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

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Abstract 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 constraints, 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 the high-dimensional sphere and then improve it by providing index-robust error analysis in an averaged norm by adjusting the relaxation parameters. The developed results provide mathematical support for the accuracy of numerical computations.

Keywords saddle dynamics, saddle point, solution landscape, error estimate, index-robust

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\section{Introduction}

High-index saddle dynamics provides a powerful instrument for systematically finding the high-index saddle points and constructing the solution landscape (see \cite{3, 8, 32–34, 40}). It has been applied to study various applications in physical and engineering problems (see \cite{12–14, 23, 25, 28, 29, 32} and \cite{35, 36, 38, 39, 41}). Here, the index of saddle points refers to the Morse index characterized by the maximal dimension of a subspace on which its Hessian operator is negative definite (see \cite{22}). Under
the additional nonlinear equality constraints, e.g., the energy functional is defined only on the high-dimensional unit sphere, the constrained high-index saddle dynamics for an index-$k$ saddle point of $E(x)$ on the unit sphere $S^{d-1}$ (see [30])

\[
\begin{align*}
\frac{dx}{dt} &= \alpha \left( I - xx^\top - 2 \sum_{j=1}^{k} v_j v_j^\top \right) F(x), \\
\frac{dv_i}{dt} &= \beta \left( I - xx^\top - v_i v_i^\top - 2 \sum_{j=1}^{i-1} v_j v_j^\top \right) H(x)v_i + \beta xv_i^\top F(x), \quad 1 \leq i \leq k
\end{align*}
\]

was proposed for solving the constrained saddle point problems such as the Thomson problem (see [27]) and the Bose-Einstein condensation (see [2]). Here, $E(x)$ is a $C^3$ function with $x \in \mathbb{R}^d$, $\alpha$ and $\beta$ are positive relaxation parameters, and the corresponding natural force $F: \mathbb{R}^d \to \mathbb{R}^d$ and the negative Hessian $H \in \mathbb{R}^{d \times d}$ are given respectively as $F(x) = -\nabla E(x)$ and $H(x) = -\nabla^2 E(x)$ with $H(x) = H(x)^\top$. However, due to the strong nonlinearities of the coupled equations in high-index saddle dynamics, rigorous numerical analysis is 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 (see [1, 4, 6, 7, 9–11, 15] and [16–19, 21, 24, 37, 43]). In contrast, conventional error analysis between the exact solutions to 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 ensures the accuracy of construction of the solution landscape (see [14, 33, 42]). In [42], a first-order numerical scheme for the high-index saddle dynamics without constraints was rigorously analyzed. However, due to the nonlinear equality constraints in the constrained high-index saddle dynamics, a more complex dynamical form is encountered and additional operations in the numerical scheme such as the retraction and vector transport are required (see [30]), which significantly complicate the numerical scheme and the corresponding numerical analysis. Furthermore, the pointwise-in-time error estimate

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

was proved in [42], where $\{x_n, v_1, \ldots, v_k\}$ serve as the numerical approximations of the state variable and corresponding eigenvectors $\{x(t), v_1(t), \ldots, v_k(t)\}$ at the time step $t_n$. However, the proof in [42] indicates that the positive constant $Q$ depends on the index $k$ of the saddle points. 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 (see [26, 27]), the dimension of the energy function and the index $k$ of saddle points can be very high. In this case, the accuracy in (1.3) 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 distinguish the numerical analysis of saddle dynamics from that for ordinary differential equations. We then derive a different error estimate from (1.3) by developing an index-robust estimate, i.e., the constant $K$ in the following estimate is independent of the index $k$, in an averaged sense under the restriction $\alpha = \beta = O(1/k)$ in (1.1):

\[
\|x(t_n) - x_n\| + \frac{1}{k} \sum_{i=1}^{k} \|v_i(t_n) - v_{i,n}\| \leq K\tau.
\]

The role of relaxation parameters $\alpha$ and $\beta$ is the rescaling factor of the time step size in the numerical discretization, and thus this restriction essentially states a decreasing step size with the increment of
the index $k$. These results provide theoretical support for the numerical accuracy of discretization of constrained high-index saddle dynamics and construction of solution landscapes for complex systems.

