AUTOMATIC DISCRETE DIFFERENTIATION AND ITS APPLICATIONS

A PREPRINT

Ai Ishikawa
Department of Computational Science,
Graduate School of System Informatics, Kobe University
1-1 Rokkodai-cho, Nada-ku, Kobe 657-8501, Japan
a-ishikawa@stu.kobe-u.ac.jp

Takaharu Yaguchi
Department of Computational Science,
Graduate School of System Informatics, Kobe University
1-1 Rokkodai-cho, Nada-ku, Kobe 657-8501, Japan
yaguchi@pearl.kobe-u.ac.jp

May 22, 2019

ABSTRACT

In this paper, a method for automatically deriving energy-preserving numerical methods for the Euler–Lagrange equation and the Hamilton equation is proposed. The derived energy-preserving scheme is based on the discrete gradient method. In the proposed approach, the discrete gradient, which is a key tool for designing the scheme, is automatically computed by a similar algorithm to the automatic differentiation. Besides, the discrete gradient coincides with the usual gradient if the two arguments required to define the discrete gradient are the same. Hence the proposed method is an extension of the automatic differentiation in the sense that the proposed method derives not only the discrete gradient but also the usual gradient. Due to this feature, both energy-preserving integrators and variational (and hence symplectic) integrators can be implemented in the same programming code simultaneously. This allows users to freely switch between the energy-preserving numerical method and the symplectic numerical method in accordance with the problem-setting and other requirements. As applications, an energy-preserving numerical scheme for a nonlinear wave equation and a training algorithm of artificial neural networks derived from an energy-dissipative numerical scheme are shown.

Keywords geometric integration · energy-preserving numerical scheme · discrete gradient method · discrete differential · automatic differentiation · automatic discrete differentiation

1 Introduction

Structure-preserving numerical methods are numerical methods that discretize differential equations while preserving good properties of the equations [4, 10, 13, 14, 17]. The main target equations of these methods are differential equations derived using analytical mechanics, i.e., the Hamilton equations and the Euler–Lagrange equations. These equations have properties such as the energy conservation law and symplecticity. A numerical scheme that preserves the latter property is called a symplectic integrator and a scheme that preserves the energy conservation law is called an energy-preserving numerical method. In this paper, energy-preserving numerical methods are mainly of interest.

Energy-preserving numerical methods conserve the energy within the rounding errors. For such numerical methods, the discrete gradient method (e.g. [15]), the discrete variational derivative method (e.g. [14]), the Hamiltonian boundary value method (e.g. [11]), continuous-stage Runge–Kutta methods (e.g. [22]) are known. In addition, in many methods,
not only the energy conservation law but also the energy dissipation law can be reproduced. However, these schemes are often implicit and therefore computationally expensive. Therefore, it has been often considered to be inferior to symplectic numerical methods in practical usefulness. Against this background, recent studies have made it possible to derive linearly implicit or even explicit schemes based on the discrete gradient method (e.g. [11, 19, 21, 23]), and thereby the discrete gradient method became a sufficiently practical technique. In particular, dissipative differential equations lead to optimization techniques, including steepest descent methods, which is called “the backpropagation” and is employed for training artificial neural networks in machine learning. Therefore, application to artificial neural networks, which has been rapidly developed in recent years, can be expected.

Meanwhile, the discrete gradient method requires a discrete version of the gradient vector called a discrete gradient. Because of this requirement, the discrete gradient method is difficult to use for non-expert users, compared to symplectic numerical methods which have a wealth of numerical libraries. The need to derive discrete gradients is a major barrier to the use for practical users, in particular, those of artificial neural networks.

In order to improve this situation, in this paper, we propose a method to automatically derive a discrete gradient of a given function. Out method is based on the idea of the automatic differentiation [16], which is, roughly, a way to automatically derive a computer program that computes the derivative of a certain function that is given as a program. The proposed approach applies this idea to discrete gradients and derives from a given program a program that computes the discrete gradients. Besides, the discrete gradient coincides with the usual gradient if the two arguments required in the evaluation of the discrete gradient are the same. Hence the proposed method is an extension of the automatic differentiation in the sense that the method computes not only the discrete gradient but also the usual gradient. In summary, the significances of the paper are as follows.

- The automatic differentiation is extended to “automatic discrete differentiation,” which automatically computes the discrete gradient and the usual gradient as a special case of the discrete gradient.
- This algorithm allows ones to implement energy-preserving numerical schemes and symplectic integrators simultaneously in the same programming code;
- just by specifying the energy functions, more precisely the Hamiltonian or the Lagrangian, of the target systems.

This paper is organized as follows. In Section 2, we will briefly explain energy-preserving numerical methods, particularly the discrete gradient method. In Section 3, the algorithms of the automatic differentiation and the automatic discrete differentiation will be explained. In Section 4, as an illustration, we will derive an energy-preserving numerical method for a nonlinear wave equation, which is used in a model of a nonlinear piano string [9]. Besides, a dissipative system called the heavy ball with friction system [1] will be discretized to derive a learning algorithm for multi-layer perceptrons. In Section 5, we will make concluding remarks.

