apply standard results for symplectic integrators to derive conclusions about presymplectic integrators and thereby derive properties of systems without an underlying conservation law.

**Theorem 3.3.** A presymplectic integrator $\phi_h$ of order $r$ preserves the time-varying Hamiltonian (assumed to be Lipschitz) up to
\[ H \circ \phi_h^t = H \circ \varphi_{th} + \mathcal{O}(h^r), \tag{3.17} \]

for exponentially large simulation times $s_t = h\ell = \mathcal{O}(h^r e^{r\rho_h/h})$.

**Proof.** Let $\Phi_h : \mathbb{R}^{2n+2} \to \mathbb{R}^{2n+2}$ be a symplectic integrator for the the higher-dimensional Hamiltonian system (3.7). Since $\mathcal{H}$ is conserved, Theorem 2.6 implies
\[ \mathcal{H} \circ \Phi_h^t = \mathcal{H} \circ \Psi_{th} + \mathcal{O}(h^r), \tag{3.18} \]
Figure 2: A presymplectic integrator closely preserves the time-varying Hamiltonian; see Theorem 3.3. The numerical trajectories lie on the same presymplectic manifold as the continuous dissipative system and the numerical value $H(t_\ell, q_\ell, p_\ell)$ exhibits a small and bounded error with respect to the true value, $H(t_\ell, q(t_\ell), p(t_\ell))$, of size $O(h^r)$.

with $s_\ell = O(h^r e^{c h_0/h})$ and where $\Psi_s$ denotes the true flow. With the gauge choice (3.11) and (3.13) the system is projected into the hypersurface (3.10), thus $\Psi_s$ reduces to $\varphi_s$, which is the true flow of (3.3), and $\Phi_h$ reduces to $\phi_h : \mathbb{R}^{2n+1} \to \mathbb{R}^{2n+1}$, which approximates $\varphi_s$. Thus, using these maps together with the substitution of (3.10) into (3.18), we conclude:

$$H \circ \phi_h^\ell + p_0(\ell h) = H \circ \varphi_h^\ell + p_0(\ell h) + O(h^r).$$

(3.19)

It is important to recall that $p_0$ is a fixed function of time and this is why it can be canceled on both sides to finally give (3.17).

Theorem 3.3 is an extension of Theorem 2.6 to dissipative Hamiltonian systems. The numerical solutions of presymplectic integrators are thus within a small and bounded error $O(h^r)$ from the hypersurface (3.10); see Fig. 2. Hence, whatever convergence or decay properties the system may have, a presymplectic integrator will closely reproduce its behavior.

In Appendix C we provide a step-by-step procedure for constructing presymplectic integrators. The procedure is straightforward, essentially involving an application of symplectic integrators with a natural choice for incorporating the time variable.

### 3.3 Preserving convergence rates in optimization

We now consider how presymplectic integrators can be used to construct rate-matching optimization algorithms. We consider a standard optimization problem:

$$\min_{q \in \mathcal{M}} f(q),$$

(3.20)

and we study dissipative systems obtained from the Hamiltonian (1.3), which we repeat here for convenience:

$$H = e^{-\eta(t)} T(t, q, p) + e^{\eta(t)} f(q),$$

(3.21)
where the functions $\eta_1$ and $\eta_2$ are positive and nondecreasing. They are responsible for introducing dissipation in the system. We assume that the kinetic energy $T$ is Lipschitz continuous. As an example, the well-known Caldirola-Kanai Hamiltonian in physics (Caldirola, 1941; Kanai, 1948) is a particular case of (3.21). The Bregman Hamiltonian in optimization (Wibisono et al., 2016) is also a particular case.

Given a specific system, we assume that a convergence rate $f(q(t)) - f^*$ is known, where $f^*$ is a minimum of $f$ in a neighborhood of the initial conditions. We are now able to prove Theorem 1.1 stated in the introduction as a consequence of Theorem 3.3.

**Proof of Theorem 1.1.** Substituting (3.21) into (3.17), where we now fix $s = t$, yields:

$$f(q_{\ell}) \leq f(q(t_{\ell})) + e^{-\eta_1(t_{\ell}) - \eta_2(t_{\ell})} \left\{ T(t_{\ell}, q(t_{\ell}), p(t_{\ell})) - T(t_{\ell}, q_{\ell}, p_{\ell}) \right\} + Kh_r e^{-\eta_2(t_{\ell})},$$  

(3.22)

for all $t_{\ell} = O(h_r e^{h_0/h})$ and for some constant $K > 0$. Recall that $q_{\ell}$ and $q(t_{\ell})$ are the discrete and continuous trajectories, respectively. Let $L_T$ be the Lipschitz constant of $T$. Substituting the global error (2.5) into the second term yields:

$$|f(q_{\ell}) - f(q(t_{\ell}))| \leq h_r e^{-\eta_2(t_{\ell})} \left( K + L_T C(e^{L_{\phi^t}} - 1)e^{-\eta_1(t_{\ell})} \right).$$  

(3.23)

We thus conclude that

$$f(q_{\ell}) = f(q(t_{\ell})) + O(h_r e^{-\eta_2(t_{\ell})}),$$  

(3.24)

provided

$$e^{L_{\phi^t}} - 1)e^{-\eta_1(t_{\ell})} < \infty,$$  

(3.25)

for all sufficiently large $t$.

Therefore, under suitable conditions, presymplectic integrators reproduce the continuous rates of convergence of dissipative Hamiltonian systems. We make several remarks:

- As mentioned earlier, the assumptions of Theorem 1.1 are mild; the kinetic energy being Lipschitz is naturally satisfied in a range of applications, and the Lipschitz condition (1.7) is also satisfied for a large class of integrators. The underlying reason is because $\mathcal{M}$ is a smooth manifold.

