Discretization and index-robust error analysis for constrained high-index saddle dynamics on high-dimensional sphere

LEI ZHANG

Beijing International Center for Mathematical Research, Center for Quantitative Biology, Center for Machine Learning Research, Peking University, Beijing, 100871, China

PINGWEN ZHANG

School of Mathematical Sciences, Laboratory of Mathematics and Applied Mathematics, Peking University, Beijing, 100871, China

AND

XIANGCHENG ZHENG*

School of Mathematical Sciences, Peking University, Beijing, 100871, China
*Corresponding author: zhengxch@math.pku.edu.cn

We develop and analyze numerical discretization to the constrained high-index saddle dynamics, the dynamics searching for the high-index saddle points confined on the high-dimensional unit sphere. Compared with the saddle dynamics without constraints, the constrained high-index saddle dynamics has more complex dynamical forms, and additional operations such as the retraction and vector transport are required due to the constraint, which significantly complicate the numerical scheme and the corresponding numerical analysis. Furthermore, as the existing numerical analysis results usually depend on the index of the saddle points implicitly, the proved numerical accuracy may be reduced if the index is high in many applications, which indicates the lack of robustness with respect to the index. To address these issues, we derive the error estimates for numerical discretization of the constrained high-index saddle dynamics on high-dimensional sphere, and then improve it by providing an index-robust error analysis in an averaged norm by adjusting the relaxation parameters. The developed results provide mathematical supports for the accuracy of numerical computations.

Keywords: saddle dynamics; saddle point; solution landscape; error estimate; index-robust.

1. Introduction

High-index saddle dynamics provides a powerful instrument in systematically finding the high-index saddle points and construction of the solution landscape [3, 8, 29, 30, 31, 36]. It has been applied to study various applications in physical and engineering problems [12, 13, 14, 25, 26, 29, 32, 34, 35, 37]. Here the index of saddle point refers to the Morse index characterized by the maximal dimension of a subspace on which its Hessian operator is negative definite [21]. If the additional nonlinear equality constraints exist, the constrained high-index saddle dynamics [27] was proposed for solving the constrained saddle point problems such as the Thomson problem [24] and the Bose–Einstein Condensation [2]. However, due to the strong nonlinearities of the coupled equations in high-index saddle dynamics, rigorous numerical analysis are less considered compared with the growing numerical implementations in applications.

There exist a couple of works investigating the convergence rate of the numerical saddle point to the target saddle point via sophisticated derivations [1, 4, 6, 7, 9, 10, 11, 15, 16, 17, 18, 20, 22, 33]. In

contrast, conventional error analysis between the exact solutions of the continuous saddle dynamics and their numerical approximations in terms of the step size provides the dynamical convergence of numerical solutions to the saddle dynamics, which provides important physical information such as transition pathway and theoretically ensure the accuracy of construction of the solution landscape [13, 31, 38]. In [38], a first-order numerical scheme for the high-index saddle dynamics without constraints was rigorously analyzed. However, due to the nonlinear equality constraint in the constrained high-index saddle dynamics, more complex dynamical form is encountered and additional operations in the numerical scheme such as the retraction and vector transport are required [27], which significantly complicate the numerical scheme and the corresponding numerical analysis. Furthermore, the pointwise-in-time error estimate

$$\|x(t_n) - x_n\| + \sum_{i=1}^{k} \|v_i(t_n) - v_{i,n}\| \leq Q\tau \tag{1.1}$$

was proved in [38], where $\{x_n, v_{1,n}, \cdots, v_{k,n}\}$ serve as the numerical approximations of the state variable and corresponding eigenvectors $\{x(t), v_1(t), \cdots, v_k(t)\}$ at the time step t_n. However, the proof in [38] indicates that the positive constant Q depends on the index k of saddle point. In some practical applications such as the Thomson problem, which considers the minimal-energy configuration of a group of classical charged particles confined on a sphere which interact with each other via a Coulomb potential [23, 24], the dimension of the energy function and the index k of saddle point can be very high. In this case, the accuracy in (1.1) could be reduced by the large factor Q.

Concerning the aforementioned issues, we aim to prove the error estimates of the numerical discretization to constrained high-index saddle dynamics on the high-dimensional unit sphere. The main difficulties we overcome lie in the complicated (nonlinear) forms of this dynamical system and the corresponding numerical scheme, which contains the retraction of the position x and the transport and orthonormalization procedure of the vectors due to the sphere constraint. In particular, these features distinguishes the numerical analysis of saddle dynamics from those for ordinary differential equations. We then improve the analysis by developing an index-robust error estimate, i.e., the constant Q in (1.1) is independent from k, in an averaged norm by adjusting the relaxation parameters α and β. These results provide theoretical supports for the numerical accuracy of discretization of constrained high-index saddle dynamics and construction of solution landscapes for complex systems.

The rest of the paper is organized as follows: In Section 2 we present formulations of the constrained high-index saddle dynamics and its numerical scheme. In Section 3 we prove auxiliary estimates, based on which we derive error estimates for the discretization of constrained high-index saddle dynamics in Section 4. Numerical experiments are performed in Section 5 to substantiate the theoretical findings. In Section 6, we prove index-robust error estimates for the numerical scheme in an averaged norm by adjusting the relaxation parameters. We finally address concluding remarks in the last section.

2. Discretization of constrained high-index saddle dynamics

In this section we present the constrained high-index saddle dynamics on the high-dimensional unit sphere, as well as the corresponding numerical scheme.

2.1. *Formulation of constrained high-index saddle dynamics*

Given a C^3 function $E(x)$ with $x \in \mathbb{R}^d$ and define the corresponding natural force $F : \mathbb{R}^d \to \mathbb{R}^d$ and the negative Hessian $H \in \mathbb{R}^{d \times d}$ by $F(x) = -\nabla E(x)$ and $H(x) = -\nabla^2 E(x)$. It is clear that $H(x) = H(x)^\top$.

