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# Construction and Analysis for Adams Explicit Discretization of High-Index Saddle Dynamics

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**Abstract.** Saddle points largely exist in complex systems and play important roles in various scientific problems. High-index saddle dynamics (HiSD) is an efficient method for computing any-index saddle points and constructing solution landscape. In this paper, we propose a two-step Adams explicit scheme for HiSD and analyze its error estimate versus time step. Through careful argumentation and overcoming the difficulties caused by nonlinear coupling and orthogonalisation, we prove that the two-step Adams explicit scheme has second-order accuracy. The theoretical results are further verified by two numerical experiments.

**AMS subject classifications**: 37M05, 37N30, 65L20

**Key words**: Saddle point, saddle dynamics, solution landscape, Adams scheme, error estimate.

## 1 Introduction

Finding the stationary point of the nonlinear multivariate energy function $E(x)$ has been an important concern in many fields of science over the last decades. It has special significance and a wide range of applications in physics, chemistry, and biology, such as critical

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nuclei in phase transitions [10,38], molecular clusters [1,6], protein folding [23,27], artificial neural networks [8], and soft matter [5,15]. For example, an index-1 saddle point is called a transition state, which means that at a stationary point, the Hessian matrix has and only has one negative eigenvalue. According to Morse theory [25], the Morse index of a non-degenerate saddle point is the maximum dimension of the negative definite subspace of its Hessian matrix $\nabla^2 E(x)$, i.e. the number of negative eigenvalues of the Hessian matrix $\nabla^2 E(x)$.

How to compute the saddle point of $E(x)$ is a very challenging problem [21]. Because of the clear meaning and wide application of index-1 saddle point, extensive methods have been developed in recent decades to find index-1 saddle point. One popular approach is the path-finding method, such as the nudged elastic band method [19,28] and the string method [7,9]. The other type method is the surface-walking method, such as the gentlest ascent dynamics (GAD) [11], the dimer-type methods [18,37,39], and the activation-relaxation technique [4], etc. In 2013, [2] extended the GAD method to find high-index saddle points. More comprehensive overview can be found in [10,17,40]. In 2019, high-index saddle dynamics was proposed to compute any-index saddle points [35], inspired by the optimization-based shrinking dimer method [39]. The HiSD method presents an effective tool for constructing the solution landscape and describes a pathway map starting with a parent state, the highest-index saddle point, that relates to the low-index saddle points and all the minimisers [33]. The solution landscape approach has been applied to investigate several physical systems [16,29,30,32,36]. In addition, the HiSD method is not limited to the gradient systems, and has been extended to the non-gradient systems by using a generalized high-index saddle dynamics (GHiSD), enabling the calculation of any-index saddle points and solution landscapes of non-gradient systems [34].

Theoretical analyses are essential to improve the confidence of the algorithms. In recent years some scholars have developed some theoretical analyses of saddle point search algorithms. For example, the asymptotic stability and convergence rate of the shrinking dimer dynamics in several different time discretization modes are analysed in [37]. The linear stability and error estimation of the dimer method with preconditioners and line search algorithms are analysed in [13]. Recently, the rate of convergence of numerical scheme for HiSD [35] has been analysed in [22] and it was found that the rate of convergence is mainly related to the local curvature around the saddle-points and the accuracy of the eigenvector computation. There are some other numerical analysis results we present here [12,14,20].

The above-mentioned works provide asymptotic convergence results of, e.g. $x_n - x_*$, where $x_n$ and $x_*$ refer to the numerical solution at the $n$-th iteration and the limit (target saddle point) of the scheme, respectively. By contrast, the difference between $x_n$ and $x(t_n)$ provides an objective measure of the error, whereby $x(t_n)$ represents the exact solution of HiSD at step $t_n$. This approach allows for the assessment of the convergence of numerical solutions to saddle dynamics, and provides valuable physical insights, including the transition pathway [32,33]. Incorrect computation of the dynamical pathway may