The rest of this 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 numerical discretization of the constrained high-index saddle dynamics (1.1). In the original work [30] on the model (1.1) with $\alpha = \beta = 1$ and the initial conditions

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

it was proved that a linearly stable steady state of (1.1) is an index-$k$ saddle point of $E(x)$ and the solutions $x$ and $\{v_i\}_{i=1}^k$ of (1.1) satisfy

$$x \in S^{d-1}, \quad v_i^T x = 0, \quad v_i^T v_j = \delta_{ij}, \quad 1 \leq i, j \leq k, \quad t \geq 0. \quad (2.1)$$

Therefore, we aim to construct the numerical scheme that preserves these properties, which are not encountered in numerical methods of unconstrained high-index saddle dynamics (see, e.g., [42]).

For $k \geq 1$ and the terminal time $T > 0$, define a uniform partition $\{t_n\}_{n=0}^N$ of $[0, T]$ with the mesh size $\tau$. We discretize the first-order derivative by the explicit Euler scheme to get the reference equations for constrained index-$k$ saddle dynamics (1.1):

$$x(t_n) = x(t_{n-1}) + \tau \alpha \left( I - x(t_{n-1}) x(t_{n-1})^T \right) + O(\tau^2),$$

$$v_i(t_n) = v_i(t_{n-1}) + \tau \beta \left( I - x(t_{n-1}) x(t_{n-1})^T \right) v_i(t_{n-1})^T + O(\tau^2), \quad 1 \leq i \leq k. \quad (2.2)$$

Then we drop the truncation errors to obtain a first-order scheme of (1.1)

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

$$x_{n+1} \left\| \hat{x}_n \right\|,$$

$$\tilde{v}_{i,n} = v_{i,n} + \tau \beta \left( I - x_{n-1} x_{n-1}^T - v_{i,n-1} v_{i,n-1}^T \right) F(x_{n-1}),$$

$$1 \leq i \leq k, \quad (2.3)$$

$$\tilde{v}_{i,n} = \tilde{v}_{i,n} - \tilde{v}_{i,n}^T x_n x_n, \quad 1 \leq i \leq k,$$

$$v_{i,n} = \frac{1}{N_{i,n}} \left( \tilde{v}_{i,n} - \sum_{j=1}^{i-1} (\tilde{v}_{i,n}^T v_j,n) v_j,n \right), \quad 1 \leq i \leq k.$$
for $1 \leq n \leq N$ and
\[ x_0 = X_0, \quad v_{i,0} = V_{i,0}, \quad Y_{i,n} := \left( \|\hat{\varphi}_{i,n}\|^2 - \sum_{j=1}^{i-1} (\hat{\varphi}_{i,n}^T v_{j,n})^2 \right)^{1/2}, \quad 1 \leq i \leq k. \]

The second equation of (2.3) represents the retraction in order to ensure that $x_n \in S^{d-1}$. The last two equations of (2.3), which stand for the vector transport and the Gram-Schmidt orthonormalization procedure [30], respectively, aim to ensure the last two properties of (2.1), i.e.,
\[ v_{i,n}^T x_n = 0, \quad v_{i,n}^T v_{j,n} = \delta_{ij}, \quad 1 \leq i, j \leq k, \quad 0 \leq n \leq N. \] (2.4)

Compared with the numerical schemes for index-$k$ saddle dynamics without constraints (see, e.g., [42]), the additional operations like the retraction and vector transport in (2.3) caused by 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.

Throughout this paper, we make the following regular assumptions on the force and the Hessian.

**Assumption A.** There exist constants $L_1, L_2 \geq 0$ such that the linear 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 $S^{d-1}$,
\[
\max_{x \in S^{d-1}} (\|F(x)\| + \|H(x)\|) \leq L_2,
\]
hold. Here, $\| \cdot \|$ refers to the standard $l^2$ norm of a vector or a matrix.

### 3 Auxiliary estimates

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

**Lemma 3.1.** Under Assumption A, the following estimate holds for $1 \leq n \leq N$:
\[ \|x_n - \tilde{x}_n\| = |1 - \|\tilde{x}_n\|| \leq 2\alpha^2 L_2^2 \tau^2. \]