2 Outline of the Discrete Gradient Method

The equations of motion of analytical mechanics are the Hamilton equation

\[
\frac{du}{dt} = S(u)\nabla H(u)
\]  

(1)

and the Euler–Lagrange equation

\[
\frac{\partial L}{\partial u} - \frac{d}{dt} \frac{\partial L}{\partial \dot{u}} = 0.
\]

(2)

Here, \( u \) is a variable representing a state of the system. \( u \) is generally a point on a manifold, but for simplicity, we assume \( u \in \mathbb{R}^n \) in this paper. \( H \) is Hamiltonian and represents the energy of the system. \( S \) is a skew-symmetric matrix that depends on \( u \). \( S \) is usually assumed to be non-degenerate, but may be degenerate if only the energy conservation law is considered. \( L \) is a Lagrangian, which is a function of \( u \) and \( \dot{u} \), where \( \dot{u} = du/dt \).

\[ \text{(1) and (2) has the energy-conservation property, that is,} \]

\[ \frac{dH}{dt} = 0 \]

for the Hamilton equation and

\[ \frac{d}{dt} \left( L - \dot{u} \cdot \frac{\partial L}{\partial \dot{u}} \right) = 0 \]
for the Euler–Lagrange equation.

Among several energy-preserving numerical schemes proposed in literature (see, e.g., [17]), a typical method is the discrete gradient method [15]. The discrete gradient method is a method to discretize an equation by replacing a gradient in the equation with a vector called a discrete gradient. A discrete gradient is defined as follows.

Definition 1. For $H : \mathbb{R}^n \rightarrow \mathbb{R}$, $\nabla H : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}^n$ that satisfies the following conditions is called a discrete gradient of $H$:

$$H(u) - H(v) = \nabla H(u,v) \cdot (u - v), \quad \nabla H(u,u) = \nabla H(u).$$

The first condition corresponds to the property $dH(\Delta u) = \nabla H \cdot \Delta u$ for $\Delta u \in \mathbb{R}^n$, which is the characteristic condition of the gradient vector of $H$. Here, $dH$ represents the Fréchet derivative of $H$, and $\Delta u$ represents an infinitesimal change of $u$. Because discrete gradients are not uniquely determined, several methods for derivation are known (see, e.g., [4, 6, 7, 11, 14, 15, 17]). In the discrete gradient method, the numerical scheme for the Hamilton equation is defined as follows:

$$\frac{u^{(n+1)} - u^{(n)}}{\Delta t} = S(u^{(n+1)}, u^{(n)}) \nabla (u^{(n+1)}, u^{(n)}),$$

where $u(n)$ represents an approximation of $u(n\Delta t)$ and $\Delta t$ is the time-step size. $S(u^{(n+1)}, u^{(n)})$ is a consistent and skew-symmetric approximation of $S$. This numerical scheme preserves the energy conservation law in the sense that

$$\frac{H(u^{(n+1)}) - H(u^{(n)})}{\Delta t} = 0.$$

Similarly, energy-preserving numerical schemes can be derived for the Euler–Lagrange equation [23]. For simplicity, we consider a natural system, which is the Euler–Lagrange equation derived using the Lagrangian of the following form:

$$L(u, \dot{u}) = \frac{1}{2} |\dot{u}|^2 - V(u),$$

where $M$ is a mass matrix and $V$ is a potential function. Suppose that an approximation of the Lagrangian $L(u, \dot{u})$ is given as

$$L_d(u^{(n)}, u^{(n+1)}) = \left( \frac{u^{(n+1)} - u^{(n)}}{\Delta t} \right)^2 - \nabla (u^{(n)}, u^{(n+1)}).$$

$V(u^{(n)}, u^{(n+1)})$ is an approximation of $V(u)$. Then, the following scheme

$$\frac{u^{(n+1)} - u^{(n)} - u^{(n-1)} + u^{(n-2)}}{2\Delta t^2} = -\nabla V(u^{(n+1)}, u^{(n)})$$

preserves the energy conservation law:

$$\frac{u^{(n+1)} - u^{(n)}}{\Delta t} - \frac{u^{(n-1)} - u^{(n-2)}}{\Delta t} = \frac{L_d(u^{(n)}, u^{(n+1)})}{\Delta t}.$$

### 3 Automatic Differentiation and Automatic Discrete Differentiation

As we have seen in the previous section, if a discrete gradient can be derived, the design of numerical schemes is straightforward for both the Lagrangian and Hamiltonian formalisms. Although a number of methods to derive discrete gradients have been established, the derivation may not be easy for non-experts, especially when the given Hamiltonian and Lagrangian are complicated functions. Against this background, we propose a method for automatically deriving a discrete gradient. The proposed algorithm is obtained by redesigning the automatic differentiation (see, e.g., [16]) for computing discrete gradients. Although the automatic differentiation has the forward mode and the reverse mode, we consider only the reverse mode because this mode is for calculating the gradient of a given function. Besides, the description of the automated differentiation is simpler for computing the Fréchet derivative than the gradient. Hence, in the following, we consider the discrete counter part of the Fréchet derivative, which is called the discrete differential [8].
Definition 2. A discrete differential \( \overline{\alpha} H : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R} \) of a function \( H : \mathbb{R}^n \to \mathbb{R} \) is a function that satisfies the following conditions:

- \( \overline{\alpha} H \) is linear with respect to the first variable if the other two are held constant,
- \( H(u) - H(v) = \overline{\alpha} H(u - v; u, v) \),
- \( \overline{\alpha} H(\cdot; u, u) = \alpha H_u(\cdot) \),

where \( \alpha H_u \) denotes the Fréchet derivative of \( H \) at \( u \).

Because \( \overline{\alpha} H(w; u, v) \) with \( u, v \) fixed is a linear function with respect to \( w \), there exists a vector \( \nabla H \) such that

\[
\nabla H \cdot w = \overline{\alpha} H(w; u, v).
\]

This vector \( \nabla H \) is a discrete gradient of \( H \). Therefore it is sufficient to compute a discrete differential in order to obtain a discrete gradient.

