Solution landscape of space-fractional problems and model comparison

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

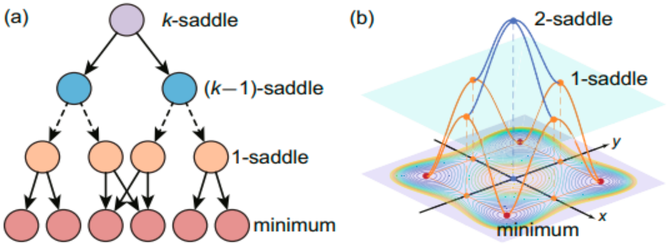


Figure: (a) A diagram of the solution landscape; (b) The solution landscape of $E(x,y) = (x^2-1)^2 + (y^2-1)^2$ [Yin-Yu-Zhang Sci. China Math. 21]

- 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.

- Computing the ith 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

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

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

- 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

$$\frac{dx}{dt} = \beta\big(I - 2P_V\big)F(x).$$

- $P_V = \sum_{i=1}^{k} v_i v_i^\top \Longrightarrow \dfrac{dx}{dt} = \beta\left(I - 2\sum_{i=1}^{k} v_i v_i^\top\right)F(x).$

- **High-index saddle dynamics for gradient systems**

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

- Relaxation parameters β, $\gamma > 0$. 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 $1 \le i, j \le k$.
- A linear stable steady state $\Longrightarrow$ A k-saddle. Orthonormal-preservation: $v_i(t)^\top v_j(t) = \delta_{i,j}$ for $t \ge 0$.
- **High-index saddle dynamics for non-gradient systems** replace the equations of $\{v_i\}$ by

$$\frac{dv_i}{dt} = \gamma\big(I - v_i v_i^\top\big)J(x)v_i - \gamma\sum_{j=1}^{i-1} v_j v_j^\top\big(J(x) + J^\top(x)\big)v_i, \quad 1 \le i \le k.$$

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 τ 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 $n \geq 1$.

$$\begin{cases} \dfrac{x_n - x_{n-1}}{\tau} = \beta\Big(I - 2\sum_{j=1}^{k} v_{j,n-1}v_{j,n-1}^\top\Big)F(x_{n-1}), \\ \dfrac{v_{i,n} - v_{i,n-1}}{\tau} = \gamma\Big(I - v_{i,n-1}v_{i,n-1}^\top \\ \qquad\qquad -2\sum_{j=1}^{i-1} v_{j,n-1}v_{j,n-1}^\top\Big)H(x_{n-1})v_{i,n-1}, \quad 1 \le i \le k. \end{cases}$$

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

$$\begin{cases} \dfrac{\tilde{v}_{i,n} - v_{i,n-1}}{\tau} = \gamma\Big(I - v_{i,n-1}v_{i,n-1}^\top \\ \qquad\qquad -2\sum_{j=1}^{i-1} v_{j,n-1}v_{j,n-1}^\top\Big)H(x_{n-1})v_{i,n-1}, \quad 1 \le i \le k, \\ \{v_{i,n}\}_{i=1}^k = \text{GramSchmidt}\{\tilde{v}_{i,n}\}_{i=1}^k. \end{cases}$$

$$\begin{cases} \text{Numerical scheme: } \dfrac{\tilde{v}_{i,n} - v_{i,n-1}}{\tau} = \cdots, \quad 1 \le i \le k; \\ \text{Reference equation: } \dfrac{v_i(t_n) - v_i(t_{n-1})}{\tau} = \cdots + O(\tau), \quad 1 \le i \le k. \end{cases}$$

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

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

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

Lemma

The following estimates hold for $1 \le n \le N$

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

Here the positive constant M *is independent from* n, N *and* τ.

