Geometric investigation of the discrete gradient method for the Webster equation with a weighted inner product

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Abstract

We consider application of the discrete gradient method for the Webster equation, which models sound waves in tubes. Typically Hamilton equations are described by the use of gradients of the Hamiltonian and it is indispensable to introduce an inner product to define a gradient. We first apply the discrete gradient method to design an energy-preserving method by using a weighted inner product. Comparing with another scheme that is derived by a standard inner product, we show that the discrete gradient method has a geometric invariance, which implies that the method reflects the symplectic geometric aspect of mechanics.

Keywords discrete gradient method, Webster equation, Hamiltonian mechanics

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1. Introduction

In this paper, we consider the Webster equation:

$$Sp_t = -\gamma u_x, \quad \frac{1}{S}u_t = -\gamma p_x. \quad (1)$$

This equation models sound waves in vocal tracts or bodies of wind instruments. This equation has been studied in research concerning speaker recognition or devices for the hearing-impaired in the field of voice recognition and synthesis [1]. $p$ and $u$ denote the value of pressure in the tube and that of volume velocity, respectively. $S(x)$ is the cross-sectional area of the tube at $x$. $\gamma$ is defined by $\gamma = c/L$, where $c$ is the air velocity and $L$ is the length of the tube. We assume that (1) is made dimensionless and the domain of this equation is normalized to $[0, 1]$. Although in applications we need to impose practical boundary conditions that describe, for example, radiation from the tube to external air, in this paper we assume for simplicity that boundary conditions are given appropriately so that energy is conserved. These boundary conditions include the Dirichlet boundary condition, for example.

Simulation of sound waves requires long-time numerical calculation compared with the time-scale of phenomena. For this reason, structure-preserving numerical methods are required to obtain meaningful numerical solutions. Regarding numerical methods for this equation, Bilbao proposed a method by using the staggered grid. Although energy behaviors of the scheme are considered in [2], the derivation is rather technical; the scheme was not derived in the systematic way that uses the geometric mechanical structure of the equation.

In this paper, we reveal Hamiltonian structures of (1) and then derive energy-preserving schemes by using the discrete gradient method. The discrete gradient method is a typical method to design numerical schemes for a Hamiltonian equation that preserve the energy-conservation law. It is well-known that preservation of this fundamental law of physics often makes numerical schemes stable and of good quality regarding long-time behaviors of numerical solutions.

A remarkable point of the Webster equation is the existence of $S(x)$, which is a function of $x$. Because the discrete gradient method requires the phase space to be equipped with an inner product to define a discrete gradient, it would be natural to design the numerical scheme by introducing the weighted inner product with $S(x)$ as the weight function. In fact, it is shown in [3] that if a certain weighted inner product is introduced, the Hamiltonian equation is formed in a simple equation where just a few coefficients appear. Since simpler schemes often give better numerical results, it is expected that the discrete gradient method with this natural inner product would yield a numerical scheme of high quality. In this paper, we aim to obtain such a scheme by using the natural weighted inner product and then compare this scheme with the scheme derived by the standard inner product.

2. The discrete gradient method

The discrete gradient method uses the Hamiltonian structure of the equation to derive numerical schemes. The equation of motion in Hamiltonian mechanics is described as

$$v_t = M \nabla_G H, \quad (2)$$

where $H$ is a Hamiltonian. $v$ is the dependent variable and $v = (p, u)^T$ in the case of the Webster equation. We
write the gradient of \( H \) in the inner product space with a metric tensor \( G \) as \( \nabla_G H \) which is defined by requiring
\[
\begin{align*}
\frac{dH(V)}{dt} &= \langle \nabla_G H, v \rangle.
\end{align*}
\]

Here \( dH(V) \) is the Fréchet derivative of \( H \), which is obtained by expanding \( H(v + \Delta v) - H(v) \) formally in powers of \( \Delta v \) and then truncating it to the first order. \( \langle \cdot, \cdot \rangle \) is the inner product defined by \( G \). We use the same notation \( G \) for the matrix that represents the metric tensor \( G \). Geometrically, \( \nabla_G H \) is a vector that is perpendicular to the level set of \( H \); hence we need an inner product, or in other words a Riemannian structure, to introduce a concept of “angles”. \( M \) is a skew-adjoint operator under this Riemannian structure:
\[
\begin{align*}
\left\langle M \left( \begin{array}{c} p_1 \\ u_1 \\ p_2 \\ u_2 \\ \end{array} \right), \left( \begin{array}{c} p_1 \\ u_1 \\ p_2 \\ u_2 \\ \end{array} \right) \right\rangle &= \left\langle \begin{array}{c} p_1 \\ u_1 \\ p_2 \\ u_2 \\ \end{array} \right|_{\cdot} M \left( \begin{array}{c} p_2 \\ u_2 \\ \end{array} \right).
\end{align*}
\]