Automatic differentiation is a technique for converting a program for calculating a function into a program for calculating a derivative of the function. In particular, this method is characterized in that the evaluation of the differential value is accurate and fast as compared with, for example, the finite difference method [16]. Indeed, computational results do not include truncation errors. The computational amount necessary for the calculation of the gradient is about three or four times the amount of the evaluation of the function. In this section, the idea of this algorithm in the case of the computation of the gradient will be explained. The basic idea is to use the chain rule and the product rule to replace differentiations of compositions of functions and products of functions with corresponding operations. For example, for two functions \( f : \mathbb{R} \to \mathbb{R}, g : \mathbb{R} \to \mathbb{R} \), the derivative of the composite function is calculated by the chain rule as follows:

\[
\frac{\partial}{\partial x}(f \circ g)(x) = \frac{\partial f}{\partial g} \frac{\partial g}{\partial x}.
\]

Similarly, the sum or product of \( f \) and \( g \) is processed as below:

\[
\frac{\partial}{\partial x}(f + g) = \frac{\partial f}{\partial x} + \frac{\partial g}{\partial x}, \quad \frac{\partial}{\partial x}(fg) = g \frac{\partial f}{\partial x} + f \frac{\partial g}{\partial x}.
\]

Suppose now that a procedure for computing a function is provided and one wishes to compute the derivative of that function. Based on the above-described rules of differential calculation, basic operations such as a sum, a product or a composition of functions that appear in the calculation procedure of the function may be replaced with corresponding differential versions.

More precisely, in the automatic differentiation, evaluation of a function, which is assumed to be given as a procedure in a computer program, is decomposed into a series of smaller atomic operations. Suppose that the gradient of a function \( y : \mathbb{R}^n \to \mathbb{R} \) is needed to be computed. In the computation of the function, the \( n \) input variables \( (x_1, \ldots, x_n) \) are transformed into intermediate variables \( v_1, \ldots, v_l \) by applying elementary operations, e.g., addition, multiplication, sin, cos, exp, and other elementary functions. Each elementary operation is denoted by \( \phi_j \). Each intermediate variable \( v_j \) is the output value of \( \phi_j \). For simplicity, all variables including the output variable \( y \) are written as a vector:

\[
v = (v_{n+1}, v_{n+2}, \ldots, v_{l+1}) \in \mathbb{R}^{l+n+1},
\]

\[
v_{n+1} = x_n, v_{n+2} = x_{n-1}, \ldots, v_0 = x_1, v_{l+1} = y.
\]

In this representation, each elementary operation \( \phi_j \) is extended to a transformation \( \Phi : \mathbb{R}^n \to \mathbb{R}^{l+n} \) of the state variable \( v \), that is,

\[
y = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \cdot \Phi_{l} \circ \Phi_{l-1} \circ \Phi_{l-2} \circ \cdots \circ \Phi_1(v).
\]

Differentiating this expression gives for an infinitesimal change \( \Delta v \) of \( v \)

\[
dy = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \cdot d\Phi_l \cdot d\Phi_{l-1} \cdot d\Phi_{l-2} \cdots d\Phi_1(\Delta v).
\]
We apply the idea of this method to computation of the discrete differential and thereby the discrete gradient.

**Example 1.** For example, the value of a function
\[ f = \sin(w_1x_1 + w_2x_2), \quad f : \mathbb{R} \to \mathbb{R}, \quad x_1, x_2, w_1, w_2 \in \mathbb{R} \]
is computed in the following manner:

1. \( v_0 = x_1, v_{-1} = x_2 \),
2. \( v_1 = \phi_1(w_1, v_0) \),
3. \( v_2 = \phi_2(w_2, v_{-1}) \),
4. \( v_3 = \phi_3(v_1, v_2) \),
5. \( v_4 = \phi_4(v_3) \),
6. \( y = v_4 \).

where
\[ \phi_1(a, b) = ab, \quad \phi_2(a, b) = ab, \quad \phi_3(a, b) = a + b, \quad \phi_4(a) = \sin(a). \]

To compute the gradient vector of the function \( f \), the above procedure is executed in the reverse order:

1. \( dy = dv_4 \),
2. \( dv_4 = d\phi_4(v_3) = d(\sin(v_3)) = \cos(v_3)dv_3 \),
3. \( dv_3 = d\phi_3(v_1, v_2) = dv_1 + dv_2 \),
4. \( dv_2 = d\phi_2(w_2, v_{-1}) = w_2dv_{-1} \),
5. \( dv_1 = d\phi_1(w_1, v_0) = w_1dv_0 \),
6. \( dv_0 = dx_1, dv_{-1} = dx_2 \).

Next, successive substitution of the above results gives
\[
\begin{align*}
df(\delta x_1, \delta x_2) &= dy(\delta x_1, \delta x_2) \\
&= \cos(v_3)dv_3(\delta x_1, \delta x_2) \\
&= \cos(v_3)(dv_1(\delta x_1, \delta x_2) + dv_2(\delta x_1, \delta x_2)) \\
&= \cos(v_3)(w_1dv_0(\delta x_1, \delta x_2) + w_2dv_{-1}(\delta x_1, \delta x_2)) \\
&= \cos(v_3)(w_1\delta x_1 + w_2\delta x_2).
\end{align*}
\]

In particular, the gradient vector of \( f \) is obtained as
\[
\begin{align*}
\frac{\partial f}{\partial x_1} &= w_1 \cos(v_3), \\
\frac{\partial f}{\partial x_2} &= w_2 \cos(v_3).
\end{align*}
\]

We apply the idea of this method to computation of the discrete differential and thereby the discrete gradient. The application is straightforward; in fact, the important tools \( \bar{\Delta} \) and \( \bar{\Delta}^2 \) also hold for the discrete differential.