- We used a conservative global error (2.5) to bound the kinetic term in (3.22). A specialized analysis may yield a better bound, which could allow condition (3.25) to be relaxed. However, this would have to be justified by a dedicated backward-error analysis.

- Increasing the order of accuracy $r$ influences (3.24) in a beneficial way. The error is dominated by $e^{-\eta_2}$, however, which suggests that, in this optimization context, using higher-order integrators may not be of practical importance. That said, higher-order methods tend to be more stable so there may be other benefits in their use.
• Interestingly, the error in (3.24) is even smaller than the error in approximating the Hamiltonian (3.17), thanks to the function $\eta_2$. If $\eta_2$ grows just enough, this error may become completely negligible, even for large step sizes and integrators of low order.

• We recall that the restriction $t_\ell = h\ell \sim h_0 e^{\eta_0/h}$ may be irrelevant. To give an idea, with $r = 1$, $h_0 = 1$, and $h = 0.1$ we have iterations $\ell \sim 6 \cdot 10^4$, and with $h = 0.01$ we have $\ell \sim 10^{13}$.

### 3.3.1 The choice of damping

Let us comment on some consequences of the condition (3.25), which can impose some limitations. There are two ways to satisfy it. The first is if the method converges quickly so $e^{L_\phi t_\ell - \eta_1(t_\ell)}$ remains bounded regardless of $\eta_1$, or equivalently we enforce $t_\ell \leq \bar{t}$ where $\bar{t}$ is a solution to

$$L_\phi \bar{t} - \eta_1(\bar{t}) \leq C,$$

for some constant $C > 0$. The second way to satisfy (3.25) is if $\eta_1$ grows fast enough, allowing $t_\ell$ to be arbitrarily large. For instance, setting:

$$\eta_1(t) = \gamma t,$$

for some constant $\gamma \geq L_\phi$ suffices for all $t \geq 0$. Curiously, this choice implies constant damping and can be related to the heavy-ball method (Polyak, 1963); see also França et al. (2019).  

As an alternative, from (3.25) we have

$$\left(1 + L_\phi t + \frac{1}{2}(L_\phi t)^2 + \cdots\right) e^{-\eta_1(t)} < \infty,$$

which is satisfied if $(L_\phi t)^m e^{-\eta_1(t)} < \infty$ for all powers $m$; i.e., $\eta_1(t) \sim m \log(L_\phi t)$. Thus, one can choose

$$\eta_1(t) = \gamma \log t,$$

with a suitable $\gamma > 0$ to ensure that (3.28) holds up to some high-order term. Also curiously, the choice (3.29) is related to the damping of Nesterov’s method (Nesterov, 1983) which attains the optimal convergence rate for convex functions $f$.  

Note that the choice (3.29) can guarantee (3.28) only up to a finite power $m$, thus we are on the edge of violating this condition—in fact we are formally violating it but in practice

---

7 With $\eta_1 = \eta_2 = \gamma t$ and $T = \frac{1}{2}||p||^2$ into (3.21) the equations of motion give $\ddot{q} + \gamma \dot{q} = -\nabla f(q)$, which is a nonlinear generalization of the damped harmonic oscillator. The heavy-ball method (Polyak, 1963) is actually a structure-preserving—a conformal symplectic—discretization of this system (França et al., 2019).

8 Choosing $\eta_1 = \eta_2 = \gamma \log t$ yields the differential equation $\ddot{q} + \frac{\gamma}{t} \dot{q} = -\nabla f(q)$. Nesterov’s method can be seen as a discretization of this system (Su et al., 2016).
this may yield a viable algorithm. On the other hand, the choice (3.27) may be overkill. It may be more reasonable to consider an intermediate alternative:

$$\eta_1(t) = \gamma_1 \log t + \gamma_2 t^\delta,$$

(3.30)

for constants $0 < \delta \leq 1$ and $\gamma_1, \gamma_2 > 0$. With this choice the condition on the $m$th term in the series (3.28) becomes $L_m t^m e^{-\gamma_1 t^\delta} < \infty$, which can be guaranteed even if $\gamma_1 < m$ with suitable choices of $\gamma_2$ and $\delta$.

Summing up, presymplectic integrators are able to match the continuous rates provided the condition (3.25) is satisfied, which involves an appropriate choice of damping. If the system is overdamped this condition is more likely to hold, however the system would tend to be slower. On the other hand, if the damping is weak the system tends to be fast, but at the cost of violating (3.25). We thus see a delicate tradeoff and the ideal choice is problem-dependent, given that $L_\phi$ in (3.25) is related to the Lipschitz constant of the original vector field; i.e., to the Lipschitz constant of $\nabla f$.

## 4 Bregman Dynamics

Given that the Bregman Hamiltonian (Wibisono et al., 2016) provides a general framework for deriving continuous-time optimization procedures, we consider this case in some detail. The Hamiltonian has the form

$$H = e^{\alpha + \gamma} \{ D_{h^*}(\nabla h(q) + e^{-\gamma p}, \nabla h(q)) + e^\beta f(q) \},$$

(4.1)

where $\alpha$, $\beta$, and $\gamma$ are all functions of time $t$, and are required to satisfy the following scaling conditions:

$$\frac{d\beta}{dt} \leq e^\alpha, \quad \frac{d\gamma}{dt} = e^\alpha.$$

(4.2)