Most structure-preserving methods for mechanics are designed for (2). If we can rewrite a dynamical model to the form of (2), we can use any structure-preserving numerical method for Hamiltonian systems. We discretize (2) by using the discrete gradient method and obtain the following scheme
\[
\begin{align*}
\frac{v^{n+1} - v^n}{\Delta t} &= M_d \nabla_d H_d,
\end{align*}
\]
where \( v^n \) represents an approximation of \( v(n \Delta t) \). \( \nabla_d H_d \) is a discrete gradient and defined by using an inner product so that it possesses a discrete analogue of the important property of the gradient:
\[
\begin{align*}
\frac{dH}{dt} &= \langle \nabla_G H, v \rangle;
\end{align*}
\]
however, in most previous work, the inner product was implicitly assumed to be Hermitian or \( L^2 \). Although generalization of the definition of discrete gradients to general inner product spaces is straightforward, for the sake of clarity, we give a definition of discrete gradients on a general inner product space.

**Definition 1** Let a discrete gradient \( \nabla_d H_d \) be defined on an inner product space with an inner product \( \langle \cdot, \cdot \rangle_d \) by requiring
\[
\begin{align*}
\left\langle H_d(v) - H_d(u), v - u \right\rangle_d &= \langle \nabla_d H_d(v, w), v - w \rangle_d, \\
\nabla_d H_d(v, v) &= \nabla H_d(v).
\end{align*}
\]

3. Hamiltonian structures of the Webster equation

We investigate Hamiltonian structures of the Webster equation. Energy of the Webster equation is given as
\[
\begin{align*}
H(p, u) &= \frac{\gamma^2}{2} \int_0^1 (Sp^2 + \frac{1}{S} u^2) dx.
\end{align*}
\]

As mentioned above, we need an inner product to find a Hamiltonian structure. We use the following inner product
\[
\begin{align*}
\left\langle \begin{array}{c} p_1 \\ u_1 \\ p_2 \\ u_2 \\ \end{array} \right|_{\cdot} \left( \begin{array}{c} p_1 \\ u_1 \\ p_2 \\ u_2 \\ \end{array} \right) &= \gamma^2 \int_0^1 (Sp_1 p_2 + \frac{1}{S} u_1 u_2) dx,
\end{align*}
\]
where \( \gamma \) and \( S(x) \) are used as the weight function. In this paper we call (8) the weighted inner product. We denote by \( G \) the metric tensor that defines this inner product. To obtain the gradient of \( H \), we calculate a gap of \( H \):
\[
\begin{align*}
H(p + \Delta p, u + \Delta u) - H(p, u) &= \gamma^2 \int_0^1 (Sp\Delta p + \frac{1}{S} u \Delta u) dx + O(\Delta t^2) \\
&= \left\langle \begin{array}{c} p \\ u \\ \end{array} \right|_{\cdot} (\Delta p) + O(\Delta t^2).
\end{align*}
\]

From this result we have
\[
\nabla_G H = \begin{pmatrix} p \\ u \end{pmatrix}.
\]

We define a matrix \( M \) by
\[
\begin{align*}
M &= -\left( \begin{array}{cc} 0 & \gamma S \partial_x \\ \gamma S \partial_x & 0 \end{array} \right).
\end{align*}
\]
By using the gradient (10) and the matrix (11), we rewrite (1) to the form of (2):
\[
\begin{align*}
\left( \begin{array}{c} p_1 \\ u_1 \\ p_2 \\ u_2 \\ \end{array} \right) &= -\left( \begin{array}{cc} 0 & \gamma S \partial_x \\ \gamma S \partial_x & 0 \end{array} \right) \left( \begin{array}{c} p \\ u \end{array} \right).
\end{align*}
\]

It is worthy to point out that the obtained gradient is of a very simple form. As noted above, numerical schemes of simple forms often show good numerical behavior. In the next section, we apply the discrete gradient method to this simple Hamiltonian equation in expectation of good numerical schemes.