**Theorem 1.** For any \( x_1, x_2 \in \mathbb{R} \) and functions \( f : \mathbb{R} \to \mathbb{R}, g : \mathbb{R} \to \mathbb{R}, g_1 : \mathbb{R} \to \mathbb{R}, g_2 : \mathbb{R} \to \mathbb{R}, \)
\[ f(g_1(x_1)) - f(g_2(x_2)) = \bar{\Delta} f(\cdot; g_1(x_1), g_2(x_2)) \circ \bar{\Delta} g(x_1 - x_2; x_1, x_2). \]

Besides, if \( \bar{\Delta} f(\cdot; x_1, x_2) \) and \( \bar{\Delta} g(\cdot; x_1, x_2) \) are discrete differentials for \( f \) and \( g \) respectively, then the following \( \bar{\Delta}(f + g) \) and \( \bar{\Delta}(fg) \) are discrete differentials for \( f + g \) and \( fg \):
\[
\begin{align*}
\bar{\Delta}(f + g)(\cdot; x_1, x_2) &= \bar{\Delta} f(\cdot; x_1, x_2) + \bar{\Delta} g(\cdot; x_1, x_2), \\
\bar{\Delta}(fg)(\cdot; x_1, x_2) &= \frac{f(x_1) + f(x_2)}{2} \bar{\Delta} g(\cdot; x_1, x_2) + \frac{g(x_1) + g(x_2)}{2} \bar{\Delta} f(\cdot; x_1, x_2).
\end{align*}
\]
Example 2. The discrete differential is computed by the successive substitution of the results. The following example illustrates this.

\[ f(x_1)g(x_1) - f(x_2)g(x_2) = \frac{f(x_1) + f(x_2)}{2}(g(x_1) - g(x_2)) + \frac{g(x_1) + g(x_2)}{2}(f(x_1) - f(x_2)). \]

\[ \phi(x_1, x_2) = \frac{f(x_1) + f(x_2)}{2}(g(x_1) + g(x_2)) + \frac{g(x_1) - g(x_2)}{2}(f(x_1) - f(x_2)). \]

In addition, for a general nonlinear elementary function \( f : \mathbb{R} \to \mathbb{R} \)

\[ df(\delta x; x_1, x_2) = \begin{cases} \frac{f(x_1) - f(x_2)}{x_1 - x_2} \delta x & (x_1 \neq x_2) \\ df(\delta x; x_1) & (x_1 = x_2) \end{cases} \]

is a discrete differential of \( f \), where \( x_1, x_2, \delta x \in \mathbb{R} \). By using all the above tools, a discrete gradient is obtained in the exactly same way as the automatic differentiation; what must be done is just to replace the differentials of elementary operations with the discrete differentials shown above.

Suppose again that for a given function \( f \), each elementary operation is represented by a function \( \phi_j \) and each intermediate variable \( v_j \) is the output value of \( \phi_j \). All variables are again written as a vector

\[ v = (v_{n+1}, \ldots, v_0, v_1, \ldots, v_{l+1}) \in \mathbb{R}^{l+n+1}, \quad (7) \]

\[ v_{n+1} = x_n, \quad v_{n+2} = x_{n-1}, \ldots, v_0 = x_1, \quad v_{l+1} = y. \quad (8) \]

In the computation of the discrete differential \( df(\cdot; x_1, \ldots, x_{n+1}, \ldots, x_{n+1}) \), we have two input variable vectors \((x_1, \ldots, x_{n,1})^T\) and \((x_2, \ldots, x_{n,2})^T\). Therefore all variables in (7) must be replaced by corresponding pairs of variables:

\[ ((v_{n+1}, v_{n+1}), \ldots, (v_0, v_0), (v_1, v_1), \ldots, (v_{l+1}, v_{l+1})) \in \mathbb{R}^{2 \times \cdots \times \mathbb{R}^{2}}, \]

\[ v_{n+1} = x_n, \quad v_{n+2} = x_{n-1}, \ldots, v_0 = x_1, \quad v_{l+1} = y. \]

The pairs of intermediate variables are computed by applying the elementary operations \( \phi_j \)'s to each elements of the input pairs; for example, if \( v_j = \phi_j(v_j-1, v_j-2) \) then \( v_{1,1} = \phi_1(v_{1,1-1}, v_{1,1-2}) \) and \( v_{1,2} = \phi_1(v_{1,2-1}, v_{1,2-2}) \). In the same way as the automatic differentiation, first the value of the function \( f \) is evaluated for the both input vectors \((x_1, \ldots, x_{n,1})^T\) and \((x_2, \ldots, x_{n,2})^T\), along with the discrete differential of the elementary operations. Then the discrete differential is computed by the successive substitution of the results. The following example illustrates this procedure.