**Proof.** We multiply both sides of the first equation of (2.3) by $x_{n-1}^T$ and use (2.4) to obtain $x_{n-1}^T \tilde{x}_n = 1$. We then multiply both sides of the first equation of (2.3) by $\tilde{x}_n^T$ and use $x_{n-1}^T v_{j,n-1} = 0$ for $1 \leq j \leq k$ and the above equation to obtain
\[
\|\tilde{x}_n\|^2 = 1 + \tau\alpha \left( \tilde{x}_n^T x_{n-1} - 2 \sum_{j=1}^{k} (\tilde{x}_n^T x_{n-1}) v_{j,n-1}^T v_{j,n-1} \right) F(x_{n-1}),
\]
which, together with Assumption A and the norm-preserving property of
\[
I - 2 \sum_{j=1}^{k} v_{j,n-1} v_{j,n-1}^T, \quad (3.1)
\]
yields $\|\tilde{x}_n\|^2 - 1 \leq \tau\alpha L_2 \|\tilde{x}_n - x_{n-1}\|$. Similarly, by the first equation of (2.3) again, we have
\[
\|\tilde{x}_n - x_{n-1}\| \leq \tau\alpha \left( I - x_{n-1} x^T_{n-1} - 2 \sum_{j=1}^{k} v_{j,n-1} v_{j,n-1}^T \right) F(x_{n-1}) \| \leq 2\tau\alpha L_2.
\]
Combining the above two equations yields $\|\tilde{x}_n\|^2 - 1 \leq \|\tilde{x}_n\|^2 - 1 \leq 2\alpha^2 L_2^2 \tau^2$, and we incorporate this with
\[
\|x_n - \tilde{x}_n\| = \|\tilde{x}_n\| (1 - \|\tilde{x}_n\|) = |1 - \|\tilde{x}_n\||
\]
to complete the proof. \(\square\)
Lemma 3.2. Under Assumption A, the following estimates hold for $1 \leq n \leq N$:

$$
\|\tilde{v}_{m,n}^T \hat{v}_{i,n}\| \leq Q\beta^2 \tau^2, \quad 1 \leq m < i \leq k,
$$

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

Here, the positive constant $Q$ is independent of $n$, $N$, $\tau$, $k$, $\alpha$ and $\beta$.

Proof. To prove the first estimate, we apply the properties in (2.4) to calculate the product $\tilde{v}_{m,n}^T \hat{v}_{i,n}$ for $1 \leq m < i \leq k$, i.e.,

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

where we used the fact that the 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 $\hat{v}_{i,n}$) in (2.3) that relates to $k$ is $\sum_{j=1}^{n-1} v_{j,n-1}^T H(x_{n-1}) v_{i,n-1}$, which could be considered as a projection of $H(x_{n-1}) v_{i,n-1}$ with the estimate $\|H(x_{n-1}) v_{i,n-1}\| \leq L_2$. By this means, the index $k$ is absorbed and the estimate of $(\cdots)$ is independent of $k$, which leads to the following estimate:

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

To estimate $\|\hat{v}_{i,n}\|$, we multiply both sides of the third equation of (2.3) by $v_{i,n-1}^T$ and apply (2.4) to obtain for $1 \leq i \leq k$,

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

We then multiply both sides of the third equation of (2.3) by $x_{n-1}$ and apply (2.4) to obtain for $1 \leq i \leq k$,

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

which implies

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

We finally multiply $\hat{v}_{i,n}^T$ on both sides of the third equation of (2.3) and apply (2.4), (3.3), (3.4) and (3.5) to obtain

$$
\hat{v}_{i,n}^T \hat{v}_{i,n} = 1 + \tau \beta \left( \hat{v}_{i,n}^T - \tau \beta v_{i,n-1}^T F(x_{n-1}) x_{n-1}^T - v_{i,n-1}^T \right)
$$

$$
- 2 \sum_{j=1}^{n-1} (\hat{v}_{i,n}^T - v_{i,n-1}^T) v_{j,n-1}^T v_{j,n-1}^T H(x_{n-1}) v_{i,n-1} + \tau^2 \beta^2 (v_{i,n-1}^T F(x_{n-1}))^2,
$$

which, together with

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

implies

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

As this equation leads to

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

we incorporate this with (3.6) and (3.7) to find that $|\hat{v}_{i,n}^T \hat{v}_{i,n} - 1| \leq Q\beta^2 \tau^2$, which completes the proof. \qed

Lemma 3.3. Suppose that Assumption A holds, $\alpha = \beta$ and $\sqrt{2}/L_2 \tau \leq 1 - \theta$ for some $0 < \theta < 1$. Then the following estimates hold for $1 \leq n \leq N$:

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

$$
\|\tilde{v}_{m,n} \hat{v}_{i,n}\| \leq Q(\beta^2 + \beta^3) \tau^2, \quad 1 \leq m < i \leq k,
$$

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

Here, the positive constant $Q$ is independent of $n$, $N$, $\tau$, $k$, $\alpha$ and $\beta$. 