Then the saddle dynamics for an index-k saddle point of $E(x)$ with $1 \leq k \in \mathbb{N}$ on the unit sphere S^{d-1} reads [27]

$$\begin{cases} \dfrac{dx}{dt} = \alpha \left(I - xx^\top - 2 \sum_{j=1}^{k} v_j v_j^\top \right) F(x), \\ \dfrac{dv_i}{dt} = \beta \left(I - xx^\top - v_i v_i^\top - 2 \sum_{j=1}^{i-1} v_j v_j^\top \right) H(x)v_i + \beta x v_i^\top F(x), \quad 1 \leq i \leq k, \end{cases} \tag{2.1}$$

equipped with the initial conditions

$$x = X_0 \in S^{d-1}, \quad v_i(0) = V_{i,0} \text{ such that } V_{i,0}^\top V_{j,0} = \delta_{ij}, \quad 1 \leq i, j \leq k.$$

Here α and β are positive relaxation parameters. In the original work [27], these parameters are chosen as $\alpha = \beta = 1$, and it was proved that the solutions x and $\{v_i\}_{i=1}^{k}$ of (2.1) satisfy

$$x \in S^{d-1}, \quad v_i^\top x = 0, \quad v_i^\top v_j = \delta_{ij}, \quad 1 \leq i, j \leq k, t \geq 0, \tag{2.2}$$

and a linearly stable steady state of (2.1) is an index-k saddle point of $E(x)$.

Compared with the classical high-index saddle dynamics without constraints [30],

$$\begin{cases} \dfrac{dx}{dt} = \alpha \left(I - 2 \sum_{j=1}^{k} v_j v_j^\top \right) F(x), \\ \dfrac{dv_i}{dt} = \beta \left(I - v_i v_i^\top - 2 \sum_{j=1}^{i-1} v_j v_j^\top \right) H(x)v_i, \quad 1 \leq i \leq k, \end{cases} \tag{2.3}$$

constrained high-index saddle dynamics (2.1) exhibits a stronger coupling between $x(t)$ and $\{v_i(t)\}_{i=1}^{k}$ with several additional terms and has more properties (cf. (2.2)) that we need to preserve in designing numerical methods, which distinguishes the current work from the existing numerical analysis for (2.3).

Throughout the paper we make the following regular assumptions on the force and the Hessian:

Assumption A: There exists constants $L_1, L_2 \geq 0$ such that the following linearly growth and local Lipschitz conditions

$$\|H(x_2) - H(x_1)\| + \|F(x_2) - F(x_1)\| \leq L_1 \|x_2 - x_1\|,$$

$$\|F(x)\| \leq L_1(1 + \|x\|), \quad x, x_1, x_2 \in S^{d-1},$$

as well as the boundedness of F and H on S^{d-1}

$$\max_{x \in S^{d-1}} \left(\|F(x)\| + \|H(x)\| \right) \leq L_2$$

hold. Here $\| \cdot \|$ refers to the standard l^2 norm of a vector or a matrix.

2.2. *Numerical scheme*

We consider the numerical approximation of the constrained index-k saddle dynamics (2.1) for some $k \geq 1$ on the time interval $(0, T]$ for some $T > 0$. Define a uniform partition $\{t_n\}_{n=0}^{N}$ of $[0, T]$ with the

mesh size τ. We discretize the first-order derivative by the explicit Euler scheme to get the reference equations for constrained index-k saddle dynamics (2.1)

$$
\begin{cases}
x(t_n) = x(t_{n-1}) + \tau\alpha\Big(I - x(t_{n-1})x(t_{n-1})^\top \\
\qquad\qquad -2\sum_{j=1}^{k} v_j(t_{n-1})v_j(t_{n-1})^\top\Big)F(x(t_{n-1})) + O(\tau^2), \\
v_i(t_n) = v_i(t_{n-1}) + \tau\beta\Big(I - x(t_{n-1})x(t_{n-1})^\top - v_i(t_{n-1})v_i(t_{n-1})^\top \\
\qquad\qquad -2\sum_{j=1}^{i-1} v_j(t_{n-1})v_j(t_{n-1})^\top\Big)H(x(t_{n-1}))v_i(t_{n-1}) \\
\qquad\qquad +\tau\beta x(t_{n-1})v_i(t_{n-1})^\top F(x(t_{n-1})) + O(\tau^2), \ \ 1 \le i \le k.
\end{cases}
\tag{2.4}
$$

Then we drop the truncation errors to obtain a first-order scheme of (2.1)

$$
\begin{cases}
\tilde{x}_n = x_{n-1} + \tau\alpha\Big(I - x_{n-1}x_{n-1}^\top - 2\sum_{j=1}^{k} v_{j,n-1}v_{j,n-1}^\top\Big)F(x_{n-1}), \\
x_n = \dfrac{\tilde{x}_n}{\|\tilde{x}_n\|}, \\
\tilde{v}_{i,n} = v_{i,n-1} + \tau\beta\Big(I - x_{n-1}x_{n-1}^\top - v_{i,n-1}v_{i,n-1}^\top \\
\qquad\qquad\qquad -2\sum_{j=1}^{i-1} v_{j,n-1}v_{j,n-1}^\top\Big)H(x_{n-1})v_{i,n-1} \\
\qquad\qquad\qquad +\tau\beta x_{n-1}v_{i,n-1}^\top F(x_{n-1}), \ \ 1 \le i \le k, \\
\hat{v}_{i,n} = \tilde{v}_{i,n} - \tilde{v}_{i,n}^\top x_n x_n, \ \ 1 \le i \le k, \\
v_{i,n} = \dfrac{1}{Y_{i,n}}\Big(\hat{v}_{i,n} - \sum_{j=1}^{i-1}(\hat{v}_{i,n}^\top v_{j,n})v_{j,n}\Big), \ \ 1 \le i \le k
\end{cases}
\tag{2.5}
$$

for $1 \le n \le N$ and

$$
x_0 = X_0, \ \ v_{i,0} = V_{i,0}, \ \ Y_{i,n} := \Big(\|\hat{v}_{i,n}\|^2 - \sum_{j=1}^{i-1}(\hat{v}_{i,n}^\top v_{j,n})^2\Big)^{1/2}, \ \ 1 \le i \le k.
$$

The second equation of (2.5) represents the retraction in order to ensure that $x_n \in S^{d-1}$. The last two equations of (2.5), which stand for the vector transport and the Gram-Schmidt orthonormalization procedure [27], respectively, aim to ensure the last two properties of (2.2), that is,

$$
v_{i,n}^\top x_n = 0, \ \ v_{i,n}^\top v_{j,n} = \delta_{ij}, \ \ 1 \le i,j \le k, \ \ 0 \le n \le N.
\tag{2.6}
$$

Compared with the numerical schemes for index-k saddle dynamics without constraints, see e.g. [38], the additional operations like the retraction and vector transport in (2.5) caused from the sphere constraint make this scheme more complex and intensify the coupling of x and $\{v_i\}_{i=1}^{k}$ that will significantly complicate the numerical analysis in subsequent sections.

