Computational enhancement of discrete gradient method

Artur Kobus
Uniwersytet w Białymstoku, Wydział Fizyki
ul. Ciolkowskiego 1L, 15-245 Białystok, Poland

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We propose new numerical approach to non-conservative dynamical systems. Our method being of low order, enhances qualitative performance of standard discrete gradient algorithm, than to new concept of a reservoir. Paper is of explanatory character, focusing on concrete non-linear physical systems. Superiority of our new method with respect to standard discrete gradient method is observed.

Keywords: Geometric Numerical Integration; Discrete Gradient Method; Non-conservative Systems

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I. INTRODUCTION

Non-trivial task of engaging the proper numerical algorithm for solving approximately target differential equation could be handled in two ways: using standard, general purpose integrators of high order as various Runge-Kutta-type methods, multi-step methods, or collocation methods, to name just a few [7, 10], or geometric methods exactly preserving qualitative properties like time-inversion symmetry, symplecticity or constants of motion [1][6], eventually reaching high order through composition and other tricks (see e.g. [4][6]).

We propose new method designed for the usual IVP treated in a very non-usual way. Here we picked system of autonomous form, but we could as well choose non-autonomous one.

We generalize already quite general approach of discrete gradient method [9][11] as constructed for Hamiltonian, Poisson and Lyapunov type systems, beyond the original scope. Especially we emphasize the application to non-linear, non-conservative dynamical systems. Convenient and effective treatment of these is possible than to introducing novel kind of conserved quantity, the so-called “computational invariant of motion”.

Before we proceed to new results, we think a quick reminder on the classical discrete gradient method (only for the Hamiltonian case!) should be useful [9]:

1. We discretize the problem on the time-grid \( t_i = t_0 + ih_i \), where \( t_0 \) is a chosen constant and \( h_i \) is (possibly variable) time step.

2. We use the scheme

\[
\frac{x_{i+1} - x_i}{h_i} = \frac{H(x_{i+1}, y_{i+1}) - H(x_{i+1}, y_i)}{y_{i+1} - y_i}, \quad \frac{y_{i+1} - y_i}{h_i} = \frac{H(x_{i+1}, y_{i+1}) - H(x_{i}, y_i)}{x_{i+1} - x_i},
\]

(I.2)

3. Cross-multiplying above equations leads to instantaneous conclusion

\[
H(x_{i+1}, y_{i+1}) = H(x_i, y_i).
\]

II. COMPUTATIONALLY CONSERVED QUANTITIES AND NEW NUMERICAL SCHEME

Let us consider a basic example

\[
\dot{x} = y, \quad \dot{y} = -x - D(x, y),
\]

(II.1)

which is essentially harmonic oscillator with some damping/forcing included, permitting non-conservative behavior to occur (dependence on \( y \) is crucial-otherwise we still get Hamiltonian case). Pure harmonic oscillator would possess a constant of motion \( H(x, y) = \frac{1}{2}x^2 + \frac{1}{2}y^2 \), but due to (II.1) there is

\[
\dot{H} = -yD(x, y).
\]

(II.2)

Now we search for a quantity with exactly opposite behavior of the time derivative, in other words we need a function \( z \) such that

\[
\dot{z} = yD(x, y),
\]

(II.3)

and of course, we can formally solve above equation with the integral

\[
z = - \int D(x, y)y dt,
\]

(II.4)
since \((x, y)\) are of course functions of independent variable \(t\).

With definition of computationally conserved quantity

\[
K = H + z \tag{II.5}
\]

we can directly check it is conserved.

Note that \(z\) nor \(K\) are not well-defined functions, since they depend on the path of integration in \([1.4]\). Moreover, to find \(z\), we would need to explicitly know \(x\) and \(y\) as functions of time. Hence the anticipated redundancy of \(z\) variable. We will call \(z\) the reservoir variable.

New scheme is of the form:

\[
\begin{align*}
\frac{x_{i+1} - x_i}{h} &= \frac{K(x_{i+1}, y_{i+1}, z_{i+1}) - K(x_{i+1}, y_i, z_i)}{h}, \\
\frac{y_{i+1} - y_i}{h} &= \frac{K(x_{i+1}, y_{i+1}, z_{i+1}) - K(x_{i}, y_i, z_i)}{h}, \\
w_{i+1} &= w_i + D(x^*_i, y^*_i)(x_{i+1} - x_i),
\end{align*}
\tag{II.6}
\]

the last equation appears since \(y dt = dx\), due to \([1.1]\). \((x^*, y^*)\) is a point calculated arbitrarily, but consequently throughout solving the equations of motion. Cross-multiplying first two equations of above scheme yields

\[
K(x_{i+1}, y_{i+1}, z_{i+1}) = K(x_i, y_i, z_i). \tag{II.7}
\]

III. EXAMPLE OF THE SIMPLE HARMONIC OSCILLATOR

Having established new tools, we begin testing with simple example

\[
\begin{align*}
\dot{x} &= y, \\
\dot{y} &= -x - by,
\end{align*} \tag{III.1}
\]

where \(b\) is the damping parameter.

As in former section, we adjoin the reservoir variable to the system

\[
z = b \int y^2 dt, \tag{III.2}
\]

so that \(K = H(x, y) + z\) is conserved due to equations of motion.