Proof. By the fourth equation of (2.3), we have \( ||\tilde{v}_{i,n} - \hat{v}_{i,n}|| = ||\hat{v}_{i,n}^T x_n|| \). By the first three equations of (2.3), we apply the conditions \( x_{n-1}x_{n-1} = 0 \) for \( 1 \leq i \leq k \) and \( v_{i,n-1}v_{j,n-1} = \delta_{ij} \) for \( 1 \leq i, j \leq k \) to calculate \( \tilde{v}_{i,n}^T x_n \) in the following equation via the term-by-term product:

\[
|\tilde{v}_{i,n}^T x_n| = \left| \frac{\tilde{v}_{i,n}^T x_n}{||x_n||} \right|
= \left| v_{i,n-1} + \tau \beta \left( I - x_{n-1}x_{n-1} - v_{i,n-1}v_{i,n-1}^T - 2 \sum_{j=1}^{k-1} v_{j,n-1}v_{j,n-1}^T \right) H(x_{n-1})v_{i,n-1} \right|
+ \tau \beta x_{n-1}v_{i,n-1}^TF(x_{n-1})
\]

\[
= \frac{1}{||x_n||} |\tau(\beta v_{i,n-1}^TF(x_{n-1}) + \alpha F(x_{n-1})v_{i,n-1} - 2\alpha v_{i,n-1}^TF(x_{n-1})) + \tau^2 \beta (\cdots)|,
\]

where we list all the first-order terms with respect to \( \tau \) for the further process while omitting the second-order terms in \( (\cdots) \) since they are all bounded. Note that the first-order term in this equation is exactly zero if \( \alpha = \beta \). By Lemma 3.1, we have

\[
1 \leq \frac{1}{1 - 2\alpha^2L_2^2}\tau^2 \leq \frac{1}{1 - (1 - \theta)^2} \leq \frac{1}{\theta}
\]

Thus we obtain from the above equations that

\[
||\tilde{v}_{i,n} - \hat{v}_{i,n}|| = ||\hat{v}_{i,n}^T x_n|| \leq Q\beta^2\tau^2.
\]  

(3.8)

For \( 1 \leq m \leq i \leq k \), we get \( \tilde{v}_{i,n,\hat{m}}^T \hat{v}_{i,n} = \hat{v}_{m,n}^T \hat{v}_{i,n} - x_n^T \tilde{v}_{i,n} x_n^T \hat{v}_{m,n} \). If \( m < i \), we apply Lemma 3.2 and (3.8) to obtain \( ||\tilde{v}_{i,n,\hat{m}}^T \hat{v}_{i,n}|| \leq Q(\beta^2 + \beta^4)\tau^2 \). If \( m = i \), we again employ Lemma 3.2 and (3.8) to get

\[
||\tilde{v}_{i,n}||^2 - 1 = ||\tilde{v}_{i,n}||^2 - 1 - (x_n^T \tilde{v}_{i,n})^2 \leq Q(\beta^2 + \beta^4)\tau^2.
\]

Thus we complete the proof. \( \square \)

**Lemma 3.4.** Suppose that 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 sufficiently small \( \tau \):

\[
||v_{i,n} - \hat{v}_{i,n}|| \leq C_0\tau^2, \quad 1 \leq i \leq k.
\]

(3.9)

Here, the positive constant \( C_0 \) is independent of \( n, N \) and \( \tau \) but may depend on \( k, \alpha \) and \( \beta \).

**Proof.** Based on Lemma 3.3, the proof could be performed by the same techniques as [42, Lemma 4.2] and is thus omitted. \( \square \)

## 4 Index-dependent error estimates

We present error estimates for the scheme (2.3). 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

\[
e_n^x := x(t_n) - x_n, \quad e_n^v := v_i(t_n) - v_{i,n}, \quad 1 \leq n \leq N, \quad 1 \leq i \leq k,
\]

based on the following lemma.

**Lemma 4.1.** Suppose that there exists a non-negative sequence \( \{Z_n\}_{n=0}^N \) with \( Z_0 = 0 \) satisfying

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

(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:

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

Proof. We first prove by induction that

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

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

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

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

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

i.e., (4.2) holds for $n = \tilde{n}$ and thus for any $1 \leq n \leq N$ by mathematical induction. We then apply the estimate $(1 + A\tau + BT\tau)^n = (1 + (A\tau + BT\tau)^{\tilde{n}}) + (A\tau + BT\tau)^{\tilde{n}}$ to complete the proof. \square

Theorem 4.2. Suppose that 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:

$$\|e_n\| + \mathcal{E}_n \leq Q\tau, \quad 1 \leq n \leq N, \quad \mathcal{E}_m := \sum_{j=1}^{k} ||e_{nm}||.$$

Here, $Q$ is independent of $\tau$, $n$ and $N$ but may depend on $k$, $\alpha$ and $\beta$.

