CSIAM Trans. Appl. Math.
doi: 10.4208/csiam-am.SO-2022-0010

Vol. **4**, No. 1, pp. 157-176
March 2023

Mathematical and Numerical Analysis to Shrinking-Dimer Saddle Dynamics with Local Lipschitz Conditions

Lei Zhang[1], Pingwen Zhang[2] and Xiangcheng Zheng[3,*]

[1] *Beijing International Center for Mathematical Research, Center for Machine Learning Research, Center for Quantitative Biology, Peking University, Beijing 100871, China.*
[2] *School of Mathematical Sciences, Laboratory of Mathematics and Applied Mathematics, Peking University, Beijing 100871, China.*
[3] *School of Mathematics, Shandong University, Jinan 250100, China.*

Received 14 March 2022; Accepted 20 July 2022

Abstract. We present a mathematical and numerical investigation to the shrinking-dimer saddle dynamics for finding any-index saddle points in the solution landscape. Due to the dimer approximation of Hessian in saddle dynamics, the local Lipschitz assumptions and the strong nonlinearity for the saddle dynamics, it remains challenges for delicate analysis, such as the boundedness of the solutions and the dimer error. We address these issues to bound the solutions under proper relaxation parameters, based on which we prove the error estimates for numerical discretization to the shrinking-dimer saddle dynamics by matching the dimer length and the time step size. Furthermore, the Richardson extrapolation is employed to obtain a high-order approximation. The inherent reason of requiring the matching of the dimer length and the time step size lies in that the former serves a different mesh size from the later, and thus the proposed numerical method is close to a fully-discrete numerical scheme of some space-time PDE model with the Hessian in the saddle dynamics and its dimer approximation serving as a "spatial operator" and its discretization, respectively, which in turn indicates the PDE nature of the saddle dynamics.

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

Key words: Saddle dynamics, solution landscape, saddle points, local Lipschitz condition, error estimate, Richardson extrapolation.

*Corresponding author. *Email addresses:* zhangl@math.pku.edu.cn (L. Zhang), pzhang@pku.edu.cn (P. Zhang), zhengxch@outlook.com (X. Zheng)

1 Introduction

One of the major challenges in computational physical and chemistry is how to efficiently calculate saddle points on a complicated energy landscape. In comparison with finding local minima, the computation of saddle points is generally more difficult due to their unstable nature. Nevertheless, saddle points provide important information about the physical and chemical properties. For instance, the index-1 saddle point represents the transition states connecting two local minima according to the transition state theory [19, 35], and the index-2 saddle points are particularly interesting in chemical systems for providing valuable information on the trajectories of chemical reactions [15]. The applications of saddle points include nucleation in phase transformations [5, 32, 33], transition rates in chemical reactions and computational biology [11, 12, 21, 23, 25], etc.

The saddle points can be classified by the (Morse) index, which is characterized by the maximal dimension of a subspace on which the Hessian $H(x)$ is negative definite, according to the Morse theory [20]. Most existing searching algorithms focus on finding the index-1 saddle points, e.g. [1, 4, 6, 7, 9, 16, 17, 31]. However, the computation of high-index (index$>$1) saddle points receive less attention despite of the fact that the number of high-index saddles are much larger than the number of local minima and index-1 saddles on the complicated energy landscapes [2, 18].

The original saddle dynamics (SD) aims to find an index-k ($1\leq k\in\mathbb{N}$) saddle point of an energy function $E(x)$ [28]

$$\begin{cases} \dfrac{dx}{dt}=\beta\left(I-2\sum\limits_{j=1}^{k}v_jv_j^\top\right)F(x), \\ \dfrac{dv_i}{dt}=\gamma\left(I-v_iv_i^\top-2\sum\limits_{j=1}^{i-1}v_jv_j^\top\right)H(x)v_i, \quad 1\leq i\leq k. \end{cases} \tag{1.1}$$

Here the natural force $F:\mathbb{R}^N\to\mathbb{R}^N$ is generated from an energy $E(x)$ by $F(x)=-\nabla E(x)$, $H(x):=-\nabla^2E(x)$ corresponds to the Hessian of $E(x)$, β, $\gamma>0$ are relaxation parameters, x represents the position variable and direction variables $\{v_i\}_{i=1}^k$ form a basis for the unstable subspace of the Hessian at x.

Because the Hessians are often expensive to calculate and store, one can apply first derivatives to approximate the Hessians in Eq. (1.1) by using k dimers centered at x. To be specific, $H(x)v_i$ is approximated by

$$\hat{H}(x,v_i,l):=\frac{1}{2l}\big(F(x+lv_i)-F(x-lv_i)\big) \tag{1.2}$$

with the direction v_i and the dimer length $2l$ for some $l>0$.

Following the idea of the shrinking dimer dynamics [31, 34], we obtain the shrinking-dimer saddle dynamics (SSD) [28] as follows: