Reaction-diffusion models: dynamics, control and numerics

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Based on joint work with I. Mazari, C. Pouchol, D. Ruiz-Balet, E. Trélat, Y. Zhu

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Often the mathematical treatment of real life problems not only involves

1. Modelling
2. Analysis
3. Simulation

but also

1. Design
2. Optimisation
3. Parameter identification
4. Uncertainty quantification
5. Control (passive or active)

Nowadays this fact is enhanced by the frequent need of **data driven modelling**.

Our original motivation: multilinguism

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A Game-Theoretic Analysis of Minority Language Use in Multilingual Societies

José-Ramón Uriarte

The Palgrave Handbook of Economics and Language, 2016 - Springer

Why, often, minority languages are used less than expected, in view of the percentage of population that masters them?

A "politeness equilibrium" emerges as a consequence of a variety of factors, including the fact we try not to annoy the other.

This and many other problems in social sciences require a significant mathematical effort and a variety of modelling paradigms can be employed:

1. ODE
2. Stochastic systems of interacting particles
3. Reaction-diffusion equations
4. Mean Field games
5. Kinetic models
6. PDEs on networks

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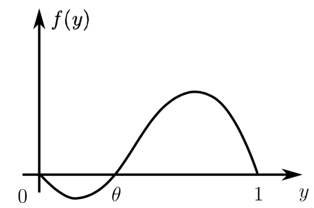
E. Trélat, J. Zhu & E. Zuazua, M3AS, 2018

The **bistable** Cauchy problem: 

$$y_t - y_{xx} = ay(1-y)(y-\theta), \quad y(0,\cdot) = y_0.$$

- The state $0 \le y \le 1$ represents the = density of individuals (or of some of their features).
- $a > 0$: reproductive rate ($a = 1$ without loss of generality).
- $\theta \in (0,1)$: local critical density or *Allee threshold* [1] that determines the sign (positive or negative) the population growth.
- Applications : spread of invading organisms in ecology,[2] population genetics (biology), propagation of nerve tension (neurobiology), waves in chemical reactors (chemistry), etc.

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[1] Warder Clyde Allee, 30's
[2] M.A. Lewis and P. Kareiva, 1993

Allee effect regulation

$$y_t - y_{xx} = ay(1-y)(y-\theta),$$

- Allee effect (ODE Mechanism):
  - Negative population growth (leading to the extinction) when $y < \theta$
  - Population grows towards carrying capacity when $y > \theta$.

Regulation :

- increase θ, by the sterile male technique, the mating disruption (pest management technique), etc.
- decrease θ, providing protection (e.g. vaccines, feeding, suppressing natural enemies)

Distinguished solutions of the system :

- **Steady state** constant solutions : $y \equiv 0$ or θ or 1.
- **Traveling wave (TW)** solutions : link two of the three steady state constant solutions, 0 and 1, through a front that propagates in space with a constant velocity.

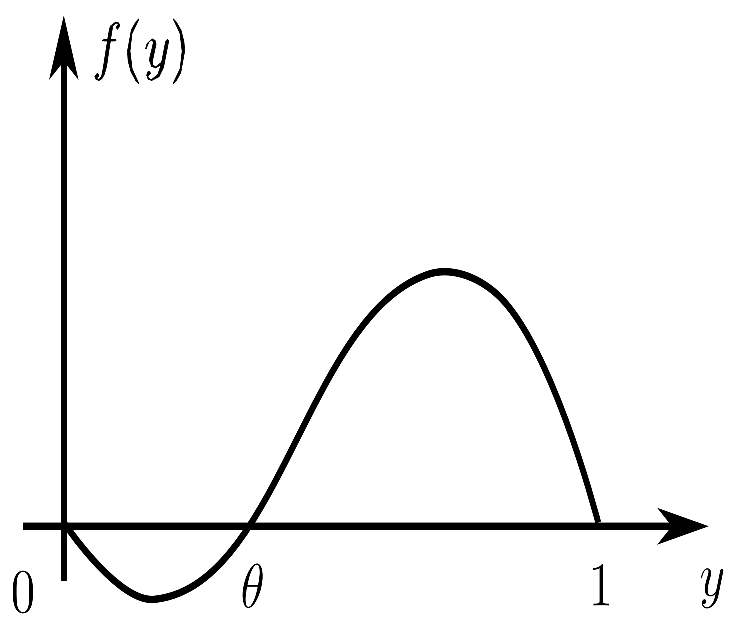
Traveling waves (TW)

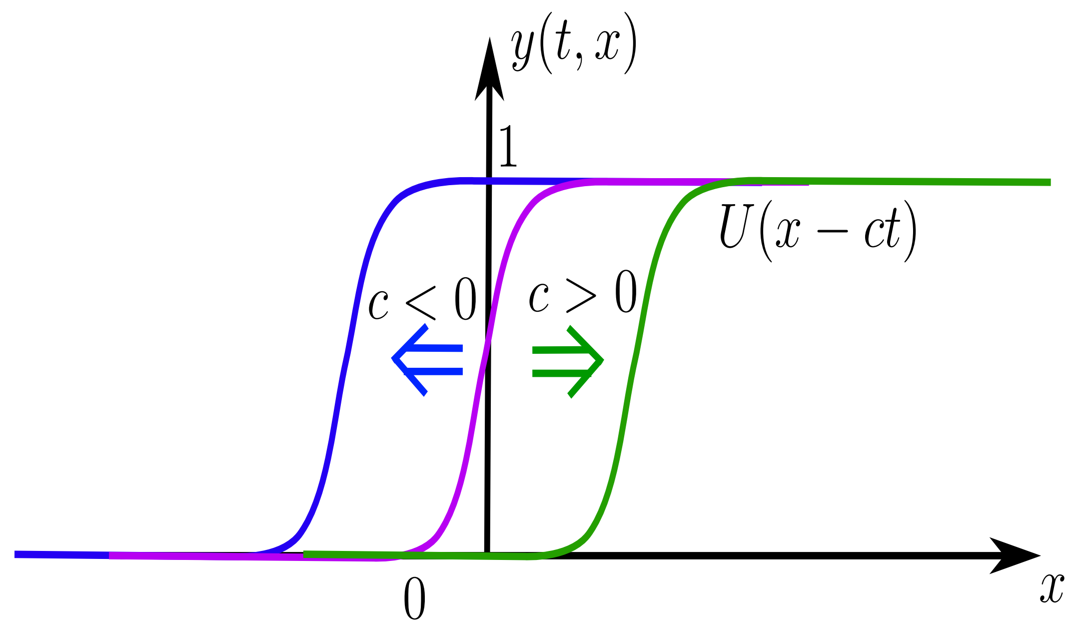
- solution of the form

$$\color{red}{y(t,x) = U(x-ct)},\, U(\pm\infty) = U_{\pm},\ U(\pm\infty)' = 0$$

where $U(x)$ is the wave profile and c is the wave speed.

- sign of the wave speed : $\mathrm{sign} c = -\int_0^1 f(t)dt$





Traveling wave

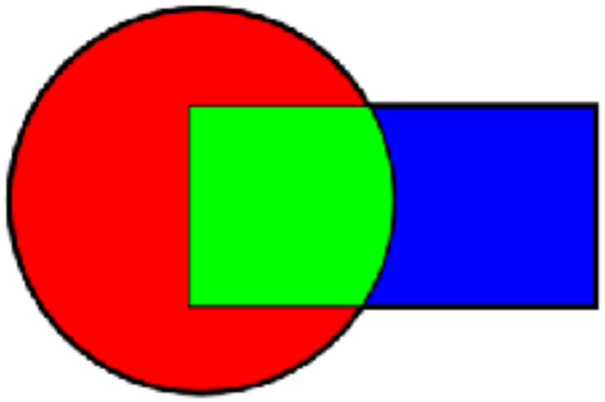
- The profile U is independent of θ: $U(x) = \frac{e^{\sqrt{a/2}x}}{1+e^{\sqrt{a/2}x}}$
- The Allee parameter θ determines the wave speed: $c = \sqrt{a/2}(2\theta - 1)$.

"La ola" / The wave

Operator splitting and TWs

$$y_t - y_{xx} = y(1-y)(y-\theta)$$

$$=$$



$$y' = y(1-y)(y-\theta)$$

$$+$$

$$y_t = y_{xx}$$

Control through known dynamical properties

Actively and dynamically controlling a system requires, first, to understand its fundamental dynamical properties, and their dependence on the control parameters.