Proof. We subtract the first equation of (2.2) from that of (2.3) to obtain

$$e_n^* = e_{n-1}^* - \tau\alpha \left( I - x(t_{n-1})x(t_{n-1})^\top - 2 \sum_{j=1}^{k} v_j(t_{n-1})v_j(t_{n-1})^\top \right) F(x(t_{n-1}))$$

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

$$= e_{n-1}^* + \tau\alpha (F(x(t_{n-1})) - F(x_{n-1})) - \tau\alpha (x(t_{n-1})x(t_{n-1})^\top F(x(t_{n-1})) - x_{n-1}x_{n-1}^\top F(x_{n-1}))$$

$$- 2\tau\alpha \sum_{j=1}^{k} (v_j(t_{n-1})v_j(t_{n-1})^\top F(x(t_{n-1})) - v_{j,n-1}v_{j,n-1}^\top F(x_{n-1})) + O(\tau^2) + (\bar{x}_n - x_n). \quad (4.3)$$

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

$$\left\| \tau \sum_{j=1}^{k} (v_j(t_{n-1})v_j(t_{n-1})^\top F(x(t_{n-1})) - v_{j,n-1}v_{j,n-1}^\top F(x_{n-1})) \right\|$$

$$\leq \tau \sum_{j=1}^{k} ||e_{n-1}v_j(t_{n-1})^\top F(x(t_{n-1})) + v_{j,n-1}(e_{n-1}v_j(t_{n-1})^\top F(x(t_{n-1}))$$

$$+ v_{j,n-1}(F(x(t_{n-1})) - F(x_{n-1}))|| \leq Q\tau (\mathcal{E}_{n-1} + ||e_{n-1}||),$${
where 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 of $k$. The other right-hand side terms could be bounded in a similar manner. We thus obtain from (4.3) and Lemma 3.1 that
\[
\|e_{n}^{\alpha}\| \leq \|e_{n-1}^{\alpha}\| + Q\tau\|e_{n-1}^{\beta}\| + Q\tau E_{n-1} + O(\tau^2) + 2\alpha^2 L_2^2 \tau^2,
\]
which, together with $O(\tau^2) + 2\alpha^2 L_2^2 \tau^2 \leq Q\tau^2$, leads to $\|e_{n}^{\alpha}\| \leq Q\tau \sum_{n=1}^{m} \|e_{n-1}^{\alpha}\| + Q\tau \sum_{n=1}^{m} E_{n-1} + Q\tau$. An application of the standard discrete Gronwall inequality yields
\[
\|e_{n}^{\alpha}\| \leq Q\tau \sum_{m=1}^{n} E_{m} + Q\tau, \quad 1 \leq n \leq N.
\]

We then subtract the third equation of (2.2) from that of (2.3) and split $v_i(t_n) - \hat{v}_i,n$ as
\[
v_i(t_n) - \hat{v}_i,n = e_i^{\alpha} + (v_i,n - \hat{v}_i,n) + (\hat{v}_i,n - \hat{v}_i,n)
\]
to obtain
\[
e_i^{\alpha} = e_{n-1}^{\alpha} + \tau \beta(H(x(t_{n-1}))v_i(t_{n-1}) - H(x_{n-1})v_i,n)
- \tau \beta x_i(t_{n-1})v_i(t_{n-1}) H(x(t_{n-1}))v_i(t_{n-1}) - v_i,n-1 v_i,n H(x_{n-1})v_i,n-1
- \tau \beta_x(x(t_{n-1})x(t_{n-1})^T H(x(t_{n-1}))v_i(t_{n-1}) - x_{n-1} x_{n-1} H(x_{n-1})v_i,n-1)
- 2\tau \beta \sum_{j=1}^{i-1} v_j(t_{n-1})v_j(t_{n-1})^T H(x(t_{n-1}))v_i(t_{n-1}) - v_j,n-1 v_j,n H(x_{n-1})v_i,n-1
+ \tau \beta [x(t_{n-1})v_i(t_{n-1})^T F(x(t_{n-1})) - x_{n-1} v_{i,n-1}^T F(x(t_{n-1}))]
- (v_i,n - \hat{v}_i,n) - (\hat{v}_i,n - \hat{v}_i,n) + O(\tau^2).
\]
We apply Lemmas 3.3 and 3.4 and similar derivations to (4.3) to get
\[
\|e_{n}^{\alpha}\| \leq \|e_{n-1}^{\alpha}\| + Q\tau (\|e_{n-1}^{\alpha}\| + \|e_{n-1}^{\beta}\|) + Q\tau E_{n-1} + C\tau + Q\beta^2 \tau^2 + O(\tau^2).
\]
Adding this equation from $i = 1$ to $k$ and using (4.6) and $C\tau + Q\beta^2 \tau^2 + O(\tau^2) \leq Q\tau^2$, we obtain
\[
E_n \leq E_{n-1} + Q\tau E_{n-1} + Q\tau^2 \sum_{m=1}^{n-1} E_{m} + Q\tau^2.
\]
Then an application of Lemma 4.1 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 (2.3). For practical applications of the constrained high-index saddle dynamics (1.1) we refer to [30] for more details. Let
\[
T = \alpha = \beta = 1, \quad \|e^\alpha\| := \max_{1 \leq n \leq N} \|x(t_n) - x_n\|, \quad \|e^\beta\| := \max_{1 \leq n \leq N} \|v_i(t_n) - v_i,n\| \quad \text{for} \quad 1 \leq i \leq k,
\]
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 tests