The kinetic energy in (4.1) is given in terms of the Bregman divergence,

$$D_h(y, x) \equiv h(y) - h(x) - \langle \nabla h(x), y - x \rangle,$$

(4.3)

which is nonnegative for a given convex function $h : \mathcal{M} \to \mathbb{R}$. Recalling the definition of the convex dual, $h^*$ of $h$, defined by the Legendre-Fenchel transformation:

$$h^*(p) \equiv \sup_v \{ \langle p, v \rangle - h(v) \},$$

(4.4)
one can show that Hamilton’s equations are given by:

\begin{align}
\dot{q} &= e^\alpha \left\{ \nabla h^* \left( \nabla h(q) + e^{-\gamma} p \right) - q \right\}, \\
\dot{p} &= -e^{\alpha + \gamma} \nabla^2 h(q) \left\{ \nabla h^* \left( \nabla h(q) + e^{-\gamma} p \right) - q \right\} + e^\alpha p - e^{\alpha + \beta + \gamma} \nabla f(q). 
\end{align}

(4.6a)

(4.6b)

In the case where the function \( f \) is convex, Wibisono et al. (2016) show that the convergence rate of this system is given by:

\[ f(q(t)) - f^* = O \left( e^{-\beta(t)} \right). \]

(4.7)

Moreover, for a given \( \alpha \), the optimal rate is obtained with \( \dot{\beta} = e^\alpha \), thus \( \beta = \gamma + C \), for some constant \( C \), and both are determined in terms of \( \alpha \). We thus have

\[ f(q(t)) - f^* = O \left( e^{-\beta(t)} \right), \quad \beta(t) = \int^t e^{\alpha(t')}dt', \quad \gamma(t) = \beta(t) + C. \]

(4.8)

A choice considered by Wibisono et al. (2016) is:

\[ \alpha = \log c - \log t, \quad \beta = c \log t + C, \quad \gamma = c \log t \quad (c > 0), \]

(4.9)

whereby the convergence rate (4.8) becomes polynomial \( O \left( t^{-c} \right) \). Another possibility is

\[ \alpha = \log c, \quad \beta = ct, \quad \gamma = ct + C \quad (c > 0), \]

(4.10)

leading to an exponential rate \( O(e^{-ct}) \).

4.1 Separable case

To consider a case where the Bregman Hamiltonian is separable, let us start with the choice \( h(x) = \frac{1}{2} x \cdot M x \), for a symmetric positive semidefinite matrix \( M \), so that \( h^*(x) = \frac{1}{2} x \cdot M^{-1} x \) and the Bregman divergence is given by \( D_{h^*}(y, x) = \frac{1}{2} (y - x) \cdot M^{-1} (y - x) \). In this case the Hamiltonian (4.1) takes the form

\[ H = \frac{1}{2} e^{-\eta_1(t)} p \cdot M^{-1} p + e^{\eta_2(t)} f(q), \]

(4.11)

where we defined

\[ \eta_1 \equiv \gamma - \alpha, \quad \eta_2 \equiv \alpha + \beta + \gamma. \]

(4.12)

\[ \dot{q} + \left( e^\alpha - \dot{\alpha} \right) \dot{q} + e^{2\alpha + \beta} \left[ \nabla^2 h \left( q + e^{-\alpha} \dot{q} \right) \right]^{-1} \nabla f(q) = 0. \]

(4.5)

We see that \( \alpha \) basically controls the damping, while \( 2\alpha + \beta \) increases the strength of the force \( \nabla f \). Both play a major role in the stability of the system, and they are not independent since \( \dot{\beta} \leq e^\alpha \).
The quadratic kinetic energy is standard in classical mechanics and we see that $M$ plays the role of a mass matrix. We thus have the following equations of motion:

$$
\dot{q} = e^{-\eta_1(t)} M^{-1} p, \quad \dot{p} = -e^{\eta_2(t)} \nabla f(q).
$$  \hspace{1cm} (4.13)

One can now use any presymplectic integrator to obtain an optimization algorithm; see Appendix C. Because the Hamiltonian (4.11) is separable, standard approaches yield explicit methods which are convenient in practice. Assuming that we use a presymplectic integrator of order $r$, Theorem 1.1 tells us that the continuous rate of convergence will be preserved as

$$
f(q_{\ell}) - f^* = O \left( e^{-\beta(t_{\ell})} \right) + O \left( h^r e^{-\alpha(t_{\ell}) - 2\beta(t_{\ell})} \right)
\sim e^{-\beta(t_{\ell})} \left( 1 + h^r e^{-\alpha(t_{\ell}) - \beta(t_{\ell})} \right)
\sim e^{-\beta(t_{\ell})},
$$  \hspace{1cm} (4.14)

provided $\eta_1$ as defined in (4.12) obeys the condition (3.25).

We present two explicit methods. Using the presymplectic Euler method given by (C.2), which is of order $r = 1$, we obtain:

$$
\begin{align*}
p_{\ell+1} &= p_{\ell} - h e^{\eta_2(t_{\ell})} \nabla f(q_{\ell}), \\
t_{\ell+1} &= t_{\ell} + h, \\
q_{\ell+1} &= q_{\ell} + h e^{-\eta_1(t_{\ell})} M^{-1} p_{\ell+1}.
\end{align*}
$$  \hspace{1cm} (4.15)

This algorithm requires only one gradient computation per iteration. In a similar way, using the presymplectic leapfrog method (C.9), which is of order $r = 2$, we obtain:

$$
\begin{align*}
t_{\ell+1/2} &= t_{\ell} + h/2, \\
q_{\ell+1/2} &= q_{\ell} + (h/2) e^{-\eta_1(t_{\ell+1/2})} M^{-1} p_{\ell}, \\
p_{\ell+1} &= p_{\ell} - h e^{\eta_2(t_{\ell+1/2})} \nabla f(q_{\ell+1/2}), \\
t_{\ell+1} &= t_{\ell+1/2} + h/2, \\
q_{\ell+1} &= q_{\ell+1/2} + (h/2) e^{-\eta_1(t_{\ell+1/2})} M^{-1} p_{\ell+1}.
\end{align*}
$$  \hspace{1cm} (4.16)

This method again only requires one gradient computation per iteration, and it is more accurate. One can now choose any suitable scaling functions in (4.12) and substitute into either (4.15) or (4.16) to obtain a specific optimization algorithm.