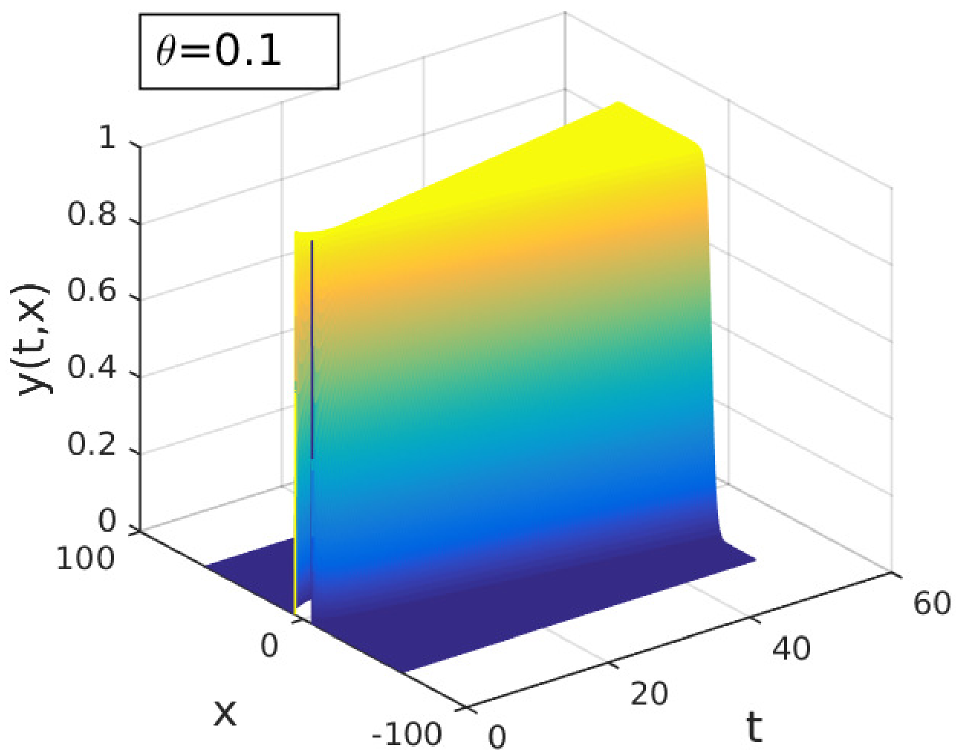
Learn about the response to parameter changes = *sensitivity analysis*. [3][4]

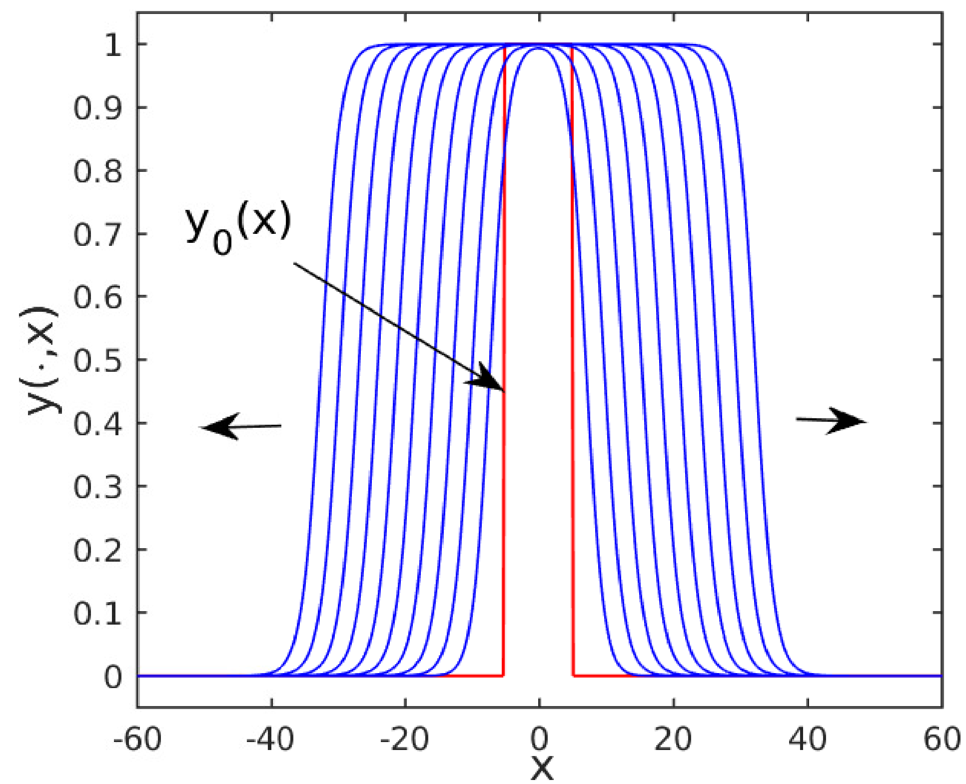
[3] D.G. Aronson, H.F. Weinberger, Nonlinear diffusion in population genetics, combustion, and nerve pulse propagation, in PDE and Related Topics, Lecture Notes in Math., vol. 446, Springer, Berlin, 1975, pp. 5-49.

[4] P.C. Fife, J.B. McLeod, The approach of solutions of nonlinear diffusion equations to travelling front solutions. Arch. Ration. Mech. Anal. **65** (1977) 335-361.

Invasion

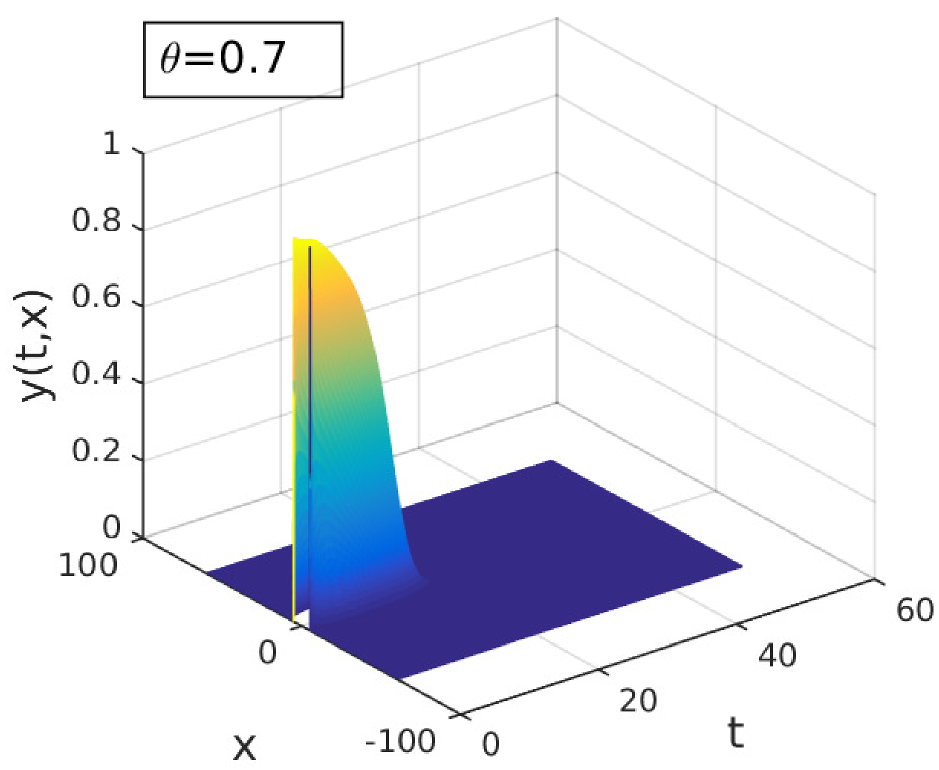
- $\theta = 0.1$: invasion of the population

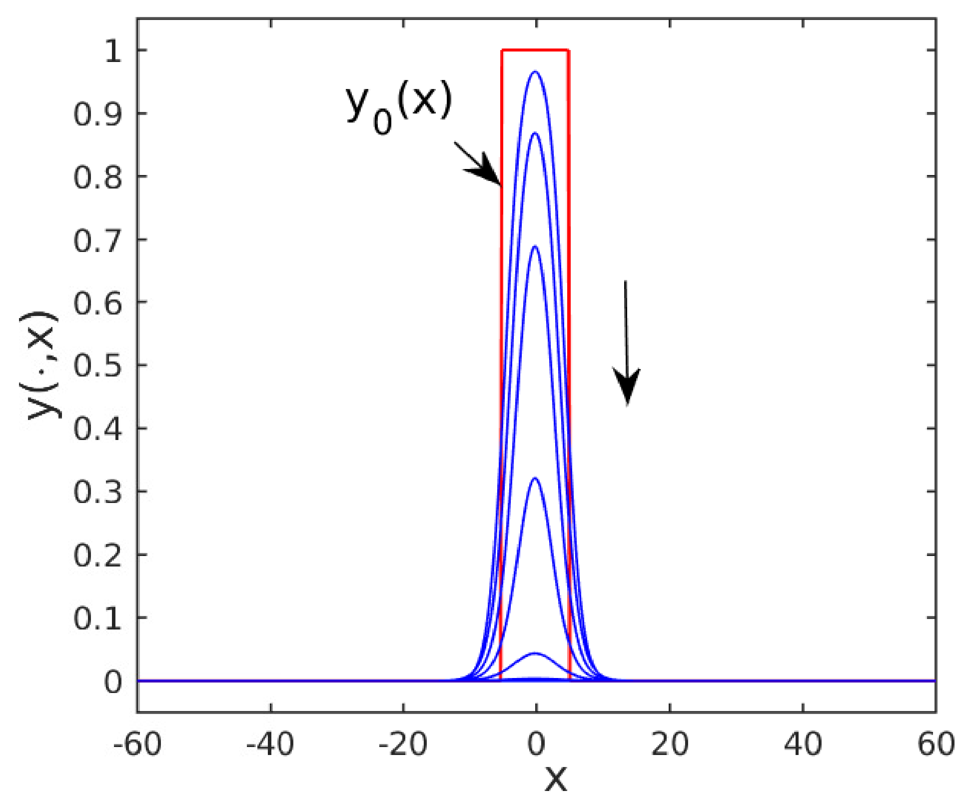




Extintion

- $\theta = 0.7$: extinction of the population





Attractiveness of TW

Theorem

(D.G. Aronson, H.F. Weinberger & P.C. Fife, J.B. McLeod)