3. Auxiliary estimates

We first prove several auxiliary estimates to support the error estimates.

Lemma 1 *Under the Assumption A, the following estimate holds for $1 \leq n \leq N$*

$$\|x_n - \tilde{x}_n\| = \left|1 - \|\tilde{x}_n\|\right| \leq 2\alpha^2 L_2^2 \tau^2.$$

Proof. We multiply $x_{n-1}^\top$ on both sides of the first equation of (2.5) and use (2.6) to obtain

$$x_{n-1}^\top \tilde{x}_n = 1.$$

We then multiply $\tilde{x}_n^\top$ on both sides of the first equation of (2.5) and use $x_{n-1}^\top v_{j,n-1} = 0$ for $1 \leq j \leq k$ and the above equation to obtain

$$\|\tilde{x}_n\|^2 = 1 + \tau\alpha\left(\tilde{x}_n^\top - x_{n-1}^\top - 2\sum_{j=1}^k (\tilde{x}_n^\top - x_{n-1}^\top)v_{j,n-1}v_{j,n-1}^\top\right)F(x_{n-1}),$$

which, together with the Assumption A and the norm-preserving property of

$$I - 2\sum_{j=1}^k v_{j,n-1}v_{j,n-1}^\top, \tag{3.1}$$

yields

$$\left|\|\tilde{x}_n\|^2 - 1\right| \leq \tau\alpha L_2\|\tilde{x}_n - x_{n-1}\|.$$

Similarly, by the first equation of (2.5) again we have

$$\|\tilde{x}_n - x_{n-1}\| = \left\|\tau\alpha\left(I - x_{n-1}x_{n-1}^\top - 2\sum_{j=1}^k v_{j,n-1}v_{j,n-1}^\top\right)F(x_{n-1})\right\| \leq 2\tau\alpha L_2.$$

Combining the above two equations yields

$$\left|\|\tilde{x}_n\| - 1\right| \leq \left|\|\tilde{x}_n\|^2 - 1\right| \leq 2\alpha^2 L_2^2 \tau^2,$$

and we incorporate this with

$$\|x_n - \tilde{x}_n\| = \left\|\frac{\tilde{x}_n}{\|\tilde{x}_n\|}(1 - \|\tilde{x}_n\|)\right\| = \left|1 - \|\tilde{x}_n\|\right|$$

to complete the proof.   □

Lemma 2 *Under the Assumption A, the following estimates hold for $1 \leq n \leq N$*

$$\left|\tilde{v}_{m,n}^\top \tilde{v}_{i,n}\right| \leq Q\beta^2\tau^2, \ \ 1 \leq m < i \leq k;$$

$$\left|\|\tilde{v}_{i,n}\|^2 - 1\right| \leq Q\beta^2\tau^2, \ \ 1 \leq i \leq k.$$

Here the positive constant Q is independent from n, N, τ, k, α and β.

Proof. To prove the first estimate, we apply the properties in (2.6) to calculate the product $\tilde{v}_{m,n}^\top \tilde{v}_{i,n}$ for $1 \leq m < i \leq k$

$$\tilde{v}_{m,n}^\top \tilde{v}_{i,n} = \tau\beta \left(v_{m,n-1}^\top H(x_{n-1}) v_{i,n-1} - 2v_{m,n-1}^\top H(x_{n-1}) v_{i,n-1} \right.$$
$$\left. + v_{m,n-1}^\top H(x_{n-1})^\top v_{i,n-1} \right) + \tau^2\beta^2(\cdots) = \tau^2\beta^2(\cdots)$$

where we used the fact that first-order term is exactly zero by the symmetry of H. In order to specify the dependence of the estimates of the terms in $(\cdots)$ on k, we observe that the only factor in the scheme of $\tilde{v}_{i,n}$ (or $\tilde{v}_{m,i}$) in (2.5) that relates to k is

$$\sum_{j=1}^{i-1} v_{j,n-1} v_{j,n-1}^\top H(x_{n-1}) v_{i,n-1},$$

which could be considered as a projection of $H(x_{n-1})v_{i,n-1}$ with the norm less or equal to $\|H(x_{n-1})v_{i,n-1}\| \leq L_2$. By this means, the index k is absorbed and the estimate of $(\cdots)$ is independent from k, which leads to

$$\left| \tilde{v}_{m,n}^\top \tilde{v}_{i,n} \right| \leq Q\beta^2\tau^2, \ \ 1 \leq m < i \leq k. \tag{3.2}$$

To estimate $\|\tilde{v}_{i,n}\|$, we multiply $v_{i,n-1}^\top$ on both sides of the third equation of (2.5) and apply (2.6) to obtain for $1 \leq i \leq k$

$$v_{i,n-1}^\top \tilde{v}_{i,n} = 1. \tag{3.3}$$

We then multiply x_{n-1} on both sides of the third equation of (2.5) and apply (2.6) to obtain for $1 \leq i \leq k$

$$x_{n-1}^\top \tilde{v}_{i,n} = \tau\beta v_{i,n-1}^\top F(x_{n-1}), \tag{3.4}$$

which implies

$$\tilde{v}_{i,n}^\top x_{n-1} x_{n-1}^\top = \tau\beta v_{i,n-1}^\top F(x_{n-1}) x_{n-1}^\top. \tag{3.5}$$

