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Probabilistic Error Estimate for Numerical Discretization of High-Index Saddle Dynamics with Inaccurate Models

Lei Zhang[1], Pingwen Zhang[2,3] and Xiangcheng Zheng[4,*]

[1] *Beijing International Center for Mathematical Research, Center for Machine Learning Research, Center for Quantitative Biology, Peking University, Beijing 100871, China*
[2] *School of Mathematics and Statistics, Wuhan University, Wuhan, Hubei 430072, China*
[3] *School of Mathematical Sciences, Laboratory of Mathematics and Applied Mathematics, Peking University, Beijing 100871, China*
[4] *School of Mathematics, Shandong University, Jinan, Shandong 250100, China*

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Abstract. We prove probabilistic error estimates for high-index saddle dynamics with or without constraints to account for the inaccurate values of the model, which could be encountered in various scenarios such as model uncertainties or surrogate model algorithms via machine learning methods. The main contribution lies in incorporating the probabilistic error bound of the model values with the conventional error estimate methods for high-index saddle dynamics. The derived results generalize the error analysis of deterministic saddle dynamics and characterize the affect of the inaccuracy of the model on the convergence rate.

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Key words: Saddle point, saddle dynamics, solution landscape, Gaussian process, probabilistic error estimate.

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*Corresponding author.
Emails: zhangl@math.pku.edu.cn (L. Zhang), pzhang@pku.edu.cn (P. Zhang), xzheng@sdu.edu.cn (X. Zheng)

1 Introduction

High-index saddle points of complex systems contain ample physical and chemical information and thus attract extensive attentions [4, 15, 27, 46]. Here the index of the saddle point refers to the Morse index characterized by the maximal dimension of a subspace on which its Hessian operator is negative definite [28]. There exist several successful algorithms for finding saddle points [5, 6, 8, 10, 11, 19, 47, 50]. For instance, the search extension method [2, 37] has been applied to find multiple solutions of nonlinear problems. The iterative minimization formulation [9] and the local minimax method [20, 21, 23] have been developed to search high-index saddle points. Recently, a high-index saddle dynamics is proposed in [43] to compute an index-k saddle point

$$\begin{cases} \dfrac{dx}{dt} = \beta\left(I - 2\displaystyle\sum_{j=1}^{k} v_j v_j^\top\right) F(x), \\ \dfrac{dv_i}{dt} = \gamma\left(I - v_i v_i^\top - 2\displaystyle\sum_{j=1}^{i-1} v_j v_j^\top\right) J(x) v_i, \quad 1 \le i \le k. \end{cases} \tag{1.1}$$

Here $x \in \mathbb{R}^d$ represents the state variable, $\{v_i\}_{i=1}^k$ are directional variables, β, $\gamma > 0$ are relaxation parameters, $F(x): \mathbb{R}^d \to \mathbb{R}^d$ represents the force generated from the energy $E(x)$ by $F(x) = -\nabla E(x)$ and $J(x)$ is the negative Hessian of $E(x)$, i.e., $J(x) = -\nabla^2 E(x)$. This high-index saddle dynamics could be further combined with the downward and upward algorithms [42] to construct solution landscapes of complex systems, the pathway map consisting of all stationary points and their connections [36], that arises several successful applications [13, 14, 24, 30, 38, 40, 41, 44, 45, 48, 49, 51].

In most previous studies, exact model values such as F and J used in the high-index saddle dynamics (1.1) are assumed to be given a priori. However, this is not the case in many practical problems. For instance, a surrogate model based saddle dynamics is proposed in [12, 55] to reduce the number of queries of model values that may be expensive or time-consuming, where the model values are predicted via the Gaussian process learning. In this scenario, the model value may not be accurate but instead follows a probabilistic distribution. For such complicated cases, deterministic error estimates for numerical approximations to high-index saddle dynamics in, e.g., [52, 54] are not applicable and instead the probabilistic error estimates are natural to be considered, which motivates the current study.

In this work we prove probabilistic error estimates for high-index saddle dynamics with or without constraints. The main contribution lies in incorporating the probabilistic error bound of the model values with the conventional error estimate