Solution landscape of space-fractional problems and model comparison

Yue Luo, Bing Yu, Lei Zhang, Pingwen Zhang, Xiangcheng Zheng

School of Mathematical Sciences, Peking University
zhengxch@outlook.com

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Critical point \( x^* \in \mathbb{R}^N \) of the energy \( E(x) \) implies \( \nabla E(x^*) = 0 \).

A critical point of \( E(x) \) that is not a local minimum is called a saddle point.

Morse index of a critical point \( x^* \) is the maximal dimension of a subspace on which \( \nabla^2 E(x^*) \) is negative definite. Denote a saddle point of Morse index \( k \) by \( k\text{-saddle} \).

Solution landscape is a pathway map consisting of all critical points and their connections.

Figure: (a) A diagram of the solution landscape; (b) The solution landscape of \( E(x, y) = (x^2 - 1)^2 + (y^2 - 1)^2 \) [Yin-Yu-Zhang Sci. China Math. 21]
To construct the solution landscape, we need to find the any-index saddle points of a given system, and we will focus on a k-saddle for illustration.

For a k-saddle $x^*$, $\nabla^2 E(x^*)$ has exactly $k$ negative eigenvalues $\lambda_1 \leq \cdots \leq \lambda_k$ with corresponding orthonormal eigenvectors $v_1, \cdots, v_k$.

Let $V = \text{span}\{v_1, \cdots, v_k\}$, $x^*$ is a local maximum on $x^* + V$ and a local minimum on $x^* + V^\perp$, where $V^\perp$ is the orthogonal complement space of $V$.

Let $P_V$ be the **orthogonal projection operator** on the finite-dimensional subspace $V$.

**Force** $F(x) = -\nabla E(x)$ and **negative Hessian** $H(x) = -\nabla^2 E(x)$.

For autonomous system $\dot{x} = F(x)$, the **stationary point** $x^*$ implies $F(x^*) = 0$. If this is a **gradient system** there exists an energy $E(x)$ such that $F(x) = -\nabla E(x)$, and the Jacobian $J(x) = \nabla F(x)$ coincides with $H(x)$. For **non-gradient system** we could not find the corresponding $E(x)$, while the Jacobian $J(x)$ still exists. This motivates the high-index saddle dynamics for both gradient and non-gradient systems using the Jacobian $J(x)$, though we derive the saddle dynamics for gradient systems for illustration.
Construction of subspace $V$ for a $k$-saddle

- Computing the $i$th eigenvector could be transformed into a constrained optimization problem (Rayleigh-Ritz theorem)

$$\min_{v_i} v_i^\top \nabla^2 E(x)v_i, \quad v_i^\top v_j = \delta_{i,j}, \quad 1 \leq j \leq i.$$ 

- Corresponding Lagrangian function

$$\mathcal{L}_i(v_i, \xi_1, \cdots, \xi_i) = v_i^\top \nabla^2 E(x)v_i - \xi_i(v_i^\top v_i - 1) - \sum_{j=1}^{i-1} \xi_j v_i^\top v_j.$$ 

- Dynamics of $v_i$

$$\frac{dv_i}{dt} = -\gamma \frac{\partial \mathcal{L}_i}{\partial v_i} = -\gamma \left( \nabla^2 E(x)v_i - \xi_i v_i - \frac{1}{2} \sum_{j=1}^{i-1} \xi_j v_j \right).$$ 

- Parameters $\{\xi_i\}$ are determined by the orthonormal condition: $v_i^\top v_j = \delta_{i,j}$ for $1 \leq i, j \leq k$. 
Construction of saddle dynamics

- Ascent direction on $V$: $P_V(-F(x))$.
- Descent direction on $V^\perp$: $(I - P_V)F(x)$.
- Corresponding gradient dynamics:
  \[
  \frac{dx}{dt} = \beta_1 P_V(-F(x)) + \beta_2 (I - P_V)F(x), \quad \beta_1, \beta_2 > 0.
  \]
- $\beta_1 = \beta_2 = \beta > 0$, then
  \[
  \frac{dx}{dt} = \beta (I - 2P_V)F(x).
  \]
- $P_V = \sum_{i=1}^k v_i v_i^\top \implies \frac{dx}{dt} = \beta \left( I - 2 \sum_{i=1}^k v_i v_i^\top \right)F(x)$. 