We finally multiply $\tilde{v}_{i,n}^\top$ on both sides of the third equation of (2.5) and apply (2.6), (3.3), (3.4) and (3.5) to obtain

$$\tilde{v}_{i,n}^\top \tilde{v}_{i,n} = 1 + \tau\beta \left(\tilde{v}_{i,n}^\top - \tau\beta v_{i,n-1}^\top F(x_{n-1}) x_{n-1}^\top - v_{i,n-1}^\top \right.$$
$$\left. -2\sum_{j=1}^{i-1} (\tilde{v}_{i,n}^\top - v_{i,n-1}^\top) v_{j,n-1} v_{j,n-1}^\top \right) H(x_{n-1}) v_{i,n-1}$$
$$+ \tau^2\beta^2 \left(v_{i,n-1}^\top F(x_{n-1}) \right)^2,$$

which, together with

$$\|\tilde{v}_{i,n} - v_{i,n-1}\|^2 = \tilde{v}_{i,n}^\top \tilde{v}_{i,n} - 2\tilde{v}_{i,n}^\top v_{i,n-1} + 1 = \tilde{v}_{i,n}^\top \tilde{v}_{i,n} - 1, \tag{3.6}$$

implies

$$\|\tilde{v}_{i,n} - v_{i,n-1}\|^2 \leq Q\tau\beta \|\tilde{v}_{i,n} - v_{i,n-1}\| + Q\tau^2\beta^2. \tag{3.7}$$

As this equation leads to

$$\|\tilde{v}_{i,n} - v_{i,n-1}\| \leq \frac{Q\tau\beta + \sqrt{Q^2\tau^2\beta^2 + 4Q\tau^2\beta^2}}{2} \leq Q\beta\tau,$$

we incorporate this with (3.6) and (3.7) to find that

$$\left|\tilde{v}_{i,n}^{\top}\tilde{v}_{i,n} - 1\right| \leq Q\beta^2\tau^2,$$

which completes the proof. □

Lemma 3   *Suppose the Assumption A holds, $\alpha = \beta$ and $\sqrt{2}\beta L_2\tau \leq 1 - \theta$ for some $0 < \theta < 1$, then the following estimates hold for $1 \leq n \leq N$*

$$\|\hat{v}_{i,n} - \tilde{v}_{i,n}\| \leq Q\beta^2\tau^2, \ \ 1 \leq i \leq k;$$

$$\left|\hat{v}_{m,n}^{\top}\hat{v}_{i,n}\right| \leq Q(\beta^2 + \beta^4)\tau^2, \ \ 1 \leq m < i \leq k;$$

$$\left|\|\hat{v}_{i,n}\|^2 - 1\right| \leq Q(\beta^2 + \beta^4)\tau^2, \ \ 1 \leq i \leq k.$$

Here the positive constant Q is independent from n, N, τ, k, α and β.

Proof . By the fourth equation of (2.5) we have

$$\|\hat{v}_{i,n} - \tilde{v}_{i,n}\| = \left|\tilde{v}_{i,n}^{\top}x_n\right|.$$

By the first and the third equations in (2.5), direct calculations show that

$$\left|\tilde{v}_{i,n}^{\top}x_n\right| = \frac{1}{\|\tilde{x}_n\|}\left|\tau\big(\beta v_{i,n-1}^{\top}F(x_{n-1}) + \alpha F(x_{n-1})^{\top}v_{i,n-1}\right.$$
$$\left. -2\alpha v_{i,n-1}^{\top}F(x_{n-1})\big) + \tau^2\alpha\beta(\cdots)\right|.$$

Note that the first-order term in this equation is exact zero if $\alpha = \beta$. By Lemma 1 we have

$$\frac{1}{\|\tilde{x}_n\|} \leq \frac{1}{1 - 2\alpha^2 L_2^2\tau^2} \leq \frac{1}{1 - (1-\theta)^2} \leq \frac{1}{\theta}.$$

Thus we obtain from the above equations that

$$\|\hat{v}_{i,n} - \tilde{v}_{i,n}\| = \left|\tilde{v}_{i,n}^{\top}x_n\right| \leq Q\beta^2\tau^2. \tag{3.8}$$

For $1 \leq m \leq i \leq k$ we get

$$\hat{v}_{m,n}^{\top}\hat{v}_{i,n} = \tilde{v}_{m,n}^{\top}\tilde{v}_{i,n} - x_n^{\top}\tilde{v}_{i,n}x_n^{\top}\tilde{v}_{m,n}.$$

If $m < i$, we apply Lemma 2 and (3.8) to obtain

$$\left|\hat{v}_{m,n}^{\top}\hat{v}_{i,n}\right| \leq Q(\beta^2 + \beta^4)\tau^2.$$

If $m = i$ we again employ Lemma 2 and (3.8) to get

$$\left|\|\hat{v}_{i,n}\|^2 - 1\right| = \left|\|\tilde{v}_{i,n}\|^2 - 1 - (x_n^{\top}\tilde{v}_{i,n})^2\right| \leq Q(\beta^2 + \beta^4)\tau^2.$$

Thus we complete the proof. □

Lemma 4 *Suppose the Assumption A holds, $\alpha = \beta$ and $\sqrt{2}\beta L_2 \tau \leq 1 - \theta$ for some $0 < \theta < 1$, the following estimate holds for $1 \leq n \leq N$ and τ sufficiently small*

$$\|v_{i,n} - \hat{v}_{i,n}\| \leq Q\tau^2, \ \ 1 \leq i \leq k. \tag{3.9}$$

Here the positive constant Q is independent from n, N and τ but may depend on k, α and β.

Proof. Based on Lemma 3, the proof could be performed by the same techniques as [38, Lemma 4.2] and is thus omitted.   □

4. Index-dependent error estimate

We present error estimates for the scheme (2.5). Note that in this section, the constant Q in the main theorem may depend on the index k, which implies that the corresponding estimate is not index-robust. An improvement for analyzing an index-robust error estimate in an averaged norm is given in Section 6.

We bound the errors

$$e_n^x := x(t_n) - x_n, \ \ e_n^{v_i} := v_i(t_n) - v_{i,n}, \ \ 1 \leq n \leq N, \ \ 1 \leq i \leq k.$$

based on the following lemma.