We consider the index-1 constrained saddle dynamics for the 4-well potential proposed in [5]:
\[
E(x_1, x_2) = x_1^4 - px_1^2 + x_2^4 - x_2^2 + q x_1^2 x_2^2
\]
with the initial conditions $X_0 = \frac{1}{\sqrt{2}}(1, 1)$ and $V_1 = \frac{1}{\sqrt{2}}(-1, 1)$ and the parameters (i) $(p, q) = (5, 1)$ and (ii) $(p, q) = (10, 5)$. Numerical results are presented in Tables 1 and 2, which demonstrate the first-order accuracy of the scheme (2.3) as proved in Theorem 4.2.
Table 1  Convergence rates for the surface (5.1) under the parameter (i)

| $\tau$   | $\|e^\tau\|$  | Convergence rate | $\|e^{\tau_1}\|$  | Convergence rate |
|----------|----------------|------------------|---------------------|------------------|
| $1/2^5$  | 2.31E–02       | 1.01             | 2.31E–02            | 1.02             |
| $1/2^6$  | 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 the surface (5.1) under the parameter (ii)

| $\tau$   | $\|e^\tau\|$  | Convergence rate | $\|e^{\tau_1}\|$  | Convergence rate |
|----------|----------------|------------------|---------------------|------------------|
| $1/2^5$  | 5.40E–02       | 1.04             | 5.40E–02            | 1.04             |
| $1/2^6$  | 2.63E–02       | 1.02             | 2.63E–02            | 1.02             |
| $1/2^7$  | 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

$$E(x_1, x_2, x_3) = a(\sqrt{3}x_2 - 3x_1^2)^2 + b(\sqrt{3}x_1 - 1)^2 + a(\sqrt{3}x_3 - 3x_2^2)^2 + b(\sqrt{3}x_2 - 1)^2$$  (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 $(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$. 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 $\tau$ decreases is observed, which demonstrates that the proposed scheme is appropriate for computing the dynamic pathways for constructing the solution landscapes (see, e.g., [14, 30, 31, 33]).

![Figure 1](Color online) 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 (2.3) of the constrained high-index saddle dynamics (1.1). However, as the constant $Q$ in the estimate of Theorem 4.2 depends on $k$, the numerical accuracy could be reduced if $k$ is large enough in real applications. In other words, the estimate in Theorem 4.2 is not index-robust. Therefore, we aim to develop an index-robust error estimate in this section. To distinguish from the above index-dependent estimates, we use $K$ instead of $Q$ in this section to denote a generic constant that is independent of $n, N, \tau, \alpha, \beta$ and $k$ but may assume different values at different occurrences.

The key ideas to achieve this goal lie in imposing some constraints on the relaxation parameter and estimating the errors in the averaged norm. Suppose

$$\alpha = \beta \leq \frac{K_0}{k^p}, \quad p \geq 0$$  \hspace{1cm} (6.1)

for some positive constant $K_0$. Note that since the role of relaxation parameters is the rescaling factor of the time step size per second, this restriction essentially states a decreasing step size with the increment of the index $k$. Furthermore, the averaged norm $\| \cdot \|_A$ is defined for any sequence of vectors $\{g_i\}_{i=1}^n$, $\|g\|_A := \frac{1}{n} \sum_{i=1}^n \|g_i\|$. Based on these presumptions, we immediately obtain from Lemmas 3.1–3.3 that for $1 \leq n \leq N$,

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

$$|\bar{v}_{m,n} \bar{v}_{i,n}| \leq M \frac{\tau^2}{k^{2p}}, \quad 1 \leq m < i \leq k,$$

$$\|\bar{v}_{i,n}\|^2 - 1 \leq M \frac{\tau^2}{k^{2p}}, \quad 1 \leq i \leq k. \hspace{1cm} (6.2)$$

Here, the constant $M$ is independent of $\tau, n, N, \alpha, \beta$ and $k$. To prove the desired results, Lemma 3.4 and Theorem 4.2 need to be re-estimated in the following subsections.