If the initial datum y_0 is such that $y_0(x) \in [0, 1]$ and

$$\liminf_{x \to +\infty} y_0(x) > \theta, \quad \limsup_{x \to -\infty} y_0(x) < \theta \tag{1}$$

the solution approaches a the traveling wave $U(x - ct - x_1)$ for some x_1, uniformly in x and exponentially in time for $c = c(\theta)$, i.e.

$$\|y(t, x) - U(x - ct - x_1)\|_{L^\infty} < Ke^{-\gamma t}.$$

Formulation of the control problem: Two grids!

Control/Optimisation problem $\mathcal{P}_c$

Find $\theta(t) \in [0,1]$, $t \in [0,T]$ such that the solution of

$$y_t - y_{xx} = y(1-y)(y-\theta(t)),$$

$$y(0,\cdot) = y_0(\cdot)$$

develops into a Travelling Wave solution $U(\cdot)$ at the given time T, minimizing

$$J(\theta) = \|y(T,\cdot) - U\|^2$$

.

Even if the minimum exists, how close do we get to the target? [5]

[5] P. M. Cannarsa, G. Floridia, A.Y. Khapalov, Multiplicative controllability for semilinear reaction-diffusion equations with finitely many changes of sign, JMPA, 2017.

Theorem

For initial data that are well behaved at infinity,

$$\lim_{x\to-\infty} y_0(x) < \lim_{x\to+\infty} y_0(x),$$

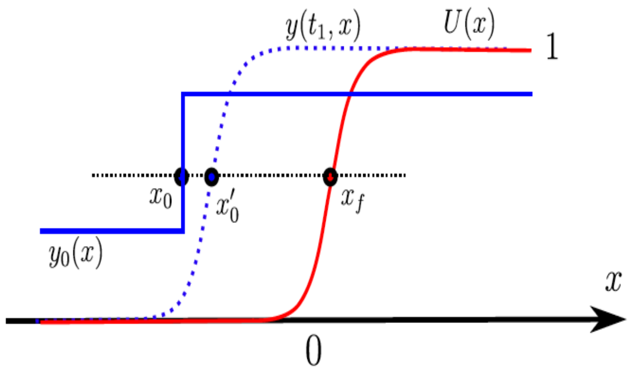
we can get arbitrarily close to the TW target in long time horizons

Two step strategy :

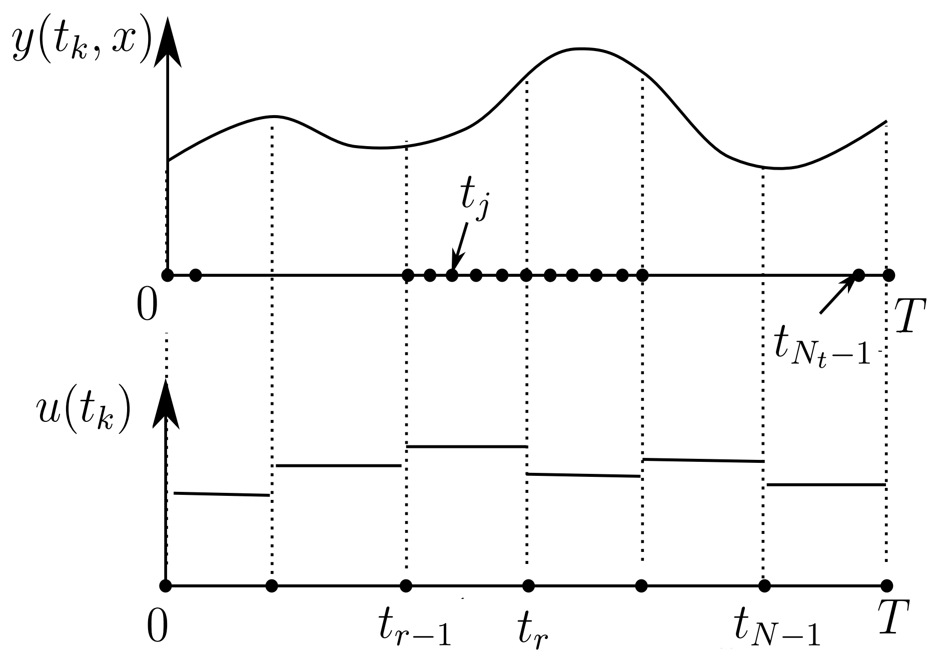
- Step 1. **Asymptotic attractiveness of the TW.** Choose θ_1 within

$$[\lim_{x\to-\infty} y_0(x), \lim_{x\to+\infty} y_0(x)]$$

  and keep it long enough $[0, T_1]$ until the solution approximates a traveling wave profile.
- Step 2. **Shift**. The location of the profile can be tuned by choosing θ_2, in the time interval $[T_1, T_1 + T_2]$.



Computational optimisation: Two-grids



- A fine **time-mesh** is employed to get a fine approximation of the state y.
- A **coarser** one suffices to approximate the control θ.

Often times optimisation (shape optimisation, control) problems are two-scale ones. This is however hard to see. We just see the scale of the PDE but not the one of the hidden pattern that emerges when solving the optimisation problem.[a]

[a] J. Casado-Diaz, C. Castro, M. Luna-Laynez & E. Z., Numerical approximation of a one-dimensional elliptic optimal design problem, SIAM J. Multiscale Analysis, 2011.

Conclusion

- Bang-bang time-dependent regulation of the **Allee parameter** $\rightarrow$ control towards a TW
- Mild effect: long time, approximately
- Weakness of the Allee threshold as control parameter
- **Boundary control** : The dynamics is confined to a bounded region and the control is applied by regulating the density of population or its flux on the boundary
- This mimics the **invasion of an external population** with specific characteristics.

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C. Pouchol, E. Trélat, E. Zuazua. Nonlinearity, 2019.

The density of individuals $0 \leq y(t,x) \leq 1$ obeys the PDE

$$\begin{cases} y_t - y_{xx} = y(1-y)(y-\theta), \\ y(0) = y_0, \\ y(t,0) = u(t), \ y(t,L) = v(t). \end{cases}$$

with $\theta < 1/2$, $x \in (0,L)$. Constrained **controls** : $0 \leq u(t), v(t) \leq 1$.

For α $(= 0,\ \theta$ ou $1)$, we say that

- *The system is controllable to α in finite time* if for all $0 \leq y_0 \leq 1$, there exist T, and controls u, v s.t.

$$y(T,\cdot) = \alpha.$$

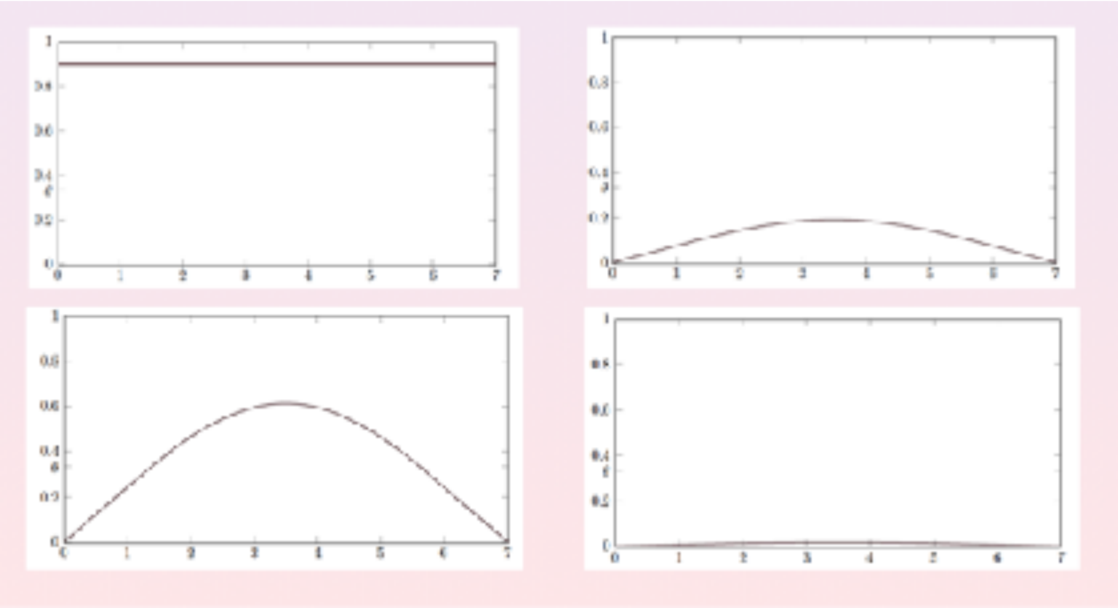
- *In infinite time* when the same occurs asymptotically as $t \to +\infty$.