Lemma 5 *Suppose there exists a non-negative sequence $\{Z_n\}_{n=0}^{N}$ with $Z_0 = 0$ satisfying*

$$Z_n \leq Z_{n-1} + A\tau Z_{n-1} + B\tau^2 \sum_{m=1}^{n-1} Z_m + C\tau^2 \tag{4.1}$$

for $1 \leq n \leq N$ and for some non-negative constants A, B and C with $A + BT \neq 0$. Then the following estimate of Z_n holds

$$Z_n \leq \frac{C}{A + BT}\left(e^{(A+BT)T} - 1\right)\tau, \ \ 1 \leq n \leq N.$$

Proof. We first prove by induction that

$$Z_n \leq \frac{C}{A + BT}\left((1 + A\tau + BT\tau)^n - 1\right)\tau, \ \ 1 \leq n \leq N. \tag{4.2}$$

It is clear that (4.2) holds for $n = 1$. Suppose (4.2) holds for $1 \leq n \leq \tilde{n} - 1$. Then we invoke these estimates in (4.1) to obtain

$$Z_{\tilde{n}} \leq \frac{C}{A + BT}\left((1 + A\tau + BT\tau)^{\tilde{n}-1} - 1\right)\tau\left(1 + A\tau + B\tau^2(\tilde{n} - 1)\right) + C\tau^2$$

$$\leq \frac{C}{A + BT}\left((1 + A\tau + BT\tau)^{\tilde{n}} - (1 + A\tau + B\tau T)\right)\tau + C\tau^2$$

$$= \frac{C}{A + BT}\left((1 + A\tau + BT\tau)^{\tilde{n}} - 1\right)\tau - \frac{C}{A + BT}(A\tau + B\tau T)\tau + C\tau^2$$

$$= \frac{C}{A + BT}\left((1 + A\tau + BT\tau)^{\tilde{n}} - 1\right)\tau.$$

That is, (4.2) holds for $n = \tilde{n}$ and thus for any $1 \leq n \leq N$ by mathematical induction. We then apply the following estimate

$$(1 + A\tau + BT\tau)^n = \left(1 + (A+BT)\tau\right)^{\frac{1}{(A+BT)\tau}(A+BT)T} \leq e^{(A+BT)T}$$

to complete the proof. $\quad\square$

Theorem 1 *Suppose the Assumption A holds, $\alpha = \beta$ and $\sqrt{2}\beta L_2 \tau \leq 1 - \theta$ for some $0 < \theta < 1$. Then the following estimate holds*

$$\|e_n^x\| + \mathscr{E}_n \leq Q\tau, \quad 1 \leq n \leq N, \quad \mathscr{E}_m := \sum_{j=1}^{k} \|e_m^{v_j}\|.$$

Here Q is independent from τ, n and N but may depend on k, α and β.

Proof . We subtract the first equation of (2.4) from that of (2.5) to obtain

$$
\begin{aligned}
e_n^x &= e_{n-1}^x + \tau\alpha\Bigg(I - x(t_{n-1})x(t_{n-1})^\top \\
&\qquad -2\sum_{j=1}^{k} v_j(t_{n-1})v_j(t_{n-1})^\top\Bigg)F(x(t_{n-1})) \\
&\qquad -\tau\alpha\Bigg(I - x_{n-1}x_{n-1}^\top - 2\sum_{j=1}^{k} v_{j,n-1}v_{j,n-1}^\top\Bigg)F(x_{n-1}) \\
&\qquad +O(\tau^2) + (\tilde{x}_n - x_n) \\
&= e_{n-1}^x + \tau\alpha\big(F(x(t_{n-1})) - F(x_{n-1})\big) \\
&\qquad -\tau\alpha\big(x(t_{n-1})x(t_{n-1})^\top F(x(t_{n-1})) - x_{n-1}x_{n-1}^\top F(x_{n-1})\big) \\
&\qquad -2\tau\alpha\sum_{j=1}^{k}\big(v_j(t_{n-1})v_j(t_{n-1})^\top F(x(t_{n-1})) \\
&\qquad\qquad -v_{j,n-1}v_{j,n-1}^\top F(x_{n-1})\big) + O(\tau^2) + (\tilde{x}_n - x_n).
\end{aligned}
\tag{4.3}
$$

We bound the forth term on the right-hand side of (4.3) as

$$
\begin{aligned}
&\left\|\tau\sum_{j=1}^{k}\big(v_j(t_{n-1})v_j(t_{n-1})^\top F(x(t_{n-1})) - v_{j,n-1}v_{j,n-1}^\top F(x_{n-1})\big)\right\| \\
&\leq \tau\sum_{j=1}^{k}\big\|e_{n-1}^{v_j}v_j(t_{n-1})^\top F(x(t_{n-1})) + v_{j,n-1}(e_{n-1}^{v_j})^\top F(x(t_{n-1})) \\
&\qquad +v_{j,n-1}v_{j,n-1}^\top\big(F(x(t_{n-1})) - F(x_{n-1})\big)\big\| \leq Q\tau\big(\mathscr{E}_{n-1} + \|e_{n-1}^x\|\big).
\end{aligned}
\tag{4.4}
$$

Here we used the projection nature of the third difference (i.e. the summation containing $F(x(t_{n-1})) - F(x_{n-1})$) such that Q is independent from k. The other right-hand side terms could be bounded in a

similar manner. We thus obtain from (4.3) and Lemma 1 that

$$\|e_n^x\| \le \|e_{n-1}^x\| + Q\tau\|e_{n-1}^x\| + Q\tau\mathscr{E}_{n-1} + Q\tau^2. \tag{4.5}$$

An application of the standard discrete Gronwall inequality yields

$$\|e_n^x\| \le Q\tau \sum_{m=1}^{n-1} \mathscr{E}_m + Q\tau, \ \ 1 \le n \le N. \tag{4.6}$$

We then subtract the third equation of (2.4) from that of (2.5) and split $v_i(t_n) - \tilde{v}_{i,n}$ as

$$v_i(t_n) - \tilde{v}_{i,n} = e_n^{v_i} + (v_{i,n} - \hat{v}_{i,n}) + (\hat{v}_{i,n} - \tilde{v}_{i,n})$$

to obtain

$$
\begin{aligned}
e_n^{v_i} = {}& e_{n-1}^{v_i} + \tau\beta\big(H(x(t_{n-1}))v_i(t_{n-1}) - H(x_{n-1})v_{i,n-1}\big) \\
& - \tau\beta\big[v_i(t_{n-1})v_i(t_{n-1})^\top H(x(t_{n-1}))v_i(t_{n-1}) \\
& \quad -v_{i,n-1}v_{i,n-1}^\top H(x_{n-1})v_{i,n-1}\big] \\
& - \tau\beta\big[x(t_{n-1})x(t_{n-1})^\top H(x(t_{n-1}))v_i(t_{n-1}) \\
& \quad -x_{n-1}x_{n-1}^\top H(x_{n-1})v_{i,n-1}\big] \\
& - 2\tau\beta\sum_{j=1}^{i-1}\big[v_j(t_{n-1})v_j(t_{n-1})^\top H(x(t_{n-1}))v_i(t_{n-1}) \\
& \quad -v_{j,n-1}v_{j,n-1}^\top H(x_{n-1})v_{i,n-1}\big] \\
& + \tau\beta\big[x(t_{n-1})v_i(t_{n-1})^\top F(x(t_{n-1})) - x_{n-1}v_{i,n-1}^\top F(x_{n-1})\big] \\
& - (v_{i,n} - \hat{v}_{i,n}) - (\hat{v}_{i,n} - \tilde{v}_{i,n}) + O(\tau^2).
\end{aligned}
\tag{4.7}
$$