We turn the system into a discrete one

\[
\begin{align*}
\frac{x_{i+1} - x_i}{h} &= \frac{1}{2}(y_i + y_{i+1}), \\
\frac{y_{i+1} - y_i}{h} &= -\frac{b}{2}(x_i + x_{i+1}) - by^*_i, \\
z_{i+1} - z_i &= b y^*_i (x_{i+1} - x_i)
\end{align*} \tag{III.3}
\]

where we will use \(y^*_i = \frac{1}{2}(y_i + y_{i+1})\) for simplicity.

Additional quantity of which error we will investigate is the energy decrement

\[
R = \frac{H(x_{i+1}, y_{i+1})}{H(x_i, y_i)} = \frac{K(x_0, y_0) - z_{i+1}}{K(x_0, y_0) - z_i}. \tag{III.4}
\]

this second form designed for en-GR scheme we use the advantage of having reservoir at our disposal. We accept initial conditions \(x_0 = 1.5, y_0 = -2.2\).

In this paper all numerical experiments are performed with simulation period \(T = 100.0\), the time-step \(h = 0.001\), and accuracy tolerance \(\varepsilon = 10^{-16}\) while solving non-linear algebraic equations by iteration. We use explicit Euler scheme as a predictor.

We compare en-GR, st-GR (standard discrete gradient), IMR and SV. As a substitute for exact solution (if it is not known) we use numerical sequences generated by th order Runge-Kutta algorithm \((3/8\) rule) with a way tinier time-step \(h_{RK} = 10^{-6}\). Also we substitute midpoint approximation in place of \(x^*_i, y^*_i\).

\[\text{Figure 3.1.: Deviation from initial value of } K.\]

We adjoined reservoir to SV to see, how it conserves \(K\).

\[\text{Figure 3.2.: Comparison of deviation from theoretical value of energy decrement. en-GR is better through six orders of magnitude. IMR yields the same results as SV. } b = 0.2.\]

IV. APPLICATION TO NON-LINEAR SYSTEMS

A. Van der Pol oscillator

Equations of motion of Van der Pol oscillator are

\[
\begin{align*}
\dot{x} &= y, \\
\dot{y} &= -x + a(1 - x^2)y,
\end{align*} \tag{IV.1}
\]

what in discrete version with a reservoir, reads

\[
\begin{align*}
x_{i+1} &= x_i + b(y_i + y_{i+1}), \\
y_{i+1} &= y_i - \frac{b}{2}(x_i + x_{i+1} - 2a(1 - (x^*_i)^2)y^*_i), \\
z_{i+1} &= z_i - a(1 - (x^*_i)^2)y^*_i(x_{i+1} - x_i)
\end{align*} \tag{IV.2}
\]
where we picked $a = 1.0$.

With midpoint approximation in place of $x_i^*, y_i^*$, en-GR becomes the same algorithm as IMR, but with computational conserved quantity $K$. Standard gradient algorithm cannot be used in this case. We apply initial conditions $x_0 = 3.42, y_0 = 2.5$.

### B. Damped Duffing oscillator

The continuous system is

$$\dot{x} = y, \quad \dot{y} = x - x^3 - by,$$

so for the conservative case Hamiltonian reads

$$H(x, y) = \frac{1}{2}y^2 - \frac{1}{2}x^2 + \frac{1}{4}x^4.$$ (IV.4)

With addition of a reservoir the enhanced discrete gradient scheme (II.6) reads

$$x_{i+1} = x_i + \frac{h}{2}(y_i + y_{i+1}),$$

$$y_{i+1} = y_i + \frac{h}{2}((x_i + x_{i+1})(1 - \frac{x_i^2 + x_{i+1}^2}{2}) + 2by_i^*),$$

$$z_{i+1} = z_i + by_i^*(x_{i+1} - x_i)$$ (IV.5)

with $b = 0.2$ again. This time $x_0 = -6.0, y_0 = 2.5$.

**Remark IV.1.** Remembering that we substitute simple midpoint approximation for $x_i^*, y_i^*$, we achieve the same form of en-GR and the standard gradient algorithm (st-GR).

All tested schemes (with exception of st-GR) point towards left minimum and this is the reason why $x$-error of this method is so huge when compared to en-GR, however we see trouble begins much earlier. Reminding now remark (IV.1) we have natural and clear understanding that gradient scheme not equipped with a conserved quantity can loose proper pace of energy decreasing.

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**V. CONCLUSIONS AND PLANS**

We introduced new numerical schemes based on novel concepts of reservoir and computationally conserved quantity. This new algorithms belong to geometric numerical integration methods, preserving some quantities by in-built mechanisms.

We performed multiple numerical tests to check if our approach yields results compatible with other well-known integrators. Enhanced discrete gradient scheme presents second order behavior and is especially useful when the
energy decrement plays important role. Moreover, it enables us to use discrete gradient procedure even if there is no constant of motion nor Lyapunov function for the system.

Future perspective of research in this direction is threefold:

1. Main focus of this paper was to briefly introduce new methods with some illustrative examples; we skipped theoretical analysis of the scheme. In fact, basic calculations suggest our approach is of close origin to [8],

2. As shown in section IV B, enhanced discrete gradient has shown some advantages in preserving trajectories of dynamical systems. There were performed numerical simulations, that further confirm this property of en-GR (good example gives the heteroclinic motions of dynamical systems). Moreover, we did not search for the optimal form of $x_i^*, y_i^*$, also interesting would be to test long-time performance of this method,

3. Higher dimensional counterpart of this method is also in preparation. It seems like matrix formulation of [9] will apply with minor changes in this case.

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