Control to 0: Lack of obstructions / L small

The *static strategy* to control to 0, L small:

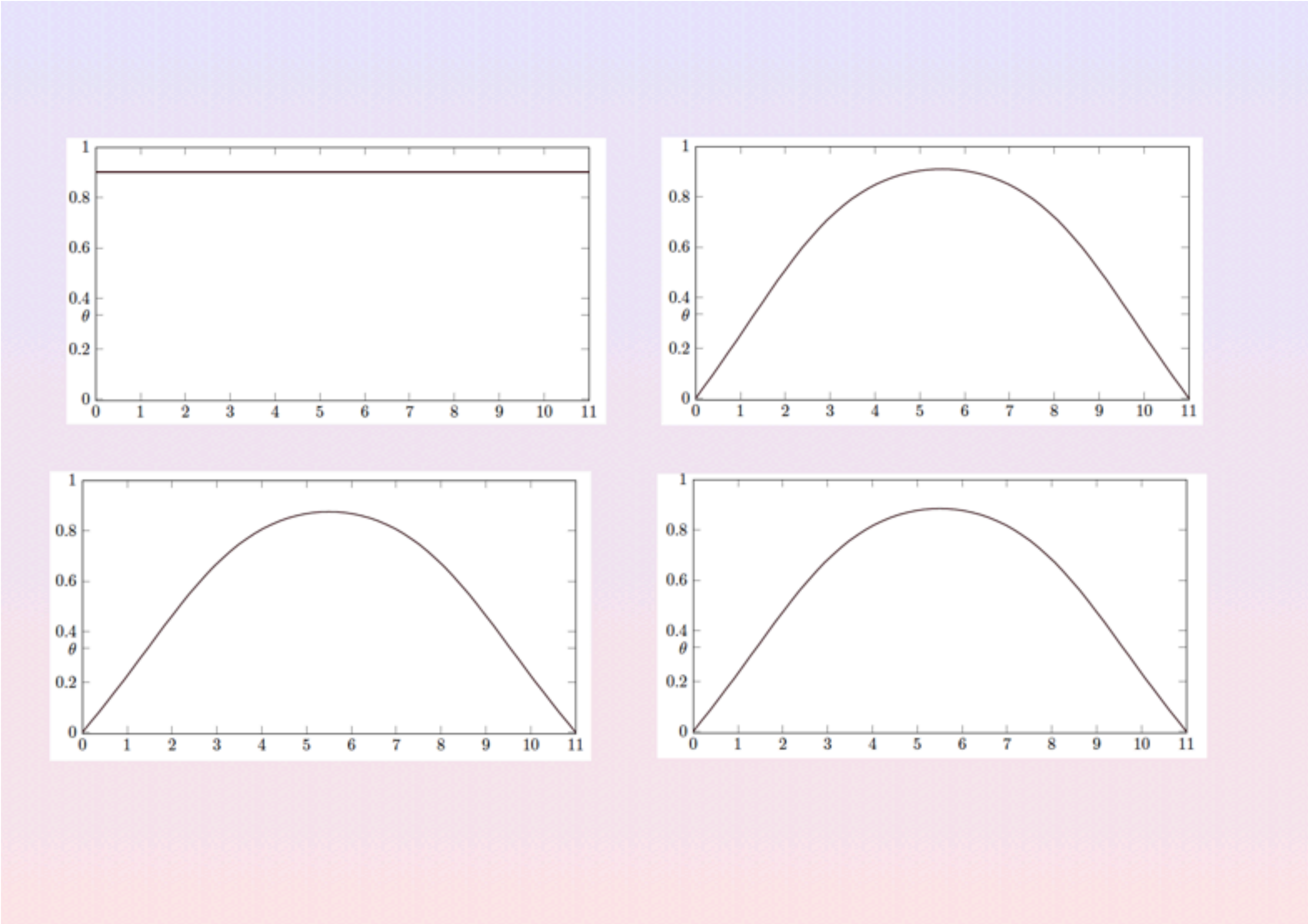
$$\begin{cases} y_t - y_{xx} = f(y), \\ y(0) = y_0, \\ y(t,0) = 0, \ \ y(t,L) = 0. \end{cases}$$

with $f(y) = y(1-y)(y-\theta)$, $\theta = 1/3$, $y_0 = 0.9$, $L = 7$. [6]



[6] One could argue that taking 0 as boundary control is not a very sophisticated control strategy. But, it is the best possible one, due to the comparison principle.

Control to 0: Obstructions / L large ($L = 11$)



Known facts

The **static strategy** to reach $\alpha = 0$, θ, or 1 consists on keeping the time-independent control α:

$$\begin{cases} y_t - y_{xx} = f(y), \\ y(0) = y_0, \\ y(t,0) = \alpha, \; y(t,L) = \alpha. \end{cases}$$

Matano's Theorem (1978) :
$y(t,\cdot)$ converges towards **a** steady state solution $0 \leq w \leq 1$:

$$\begin{cases} -w_{xx} = f(w), \\ w(0) = \alpha, \; w(L) = \alpha. \end{cases} \tag{2}$$

$w \equiv \alpha$ is a steady state solution for $\alpha = 0, \theta$ and 1. The only one?

P. L. Lions's Theorem (1982) : There exists a threshold L_α such that

- If $L < L_\alpha$, $w = \alpha$ is the unique steady-state solution.
- If $L > L_\alpha$, there is another non-trivial steady state solution.

Conclusion

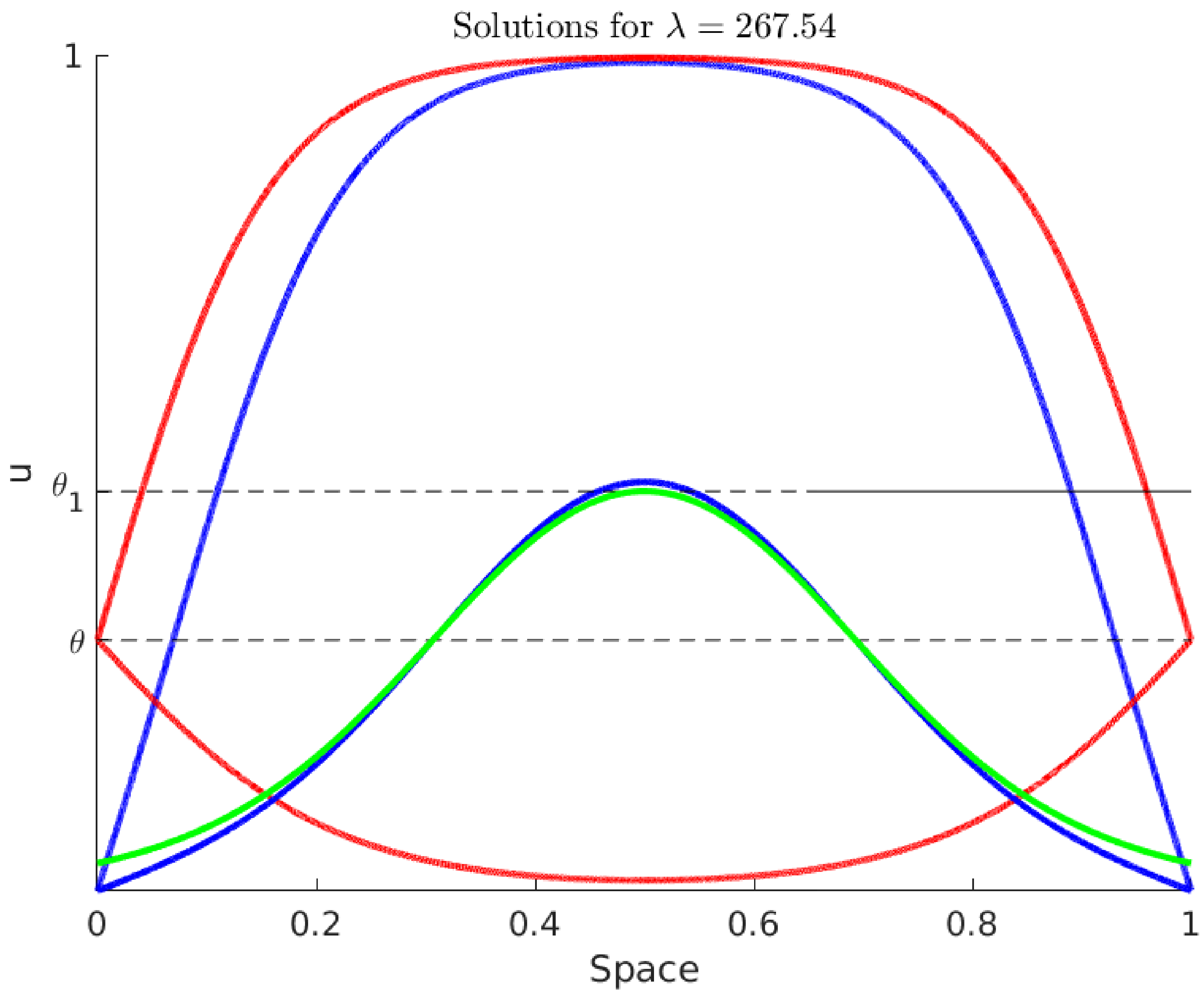
- If $L < L_\alpha$, the system is asymptotically controllable towards α.
- If $L > L_\alpha$, there is a barrier function making this impossible.