We apply Lemmas 3 and 4 and similar derivations as (4.3) to get

$$\|e_n^{v_i}\| \le \|e_{n-1}^{v_i}\| + Q\tau\big(\|e_{n-1}^x\| + \|e_{n-1}^{v_i}\|\big) + Q\tau\mathscr{E}_{n-1} + Q\tau^2.$$

Adding this equation from $i = 1$ to k and using (4.6) we obtain

$$\mathscr{E}_n \le \mathscr{E}_{n-1} + Q\tau\mathscr{E}_{n-1} + Q\tau^2 \sum_{m=1}^{n-1} \mathscr{E}_m + Q\tau^2. \tag{4.8}$$

Then an application of Lemma 5 leads to the conclusion of the theorem. □

5. Numerical experiments

In this section, we carry out numerical experiments to test the numerical accuracy of the scheme (2.5). For practical applications of the constrained high-index saddle dynamics (2.1) we refer [27] for more details. Let $T = \alpha = \beta = 1$, $\|e^x\| := \max_{1 \le n \le N}\|x(t_n) - x_n\|$, $\|e^{v_i}\| := \max_{1 \le n \le N}\|v_i(t_n) - v_{i,n}\|$ for $1 \le i \le k$ and we use numerical solutions computed under $\tau = 2^{-13}$ as the reference solutions due to the unavailability of the exact solutions.

5.1. *Accuracy test*

We consider the index-1 constrained saddle dynamics for the 4-well potential proposed in [5]

$$E(x_1, x_2) = x_1^4 - px_1^2 + x_2^4 - x_2^2 + qx_1^2 x_2^2 \tag{5.1}$$

with the initial conditions

$$X_0 = \frac{1}{\sqrt{2}}(1, 1), \quad V_1 = \frac{1}{\sqrt{2}}(-1, 1)$$

and the parameters

$$\text{(i) } (p, q) = (5, 1), \quad \text{(ii) } (p, q) = (10, 5).$$

Numerical results are presented in Tables 1-2, which demonstrate the first-order accuracy of the scheme (2.5) as proved in Theorem 1.

TABLE 1   *Convergence rates for surface (5.1) under the parameter (i).*

τ	$\|e^x\|$	conv. rate	$\|e^{v_1}\|$	conv. rate
$1/2^5$	2.31E-02		2.31E-02	
$1/2^6$	1.15E-02	1.01	1.15E-02	1.02
$1/2^7$	5.67E-03	1.02	5.67E-03	1.02
$1/2^8$	2.79E-03	1.02	2.79E-03	1.03

TABLE 2   *Convergence rates for surface (5.1) under the parameter (ii).*

τ	$\|e^x\|$	conv. rate	$\|e^{v_1}\|$	conv. rate
$1/2^5$	5.40E-02		5.40E-02	
$1/2^6$	2.63E-02	1.04	2.63E-02	1.04
$1/2^7$	1.29E-02	1.02	1.29E-02	1.02
$1/2^8$	6.31E-03	1.03	6.31E-03	1.03

5.2. *Dynamic convergence*

We consider the index-1 constrained saddle dynamics for the Rosenbrock type function

$$E(x_1, x_2, x_3) = a(\sqrt{3}x_2 - 3x_1^2)^2 + b(\sqrt{3}x_1 - 1)^2 + a(\sqrt{3}x_3 - 3x_2^2)^2 + b(\sqrt{3}x_2 - 1)^2 \tag{5.2}$$

equipped with the parameters $a = 2$, $b = -9.8$, $T = 5$ and different initial conditions

$$X_0 = \frac{1}{\sqrt{29}}(2, -3, 4), \quad X_0' = \frac{1}{\sqrt{3}}(-1, -1, 1), \quad V_{1,0} = \frac{1}{\sqrt{2}}(1, 1, 0).$$

Under the given parameters, this surface has an index-1 saddle point located at

$$\left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}} \right).$$

Numerical results are presented in Figure 1, which shows that the numerical saddle dynamics could reach the target saddle point under different initial values, even though the curvature of the Rosenbrock type function is complicated. Furthermore, the dynamic convergence of the numerical saddle dynamics as the step size τ decreases is observed, which demonstrates that the proposed scheme is appropriate for computing the dynamic pathways for constructing the solution landscapes, e.g. [13, 27, 28, 31].
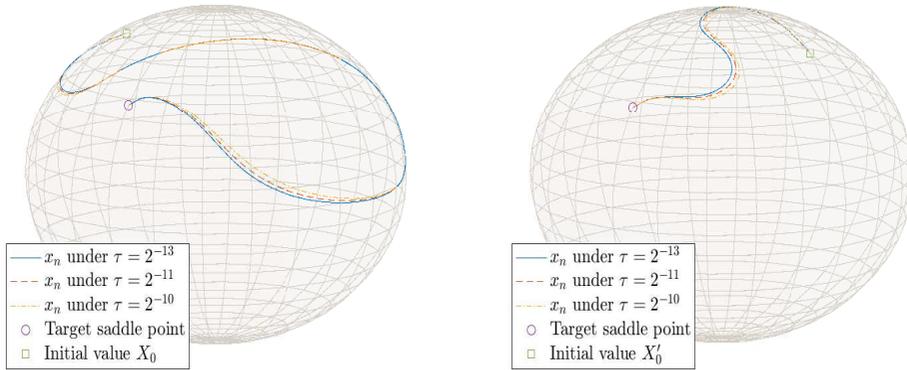
FIG. 1. Pathway convergence of constrained saddle dynamics under different initial values.