Lemma

The following estimate holds for τ small enough

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

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

Lemma

The following estimate holds for τ small enough

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

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

Theorem

The following estimate holds for τ sufficiently small

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

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

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

with the initial conditions

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

τ	$\max_n \|x(t_n) - x_n\|$	conv. rate	$\max_n \|v_1(t_n) - v_{1,n}\|$	conv. rate
$1/32$	1.41E-02		2.16E-03	
$1/64$	6.98E-03	1.01	1.09E-03	0.98
$1/128$	3.45E-03	1.01	5.46E-04	1.00
$1/256$	1.70E-03	1.02	2.70E-04	1.02

To observe the pathway convergence of saddle dynamics, we plot the trajectories of x with $k = 1$ and the initial conditions

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

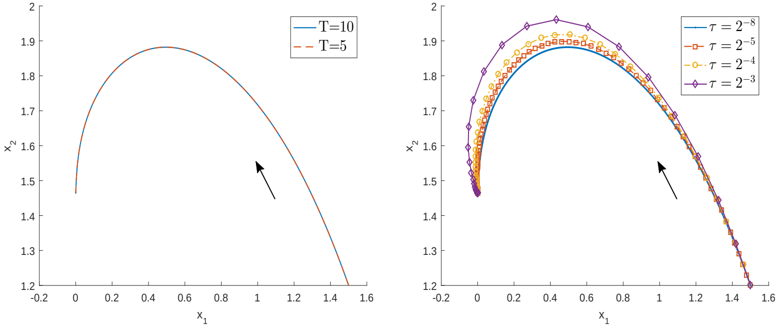


Figure: (Left) Numerical solution of $x(t)$ with $\tau = 2^{-8}$ and different terminal time T; (Right) Numerical solution of $x(t)$ with $T = 5$ and different τ. The symbols on the curves indicate the time steps.

- Scheme of x for some step size β_n

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

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:

$$\left\| V(t_n) V(t_n)^\top - V_n V_n^\top \right\| \leq \alpha \text{ for some } 0 \leq \alpha \leq 1.$$

Lemma

The scheme (1) could be reformulated as

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

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 $H(x)$.

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* $r_n < \dfrac{q}{c}$ *for some* $n \geq 0$, *then* $r_{n+1} < r_n < \dfrac{q}{c}$;

(b) *If* $r_0 < \dfrac{q}{c}$, *then* $r_{n+1} \leq \left(\dfrac{1}{1+q}\right)^{n+1} \dfrac{qr_0}{q-cr_0}$ *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 $[0,1]$

$$(-\Delta)^{\alpha(x)/2}u(x) = \sum_{k\in\mathbb{Z}} \left(4\pi^2k^2\right)^{\alpha(x)/2} u_k e^{2\pi \mathbf{i} kx}$$

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

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

- Approximation scheme

$$(-\Delta)_{N,h}^{\alpha(x_i)/2}u(x_i) = \sum_{k\in\mathbb{N}} \left(4\pi^2k^2\right)^{\alpha(x_i)/2} \hat{u}_k e^{2\pi\mathbf{i}kx_i}, \quad 0\le i<N.$$

where $\mathbb{N} := \{z\in\mathbb{Z} : -N/2 \le z \le N/2-1\}$.

We treat $\left(4\pi^2k^2\right)^{\alpha(x)/2}$ as a power function $g_k(z) := \left(4\pi^2k^2\right)^{z/2}$ for $k \neq 0$ and $0 < z \leq 2$ such that $g_k(\alpha(x)) = \left(4\pi^2k^2\right)^{\alpha(x)/2}$, and expand g_k at $z = 1$

$$\begin{aligned} g_k(z) &= \sum_{s=0}^{S} \frac{g_k^{(s)}(1)}{\Gamma(s+1)}(z-1)^s + \frac{g_k^{(S+1)}(\xi)}{\Gamma(S+2)}(z-1)^{S+1} \\ &= \sum_{s=0}^{S} \frac{\left(4\pi^2k^2\right)^{1/2}}{\Gamma(s+1)} \frac{\ln^s(4\pi^2k^2)}{2^s}(z-1)^s \\ &\quad + \frac{\left(4\pi^2k^2\right)^{\xi/2}}{\Gamma(S+2)} \frac{\ln^{S+1}(4\pi^2k^2)}{2^{S+1}}(z-1)^{S+1} =: G_k(z) + R_k(z). \end{aligned}$$