This issue is closely related to the question of whether the minimiser of the functional

$$J(y) = \frac{1}{2}\int_0^L |y_x|^2 dx - \int_0^L F(y)dx$$

in $H_0^1(0, L)$ is the trivial one $y \equiv 0$ or not.
Obviously, large L implies the first Dirichlet eigenvalue to be small, this weakens the coercivity of the H_0^1-norm, and facilitates the existence of non-trivial solutions.

Some non-trivial steady-states



$$\lambda = L^2 \text{ (by scaling), large}$$

Application

SCIENTIFIC REPORTS

OPEN

The minimum area requirements (MAR) for giant panda: an empirical study

Received: 28 July 2015
Accepted: 01 November 2016
Published: 08 December 2016

Jing Qing[1,2,*], Zhisong Yang[1,*], Ke He[1], Zejun Zhang[3], Xiaodong Gu[4], Xuyu Yang[4], Wen Zhang[5], Biao Yang[6], Dunwu Qi[7] & Qiang Dai[2]

Habitat fragmentation can reduce population viability, especially for area-sensitive species. The Minimum Area Requirements (MAR) of a population is the area required for the population's long-term persistence. In this study, the response of occupancy probability of giant pandas against habitat patch size was studied in five of the six mountain ranges inhabited by giant panda, which cover over 78% of the global distribution of giant panda habitat. The probability of giant panda occurrence was positively associated with habitat patch area, and the observed increase in occupancy probability with patch size was higher than that due to passive sampling alone. These results suggest that the giant panda is an area-sensitive species. The MAR for giant panda was estimated to be 114.7 km^2 based on analysis of its occupancy probability. Giant panda habitats appear more fragmented in the three southern mountain ranges, while they are large and more continuous in the other two. Establishing corridors among habitat patches can mitigate habitat fragmentation, but expanding habitat patch sizes is necessary in mountain ranges where fragmentation is most intensive.

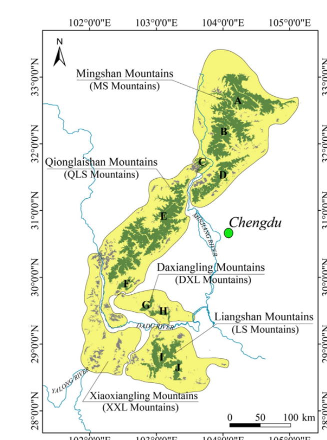


Figure 3. Distribution of habitat patches in the five mountain ranges. Yellow regio
the mountain ranges. Habitat patches greater than MAR are green and patches smalle
map is made by ArcGIS 9.1 software, http://www.arcgis.com/features.

Control to the Allee threshold θ

- For $\alpha = 0$ and $\alpha = 1$, because of the comparison principle, under the constraints $0 \leq y \leq 1$, the static strategy is the best possible one.
- When controlling towards the Allee threshold (politeness equilibrium) $z(x) = \theta$ steady state controls $u(t), v(t)$ may oscillate around θ within the bounds: $0 \leq u(t), v(t) \leq 1$
- Would that help?
  Note that $z(x) = \theta$ is an unstable equilibrium when L is large enough. But controls can cope with unstability too.

Local controllability: dynamic strategy

- Carleman estimates
- Linearisation
- Fixed point

Theorem

Fix $T = 1$ *and the target* $\alpha(x) \equiv \theta$. *Then, if*

$$||y_0 - \theta||_{L^2(0,L)} \leq \epsilon$$

with $\epsilon > 0$ *small enough, then there exist controls* $0 \leq u(t), v(t) \leq 1$ *s. t.*

$$y(\cdot, t = 1) \equiv \alpha.$$

Global control: $L < L_\alpha$. Two step strategy (Turnpike)

$L < L_\theta \to z(x) \equiv \theta$ is the unique steady state.

All initial data can be driven to θ in finite time.

Two step strategy:

- Step 1: $[0, T]$, with $T >> 1$, keep $u(t) \equiv v(t) \equiv \theta \to$

$$||y(\cdot, t = T) - \theta||_{L^2(0,L)} \leq \varepsilon.$$

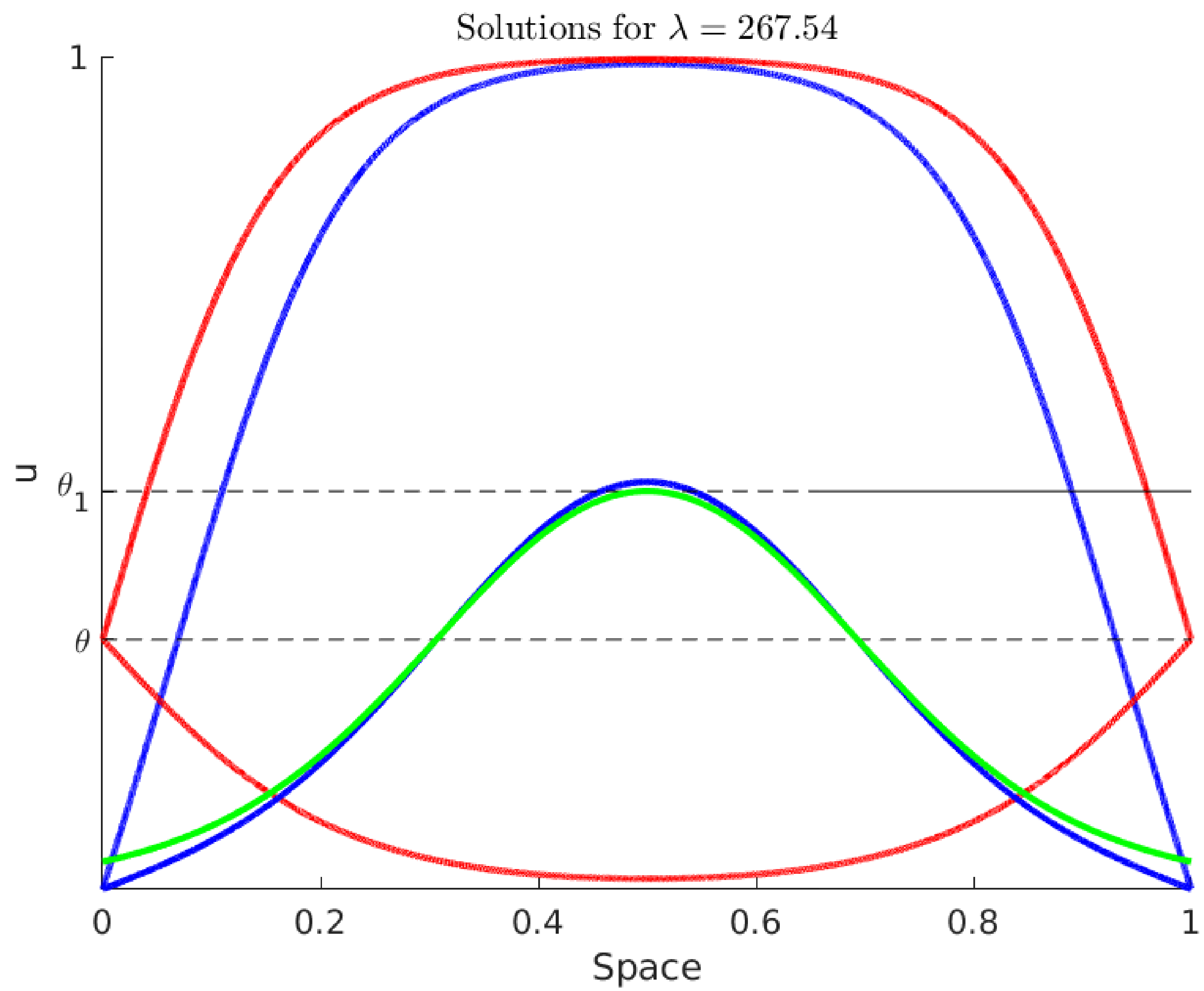
- Step 2: In $[T, T+1]$ apply the previous local control $\to$