Xiangcheng Zheng, PKU (School of Mathematical Sciences, Peking University)
zhengxch@outlook.com
High-index saddle dynamics for gradient systems

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

Relaxation parameters \( \beta, \gamma > 0 \). Initial conditions \( x(0) = x_0 \) and \( v_i(0) = v_{i,0} \) with \( v_{i,0}^\top v_{j,0} = \delta_{i,j} \) for \( 1 \leq i, j \leq k \).

A linear stable steady state \( \implies \) A \( k \)-saddle. Orthonormal-preservation: \( v_i(t)^\top v_j(t) = \delta_{i,j} \) for \( t \geq 0 \).

High-index saddle dynamics for non-gradient systems replace the equations of \( \{v_i\} \) by

\[
\frac{dv_i}{dt} = \gamma \left( I - v_i v_i^\top \right) J(x) v_i - \gamma \sum_{j=1}^{i-1} v_j v_j^\top (J(x) + J^\top(x)) v_i, \quad 1 \leq i \leq k.
\]
Problems in numerical analysis

Two kinds of numerical analysis problems in saddle dynamics:

- **Problem 1: Accuracy of pathway.**
  - The trajectory \( x(t) \) of saddle dynamics provides reasonable predictions for the transition pathway between saddle points.
  - Numerical accuracy of the pathway is characterized by, e.g.
    \[
    \|x_n - x(t_n)\| \leq Q\tau^p, \quad 1 \leq n \leq N
    \]
    for some time step size \( \tau \) and some positive integer \( N \) (i.e. for finite terminal time).

- **Problem 2: Convergence to the target saddle point.**
  - One may also interest in the convergence rate of \( x_n \) to the target saddle point \( x^* \).
  - The convergence rate is characterized by
    \[
    \|x_n - x^*\| \leq Qq^n
    \]
    for some \( 0 < q < 1 \) and for any \( n \geq 1 \).
Discretization for Problem 1

\[
\begin{aligned}
\frac{x_n - x_{n-1}}{\tau} &= \beta \left( I - 2 \sum_{j=1}^{k} v_{j,n-1} v_{j,n-1}^\top \right) F(x_{n-1}), \\
\frac{v_i,n - v_{i,n-1}}{\tau} &= \gamma \left( I - v_{i,n-1} v_{i,n-1}^\top ight. \\
& \quad \left. - 2 \sum_{j=1}^{i-1} v_{j,n-1} v_{j,n-1}^\top \right) H(x_{n-1}) v_{i,n-1}, \quad 1 \leq i \leq k.
\end{aligned}
\]

Note: $v_{i,n}^\top v_{j,n} \neq \delta_{i,j}$ due to the error of discretization. Modified schemes of $\{v_i\}_{i=1}^{k}$:

\[
\begin{aligned}
\frac{\tilde{v}_i,n - v_{i,n-1}}{\tau} &= \gamma \left( I - v_{i,n-1} v_{i,n-1}^\top ight. \\
& \quad \left. - 2 \sum_{j=1}^{i-1} v_{j,n-1} v_{j,n-1}^\top \right) H(x_{n-1}) v_{i,n-1}, \quad 1 \leq i \leq k, \\
\{v_i,n\}_{i=1}^{k} &= \text{GramSchmidt}\{\tilde{v}_i,n\}_{i=1}^{k}.
\end{aligned}
\]
Error estimate

\begin{align*}
\text{Numerical scheme:} & \quad \frac{\tilde{v}_{i,n} - v_{i,n-1}}{\tau} = \cdots, \quad 1 \leq i \leq k; \\
\text{Reference equation:} & \quad \frac{v_i(t_n) - v_i(t_{n-1})}{\tau} = \cdots + O(\tau), \quad 1 \leq i \leq k.
\end{align*}