### 4.2 Nonseparable case

We turn to the case of a nonseparable Hamiltonian, where the integrators considered thus far yield implicit updates that require solving nonlinear equations. This not only increases the computational burden but can affect the numerical stability. In particular, for the Bregman Hamiltonian (4.1), we need a construction suited to nonseparable cases. In order to obtain
explicit methods, we use the approach of Tao (2016). Given a Hamiltonian $H(t,q,p)$, we double its degrees of freedom by introducing the augmented Hamiltonian:

$$
\bar{H}(t,q,p,\bar{t},\bar{q},\bar{p}) \equiv H(t,q,\bar{p}) + H(\bar{t},\bar{q},p) + \frac{\xi}{2} \left( \|q - \bar{q}\|^2 + \|p - \bar{p}\|^2 \right).
$$

(4.17)

Here $\xi > 0$ is a coupling constant that controls the strength of the last term, which forces $q = \bar{q}$ and $p = \bar{p}$. The presymplectic structure of this system is now

$$
\Omega = -dH \wedge dt + dp \wedge dq^j - d\bar{H} \wedge d\bar{t} + d\bar{p} \wedge d\bar{q}^j \quad (j = 1,\ldots,n).
$$

(4.18)

Hamilton’s equations, obtained from (4.17), will preserve $\Omega$. The equations of motion are equivalent to those of the original system when $q = \bar{q}$, $p = \bar{p}$ and $t = \bar{t}$. We thus propose the following numerical maps:

$$
\phi^A_h \left( \begin{array}{c} t \\ q \\ p \\ \bar{t} \\ \bar{q} \\ \bar{p} \end{array} \right) = \left( \begin{array}{c} t + h \\ q + h \nabla_q H(t,q,p) \\ p - h \nabla_p H(\bar{t},\bar{q},\bar{p}) \\ \bar{t} + h \\ \bar{q} + h \nabla_{\bar{q}} H(\bar{t},\bar{q},\bar{p}) \\ \bar{p} - h \nabla_{\bar{p}} H(\bar{t},\bar{q},\bar{p}) \end{array} \right),
$$

$$
\phi^B_h \left( \begin{array}{c} t \\ q \\ p \\ \bar{t} \\ \bar{q} \\ \bar{p} \end{array} \right) = \left( \begin{array}{c} t + h \\ q + h \nabla_p H(\bar{t},\bar{q},\bar{p}) \\ p - h \nabla_q H(t,q,p) \\ \bar{t} + h \\ \bar{q} + h \nabla_{\bar{q}} H(\bar{t},\bar{q},\bar{p}) \\ \bar{p} - h \nabla_{\bar{p}} H(\bar{t},\bar{q},\bar{p}) \end{array} \right),
$$

$$
\phi^C_h \left( \begin{array}{c} t \\ q \\ p \\ \bar{t} \\ \bar{q} \\ \bar{p} \end{array} \right) = \frac{1}{2} \left( \begin{array}{c} 2t \\ q + \bar{q} + \cos(2\xi h)(q - \bar{q}) + \sin(2\xi h)(p - \bar{p}) \\ p + \bar{p} - \sin(2\xi h)(q - \bar{q}) + \cos(2\xi h)(p - \bar{p}) \\ 2\bar{t} \\ q + \bar{q} - \cos(2\xi h)(q - \bar{q}) - \sin(2\xi h)(p - \bar{p}) \\ p + \bar{p} + \sin(2\xi h)(q - \bar{q}) - \cos(2\xi h)(p - \bar{p}) \end{array} \right).
$$

(4.19)

A presymplectic integrator for any (nonseparable) time-dependent Hamiltonian system can then be constructed by composing these maps. For instance, the Strang composition,

$$
\phi^A_{h/2} \circ \phi^B_{h/2} \circ \phi^C_h \circ \phi^B_{h/2} \circ \phi^A_{h/2},
$$

(4.20)

is known to generate a method of order $r = 2$—this is the same composition as the leapfrog. Note that the maps (4.20) are completely explicit in all variables and this approach works for any general time-dependent Hamiltonian.

In particular, for the Bregman Hamiltonian (4.1) one just needs to substitute the gradients $\dot{q} = \nabla_p H$ and $\dot{p} = -\nabla_q H$ from (4.6) into (4.19), followed by the composition (4.20). This yields a completely explicit, second-order integrator for the general Bregman dynamics. Thanks to Theorem 1.1, this generates an optimization algorithm that may closely preserve the continuous rate of convergence (4.7) for suitable functions $\alpha$, $\beta$ and $\gamma$.

---

10 It is not necessary to introduce the same term for $t$ and $\bar{t}$ since they will be be equal thanks to (3.11). The constant $\xi$ has to be tuned in practice; see Tao (2016) for details.
5 Discussion

We have introduced “presymplectic integrators” as a class of discretizations that are suitable for the simulation of explicit time-dependent Hamiltonian systems. This framework accommodates a large class of dissipative dynamical systems that are appropriate for applications to optimization. We have also shown that, besides preserving the presymplectic structure of the system, such methods nearly preserve the time-varying Hamiltonian and exhibit long-term stability, despite the absence of a conservation law (see Theorem 3.3). This extends, into a dissipative setting, the most important property of symplectic integrators which are restricted to conservative systems. Thus, our approach and theoretical conclusions may be of interest not only to the field of optimization, but also to a variety of other disciplines where the simulation of dissipative systems play an important role, such as nonequilibrium statistical physics, complex systems, economics, and control theory.