6. Index-robust numerical analysis

In previous sections, we develop error estimates for the numerical discretization (2.5) of the constrained high-index saddle dynamics (2.1). However, as the constant Q in the estimate of Theorem 1 depends on k, the numerical accuracy could be reduced if k is large enough in real applications. In other words, the estimate in Theorem 1 is not index-robust. Therefore, we aim to develop an index-robust error estimate in this section to eliminate the dependence of k on Q in Theorem 1, which serves as an improvement for the previous results.

The key ideas to achieve this goal lie in adjusting the relaxation parameter and estimating the errors in the averaged norm. Suppose

$$\alpha = \beta \leq \frac{Q_0}{k} \tag{6.1}$$

for some positive constant Q_0. Furthermore, the following averaged norm $\|\cdot\|_A$ is defined for any sequence of vectors $\{g_i\}_{i=1}^{k}$

$$\|g\|_A := \frac{1}{k} \sum_{i=1}^{k} \|g_i\|.$$

Based on these presumptions, we immediately obtain from Lemmas 1–3 that for $1 \leq n \leq N$

$$\|x_n - \tilde{x}_n\| \leq M\frac{\tau^2}{k^2}, \quad \|\hat{v}_{i,n} - \tilde{v}_{i,n}\| \leq M\frac{\tau^2}{k^2}, \quad 1 \leq i \leq k,$$

$$\left|\hat{v}_{m,n}^\top \hat{v}_{i,n}\right| \leq M\frac{\tau^2}{k^2}, \quad 1 \leq m < i \leq k, \tag{6.2}$$

$$\left|\|\hat{v}_{i,n}\|^2 - 1\right| \leq M\frac{\tau^2}{k^2}, \quad 1 \leq i \leq k.$$

Here the constant M is independent from τ, n, N, α, β and k. To prove the desired results, the Lemma 4 and the Theorem 1 need to be re-estimated in the following subsections.

6.1. *Re-estimation of Lemma 4*

We re-estimate Lemma 4 such that the constant Q in (3.9) is independent from k. Though the derivations of the re-estimation follow the ideas of the proof of Lemma 4 in [38, Lemma 4.2], there are essential differences in that the condition (6.1) is invoked to eliminate the dependence of the constants Q on k throughout the derivations.

Lemma 6 *Suppose the Assumption A and (6.1) hold, then the following estimate holds for $1 \leq n \leq N$ and for τ small enough*

$$\|v_{i,n} - \hat{v}_{i,n}\| \leq Q\tau^2, \quad 1 \leq i \leq k.$$

Here the positive constant Q is independent from n, N, τ, α, β and k.

Proof. Let $G > M$ be a fixed positive number where M is defined in (6.2). Then we firstly prove that, if τ satisfies the constraint

$$\frac{M + \tau^2 G^2}{\left(1 - M\tau^2 - G^2\tau^4\right)^{1/2}} \leq G, \tag{6.3}$$

then the following estimates hold

$$|\hat{v}_{i,n}^\top v_{m,n}| \leq G\frac{\tau^2}{k^2}, \quad 1 \leq m < i \leq k. \tag{6.4}$$

Note that the condition (6.3) is independent from k and is valid if τ is sufficiently small. We prove this argument by induction on the subscription m. For $m = 1$ we apply (6.2), the last equation of (2.5) as well as (6.3) to obtain for $1 < i \leq k$

$$|\hat{v}_{i,n}^\top v_{1,n}| = \frac{|\hat{v}_{i,n}^\top \hat{v}_{1,n}|}{(\|\hat{v}_{1,n}\|^2)^{1/2}} \leq \frac{M\tau^2/k^2}{(1 - M\tau^2/k^2)^{1/2}} \leq \frac{M}{(1 - M\tau^2)^{1/2}} \frac{\tau^2}{k^2} \leq G\frac{\tau^2}{k^2}. \tag{6.5}$$

Thus, (6.4) holds with $m = 1$. Suppose (6.4) holds for $1 \leq m < m^*$ for some $1 \leq m^* < k-1$. Then we invoke (6.4) with $1 \leq m < m^*$ and (6.2) into the expression of $\hat{v}_{i,n}^\top v_{m^*,n}$ to obtain for $m^* < i \leq k$

$$
\begin{aligned}
|\hat{v}_{i,n}^\top v_{m^*,n}| &= \frac{\left| \hat{v}_{i,n}^\top \hat{v}_{m^*,n} - \sum_{j=1}^{m^*-1} (\hat{v}_{m^*,n}^\top v_{j,n})(\hat{v}_{i,n}^\top v_{j,n}) \right|}{\left(\|\hat{v}_{m^*,n}\|^2 - \sum_{j=1}^{m^*-1} (\hat{v}_{m^*,n}^\top v_{j,n})^2 \right)^{1/2}} \\
&\leq \frac{M\dfrac{\tau^2}{k^2} + (m^*-1)\dfrac{G^2\tau^4}{k^4}}{\left(1 - M\dfrac{\tau^2}{k^2} - (m^*-1)\dfrac{G^2\tau^4}{k^4} \right)^{1/2}} \\
&\leq \frac{M + G^2\tau^2}{\left(1 - M\tau^2 - \tau^4 G^2 \right)^{1/2}} \frac{\tau^2}{k^2} \leq G\frac{\tau^2}{k^2}, \quad m^* < i \leq k.
\end{aligned}
$$

That is, (6.4) holds for $m = m^*$ and thus holds for any $1 \leq m < k$ by mathematical induction.