6.1 Re-estimation of Lemma 3.4

We re-estimate Lemma 3.4 such that the constant $Q$ in (3.9) is independent of $k$. Though the derivations of the re-estimation follow the ideas of the proof of [42, Lemma 4.2], there are essential differences in the fact that the condition (6.1) is invoked to eliminate the dependence of the constant $K$ on $k$ throughout the derivations.

**Lemma 6.1.** Suppose that Assumption A and (6.1) hold with $p \geq 1/2$. Then the estimate holds for $1 \leq n \leq N$ and for $\tau$ small enough, $\|v_{i,n} - \bar{v}_{i,n}\| \leq K \tau^2, \quad 1 \leq i \leq k$. Here, the positive constant $K$ is independent of $n, N, \tau, \alpha, \beta$ and $k$.

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

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

then the following estimates hold:

$$|\bar{v}_{i,n} \bar{v}_{m,n}| \leq G \frac{\tau^2}{k}, \quad 1 \leq m < i \leq k. \hspace{1cm} (6.4)$$

Note that the condition (6.3) is independent of $k$ and is valid if $\tau$ is sufficiently small. We prove this argument by induction on the subscription $m$. For $m = 1$, we apply (6.2) with $2p \geq 1$, the last equation of (2.3) as well as (6.3) to obtain for $1 < i \leq k$,

$$|\bar{v}_{i,n} \bar{v}_{1,n}| = \frac{|\bar{v}_{i,n} \bar{v}_{1,n}|}{(\|\bar{v}_{1,n}\|)^2} \leq \frac{M \tau^2/k}{(1 - M \tau^2/k)^{1/2}} \leq \frac{M}{(1 - M \tau^2/k)^{1/2}} \frac{\tau^2}{k} \leq G \frac{\tau^2}{k} \hspace{1cm} (6.5)$$
Thus, (6.4) holds with $m = 1$. Suppose that (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 $m^* < i \leq k$,

$$
|\hat{v}_{i,n}^\top v_{m^*,n}| = \frac{|\hat{v}_{i,n}^\top \hat{v}_{m*,n} - \sum_{j=1}^{m^*-1} (\hat{v}_{m^*,n}^\top v_{j,n}) (\hat{v}_{i,n}^\top v_{j,n})|}{(\|\hat{v}_{m^*,n}\|^2 - \sum_{j=1}^{m^*-1} (\hat{v}_{m^*,n}^\top v_{j,n})^2)^{1/2}} \\
\leq \frac{M^2_k + (m^*-1)\frac{G_k^2}{k^2}}{(1 - M^2_k - (m^*-1)\frac{G_k^2}{k^2})^{1/2}} \\
\leq \frac{M + G^2\frac{\tau^2}{k}}{(1 - M\tau^2 - \tau^4 G^2)^{1/2}} \leq \frac{G^2\frac{\tau^2}{k}}{K}, \quad m^* < i \leq k,
$$
i.e., (6.4) holds for $m = m^*$ and thus for any $1 \leq m < k$ by mathematical induction.

Similar to the above derivations, there exists some constant $K > 0$ independent of $n$, $\tau$, $\alpha$, $\beta$ and $k$ such that for $1 \leq i \leq k$ and $1 \leq n \leq N$,

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

Note that this implies

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

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

$$\|v_{i,n} - \hat{v}_{i,n}\| \leq \frac{1}{|Y_{i,n}|} \left( |1 - Y_{i,n}||\hat{v}_{i,n}| + \sum_{j=1}^{i-1} |\hat{v}_{i,n}^\top v_{j,n}| v_{j,n} \right) \leq K|1 - Y_{i,n}| + Kk\tau^2_k \leq K\tau^2.$$

Thus we complete the proof. $\square$

### 6.2 Index-robust error estimates

We prove an index-robust error estimate for the numerical scheme (2.3) in the averaged norm $\|\cdot\|_A$ to the constrained high-index saddle dynamics (1.1) in the following theorem.

