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Arbitrary-order functionally fitted energy-diminishing methods for gradient systems

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ABSTRACT

It is well known that for gradient systems in Euclidean space or on a Riemannian manifold, the energy decreases monotonically along solutions. In this letter we derive and analyse functionally fitted energy-diminishing methods to preserve this key property of gradient systems. It is proved that the novel methods are energy-diminishing and can achieve damping for very stiff gradient systems. We also show that the methods can be of arbitrarily high order and discuss their implementations. A numerical test is reported to illustrate the efficiency of the new methods in comparison with three existing numerical methods in the literature.

1. Introduction

In this letter, we investigate the following gradient systems in coordinates:

$$G(y(t))\dot{y}(t) = -\nabla U(y(t)), \quad y(0) = y_0 \in \mathbb{R}^d, \quad t \in [0, T], \tag{1}$$

where the dot denotes $\frac{\mathrm{d}}{\mathrm{d}t}$, d is a positive integer, $U(y) : \mathbb{R}^d \to \mathbb{R}$ is a potential function and the symmetric matrix $G(y)$ is assumed to satisfy

$$v^{\intercal} G(y) v \geq v^{\intercal} \Gamma v > 0$$

for all vectors $v \neq 0$. Here Γ is a fixed positive definite matrix.

Gradient systems frequently arise in a wide variety of applications both in a finite-dimensional and an infinite-dimensional setting. There are many examples of this system (see, e.g. [1–7]) such as models in quantum systems, in differential geometry, in image processing, and in material science. A fundamental and

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key property of gradient systems is that along every exact solution of (1), one has

$$\frac{d}{dt}U(y(t)) = \nabla U(y(t))^{\intercal}\dot{y}(t) = -\dot{y}(t)^{\intercal}G(y(t))\dot{y}(t) \leq 0,$$

which shows that $U(y(t))$ is monotonically decreasing with t. The monotonicity is true with strict inequality except at stationary points of U. The aim of this letter is to formulate and analyse a novel kind of method preserving this monotonicity in the numerical treatment, i.e., after one step of the method starting from y_0 with a time step h one would have $U(y_1) \leq U(y_0)$.

In order to get methods with this property, Hairer and Lubich analysed various energy-diminishing methods in [8]. They showed that implicit Euler method has this property but it is only of order one. Algebraically stable Runge–Kutta methods were proved to reduce the energy in each step under a mild step-size restriction, which means that Runge–Kutta methods are not unconditionally energy-diminishing. They also showed that discrete-gradient methods, averaged vector field (AVF) methods and AVF collocation methods are energy-diminishing, but cannot achieve damping for very stiff gradient systems. For other energy-diminishing methods, we refer the reader to [9,10] as well as the references contained therein. In this letter, we will derive a novel kind of method which can be of arbitrarily high order. Moreover, the methods will be shown that they are energy-diminishing and are strongly damped even for very stiff gradient systems.

The rest of this letter is organised as follows. In Section 2, we derive the novel methods and prove that they are energy-diminishing for gradient systems. The unconditionally damping property is analysed in Section 3. We study the order of the methods in Section 4. Section 5 is devoted to the implementation issue. In Section 6, a numerical test is carried out to demonstrate the excellent qualitative behaviour. Section 7 focuses on the concluding remarks.

2. Functionally fitted energy-diminishing methods

In order to formulate the novel methods, we will use the functionally fitted technology, which is a popular approach to constructing efficient and effective methods in scientific computing (see, e.g. [11]). A functionally fitted method is generally derived by requiring it to integrate members of a given function space exactly. To this end, define a function space Y=span$\{\varphi_0(t), \ldots, \varphi_{r-1}(t)\}$ on $[0, T]$ by (see [11])

$$Y = \left\{ w : w(t) = \sum_{i=0}^{r-1} \varphi_i(t) W_i,\ t \in I,\ W_i \in \mathbb{R}^d \right\},$$

where $\{\varphi_i(t)\}_{i=0}^{r-1}$ are sufficiently smooth and linearly independent on $[0, T]$ with an integer $r \geq 1$. In this letter, we consider two finite-dimensional function spaces Y and X as follows

$$Y = \text{span}\left\{\varphi_0(t), \ldots, \varphi_{r-1}(t)\right\}, \quad X = \text{span}\left\{1, \int_0^t \varphi_0(s)ds, \ldots, \int_0^t \varphi_{r-1}(s)ds\right\}.$$

Choose a stepsize $h > 0$ and define the function spaces Y_h and X_h on $[0, 1]$ by

$$Y_h = \text{span}\left\{\tilde{\varphi}_0(\tau), \ldots, \tilde{\varphi}_{r-1}(\tau)\right\}, \quad X_h = \text{span}\left\{1, \int_0^\tau \tilde{\varphi}_0(s)ds, \ldots, \int_0^\tau \tilde{\varphi}_{r-1}(s)ds\right\},$$

where $\tilde{\varphi}_i(\tau) = \varphi_i(\tau h),\ \tau \in [0, 1]$ for $i = 0, 1, \ldots, r-1$. We remark that for all the functions throughout this letter, the notation $\tilde{f}(\tau)$ is referred to $f(\tau h)$.

We will use a projection $\mathcal{P}_h$ in the formulation of the new methods. It was defined in [11] and we summarise it here.