Define the error \( e_{n}^{v_{i}} = v_{i}(t_{n}) - v_{i,n}. \) If we subtract the numerical scheme from the reference equation, we will encounter

\[
(e_{n}^{v_{i}} \neq) v_{i}(t_{n}) - \tilde{v}_{i,n} = e_{n-1}^{v_{i}} + \cdots + O(\tau^{2}),
\]

**which is not an error equation.** A straightforward idea is to split \( v_{i}(t_{n}) - \tilde{v}_{i,n} \) as

\[
(v_{i}(t_{n}) - v_{i,n}) + (v_{i,n} - \tilde{v}_{i,n}) = e_{n}^{v_{i}} + (v_{i,n} - \tilde{v}_{i,n}),
\]

which leads to the error equation

\[
e_{n}^{v_{i}} = e_{n-1}^{v_{i}} + \cdots + O(\tau^{2}) + (v_{i,n} - \tilde{v}_{i,n}).
\]

Therefore, the main task is to show \( v_{i,n} - \tilde{v}_{i,n} = O(\tau^{2}). \)
Relation between $v_{i,n}$ and $\tilde{v}_{i,n}$ lies in the Gram-Schmidt orthonormalization

$$\tilde{v}_{i,n} = v_{i,n} - \sum_{j=1}^{i-1} (\tilde{v}_{i,n}^\top v_{j,n}) v_{j,n}$$

$$v_{i,n} = \left( \left\| \tilde{v}_{i,n} \right\|^2 - \sum_{j=1}^{i-1} (\tilde{v}_{i,n}^\top v_{j,n})^2 \right)^{1/2}, \quad 1 \leq i \leq k,$$

which requires several auxiliary estimates for the quantities involving $v_{i,n}$ and $\tilde{v}_{i,n}$.

**Lemma**

**The following estimates hold for** $1 \leq n \leq N$

$$\left| (\tilde{v}_{m,n})^\top \tilde{v}_{i,n} \right| \leq M \tau^2, \quad 1 \leq m < i \leq k;$$

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

**Here the positive constant $M$ is independent from $n$, $N$ and $\tau$.**
Error estimate

**Lemma**

The following estimate holds for $\tau$ small enough

$$|\tilde{v}_{i,n}^T v_{m,n}| \leq G\tau^2, \ 1 \leq m < i \leq k, \ 1 \leq n \leq N$$

for some positive constant $G > M$ independent from $n, N$ and $\tau$.

**Lemma**

The following estimate holds for $\tau$ small enough

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

Here the positive constant $Q$ is independent from $n, N$ and $\tau$.

**Theorem**

The following estimate holds for $\tau$ sufficiently small

$$\|x(t_n) - x_n\| + \sum_{i=1}^{k} \|v_{i}(t_n) - v_{i,n}\| \leq Q\tau, \ 1 \leq n \leq N.$$
Numerical experiments

Let $\beta = \gamma = T = 1$. Numerical solutions computed under $\tau = 2^{-13}$ serve as the reference solutions. We compute the index-1 saddle point of the Eckhardt surface

$$E(x_1, x_2) = \exp(-x_1^2 - (x_2 + 1)^2) + \exp(-x_1^2 - (x_2 - 1)^2) + 4\exp\left(-3\frac{x_1^2 + x_2^2}{2}\right) + \frac{x_2^2}{2}$$

with the initial conditions

$$x(0) = (-2, 1)^\top, \quad v(0) = \frac{1}{\sqrt{2}}(-1, 1)^\top.$$
To observe the pathway convergence of saddle dynamics, we plot the trajectories of $x$ with $k = 1$ and the initial conditions

$$x(0) = (1.5, 1.2)^\top, \quad v(0) = \frac{1}{\sqrt{5}}(-1, 2)^\top.$$

**Figure:** (Left) Numerical solution of $x(t)$ with $\tau = 2^{-8}$ and different terminal time $T$; (Right) Numerical solution of $x(t)$ with $T = 5$ and different $\tau$. The symbols on the curves indicate the time steps.
Analysis for Problem 2