Here ξ 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 $(-\Delta)_{N,h}^{\alpha(x_i)/2}u(x_i)$ and notice that $g_0(\alpha(x)) = 0$ to reach a further approximation for $0 \leq i < N$

$$\begin{aligned} (-\Delta)_{N,h,F}^{\alpha(x_i)/2}u(x_i) &= \sum_{k\in\mathbb{N}/\{0\}} G_k(\alpha(x_i))\hat{u}_k e^{2\pi\mathbf{i}kx_i} \\ &= \sum_{s=0}^{S}(\alpha(x_i)-1)^s \sum_{k\in\mathbb{N}/\{0\}} \frac{\left(4\pi^2k^2\right)^{1/2}}{\Gamma(s+1)} \frac{\ln^s(4\pi^2k^2)}{2^s}\hat{u}_k e^{2\pi\mathbf{i}kx_i}. \end{aligned}$$

Theorem

For $0 < m \in \mathbb{Z}$*, let* $S = \lceil e^{\mu+1} \ln(\pi N) - 1 \rceil$ *with* μ *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 $(-\Delta)_{N,h,F}^{\alpha(x_i)/2} u(x_i)$ *for* $0 \leq i < N$ *requires* $O(N \ln^2 N)$ *operations via the FFT, which is much faster than the evaluation of* $(-\Delta)_{N,h}^{\alpha(x_i)/2} u(x_i)$ *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.

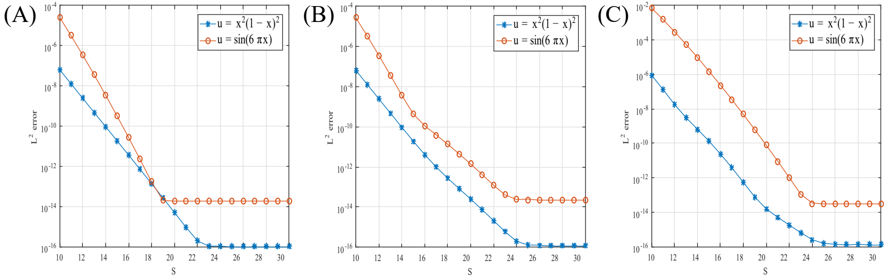


Figure: Plots of L^2 errors under (A) $\alpha = 1.5$ and $N = 2^{12}$; (B) $\alpha = 1.5$ and $N = 2^{18}$ and (C) $\alpha = 1.5 + 0.4\sin(2\pi x)$ and $N = 2^{12}$.

We then test the efficiency of the fast method with $S = 25$.

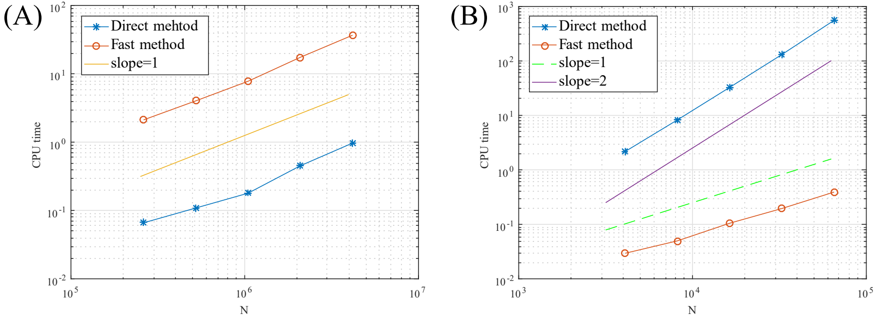


Figure: Plots of CPU times under (A) $\alpha = 1.5$ and (B) $\alpha = 1.5 + 0.4\sin(2\pi x)$.