Focusing on optimization, we showed that, for a general class of dissipative systems arising from a Hamiltonian in the form (1.3), presymplectic integrators are able to preserve the continuous rates of convergence up to a negligible error, as long as certain conditions are satisfied (see Theorem 1.1). This provides a systematic, first-principles approach to deriving “rate-matching” optimization algorithms, thereby obviating the need for a discrete-time convergence analysis.\textsuperscript{11} As a concrete example, we considered the general Bregman Hamiltonian, providing general methods from which specific optimization algorithms can be derived, in both the separable and the nonseparable case. Hopefully, this will motivate future numerical explorations.

Finally, we comment on two problems that might deserve further study. First, we showed that condition (3.25) is essential and in particular leads to the damping strategies (3.27) and (3.29) related to the heavy ball and Nesterov’s method, respectively. We also argued that a more elaborate choice (3.30) may be beneficial. Thus, finding the optimal damping for a given class of problems seems an interesting problem. Second, it would be appealing to find numerical schemes with a better global error (see Eq. (1.7)), or obtain improved bounds for existing methods, since this would automatically relax the condition (3.25).

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\textsuperscript{11}Of course, if one wants to study fine details of a specific algorithm’s performance, a discrete-time analysis, together with an appropriate backward-error analysis, may be necessary.
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### A Background on Differential Geometry

In this section we provide a brief, informal overview of those elements of differential geometry that we need for our results. For a fuller presentation see any of the excellent textbooks on the subject (e.g., Arnold et al., 2006; Abraham and Marsden, 1978; Berndt, 2001; Aebischer et al., 1994; Sternberg, 1964).

Let $\mathcal{M} \equiv \mathcal{M}^n$ be a smooth $n$-dimensional manifold. Let $p \in \mathcal{M}$ and $(U, x)$ be a chart so that $p$ can be assigned local coordinates, $x(p) \equiv (x^1(p), \ldots, x^n(p))$ in $\mathbb{R}^n$. The coordinates...
x and the point p are used interchangeably, and we often refer to the former to indicate a point on the manifold. To each x ∈ M there is an associated vector space TₓM called the tangent space. The coordinates x induces a basis ∂₁, . . . , ∂ₚ in TₓM, where ∂ᵢ = ∂/∂xᵢ. Thus, Vₓ = Vⱼ(x)∂ⱼ is a representation of the vector Vₓ ∈ TₓM.¹² The collection of all tangent vectors of M form the tangent bundle TM. One can then represent a (contravariant) vector field by the differential operator

\[ V(x) = Vⱼ(x)∂ⱼ, \]

which can be seen as a cross section of the tangent bundle TM. For a given x, the vector field V assigns a single vector, V(x) = Vₓ. Note that a point in TM has 2n coordinates, x¹, . . . , xₙ, V¹, . . . , Vₙ.

To each Vₓ there is an associated dual vector, αₓ : TₓM → ℝ; i.e., α is a linear functional. Dual vectors are called covectors or 1-forms and they live on the cotangent space denoted by Tₓ*M. The collection of all 1-forms at every point of M forms the cotangent bundle T*M. The coordinate basis x induces a dual basis dx¹, . . . , dxₙ in TXM, defined by dxⱼ(∂ⱼ) = δⱼ, where δ is the Kronecker delta. Similarly to (A.1) one can now represent a 1-form field α ∈ T*M as

\[ α(x) = αⱼ(x)dxⱼ, \]

which is a cross section of the cotangent bundle T*M. The action of dual vectors is thus α(V)|ₓ = V(α)|ₓ = αⱼ(x)Vⱼ(x). Note that T*M is a 2n-dimensional space where a point has coordinates x¹, . . . , xₙ, α₁, . . . , αₙ. The cotangent bundle T*M is very special since it can be shown that it is itself a symplectic manifold (see Theorem 2.3).

A general tensor T of rank (p, q) is a multilinear map T : ⊗ᵢ Tₓ*Μ ⊗ⱼ TₓΜ → ℝ. In a coordinate basis it is written as

\[ T = T^j₁...jₚ₁...ₖₗdx^{j₁}...dx^{jₚ}∂₁...∂ₚdx^{k₁}...dx^{kₗ}. \]

In calculations, it is useful to focus on the components T^j₁...jₚ₁...ₖₗ alone and omit the basis altogether. A contravariant tensor is a tensor of rank (p, 0), for some p ≥ 1, and a covariant tensor is a tensor of rank (0, q), for some q ≥ 1. A q-form is a (0, q)-tensor which is totally antisymmetric in its indices. In a basis it is denoted as

\[ α = \frac{1}{q!}αⱼ₁...ⱼₗdx^{j₁}...dx^{jₗ}, \]

where ∧ denotes the exterior product.¹³ Given another p-form β, one can compose the (p + q)-form α ∧ β which obeys

\[ α ∧ β = (-1)^{pq}β ∧ α. \]

¹² We use Einstein’s summation convention throughout, where a pair of upper and lower indices are summed over; e.g., Xⱼ∂ⱼ = ∑ₙ Xᵢ∂ᵢ, αⱼkTᵢjk = ∑ₙ αⱼkδᵢj, etc. Upper indices denote components of vectors—also called contravariant vectors—in TₓM, while lower indices denote components of dual vectors—also called covectors—which belong to the cotangent space Tₓ*Μ.

¹³ For two 1-forms α, β ∈ Tₓ*Μ we have (α ∧ β)(v, w) = α(v)β(w) − β(v)α(w), for v, w ∈ TₓM.
It is useful to introduce a notation to denote the space of $q$-forms at $x$, namely $\bigwedge^q T^*_x M$, and as before we obtain a bundle $\bigwedge^q T^* M$ of $q$-form fields by allowing the coefficient $\omega_{j_1\ldots j_q}(x)$ to depend on $x$.