- Scheme of $x$ for some step size $\beta_n$

$$x_{n+1} = x_n + \beta_n \left( I - 2 \sum_{i=1}^{k} v_i,n v_{i,n}^\top \right) F(x_n), \quad (1)$$

where the computed vectors $\{v_i,n\}_{i=1}^{k}$ form the approximated unstable subspace $V_n$ at the $n$-th step.

- Assumption on the approximation $V_n$ of the unstable subspace $V(t_n)$ at $t_n$:

$$\|V(t_n)V(t_n)\top - V_n V_n\top\| \leq \alpha$$

for some $0 \leq \alpha \leq 1$.

**Lemma**

The scheme (1) could be reformulated as

$$x_{n+1} - x^* = \left( I + \beta_n (I - 2V_n V_n^\perp) H(x_n) \right) (x_n - x^*) + B_n (x_n - x^*)$$

where

$$\|B_n\| \leq \frac{1}{2} \beta_n M \|I - 2V_n V_n^\perp\| \|x_n - x^*\|.$$

Here $M$ is the Lipschitz constant of $H(x)$. 

Xiangcheng Zheng, PKU (School of Mathematical Sciences, Peking University) zhengxch@outlook.com
Lemma

Let \( \{r_n\}_{n \geq 0} \) be a non-negative series satisfying

\[
r_{n+1} \leq (1 - q)r_n + cr_n^2, \quad n \geq 0, \quad q \in (0, 1), \quad c > 0.
\]

(a) If \( r_n < \frac{q}{c} \) for some \( n \geq 0 \), then \( r_{n+1} < r_n < \frac{q}{c} \);

(b) If \( r_0 < \frac{q}{c} \), then \( r_{n+1} \leq \left( \frac{1}{1 + q} \right)^{n+1} \frac{qr_0}{q - cr_0} \) for all \( n \geq 0 \).

Theorem

Suppose \( 1 - \alpha > \kappa\alpha(\alpha + 5) \) where \( \kappa = L/\mu \) and \( 0 < \mu \leq |\lambda_i| \leq L \) within \( B_\delta(x^*) \) for \( 1 \leq i \leq d \), the initial point \( x_0 \) satisfies \( r_0 := \|x_0 - x^*\| < \min\{\delta, r\} \) where \( r = 2\mu\eta/M \), \( \eta = 1 - \alpha - \kappa\alpha(\alpha + 5) > 0 \), and \( M \) is the Lipschitz constant of \( H(x) \). Then for \( \beta_n = 2/(L(1 - \alpha^2) + \mu(1 - \alpha)) \), \( x^{(n)} \) converges to \( x^* \) with

\[
\|x_n - x^*\| \leq \left( 1 - \frac{2\eta}{\kappa(1 - \alpha^2) + 1 - \alpha + 2\eta} \right)^n \frac{rr_0}{r - r_0}.
\]
1D fractional Laplacian on \([0, 1]\)

\[
(-\Delta)^{\alpha(x)/2} u(x) = \sum_{k \in \mathbb{Z}} (4\pi^2 k^2)^{\alpha(x)/2} u_k e^{2\pi i k x}
\]

where the Fourier coefficients \(\{u_k\}\) and their discretizations \(\{\hat{u}_k\}\) are given by

\[
u_k = \int_0^1 u(x) e^{-2\pi i k x} \, dx, \quad \hat{u}_k = h \sum_{i=0}^{N-1} u(x_i) e^{-2\pi i k x_i}.
\]