Example 2. For example, the discrete differential \( df(\cdot; (x_{1,1}, x_{2,1}), (x_{1,2}, x_{2,2})) \) of the function

\[ f = \sin(w_1 x_1 + w_2 x_2), \quad f : \mathbb{R} \to \mathbb{R}, \quad x_1, x_2, w_1, w_2 \in \mathbb{R} \]

is computed in the following way. First this function is evaluated for the two input vectors:

1. \((v_{0,1}, v_{0,2}) = (x_{1,1}, x_{1,2}), \quad (v_{1,1}, v_{1,2}) = (x_{2,1}, x_{2,2}).\)
2. \((v_{1,1}, v_{1,2}) = (\phi_1(w_1, v_{0,1}), \phi_1(w_1, v_{0,2})).\)
3. \((v_{2,1}, v_{2,2}) = (\phi_2(w_2, v_{1,1}, v_{1,2})).\)
4. \((v_{3,1}, v_{3,2}) = (\phi_3(v_{1,1}, v_{1,2}), \phi_3(v_{2,1}, v_{2,2})).\)
5. \((v_{4,1}, v_{4,2}) = (\phi_4(v_{3,1}), \phi_4(v_{3,2})).\)
6. \((y_1, y_2) = (v_{4,1}, v_{4,2}).\)

where

\[ \phi_1(a, b) = ab, \quad \phi_2(a, b) = ab, \quad \phi_3(a, b) = a + b, \quad \phi_4(a) = \sin(a). \]

The discrete differential of each elementary operations are calculated at the same time:
To employ a general-purpose numerical integrator such as a Runge–Kutta method, it is required to first define the Hamiltonian, or the Lagrangian of the system to be simulated and to derive the equation of motion from it. This implies that besides being easy to use, this approach is free from human errors. Using discrete differentiation, a user can automatically generate a scheme from a Lagrangian or a Hamiltonian.

Remark 1. Similarly to the automatic differentiation, the automatic discrete differentiation can be implemented by operator overloading or source transformation. Because the discrete gradient computed by the automatic discrete differentiation is based on operator overloading. Indeed, the scheme (3) becomes the scheme by the variational integrator [20] to be implemented simultaneously in a computer program. Indeed, the scheme (3) becomes the scheme by the variational integrator

\[
\frac{u^{(n+1)} - 2u^{(n)} + u^{(n-1)}}{2\Delta t^2} = -\nabla V(u^{(n)}),
\]

which is known to be symplectic, if the variables in the scheme (3) are replaced as follows:

\[
\begin{align*}
    u_j^{(n+1)} &\leftarrow u_j^{(n+1)}, \\
    u_j^{(n)} &\leftarrow u_j^{(n)}, \\
    u_j^{(n-1)} &\leftarrow u_j^{(n-1)}, \\
    u_j^{(n-2)} &\leftarrow u_j^{(n-2)}.
\end{align*}
\]

Remark 2. Since the discrete differential has the property \(\delta H(\cdot; u, v) = \delta H_u(\cdot)\), the analytical derivative of \(H\) can be obtained by computing \(\Delta H(\cdot; u, v)\) using the automatic discrete differentiation algorithm. This allows schemes by energy-preserving numerical methods and schemes by the variational integrator [20] to be implemented simultaneously in a computer program. Indeed, the scheme (3) becomes the scheme by the variational integrator

\[
\frac{u^{(n+1)} - 2u^{(n)} + u^{(n-1)}}{2\Delta t^2} = -\nabla V(u^{(n)}),
\]

which is known to be symplectic, if the variables in the scheme (3) are replaced as follows:

\[
\begin{align*}
    u_j^{(n+1)} &\leftarrow u_j^{(n+1)}, \\
    u_j^{(n)} &\leftarrow u_j^{(n)}, \\
    u_j^{(n-1)} &\leftarrow u_j^{(n-1)}, \\
    u_j^{(n-2)} &\leftarrow u_j^{(n-2)}.
\end{align*}
\]

Remark 3. Using discrete differentiation, a user can automatically generate a scheme from a Lagrangian or a Hamiltonian. In particular, it is worth noting that even derivation of the equation is not required to derive the scheme. To employ a general-purpose numerical integrator such as a Runge–Kutta method, it is required to first define the Hamiltonian or the Lagrangian of the system to be simulated and to derive the equation of motion from it. This can be done in a straightforward way by differentiating Hamiltonian or Lagrangian, which, however, often requires cumbersome calculations. On the other hand, using the proposed method, high-quality simulations by energy-preserving schemes and symplectic schemes can be performed by describing only the Hamiltonian or the Lagrangian, i.e., the energy functions of the system. This implies that besides being easy to use, this approach is free from human errors.

## 4 Applications

In this section, we derive an energy-preserving numerical method for a nonlinear wave equation and also derive an algorithm for training artificial neural networks as applications.
4.1 Energy-Preserving Scheme for a Nonlinear Wave Equation

As a simple example, we consider the nonlinear wave equation, which is used in a model of nonlinear string motion [9],

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial}{\partial x} \left( \frac{\partial u}{\partial x} \sqrt{1 + \left( \frac{\partial u}{\partial x} \right)^2} \right) = 0, \quad x \in (0, 1).$$

For simplicity, we impose the periodic boundary condition

$$u(t, x + 1) = u(t, x).$$

This equation is derived as the Euler–Lagrange partial differential equation with the Lagrangian

$$\mathcal{L}(u, \frac{\partial u}{\partial t}) = \int_0^1 \left( \frac{1}{2} \left( \frac{\partial u}{\partial t} \right)^2 - \left( 1 + \left( \frac{\partial u}{\partial x} \right)^2 \right)^{\frac{3}{2}} \right) \, dx.$$

All we need to do is to discretize the Lagrangian, for example,

$$\mathcal{L}_d(u_1^{(n)}, \ldots, u_M^{(n)}, u_1^{(n+1)}, \ldots, u_M^{(n+1)})$$

$$= \sum_{j=1}^M \left( \frac{1}{2} \left( \frac{u_j^{(n+1)} - u_j^{(n)}}{\Delta t} \right)^2 - \left[ 1 + \frac{1}{2} \left( \frac{u_{j+1}^{(n)} - u_j^{(n)}}{\Delta x} \right)^2 + \frac{1}{2} \left( \frac{u_j^{(n)} - u_{j-1}^{(n)}}{\Delta x} \right)^2 \right]^{\frac{3}{2}} \right) \Delta x,$$

where \( \Delta t \) and \( \Delta x \) are temporal and spatial step sizes respectively and \( u_j^{(n)} \) is an approximation of \( u(n \Delta t, j \Delta x) \).