4. Application of the discrete gradient method

4.1. Discrete gradient method

We use a uniform space-time mesh with the step sizes \( \Delta x \) in the space direction and \( \Delta t \) in the time direction. The number of points is denoted by \( N \). We denote the approximated value of \( p(j \Delta x, n \Delta t) \) by \( p^n \) and those for \( u \) and \( S \) by \( u^n \) and \( S^n \). We also write, e.g., \( p^n = (p_1^n, \ldots, p_N^n) \) and \( S^n = (S_1^n, \ldots, S_N^n) \). \( \Delta p^n = (p_1^{n+1}, \ldots, p_N^{n+1}) \) and \( \Delta S^n = (S_1^{n+1}, \ldots, S_N^{n+1}) \) for simplicity. \( \partial_x \) denotes the central difference operator.

As mentioned in Introduction, energy-preserving numerical schemes are obtained by applying the discrete gradient method (e.g. \cite{4}). Generally a discrete gradient is not uniquely determined and many methods for deriving a discrete gradient of a given Hamiltonian \( H \) have already been proposed in the case of the standard inner products. In this paper, we use Furihata’s discrete gradient \( \left[5\right] \) that is extended to general inner product spaces.

First we discretize the Hamiltonian of the Webster equation as follows:
\[
\begin{align*}
H_d(p^n, u^n) &= \frac{\gamma^2}{2} \sum_{j=0}^N \left( S_j (p_j^n)^2 + \frac{1}{S_j} (u_j^n)^2 \right) \Delta x.
\end{align*}
\]
We also discretize the weighted inner product (8) as
\[
\left\langle \left( \frac{p^n}{u^n}, \frac{q^n}{v^n} \right) \right\rangle_d = \gamma^2 \sum_{j=0}^{N} \left( S_j p_j^n q_j^n + \frac{1}{s_j} u_j^n v_j^n \right) \Delta x.
\]
(14)

Following Furihata [5], we have
\[
H_d(p^{n+1}, u^{n+1}) - H_d(p^n, u^n)
= \frac{\gamma^2}{2} \sum_{j=0}^{N} \left( S_j (p_j^{n+1})^2 + \frac{1}{s_j} (u_j^{n+1})^2 \right) \Delta x
- \frac{\gamma^2}{2} \sum_{j=0}^{N} \left( S_j (p_j^n)^2 + \frac{1}{s_j} (u_j^n)^2 \right) \Delta x
= \frac{\gamma^2}{2} \sum_{j=0}^{N} \left( (S_j p_j^{n+1} + p_j^n)(p_j^{n+1} - p_j^n)
+ \frac{1}{s_j} (u_j^{n+1} + u_j^n)(u_j^{n+1} - u_j^n) \right) \Delta x
= \left\langle \left( \frac{p^n}{u^n}, \left( p^{n+1} - p^n \right) \right) \right\rangle_d.
\]
Therefore from (6), we obtain
\[
\nabla_d H_d = \left( \frac{\dot{p}^n}{\dot{u}^n} \right).
\]
(16)

We discretize the skew-adjoint matrix $M$ to
\[
M_d = -\left( \begin{array}{cc} 0 & \frac{\gamma}{s_j} \delta_x \\ \frac{\gamma s_j}{\delta_x} & 0 \end{array} \right)
\]
and obtain the discretized Hamiltonian equation
\[
\begin{bmatrix} p_{j+1}^{n+1} - p_j^n \\ u_{j+1}^{n+1} - u_j^n \end{bmatrix} = \begin{bmatrix} 0 & \frac{\gamma}{s_j} \delta_x \\ \frac{\gamma s_j}{\delta_x} & 0 \end{bmatrix} \begin{bmatrix} \dot{p}_j^n \\ \dot{u}_j^n \end{bmatrix}.
\]
(18)

**Theorem 2** The scheme (18) has the discrete energy-conservation law
\[
\frac{H_d(p^{n+1}, u^{n+1}) - H_d(p^n, u^n)}{\Delta t} = 0
\]
under appropriate boundary conditions that make the operator $M$ skew-adjoint.