$$y(\cdot, t = T+1) \equiv \theta.$$

Question

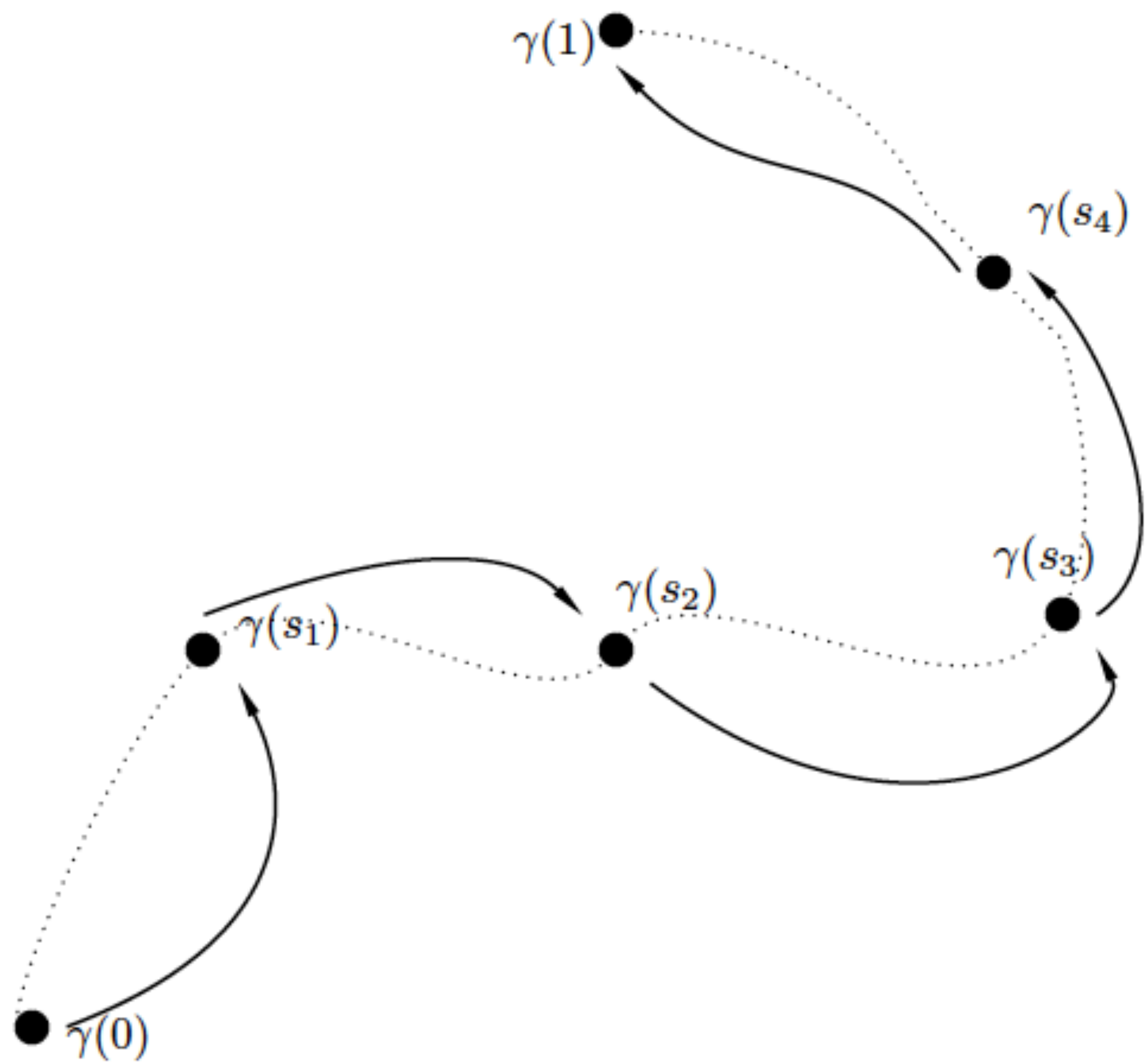
Can we get close to $z \equiv \theta$ for $L > L_\theta$ with a more complex strategy and this for all initial data?

Which barriers can be broken ?



Note that, although, one can not expect to decrease monotonically from large data to θ, in principle, one could first go down to then go up again!