If we have a discrete gradient for the potential term

$$\phi(u_1^{(n)}, \ldots, u_M^{(n)}, u_1^{(n+1)}, \ldots, u_M^{(n+1)})$$

$$= \sum_{j=1}^M \left( \left[ 1 + \frac{1}{2} \left( \frac{u_j^{(n)} - u_{j-1}^{(n)}}{\Delta x} \right)^2 \right] \left( \frac{u_j^{(n)} - u_{j-1}^{(n)}}{\Delta x} \right)^2 \right)^{\frac{1}{2}} \Delta x,$$

the energy-preserving numerical scheme is obtained from [3] immediately:

$$\frac{u_j^{(n+1)} - u_j^{(n)} - u_j^{(n-1)} + u_j^{(n-2)}}{2\Delta t^2} + (\nabla \phi(u_1^{(n)}, \ldots, u_M^{(n)}, u_1^{(n-1)}, \ldots, u_M^{(n-1)}))_j = 0,$$

where \((\nabla \phi(u_1^{(n)}, \ldots, u_M^{(n-1)}))_j\) denotes the \(j\)th component of the discrete gradient.

We implemented the algorithm of the automatic discrete differential in c++ using operator overloading so that in our implementation a pseudo-code like that shown in Algorithm [1] works. In this pseudo-code, “dd_double” denotes the class of real variables. In Step 6 the computational graph is generated; in “dd_double” class, the operators are overloaded so that a new node is generated implicitly for each operation and added to the computational tree. At the 8th step, each component of the discrete gradient is computed by the algorithm shown in the previous section and stored as a member variable of “dd_u,” which is extracted by calling a member function “discrete_differential()” at the 10th step.

We solved numerically the nonlinear wave equation by using the above procedure under the initial condition

$$u_j^{(0)} = u_j^{(-1)} = u_j^{(-2)} = \sin(2\pi j \Delta x).$$

Please note that because the scheme is a multi-step scheme we need additional initial conditions, which must be carefully set in general for accuracy and stability. The above choice is just for tests and is not recommended. For details, see, e.g., [5]. We set \( \Delta t = 0.001, \Delta x = 1.0/80 \).
Algorithm 1 Pseudo-code of the scheme for the nonlinear wave equation

1: for each time step $n$:
2:   $dd\_double\_dd\_u(N)$
3: for each $j$:
4:   Initialize $dd\_u(j)$
5: $L \leftarrow 0$
6: for each $j$:
7:   $L \leftarrow L + \sqrt{1 + 0.5 \ast (dd\_u(j + 1) - dd\_u(j))/dx \ast (dd\_u(j + 1) - dd\_u(j))/dx + 0.5 \ast (dd\_u(j) - dd\_u(j - 1))/dx \ast (dd\_u(j) - dd\_u(j - 1))/dx}$
8: $L$compute discrete differential()
9: for each $j$:
10: $u(n + 1, j) = u(n, j) + u(n - 1, j) - u(n - 2, j) + 2 \ast dt \ast dt \ast dd\_u(j).discrete\_differential()$

Figures 1 and 2 are the graph of the computed $u_j^{(n)}$’s and the discrete energy respectively. We also solved this equation by using a scheme with the discrete gradient that is derived by hand:

$$\nabla\phi(u_1^{(n)}, \ldots, u_M^{(n-1)}) =$$

$$\begin{bmatrix}
\frac{1}{2} \left( \frac{u_{n+1}^{(n)} - u_{n}^{(n)}}{\Delta x} \right) + \frac{1}{2} \left( \frac{u_{n+1}^{(n-1)} - u_{n}^{(n-1)}}{\Delta x} \right) \\
1 + \frac{1}{2} \left( \frac{u_{n+1}^{(n)} - u_{n}^{(n)}}{\Delta x} \right)^2 + \frac{1}{2} \left( \frac{u_{n+1}^{(n-1)} - u_{n}^{(n-1)}}{\Delta x} \right)^2 \\
\frac{1}{2} \left( \frac{u_{n}^{(n)} - u_{n-1}^{(n)}}{\Delta x} \right) + \frac{1}{2} \left( \frac{u_{n}^{(n-1)} - u_{n-1}^{(n-1)}}{\Delta x} \right)
\end{bmatrix}
$$

This complicated vector is certainly a discrete gradient. In fact, Figures 3 and 4 show the graph of $u_j^{(n)}$’s and the discrete energy function computed by using this vector as the discrete gradient in the scheme. Any significant difference is observed between the results by the two schemes. Although the displacement of the energy in the case of the automatic discrete differential is a little bit smaller than that by the other one, this displacement is due to the rounding errors and hence dependent on implementation. These results illustrate that the proposed automatic discrete differentiation algorithm gives the numerical results of the same quality as the scheme derived by hand, while the former does not require any knowledge of discrete gradients nor any hard calculations. Even derivation of the equation is not required; only Lagrangian or Hamiltonian, that is, energy functions are needed.
4.2 Application to Designing Training Algorithms of Artificial Neural Networks

In this section, a simple training algorithm for multi-layer perceptrons is designed as an application of the proposed approach. As an example, we consider a perceptron with $N$ inputs, a middle layer with $M$ vertices, and $L$ outputs:

$$y_j = g_j \left( \sum_{k=1}^{M} (w_{jk} h_k) \right), \quad h_k = f_k \left( \sum_{l=1}^{N} (\bar{w}_{kl} x_l) \right).$$