Similar to the above derivations, there exists a constant $Q > 0$ independent from n, N, τ, α, β and k such that for $1 \leq i \leq k$ and $1 \leq n \leq N$

$$
(1 - Q\tau^2)^{1/2} \leq |Y_{i,n}| \leq (1 + Q\tau^2)^{1/2}. \tag{6.6}
$$

Note that this implies

$$
|1 - Y_{i,n}| \leq |1 - Y_{i,n}|(1 + Y_{i,n}) = |Y_{i,n}^2 - 1| \leq Q\tau^2. \tag{6.7}
$$

Then we remain to estimate $v_{i,n} - \hat{v}_{i,n}$ for $1 \leq i \leq k$. According to the definition of $v_{i,n}$ we have

$$
v_{i,n} - \hat{v}_{i,n} = \frac{1}{Y_{i,n}} \left((1 - Y_{i,n})\hat{v}_{i,n} - \sum_{j=1}^{i-1} (\hat{v}_{i,n}^\top v_{j,n}) v_{j,n} \right),
$$

which, together with (6.2), (6.4), (6.6) and (6.7), implies

$$
\begin{aligned}
\|v_{i,n} - \hat{v}_{i,n}\| &\leq \frac{1}{|Y_{i,n}|} \left(|1 - Y_{i,n}| \|\hat{v}_{i,n}\| + \sum_{j=1}^{i-1} |\hat{v}_{i,n}^\top v_{j,n}| \right) \\
&\leq Q|1 - Y_{i,n}| + Qk\frac{\tau^2}{k^2} \leq Q\tau^2.
\end{aligned}
$$

Thus we complete the proof. $\quad \square$

Remark 1 *From the proof of Lemma 6 we note that the same conclusion could be obtained under a weaker constraint on β than (6.1), that is, the power of k on the denominator could be less than 1. However, we will show in the next proof that (6.1) is necessary.*

6.2. *Index-robust error estimate*

We prove an index-robust error estimate for the numerical scheme (2.5) in the averaged norm $\|\cdot\|_A$ to the constrained high-index saddle dynamics (2.1) in the following theorem.

Theorem 2 *Suppose the Assumption A and (6.1) hold and $\sqrt{2}\beta L_2\tau \leq 1 - \theta$ for some $0 < \theta < 1$, then the following estimate holds for τ sufficiently small*

$$\|e_n^x\| + \|e_n^v\|_A \leq Q\tau, \ \ 1 \leq n \leq N, \ \ \|e_n^v\|_A = \frac{1}{k}\sum_{j=1}^{k}\|e_n^{v_j}\| = \frac{1}{k}\mathscr{E}_n.$$

Here Q is independent from τ, n, N, α, β and k.

Proof . For the estimate of e_n^x, we observe from (4.3) that only its fourth right-hand side term could result in the dependence of Q on k. As this term was carefully estimated in (4.4), in which the constant Q is independent from k, we could apply similar derivations as those for (4.6) in the proof of Theorem 1 and the condition (6.1) to obtain

$$\|e_n^x\| \leq Q\frac{\tau}{k}\sum_{m=1}^{n-1}\mathscr{E}_m + Q\tau = Q\tau\sum_{m=1}^{n-1}\|e_m^v\|_A + Q\tau, \ \ 1 \leq n \leq N. \tag{6.8}$$

For the estimate of $e_n^{v_i}$ from (4.7), it suffices to pay attention on the difference of two summations

$$\begin{aligned}
\tau\beta\bigg\| \sum_{j=1}^{i-1} &\big[v_j(t_{n-1})v_j(t_{n-1})^\top H(x(t_{n-1}))v_i(t_{n-1})\\
&-v_{j,n-1}v_{j,n-1}^\top H(x_{n-1})v_{i,n-1}\big]\bigg\|\\
\leq \tau\beta\bigg\| \sum_{j=1}^{i-1} &\big[e_{n-1}^{v_j}v_j(t_{n-1})^\top H(x(t_{n-1}))v_i(t_{n-1})\\
&+v_{j,n-1}(e_{n-1}^{v_j})^\top H(x(t_{n-1}))v_i(t_{n-1})\\
&+v_{j,n-1}v_{j,n-1}^\top(H(x(t_{n-1})) - H(x_{n-1}))v_i(t_{n-1})\\
&+v_{j,n-1}v_{j,n-1}^\top H(x_{n-1})e_{n-1}^{v_i}\big]\bigg\|\\
\leq \frac{Q\tau}{k}&\big(\mathscr{E}_{n-1} + \|e_{n-1}^x\| + \|e_{n-1}^{v_i}\|\big).
\end{aligned} \tag{6.9}$$

Here the constant Q is independent from α, β and k. Then similar estimates as those for (4.5) yield

$$\|e_n^{v_i}\| \leq \|e_{n-1}^{v_i}\| + Q\frac{\tau}{k}\big(\|e_{n-1}^x\| + \|e_{n-1}^{v_i}\|\big) + Q\frac{\tau}{k}\mathscr{E}_{n-1} + Q\tau^2.$$

Adding this equation from $i = 1$ to k and multiplying the resulting equation by k^{-1} lead to

$$\|e_n^v\|_A \leq \|e_{n-1}^v\|_A + Q\frac{\tau}{k}\|e_{n-1}^x\| + Q\frac{\tau}{k}\|e_{n-1}^v\|_A + Q\tau\|e_{n-1}^v\|_A + Q\tau^2.$$

We invoke (6.8) to obtain

$$\|e_n^v\|_A \leq \|e_{n-1}^v\|_A + Q\frac{\tau^2}{k}\sum_{m=1}^{n-1}\|e_m^v\|_A + Q\tau\|e_{n-1}^v\|_A + Q\tau^2.$$

Then an application of Lemma 5 leads to the conclusion of the theorem. □

7. Concluding remarks

In this paper we prove error estimates for numerical approximation to constrained high-index saddle dynamics, which extends the existing results for the classical high-index saddle dynamics without constraints in the literature. We then improve the proved results by developing an index-robust error estimate for the proposed numerical scheme in an averaged norm by adjusting the relaxation parameters α and β. These results provide theoretical supports for the numerical accuracy of discretization of constrained high-index saddle dynamics.

It is worth mentioning that the current work mainly focuses on the constrained high-index saddle dynamics on the finite interval $t \in [0, T]$ and prove error estimates to show the dynamic convergence of numerical solutions. For most applications, the target saddle point x_* could be reached within a certain number of iterations, which corresponds to a finite T as imposed in the current work. Nevertheless, the convergence to the saddle point is theoretically determined by the rate of $x(t) \to x_*$ as $t \to \infty$, which suggests the error estimate of $x_n - x_*$ for $n \to \infty$ as those for optimization algorithms. In a very recent work [19] such convergence analysis for the high-index saddle dynamics without constraints is performed. However, due to the stronger coupling between x and $\{v_i\}_{i=1}^k$ in the constrained case, it is not straightforward to extend the methods in [19] to analyze the convergence of $x_n - x_*$ for numerical methods to the constrained high-index saddle dynamics (2.1) and we will investigate this interesting topic in the near future.

Acknowledgements

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