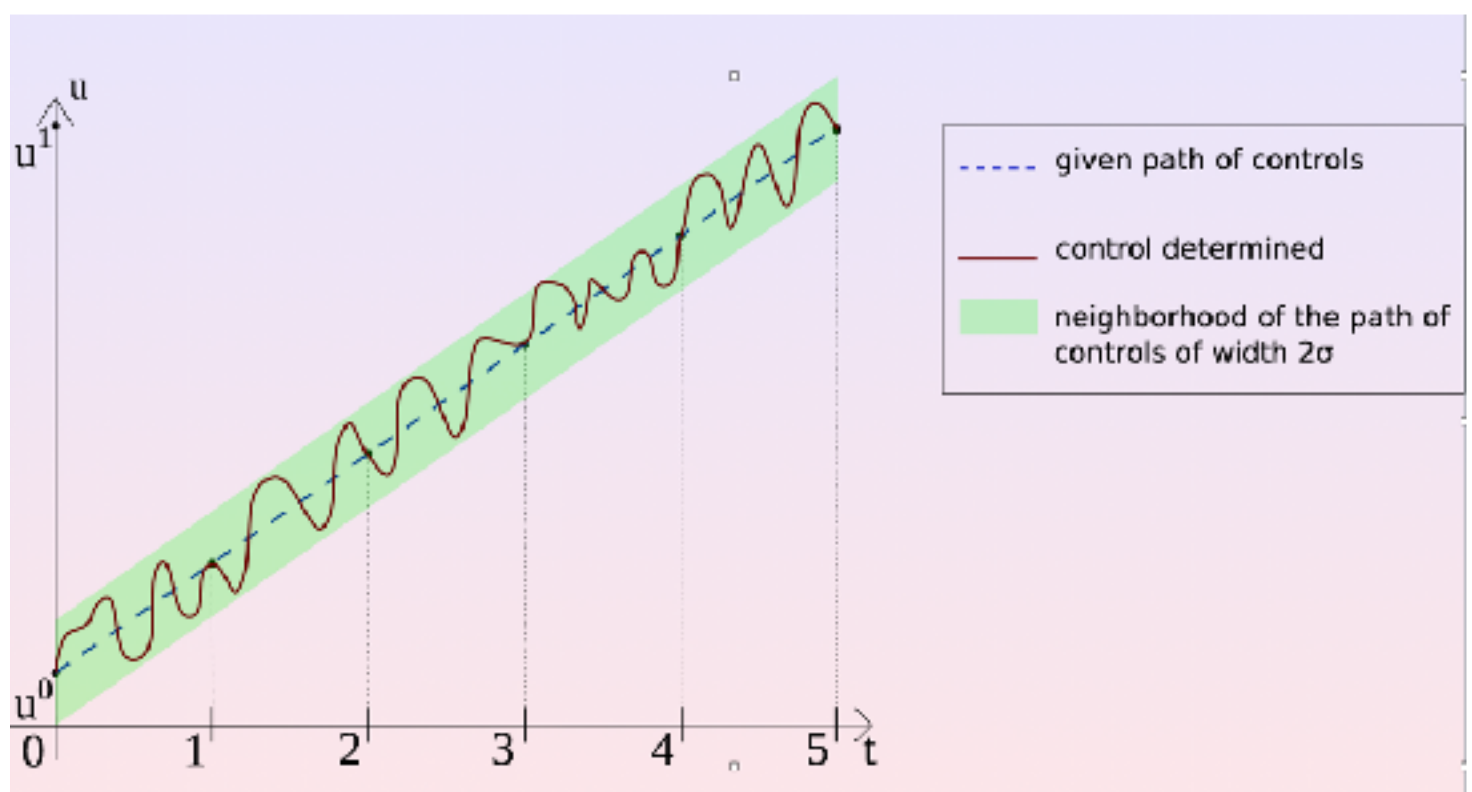
Hidden complexity of control patterns



Theorem

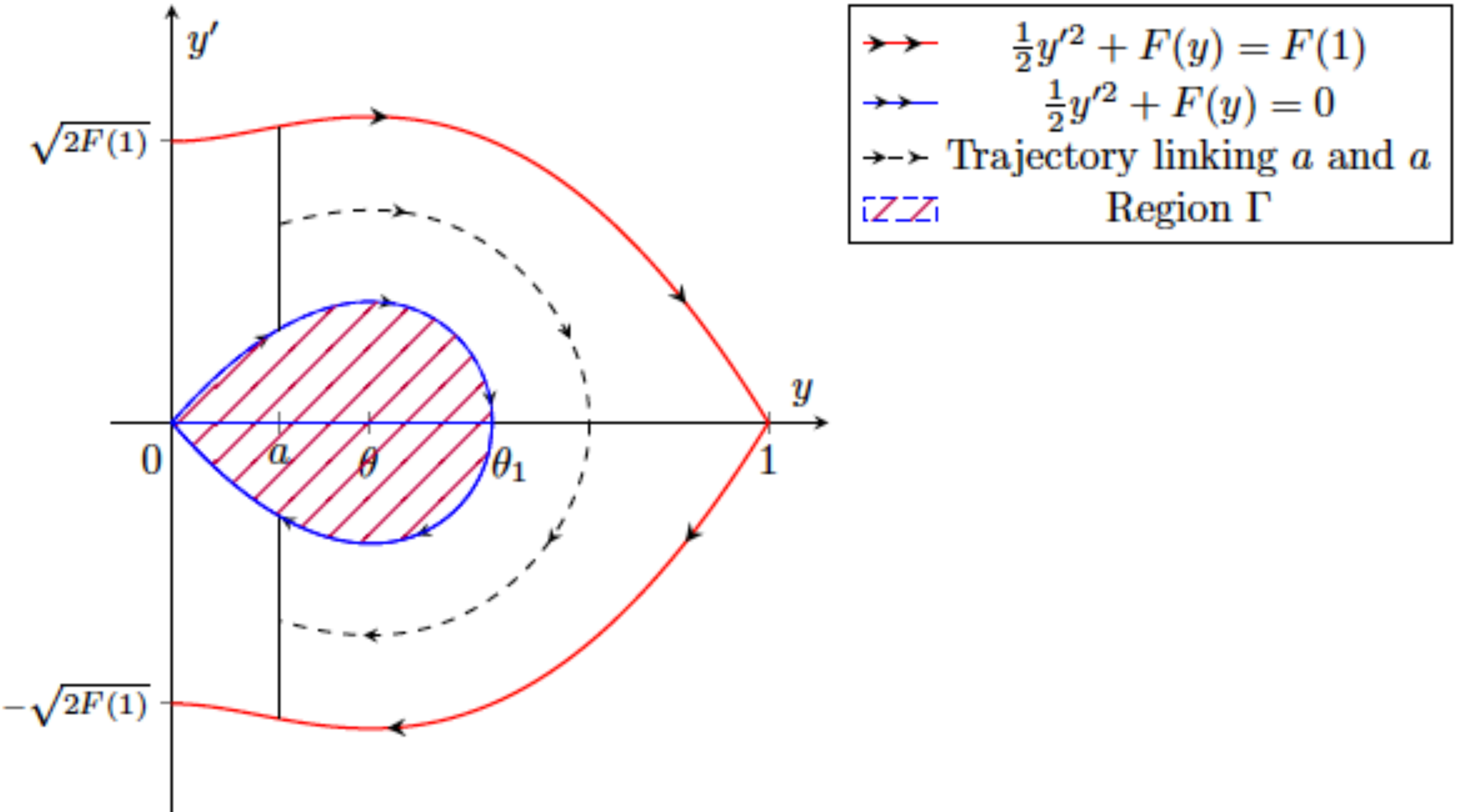
The global control to θ is possible even when $L_\theta < L < L_0$.

- The result is sharp. The barrier corresponding to the nontrivial steady state with zero Dirichlet b. c. cannot be broken.
- Two steps strategy
  - First step: Keep $u \equiv v \equiv 0$, to **cool down**.
  - Second step: Increase again following a **stair-case strategy**. Build a path of steady states and follow it slowly, so to guarantee that solutions oscillate very little. This imposes the time of control to be long.



Phase portrait for $-w'' = f(w)$

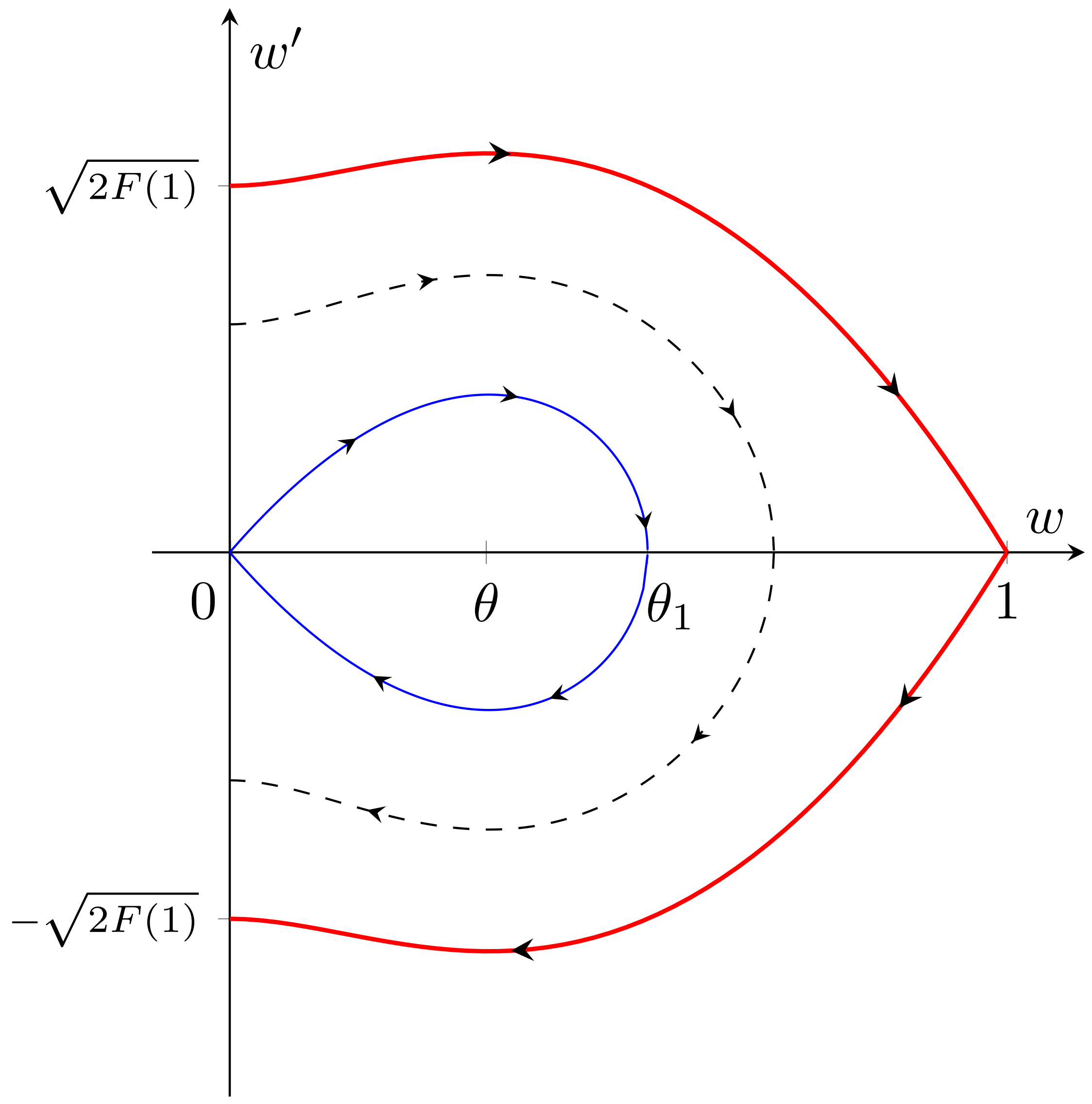
We set $F(y) := \int_0^y f(z)\,dz$, and suppose that $F(1) \geq 0$ ($\Leftrightarrow \theta \leq \frac{1}{2}$ with $f(y) = y(1-y)(y-\theta)$).



Case $\alpha = 0$: $L_0 < \infty$

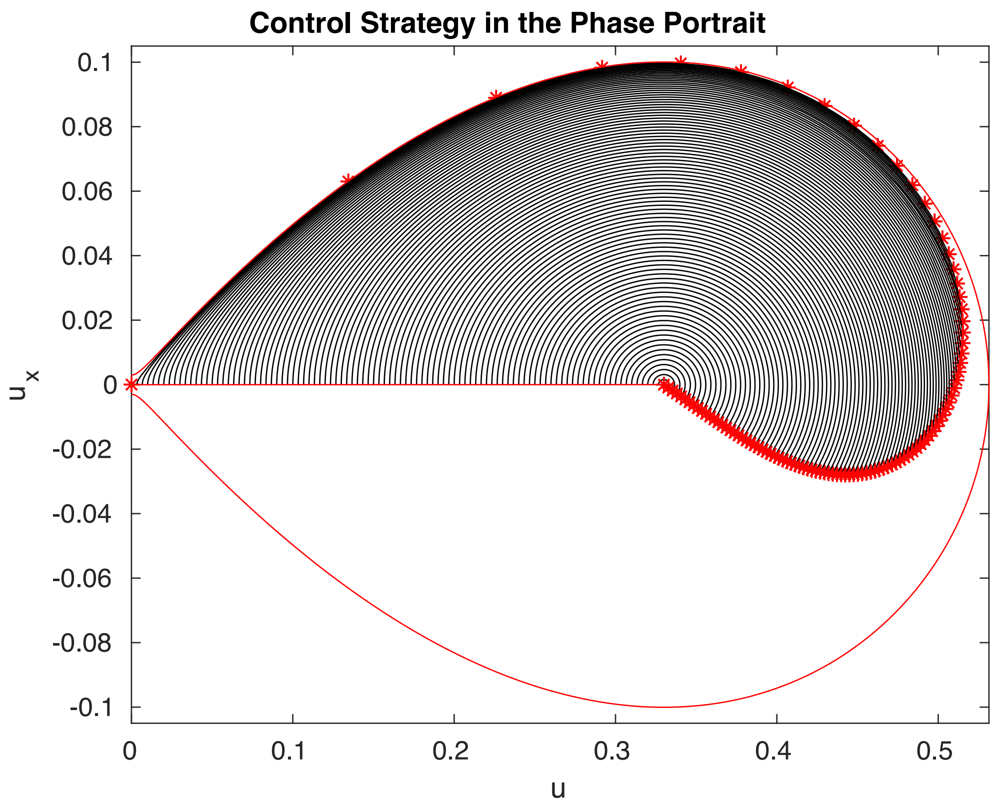
$w = 0$ is the unique steady state solution if $L < L_0 = L^\star$,