Approximation scheme

\[
(-\Delta)^{\alpha(x_i)/2} u(x_i) = \sum_{k \in \mathbb{N}} (4\pi^2 k^2)^{\alpha(x_i)/2} \hat{u}_k e^{2\pi i k x_i}, \quad 0 \leq i < N.
\]

where \(\mathbb{N} := \{z \in \mathbb{Z} : -N/2 \leq z \leq N/2 - 1\}\).
We treat \((4\pi^2 k^2)^{\alpha(x)/2}\) as a power function \(g_k(z) := (4\pi^2 k^2)^{z/2}\) for \(k \neq 0\) and \(0 < z \leq 2\) such that \(g_k(\alpha(x)) = (4\pi^2 k^2)^{\alpha(x)/2}\), and expand \(g_k\) at \(z = 1\)

\[
g_k(z) = \sum_{s=0}^{S} \frac{g_k^{(s)}(1)}{\Gamma(s + 1)} (z - 1)^s + \frac{g_k^{(S+1)}(\xi)}{\Gamma(S + 2)} (z - 1)^{S+1}
\]

\[
= \sum_{s=0}^{S} \frac{(4\pi^2 k^2)^{1/2}}{\Gamma(s + 1)} \frac{\ln^s(4\pi^2 k^2)}{2^s} (z - 1)^s
\]

\[
+ \frac{(4\pi^2 k^2)^{\xi/2}}{\Gamma(S + 2)} \frac{\ln^{S+1}(4\pi^2 k^2)}{2^{S+1}} (z - 1)^{S+1} =: G_k(z) + R_k(z).
\]

Here \(\xi\) lies in between 1 and \(z\). We could substitute \(g_k(\alpha(x))\) by \(G_k(\alpha(x))\) for \(k \in \mathbb{N}/\{0\}\) in \((-\Delta)^{\alpha(x)/2}_{N,h} u(x_i)\) and notice that \(g_0(\alpha(x)) = 0\) to reach a further approximation for \(0 \leq i < N\)

\[
(-\Delta)^{\alpha(x_i)/2}_{N,h,F} u(x_i) = \sum_{k\in\mathbb{N}/\{0\}} G_k(\alpha(x_i)) \hat{u}_k e^{2\pi ikx_i} = \sum_{s=0}^{S} (\alpha(x_i) - 1)^s \sum_{k\in\mathbb{N}/\{0\}} \frac{(4\pi^2 k^2)^{1/2}}{\Gamma(s + 1)} \frac{\ln^s(4\pi^2 k^2)}{2^s} \hat{u}_k e^{2\pi ikx_i}.
\]
Variable-order fractional Laplacian

Theorem

For $0 < m \in \mathbb{Z}$, let $S = \left\lfloor e^{\mu+1} \ln(\pi N) - 1 \right\rfloor$ with $\mu$ satisfying

$$\mu e^{\mu+1} \geq m + 2.$$

Then the truncation error can be bounded by

$$|R_k(z)| \leq N^{-m}, \quad k \in \mathbb{N}/\{0\}, \quad 0 < z \leq 2.$$

Theorem

The implementation of $(-\Delta)^{\alpha(x_i)/2}_{N,h,F} u(x_i)$ for $0 \leq i < N$ requires $O(N \ln^2 N)$ operations via the FFT, which is much faster than the evaluation of $(-\Delta)^{\alpha(x_i)/2}_{N,h} u(x_i)$ for $0 \leq i < N$ that needs $O(N^2 \ln N)$ operations.
We first measure the $L^2$ errors between the fast method and the direct method.

Figure: Plots of $L^2$ errors under (A) $\alpha = 1.5$ and $N = 2^{12}$; (B) $\alpha = 1.5$ and $N = 2^{18}$ and (C) $\alpha = 1.5 + 0.4 \sin(2\pi x)$ and $N = 2^{12}$. 
We then test the efficiency of the fast method with $S = 25$.