$x_1, \ldots, x_N$ are the input variables, $h_1, \ldots, h_M, y_1, \ldots, y_L$ are the output variables from the hidden layer and the output layer. $f_1, \ldots, f_M, g_1, \ldots, g_L$ denotes activation functions. We assume that these functions are smooth. $w_{jk}, \bar{w}_{kl}$ denote the weights, which are determined by minimizing a loss function $E\left( \{w_{jk}, \bar{w}_{kl}\} \right)$ computed using data. Methods such as the stochastic gradient method are used for the minimization. In this section, we consider a dissipative dynamical system of which potential energy is a loss function, and use a structure-preserving numerical method as an
optimization algorithm. The simplest such mechanical system is a potential system with a friction term:
\[
\frac{d^2 w}{dt^2} + \mu \frac{dw}{dt} = -\nabla V(w).
\]

This system is used for optimization in [1] and is the Euler–Lagrange equation with the following action integral [2][18]:
\[
\int_0^T \mathcal{L}(u, \frac{du}{dt})e^{\mu t} dt, \quad \mathcal{L}(u, \frac{du}{dt}) = \frac{1}{2} \left( \frac{du}{dt} \right)^2 - V(u).
\]

The energy behavior of this equation is analyzed as
\[
E(t)e^{\mu t} - E(0) = -\mu \int_0^t \mathcal{L}(u, \dot{u})e^{\mu s} ds, \quad E(t) = \frac{1}{2} \left( \frac{du}{dt} \right)^2 + V(u).
\]
by formally applying the Noether theorem. This equality corresponds to the energy-dissipation property; by differentiating the both sides of this equality, we get

\[
\frac{dE}{dt} e^{\mu t} + \mu E(t) e^{\mu t} = -\mu \mathcal{L}(u, \dot{u}) e^{\mu t} = -\mu \left( \frac{1}{2} \left( \frac{du}{dt} \right)^2 - V(u) \right) e^{\mu t}
\]

and thereby

\[
\frac{dE}{dt} = -\mu \left( \frac{du}{dt} \right)^2.
\]

A structure-preserving numerical method for this equation is

\[
\frac{1}{\Delta t} \left( \frac{u^{(n+1)} - u^{(n-1)}}{2\Delta t} - \frac{u^{(n)} - u^{(n-2)}}{2\Delta t} e^{-\mu \Delta t} \right) = -\nabla V(u^{(n)}, u^{(n-1)}),
\]

which has the dissipation property

\[
\frac{1}{2} \left( \frac{u^{(n+1)} - u^{(n)}}{\Delta t} \right)^2 + V(u^{(n)}) e^{\mu \Delta t} - \frac{u^{(n+1)} - u^{(n)}}{\Delta t} + e^{-\mu \Delta t} \frac{u^{(n+1)} - u^{(n-1)}}{2\Delta t} = \sum_{k=2}^{N} \frac{e^{\mu k \Delta t} - e^{\mu (k-1) \Delta t}}{2} \left( \mathcal{L}_d(u^{(k)}, u^{(k+1)}) + \mathcal{L}_d(u^{(k-1)}, u^{(k)}) \right),
\]

\[
\mathcal{L}_d(u^{(n)}, u^{(n+1)}) = \frac{1}{2} \left( \frac{u^{(n+1)} - u^{(n)}}{\Delta t} \right)^2 - V(u^{(n)}).
\]

Using this scheme with the loss function as the potential function, we trained a perceptron for the wine data set in UCI Machine Learning Repository [12]. In this data set the number of the input variables \( N \) is 14 and that of the output variables is 3. We set \( \Delta t = 0.1 \) and the number of the nodes in the hidden layer \( M \) to 14. All activation functions were the standard sigmoid function. We used the first 143 data for the training. The loss function was given by the squared 2-norm of the errors.

The trajectories of the loss function are shown in Figures 5 and 6. In these figures, the curve denoted by “backprop” is the result of the usual backpropagation. Firstly, it can be seen from Figure 5 that the history of the structure-preserving numerical method is smoother than in the usual backpropagation. Besides, when the algorithm based on the structure-preserving numerical method is used, the algorithm was trapped in a local optimal at the early stage of the training and then escaped from it. This is because this method is for minimizing the sum of the loss function and the kinetic energy, not for the loss function itself. If the energy eventually decays and the motion stops, the energy and the loss function coincide. However, if the motion is not stopped, i.e., the algorithm is running, the total energy is dissipated, while the loss function can be increased, which allows the algorithm to escape from local solutions.

Next, from Figure 6 it can be seen that the performance of the structure-preserving numerical method is strongly dependent on the choice of the decay rate, \( \mu \); however, the overall behaviors of the trajectories are comparable to those by the backpropagation.

5 Conclusion

In this paper, aiming at promotion of practical application of the discrete gradient method, we propose a method for automating the derivation of the discrete gradient, which is a key tool for designing energy-preserving schemes. The proposed method is a discrete gradient version of the automatic differentiation. Similar to the automatic differentiation,
a program for computing a discrete gradient is automatically derived from a given program for computing a function. Besides, it follows from the definition that the discrete gradient coincides with the usual gradient if the two arguments are the same. That is, in the proposed method, not only the discrete gradient but also the usual gradient can be calculated. In this sense, the present method is an extension of the automatic differentiation algorithm. In addition, if this property is successfully exploited, an energy-preserving numerical method and a symplectic numerical method can be implemented simultaneously in the same program. This allows users to freely switch between the energy-preserving numerical method and the symplectic numerical method in accordance with the problem-setting and other requirements. As applications, we derived an energy-preserving numerical scheme for a nonlinear wave equation using the proposed
method and compared it with a method with a hand-derived discrete gradient. The numerical results were substantially the same and no adverse influence on the results due to rounding errors was observed. Besides, by combining the proposed method with a structure-preserving numerical method for a dissipative dynamical system, we also propose a training method for multi-layer perceptrons. The decay history of the loss function by the proposed method was quite smooth. This should be because the proposed approach is based on the structure-preserving numerical method. In addition, since this method attenuates not the loss function but the sum of the loss function and the kinetic energy, it may be possible to escape from local optima.