- 2D fractional Laplacian on $[0,1]^2$

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

- Approximation for $0 \le i,j < N$

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

- Fast scheme for $0 \le i,j < N$

$$(-\Delta)_{N,h,F}^{\alpha(x_i,y_j)/2}u(x_i,y_j) := \sum_{s=0}^{S} (\alpha(x_i,y_j)-1)^s \times \sum_{k,l\in\mathbb{N},(k,l)\neq(0,0)} \frac{\left(4\pi^2(k^2+l^2)\right)^{1/2}}{\Gamma(s+1)} \frac{\ln^s(4\pi^2(k^2+l^2))}{2^s} \hat{u}_{kl} e^{2\pi\mathbf{i}(kx_i+ly_j)}.$$

- $S = \left\lceil e^{\mu+1}\ln(\sqrt{2}\pi N) - 1\right\rceil$ with $\mu e^{\mu+1} \ge m+2$ (recall that for the 1D case $S = \left\lceil e^{\mu+1}\ln(\pi N) - 1\right\rceil$).

- Variable-order constant-coefficient space-fractional phase field equation

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

- Variable-coefficient integer-order phase field model

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

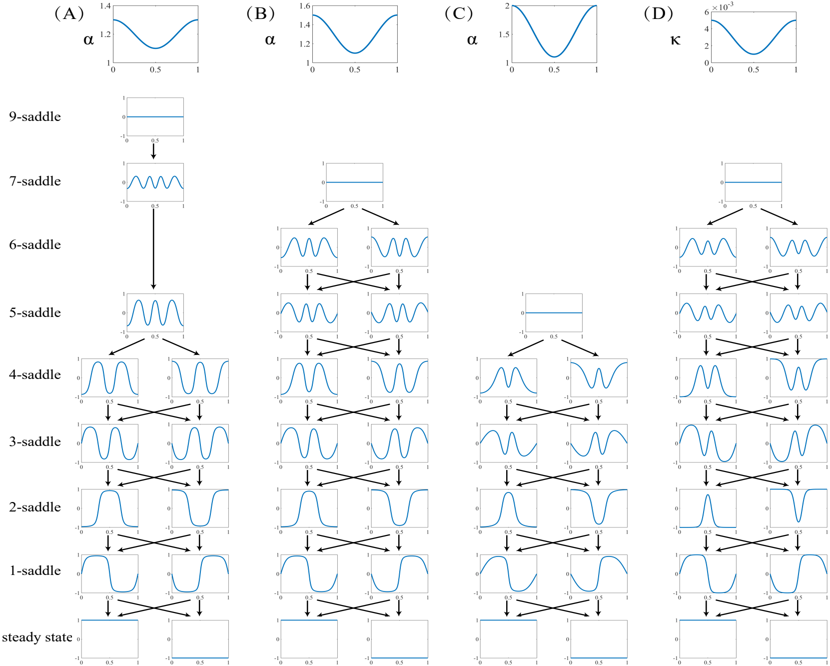
- How to compare different models? A potential criteria is the **solution landscapes of these two models** since all stationary points and their connections (transition pathways) could provide a comprehensive description for the models.

- 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

$$\kappa(x) = 3 \times 10^{-3} + 2 \times 10^{-3}\cos(2\pi x).$$


(A)
α
(B)
α
(C)
α
(D)
κ
9-saddle
7-saddle
6-saddle
5-saddle
4-saddle
3-saddle
2-saddle
1-saddle
steady state

- 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.

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- Y. Luo, **X. Zheng**, X. Cheng, L. Zhang, Convergence analysis of discrete high-index saddle dynamics. *SIAM J. Numer. Anal.* to appear.
- B. Yu, **X. Zheng**, L. Zhang, P. Zhang, Computing solution landscape of nonlinear space-fractional problems via fast approximation algorithm. *J. Comput. Phys.* https://doi.org/10.1016/j.jcp.2022.111513

Thank You

for Your Attention!