Figure: Plots of CPU times under (A) $\alpha = 1.5$ and (B) $\alpha = 1.5 + 0.4 \sin(2\pi x)$. 
2D fractional Laplacian on $[0, 1]^2$

$$(-\Delta)^{\alpha(x,y)/2} u(x, y) := \sum_{k,l \in \mathbb{Z}} \left[ 4\pi^2 (k^2 + l^2) \right]^{\alpha(x,y)/2} u_{k,l} e^{2\pi i(kx+ly)}.$$

Approximation for $0 \leq i, j < N$

$$(-\Delta)^{\alpha(x_i,y_j)/2} u(x_i, y_j) = \sum_{k,l \in \mathbb{N}} \left[ 4\pi^2 (k^2 + l^2) \right]^{\alpha(x_i,y_j)/2} \hat{u}_{k,l} e^{2\pi i(kx_i+ly_j)}.$$

Fast scheme for $0 \leq i, j < N$

$$(-\Delta)^{\alpha(x_i,y_j)/2} u(x_i, y_j) := \sum_{s=0}^{S} (\alpha(x_i, y_j) - 1)^s$$

$$\times \sum_{k,l \in \mathbb{N}, (k,l) \neq (0,0)} \frac{(4\pi^2 (k^2 + l^2))^{1/2}}{\Gamma(s + 1)} \frac{\ln^s (4\pi^2 (k^2 + l^2))}{2^s} \hat{u}_{k,l} e^{2\pi i(kx_i+ly_j)}.$$

$$S = \left[ e^{\mu+1} \ln(\sqrt{2}\pi N) - 1 \right] \text{ with } \mu e^{\mu+1} \geq m + 2 \text{ (recall that for the 1D case } S = \left[ e^{\mu+1} \ln(\pi N) - 1 \right]).$$
Variable-order constant-coefficient space-fractional phase field equation

\[ \dot{u} = F(u) := -\kappa(-\Delta)^{\alpha(x)/2}u + u - u^3. \] (2)

Variable-coefficient integer-order phase field model

\[ \dot{u} = F(u) := \kappa(x)\Delta u + u - u^3. \] (3)

How to compare different models? A potential criteria is the solution landscapes of these two models since all stationary points and their connections (transition pathways) could provide a comprehensive description for the models.

Parameter selection: model (2) with

\[ \alpha(x) = 1.2 + 0.1 \cos(2\pi x), 1.3 + 0.2 \cos(2\pi x), 1.55 + 0.45 \cos(2\pi x) \]

and \( \kappa = 0.02 \), and model (3) with

\[ \kappa(x) = 3 \times 10^{-3} + 2 \times 10^{-3} \cos(2\pi x). \]
Figure: (A)-(C) Solution landscapes of 1D variable-order phase field model with different $\alpha$. (D) Solution landscape of the integer-order phase field model with variable coefficient.

Xiangcheng Zheng, PKU (School of Mathematical Sciences, Peking University)

Solution landscape of space-fractional PDE

August 11-13, 2022 23 / 25
It seems that the solution landscape of variable-order constant-coefficient space-fractional phase field equation could be recovered by adjusting the variable coefficient in integer-order space-fractional phase field equation. That is, these two models exhibit similar behaviors under suitable parameters.

Probably the singularity of the solutions to fractional problems may distinguish the fractional models from the integer-order analogues with variable coefficients as it could be difficult to recover the boundary singularities by adjusting the variable coefficients in integer-order models, and we are currently working on this problem.

The proposed method does not work for time-fractional problems straightforwardly since the current saddle dynamics only works for the first-order autonomous systems. How to compare the time-fractional models with variable order and variable coefficient remains to be investigated.


Thank You

for Your Attention!