**Proof** By the definition of the discrete gradient in general inner product spaces (6), we have
\[
\frac{H_d(p^{n+1}, u^{n+1}) - H_d(p^n, u^n)}{\Delta t}
= \left\langle \nabla_d H_d, \left( \frac{p^{n+1} - p^n}{\Delta t}, \frac{u^{n+1} - u^n}{\Delta t} \right) \right\rangle_d.
\]
By substituting the scheme into this equation, we have
\[
\frac{H_d(p^{n+1}, u^{n+1}) - H_d(p^n, u^n)}{\Delta t} = \left\langle \nabla_d H_d, M_d \nabla_d H_d \right\rangle_d.
\]

Because $M_d$ is skew-adjoint, we get
\[
\frac{H_d(p^{n+1}, u^{n+1}) - H_d(p^n, u^n)}{\Delta t} = -\left\langle M_d \nabla_d H_d, \nabla_d H_d \right\rangle_d,
\]
which shows
\[
\frac{H_d(p^{n+1}, u^{n+1}) - H_d(p^n, u^n)}{\Delta t} = \left\langle \nabla_d H_d, M_d \nabla_d H_d \right\rangle_d = 0.
\]
(17)

**4.2 Numerical Experiment**

We compare numerical solutions by our scheme (18) with those by the scheme derived by the Heun method. We note that these schemes have the same order of accuracy in space and time. The initial conditions are given by $p(0, x) = 0, u(0, x) = \exp(-100(x - 0.5)^2)$ and the boundary condition is periodic. We also set $\Delta x = 1/90$ and $\gamma = 1050$. Fig. 1 shows the evolution of the energy. In the case of the Heun method, the energy blows up in spite of the extremely small time step size $\Delta t = 1/4410000$. If we use the scheme (18), however, the energy is preserved even when $\Delta t = 1/441000$, as is shown in Theorem 2. Fig. 2 shows the values of $u$ at $t = 0.01$ obtained under the same conditions. The numerical solution by the Heun method exhibits oscillations, which are not observed in the graph of the scheme (18). In addition, the scheme (18) remains stable even when $\Delta t = 1.0$; this result confirms a superior stability of this scheme. Details of this numerical experiment are reported elsewhere.

**Remark 3** We also tested the scheme by Bilbao [2] for wind instruments and found that this scheme is not sta-
this result, we obtain the following theorem:

From this result, we find that this scheme coincides with (18). In other words, although we need an inner product to derive a discrete gradient, the obtained scheme has invariance with respect to the inner product. By extending this result, we obtain the following theorem:

**Theorem 4** Suppose that the Webster equation is first semi-discretized to an ordinal differential equation by approximating \( S(j\Delta t) \) to a fixed value \( S_j \) and replacing differential operators with the 2nd order central difference operator. Then, the schemes obtained by applying the discrete gradient method to this ordinary differential equation has invariance under the change of the inner product.

**Proof** This theorem is shown by the fact that although different inner products yield different discrete gradients, they also affect the skew-adjoint matrices at the same time. In fact the matrix \( M \) is a hybrid tensor of rank 2 which is converted to this type of tensor from the symplectic 2-form, which is a covariant tensor of rank 2, by using the inner product.

(QED)

5. Future work

The Hamiltonian equation written as (2) is described by using a gradient vector of the Hamiltonian and hence this equation must be posed on a both symplectic and inner product space. On the other hand, the Hamiltonian equation can also be described by using only the symplectic structure \([6]\) as

\[
\omega \cdot X = dH, \quad u_t = X.
\]

In this description, introduction of an inner product is not required; indeed, this form of the Hamiltonian equation consists of a minimum geometric structure, or a pair of \((\omega, H)\), that is genuinely indispensable for mechanics. From this consideration and Theorem 4, we make the following conjecture:

**Conjecture 5** If we use the same pair of a “discrete Hamiltonian \( H_d \)” and a “discrete symplectic form \( \omega_d \)”, then the discrete gradient method derives the same schemes regardless of the choice of the inner product.

If the discrete gradient method has such invariance under the change of the inner product, this method would be reformulated to a framework only with the symplectic geometric structure, which is truly needed for mechanics. We will report on this conjecture in another opportunity.

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