Another important operation is the exterior derivative:

$$d : \bigwedge^q T^* M \rightarrow \bigwedge^{q+1} T^* M,$$

which can be defined componentwise as

$$d\alpha(x) \equiv \frac{1}{q!} \frac{\partial \omega_{j_1\ldots j_q}(x)}{\partial x^k} dx^k \wedge dx^{j_1} \wedge \cdots \wedge dx^{j_q}.$$  (A.7)

This is a linear operation, $d(c_1\alpha + c_2\beta) = c_1d\alpha + c_2d\beta$, for any forms $\alpha$ and $\beta$. Its main properties are given by the equation:

$$d(\alpha \wedge \beta) = (d\alpha) \wedge \beta + (-1)^q \alpha \wedge (d\beta),$$  (A.8)

and by the identity

$$d^2 = d \circ d = 0.$$  (A.9)

A differential form $\omega$ is said to be closed if $d\omega = 0$. A differential $q$-form $\omega$ is said to be exact if $\omega = d\lambda$ for some $(q - 1)$-form $\lambda$. Trivially, from (A.9) every exact form is closed. The Poincaré lemma ensures the converse, namely that every closed form is also exact.$^{14}$

Given a vector $v \in T_x M$ and a $q$-form $\alpha \in \bigwedge^q T^*_x M$, the interior product $i_v \alpha$ is a $(q - 1)$-form defined by

$$(i_v \alpha)(v_2, \ldots, v_q) \equiv \alpha(v, v_2, \ldots, v_q).$$  (A.10)

In components, this is simply the contraction $(i_v \alpha)_{j_2\ldots j_q} = v^k \alpha_{kj_2\ldots j_q}$. The interior product is also linear and satisfies an analogous relation to (A.8):

$$i_v(\alpha \wedge \beta) = (i_v \alpha) \wedge \beta + (-1)^q \alpha \wedge (i_v \beta).$$  (A.11)

Since one can only operate on elements of the same vector space, it is necessary to introduce a mapping that makes it possible to move geometric objects over the manifold. In particular, given a function $F : M \rightarrow N$ between two manifolds $M$ and $N$, for any function $g : \mathcal{N} \rightarrow \mathbb{R}$ one defines the pushforward—also called the differential—of $v \in T_x M$ to be the vector $F_* v \in T_{F(x)} N$ defined by the operation

$$(F_*v)(g) \equiv v(g \circ F).$$  (A.12)

The pullback goes in the opposite direction, i.e., given a $q$-form $\alpha \in T^*_{F(x)} N$ we obtain the $q$-form $F^* \alpha \in T^*_x M$ through

$$F^* \alpha(v_1, \ldots, v_q) \equiv \alpha(F_* v_1, \ldots, F_* v_q),$$  (A.13)

$^{14}$This holds for contractible manifolds, which is the case for smooth manifolds as considered in this paper.
for $v_j \in T_x \mathcal{M}$, $j = 1, \ldots, q$. The pullback allows us to move $q$-forms over the manifold. By introducing the concept of a flow: $\varphi_t : \mathcal{M} \to \mathcal{M}$ induced by a vector field $X$ of $T \mathcal{M}$, i.e., $\varphi_t = e^{tX}$, one can define the Lie derivative of a $q$-form as in (2.4). A flow $\varphi_t$ is a diffeomorphism and thus $\varphi_t^* = (\varphi_{-t})^*$. In this case, one can consider the pullback of not only $q$-forms but arbitrary $(p,q)$-tensors. Thus, the Lie derivative of a general tensor field $T$ can be defined by

$$\mathcal{L}_X T|_x \equiv \frac{d}{dt} \bigg|_{t=0} \varphi_t^* T|_{\varphi_t(x)}.$$  \hfill (A.14)

Given a differentiable form $\omega$ and a vector field $X$, we say that $X$ preserves $\omega$ if and only if

$$\mathcal{L}_X \omega = 0.$$  \hfill (A.15)

From the definition (A.14) this implies

$$\varphi_t^* \omega = \omega.$$  \hfill (A.16)

In this sense, any map $\phi : \mathcal{M} \to \mathcal{N}$ is said to be canonical if it preserves $\omega$; i.e., $\phi^* \omega = \omega$. In the case of Hamiltonian systems $\omega$ is the symplectic 2-form, and Hamiltonian flows generate canonical transformations, which are symplectomorphisms.

A very useful formula is Cartan’s magic formula

$$\mathcal{L}_X \alpha = d \circ i_X \alpha + i_X \circ d \alpha,$$  \hfill (A.17)

for any differentiable form $\alpha$. Some other useful formulas are

$$\mathcal{L}_X (\alpha \wedge \beta) = (\mathcal{L}_X \alpha) \wedge \beta + \alpha \wedge (\mathcal{L}_X \beta), \hfill (A.18)$$
$$\mathcal{L}_{[X,Y]} \alpha = [\mathcal{L}_X, \mathcal{L}_Y] \alpha, \hfill (A.19)$$
$$\mathcal{L}_X \circ d = d \circ \mathcal{L}_X, \hfill (A.20)$$
$$i_{[X,Y]} = \mathcal{L}_X \circ i_Y - i_Y \circ \mathcal{L}_X.$$  \hfill (A.21)

Here, $[\mathcal{L}_X, \mathcal{L}_Y] \equiv \mathcal{L}_X \mathcal{L}_Y - \mathcal{L}_Y \mathcal{L}_X$ is the Lie bracket. The same definition holds for $[X,Y] = XY - YX$, and in this case one refers to $[\cdot, \cdot]$ as the commutator of two vector fields.