**Theorem 6.2.** Suppose that Assumption A and (6.1) hold with $p \geq 1$ and $\sqrt{2}L_2\tau \leq 1 - \theta$ for some $0 < \theta < 1$. Then the following estimate holds for sufficiently small $\tau$:

$$\|e^p_n\| + \|e^\nu_n\|_A \leq K\tau, \quad 1 \leq n \leq N, \quad \|e^\nu_n\|_A = \frac{1}{k} \sum_{j=1}^{k} \|e^\nu_{j,n}\| = \frac{1}{k} E_n.$$ 

Here, $K$ is independent of $\tau$, $n$, $\alpha$, $\beta$ and $k$.

**Proof.** For the estimate of $e^\nu_n$, we observe from (4.3) that only its fourth right-hand side term could result in the dependence of the constant on $k$. As this term was carefully estimated in (4.4), in which the constant $Q$ is independent of $k$, we could apply the similar derivations to those for (4.6) in the proof of Theorem 4.2 and the condition (6.1) to obtain

$$\|e^\nu_n\| \leq \frac{K^2}{k} \sum_{m=1}^{n-1} E_m + K\tau = K\tau \sum_{m=1}^{n-1} \|e^\nu_m\|_A + K\tau, \quad 1 \leq n \leq N. \tag{6.8}$$

For the estimate of $e^\nu_n$ from (4.7), it suffices to pay attention to the difference between two summations, i.e.,

$$\tau\beta \left\| \sum_{j=1}^{i-1} v_j(t_{n-1})v_j(t_{n-1})^\top H(x(t_{n-1})) v_i(t_{n-1}) - v_j(t_{n-1})v_j(t_{n-1})^\top H(x(t_{n-1})) v_{i,n-1} \right\|$$
dynamics on the finite interval continue to resolve this issue in the future. For most applications, the target saddle point is independent of \( \alpha, \beta \) and \( k \). Then the similar estimates to those for (4.5) yield
\[
\| e_{n-1}^0 \| \leq \| e_{n-1}^0 \| + K_T \| e_{n-1}^x \| + K_T \| e_{n-1}^v \| + \beta \tau E_{n-1} + K \tau^2.
\]
Adding this equation from \( i = 1 \) to \( k \) and multiplying the resulting equation by \( k^{-1} \) lead to
\[
\| e_{n-1}^0 \| \leq \| e_{n-1}^0 \| + K_T \| e_{n-1}^x \| + K_T \| e_{n-1}^v \| + \beta \tau E_{n-1} + k \tau^2.
\]
We invoke (6.8) to obtain
\[
\| e_{n-1}^0 \| \leq \| e_{n-1}^0 \| + K_T \sum_{m=1}^{n-1} \| e_n^0 \| + \beta \tau E_{n-1} + \tau^2.
\]
Then an application of Lemma 4.1 leads to the conclusion of the theorem. \qed

7 Concluding remarks

In this paper, we prove error estimates for the 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 develop an index-robust error estimate for the proposed numerical scheme in an averaged norm. These results provide theoretical support for the numerical accuracy of discretization of constrained high-index saddle dynamics.

In the derivations of the index-robust error estimates, the restriction (6.1) on the relaxation parameters is imposed to support the analysis, which may essentially force a decreasing step size with the increment of the index \( k \). The application of the averaged norm partly eliminates the dependence of the result on \( k \), while it seems difficult to remove or relax the restriction (6.1). By carefully checking the proofs, we see that the main obstacle lies in the estimate of (6.9), where a \( \beta \tau E_{n-1} \) term appears on its right-hand side and finally in the error equation of \( e_{n-1}^0 \). Even if we assume the index-robust error estimate at the \((n-1)\)-th step has been proved in the averaged norm, i.e., \( E_{n-1} \leq K \tau \), the term \( \beta \tau E_{n-1} \) introduces \( K \beta \tau^2 \) in the error equation of \( e_{n-1}^0 \) and the factor \( k \) will be inherited and could not be counteracted without setting \( \beta = O(1/k) \) at the \( n \)-th step, no matter whether the averaged norm is used or not. Nevertheless, we will continue to resolve this issue in the future.

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 proves 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 [20], such convergence analysis for the high-index saddle dynamics without constraints is performed. However, due to the stronger coupling between \( x \) and \( \{v_{i,n}\}_{i=1}^k \) in the constrained case, it is not straightforward to extend the methods in [20] to analyze the convergence of \( x_n - x_* \) for numerical methods to the constrained high-index saddle dynamics (1.1), and we will investigate this interesting topic in the near future.

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