Finally, in this study, the proposed method was implemented with C++. Although this program is currently not completely optimized for execution speed, the program will be published after the optimization. For the program under development, please contact the corresponding author.

Acknowledgments

This work is supported by JST, PRESTO Grant Number JPMJPR16EC.

References

[1] H. Attouch, X. Goudou, and P. Redont, The heavy ball with friction method, I. the continuous dynamical system: Global exploration of the local minima of a real-valued function by asymptotic analysis of a dissipative dynamical system, Commun. Contemp. Math., 2 (2000), pp. 1–34.
[2] H. Bateman, On Dissipative Systems and Related Variational Principles, Phys. Rev., 38 (1931), pp. 815–819.
[3] L. Brugnano, F. Iavernaro, and D. Trigiante, Analysis of Hamiltonian Boundary Value Methods (HB-VMs): A class of energy-preserving Runge–Kutta methods for the numerical solution of polynomial Hamiltonian systems, Commun. Nonlinear Sci., 20 (2015), pp. 650–667.
[4] C. J. Budd and M. D. Piggott, Geometric Integration and its Applications, in Handbook of Numerical Analysis, vol. 11 of Handb. Numer. Anal., XI, North-Holland, Amsterdam, 2003, pp. 35–139.
[5] J. C. Butcher, Numerical Methods for Ordinary Differential Equations, Wiley, Chichester, West Sussex, United Kingdom, 3rd ed., 2016.
[6] E. Celledoni, V. Grimm, R. I. McLachlan, D. I. McLaren, D. O’Neale, B. Owren, and G. R. W. Quispel, Preserving energy resp. dissipation in numerical PDEs using the “average vector field” method, J. Comput. Phys., 231 (2012), pp. 6770–6789.
[7] E. Celledoni, R. I. McLachlan, D. I. McLaren, B. Owren, G. R. W. Quispel, and W. M. Wright, Energy-preserving Runge–Kutta methods, M2AN Math. Model. Numer. Anal., 43 (2009), pp. 645–649.
[8] E. Celledoni and B. Owren, Preserving first integrals with symmetric Lie group methods, Discrete Contin. Dyn. Syst. Ser. A, 34 (2014), pp. 977–990.
[9] J. Chabassier and A. Chaigne, Modeling and numerical simulation of a nonlinear system of piano strings coupled to a soundboard, Proceedings of 20th International Congress on Acoustics, ICA 2010, (2010), pp. 1–8.
[10] S. H. Christiansen, H. Z. Munthe-Kaas, and B. Owren, Topics in structure-preserving discretization, Acta Numer., 20 (2011), pp. 1–119.
[11] M. Dahlby and B. Owren, A general framework for deriving integral preserving numerical methods for PDEs, SIAM J. Sci. Comput., 33 (2011), pp. 2318–2340.
[12] D. Dua and C. Graff, UCI machine learning repository, 2017.
[13] K. Feng and M. Qin, Symplectic geometric algorithms for Hamiltonian systems, Zhejiang Science and Technology Publishing House, Hangzhou; Springer, Heidelberg, 2010.
[14] D. Furihata and T. Matsuo, Discrete Variational Derivative Method, Chapman & Hall/CRC Numerical Analysis and Scientific Computing, CRC Press, Boca Raton, FL, 2010.
[15] O. Gonzales, Time integration and discrete Hamiltonian systems, J. Nonlinear Sci., 6 (1996), pp. 449–467.
[16] A. Griewank and A. Walther, Evaluating derivatives: principles and techniques of algorithmic differentiation, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2nd ed., 2008.
[17] E. Hairer, C. Lubich, and G. Wanner, Geometric numerical integration, vol. 31 of Springer Series in Computational Mathematics, Springer-Verlag, Berlin, 2nd ed., 2006.
[18] L. Herrera, L. Núñez, A. Patiño, and H. Rago, A variational principle and the classical and quantum mechanics of the damped harmonic oscillator, American Journal of Physics, 54 (1986), pp. 273–277.

[19] A. Ishikawa and T. Yaguchi, Application of the variational principle to deriving energy-preserving schemes for the Hamilton equation, JSIAM Lett., 8 (2016), pp. 53–56.

[20] J. E. Marsden and M. West, Discrete mechanics and variational integrators, Acta Numer., 10 (2001), pp. 357–514.

[21] T. Matsuo, M. Sugiwhara, D. Furihata, and M. Mori, Linearly implicit finite difference schemes derived by the discrete variational method, Sūrikaisekikenkyūsho Kōkyūroku, (2000), pp. 121–129.

[22] Y. Miyatake and J. C. Butcher, A Characterization of Energy-Preserving Methods and the Construction of Parallel Integrators for Hamiltonian Systems, SIAM Journal on Numerical Analysis, 54 (2016), pp. 1993–2013.

[23] T. Yaguchi, Lagrangian approach to deriving energy-preserving numerical schemes for the Euler-Lagrange partial differential equations, ESAIM Math. Model. Numer. Anal., 47 (2013), pp. 1493–1513.