### B Generalized Conformal Hamiltonian Systems

Conformal Hamiltonian systems (McLachlan and Perlmutter, 2001) provide an alternative approach to introducing dissipation into Hamiltonian systems. In this approach, one modifies Hamilton’s equations directly by adding a linear term in the momentum. It is easy to construct structure-preserving discretizations for these systems since one can split the system into conservative and dissipative parts, then apply a standard symplectic integrator to the former, while integrating the latter exactly. This approach has been recently explored
in optimization (França et al., 2019). The purpose of this section is to show that a generalization of conformal Hamiltonian systems correspond to a particular case of the explicit time-dependent Hamiltonian formalism introduced in Section 3. As a consequence, one can construct (generalized) conformal symplectic integrators from presymplectic integrators (see Definition 3.2).

Consider a time-independent Hamiltonian, \( H = H(q, p) \), and assume a modified form of Hamilton’s equations given by
\[
\frac{dq_j}{dt} = \frac{\partial H}{\partial p_j}, \quad \frac{dp_j}{dt} = -\frac{\partial H}{\partial q_j} - \gamma(t)p_j \quad (j = 1, \ldots, n).
\] (B.1)

The conformal case (McLachlan and Perlmutter, 2001) assumes that the damping coefficient \( \gamma(t) = \gamma \) is constant. In this formulation, the Hamiltonian vector field is
\[
X_H = \frac{\partial H}{\partial q^i} \frac{\partial}{\partial q^i} + \frac{\partial H}{\partial p_i} \frac{\partial}{\partial p_i},
\] (B.2)
and by the same geometric approach previously discussed one can see that the equations of motion (B.1) are equivalent to
\[
i_X_H(\omega) = -dH - \gamma(t)\lambda,
\] (B.3)
with \( \omega \) defined in (2.11) and where \( \lambda \equiv p_j dq_j \) is the Liouville-Poincaré 1-form. From Cartan’s formula (2.13) we conclude that the symplectic structure contracts as
\[
L_X_H \omega = -\gamma(t)\omega, \quad \gamma(t) \equiv \int t_{\gamma(t')} dt',
\] (B.4)
or equivalently\(^{15}\)
\[
\varphi_t^* \omega = e^{-\eta(t)}\omega, \quad \eta(t) \equiv \int t_{\gamma(t')} dt'.
\] (B.5)

Finally, in this setting \( H \) is the energy of the system and it dissipates as
\[
\frac{dH}{dt} = -\gamma(t) \frac{\partial H}{\partial p_j} p_j.
\] (B.6)

We now show that generalized conformal Hamiltonian systems corresponds to a particular case of the time-dependent Hamiltonian formalism. Define the time-dependent Hamiltonian \( K \) by
\[
K(t, Q, P) \equiv e^{\eta(t)} H(Q, e^{-\eta(t)} P), \quad Q \equiv q, \quad P \equiv e^{\eta(t)} p,
\] (B.7)
where \( H \) is the original Hamiltonian of (B.1). The standard Hamiltonian equations (1.2) yield:
\[
\frac{dQ_j}{dt} = \frac{\partial K}{\partial P_j} = \frac{\partial H(q, p)}{\partial p_j}, \quad \frac{dP_j}{dt} = -\frac{\partial K}{\partial Q_j} = -e^{\eta(t)} \frac{\partial H(q, p)}{\partial q_j},
\] (B.8)
which when written in terms of \((q, p)\) are precisely (B.1). Therefore, one can construct discretizations that preserve the contraction of the symplectic form (B.4) through presymplectic integrators (see Definition 3.2) with the explicit time-dependent Hamiltonian \( K \).

\(^{15}\)From this one concludes that the phase-space volumes contract as \( L_{X_H} \text{vol}^{2n} = -n\gamma(t) \text{vol}^{2n} \), so that \( \varphi_t^* \text{vol}^{2n} = e^{-nC(t)} \text{vol}^{2n} \). This is a dissipative version of Liouville’s theorem; note the dimension dependency.
C Constructing Presymplectic Integrators

As stated in Definition 3.2, a presymplectic integrator is a reduction of a higher-dimensional symplectic integrator under the specific choice of coordinates (3.11) and (3.13). To follow this prescription one must perform three steps:

1. Pick a symplectic integrator and apply it to the Hamiltonian system (3.7). This results in updates for \((q^0, p_0)\) and for the spatial components \((q^j, p_j)\);
2. Set \(q^0 = t\) and ignore \(p_0\) completely—\(p_0\) is just the actual value of the Hamiltonian as a function of time and does not participate in the dynamics;
3. Set \(s = t\).

While these formal steps make clear that we are respecting the symplectification prescription, in practice, these three steps can be reduced to the following:

1. Apply any symplectic integrator to the time-dependent Hamiltonian \(H(t, q, p)\) in the “natural way.” By this we mean to simply include additional updates for the time variable \(t\) with the same rule as the coordinates \(q^j\).

We will provide some examples below that should make this procedure clear.

**Presymplectic Euler** For a conservative Hamiltonian system, one has the following version of the first-order symplectic Euler method (Hairer et al., 2006):

\[
\begin{align*}
p_{\ell+1} &= p_\ell - h \nabla_q H(q_\ell, p_{\ell+1}), \\
qu_{\ell+1} &= q_\ell + h \nabla_p H(q_\ell, p_{\ell+1}).
\end{align*}
\]

(C.1)

Considering a time-dependent Hamiltonian \(H(t, q, p)\), since \(t\) must be updated in the same way as \(q\), we immediately obtain the following presymplectic Euler method:

\[
\begin{align*}
p_{t+1} &= p_t - h \nabla_q H(t_\ell, q_\ell, p_{\ell+1}), \\
t_{\ell+1} &= t_\ell + h, \\
qu_{\ell+1} &= q_\ell + h \nabla_p H(t_\ell, q_\ell, p_{\ell+1}).
\end{align*}
\]

(C.2)

Note how we have simply added an update for \(t\), following the same structure as the update for \(q\). Also, there is a dual version of (C.1) given by (Hairer et al., 2006):

\[
\begin{align*}
qu_{\ell+1} &= q_\ell + h \nabla_p H(q_{\ell+1}, p_\ell), \\
p_{\ell+1} &= p_\ell - h \nabla_q H(q_{\ell+1}, p_\ell).
\end{align*}
\]

(C.3)
From this we obtain the following alternative to (C.2)

\begin{align*}
    t_{\ell+1} &= t_\ell + h, \\
    q_{\ell+1} &= q_\ell + h \nabla_p H(t_{\ell+1}, q_{\ell+1}, p_\ell), \\
    p_{\ell+1} &= p_\ell - h \nabla_q H(t_{\ell+1}, q_{\ell+1}, p_\ell).
\end{align*}

Both of these methods, namely (C.2) and (C.4), are of order \( r = 1 \). Note that for an arbitrary Hamiltonian \( H \) in general they are implicit; i.e., nonlinear equations have to be solved to obtain either \( q_{\ell+1} \) or \( p_{\ell+1} \). However, when the Hamiltonian is separable in the form

\[ H = T(t, p) + V(t, q) \tag{C.5} \]

these methods become completely explicit in all variables resulting in cheap implementations.

**Presymplectic leapfrog** One of the versions of the leapfrog method for a conservative Hamiltonian system is the following second-order method Hairer et al. (2006):

\begin{align*}
    p_{\ell+1/2} &= p_\ell - (h/2) \nabla_q H(q_\ell, p_{\ell+1/2}), \\
    q_{\ell+1} &= q_\ell + (h/2) \left( \nabla_p H(q_\ell, p_{\ell+1/2}) + \nabla_p H(q_{\ell+1}, p_{\ell+1/2}) \right), \\
    p_{\ell+1} &= p_{\ell+1/2} - (h/2) \nabla_q H(q_{\ell+1}, p_{\ell+1/2}). \tag{C.6}
\end{align*}

For a time-dependent Hamiltonian \( H(t, q, p) \) we include appropriate updates for time and obtain the following *presymplectic leapfrog* method:

\begin{align*}
    p_{\ell+1/2} &= p_\ell - (h/2) \nabla_q H(t_\ell, q_\ell, p_{\ell+1/2}), \\
    t_{\ell+1} &= t_\ell + h, \\
    q_{\ell+1} &= q_\ell + (h/2) \left( \nabla_p H(t_\ell, q_\ell, p_{\ell+1/2}) + \nabla_p H(t_{\ell+1}, q_{\ell+1}, p_{\ell+1/2}) \right), \\
    p_{\ell+1} &= p_{\ell+1/2} - (h/2) \nabla_q H(t_{\ell+1}, q_{\ell+1}, p_{\ell+1/2}). \tag{C.7}
\end{align*}

There is another dual version of the leapfrog method (C.6), which for conservative systems is given by (Hairer et al., 2006):

\begin{align*}
    q_{\ell+1/2} &= q_\ell + (h/2) \nabla_p H(q_{\ell+1/2}, p_\ell), \\
    p_{\ell+1} &= p_\ell - (h/2) \left( \nabla_q H(q_{\ell+1/2}, p_{\ell+1/2}) + \nabla_q H(q_{\ell+1/2}, p_{\ell+1}) \right), \\
    q_{\ell+1} &= q_{\ell+1/2} + (h/2) \nabla_p H(q_{\ell+1/2}, p_{\ell+1}). \tag{C.8}
\end{align*}

This leads to an alternative version of the presymplectic leapfrog, given by:

\begin{align*}
    t_{\ell+1/2} &= t_\ell + h/2, \\
    q_{\ell+1/2} &= q_\ell + (h/2) \nabla_p H(t_{\ell+1/2}, q_{\ell+1/2}, p_\ell), \\
    p_{\ell+1} &= p_\ell - (h/2) \left( \nabla_q H(t_{\ell+1/2}, q_{\ell+1/2}, p_\ell) + \nabla_q H(t_{\ell+1/2}, q_{\ell+1/2}, p_{\ell+1}) \right), \\
    t_{\ell+1} &= t_{\ell+1/2} + h/2, \\
    q_{\ell+1} &= q_{\ell+1/2} + (h/2) \nabla_p H(t_{\ell+1/2}, q_{\ell+1/2}, p_{\ell+1}). \tag{C.9}
\end{align*}

Again, in general these methods are implicit, but for a separable Hamiltonian (C.5) they become completely explicit in all variables. Moreover, only one gradient computation per iteration is necessary, even though these methods are of order \( r = 2 \).
Higher-order methods  Suzuki (1990) and Yoshida (1990) have presented an elegant general approach to construct arbitrarily higher-order symplectic integrators. It assumes we are given a base method $\phi_h$ of order $2r$ ($r \geq 1$). An integrator of order $2r+2$ is then obtained by the composition:

$$
\phi_{\tau_0} \circ \phi_{\tau_1} \circ \phi_{\tau_0}, \quad \tau_0 = \frac{1}{2 - 2^{r+1}/\sqrt{2}}, \quad \tau_1 = -\frac{2^{r+1}/\sqrt{2}}{2 - 2^{r+1}/\sqrt{2}}. \quad (C.10)
$$

One can start with any base method of choice, such as the leapfrog. From this new integrator of order $2r + 2$ one may proceeds recursively to construct even higher-order methods. It is easy to adapt this procedure to presymplectic integrators by carefully adding an update for time $t$. However, the number of gradient computations of the Suzuki-Yoshida approach grows very fast with increasing order, thus this approach quickly becomes unfeasible. Moreover, the truncation error of such methods tend to be rather large, although the fourth-order method obtained from the leapfrog is competitive and interesting. (See McLachlan and Quispel (2006) and especially McLachlan (2002) for an interesting discussion.)