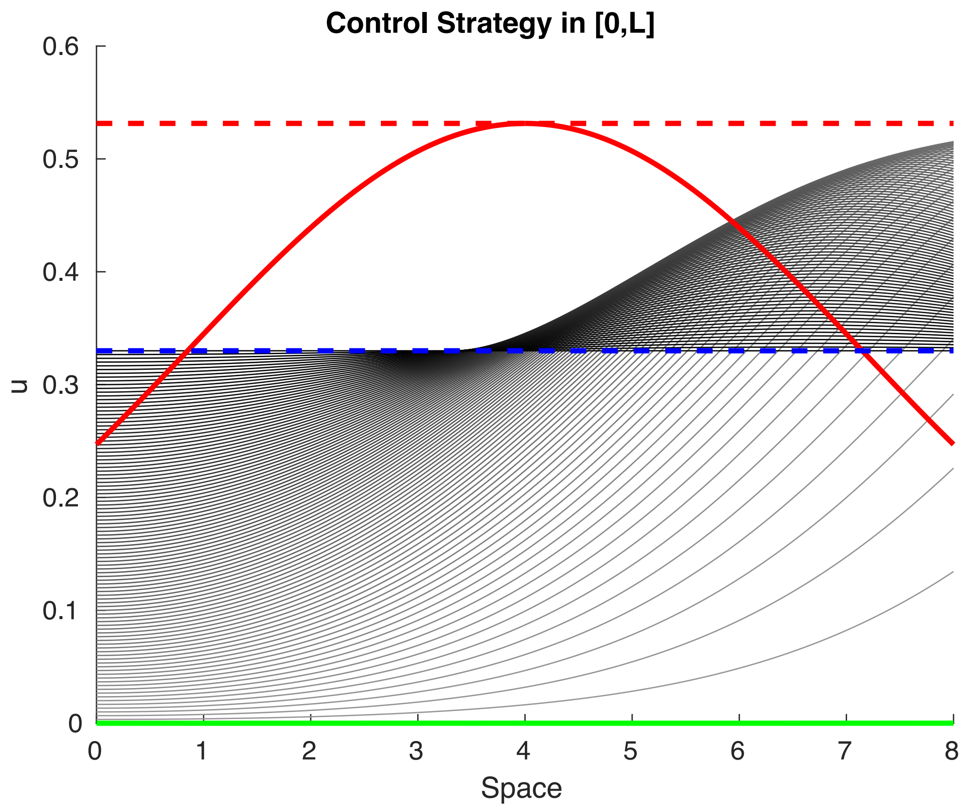
$$L^\star = \inf_{\beta \in (\theta_1, 1)} \sqrt{2} \int_0^\beta \frac{dy}{\sqrt{F(\beta) - F(y)}}.$$



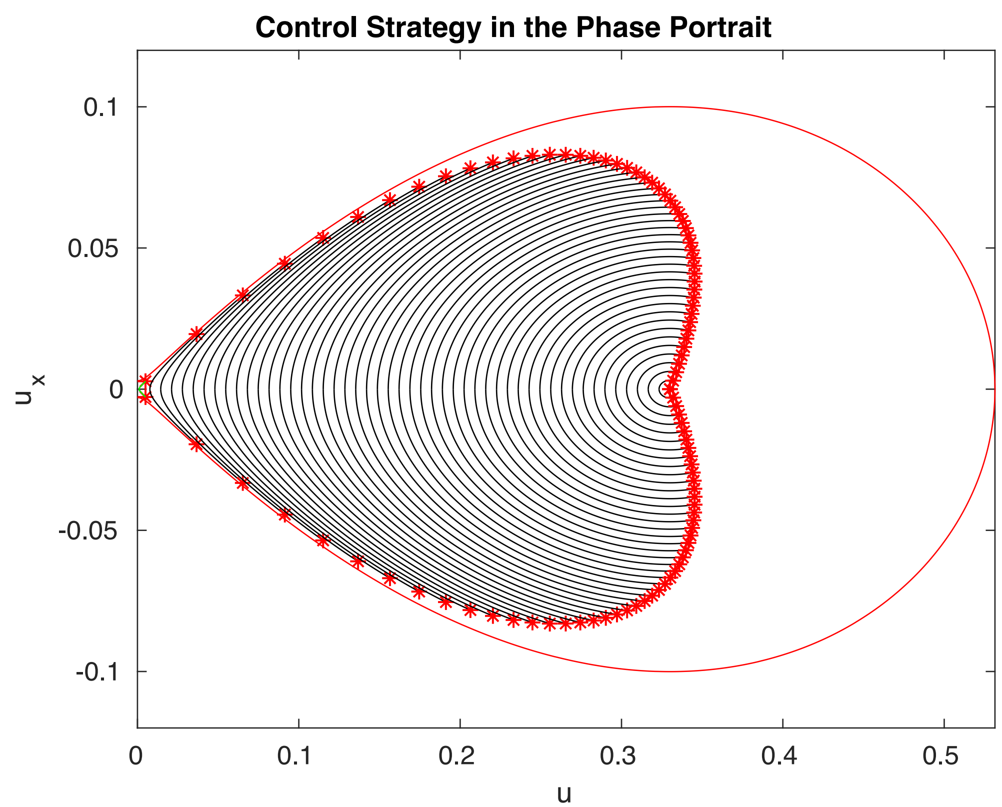
Path of steady states connecting 0 and θ

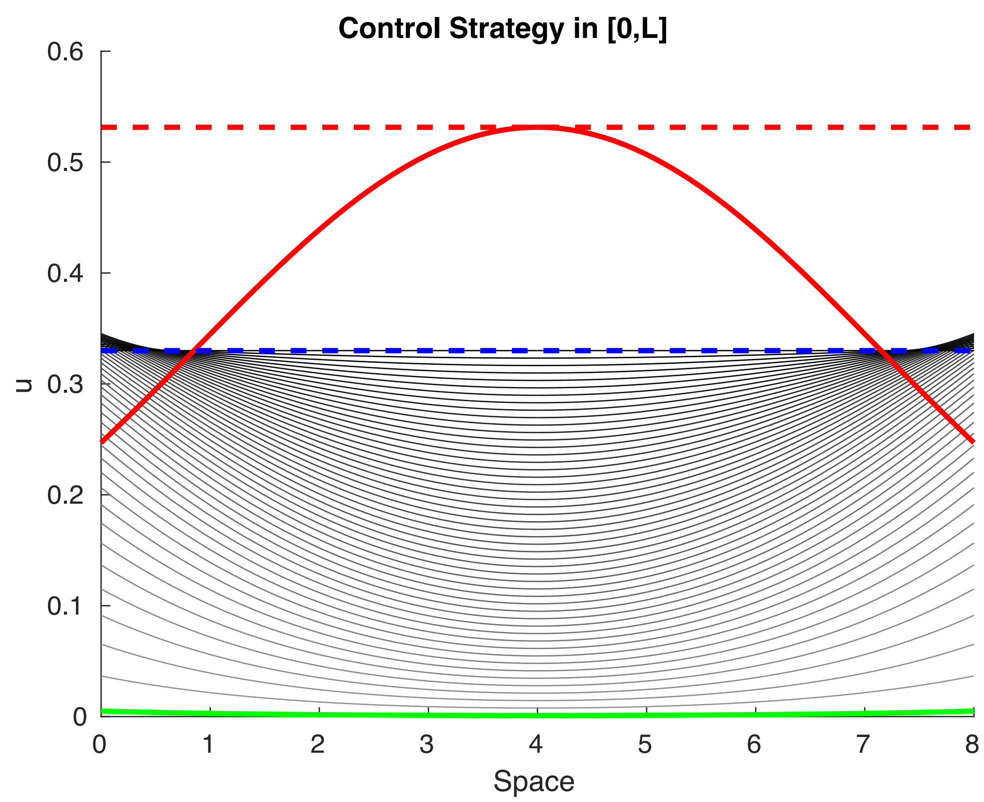
Construction of the paths in the phase portrait



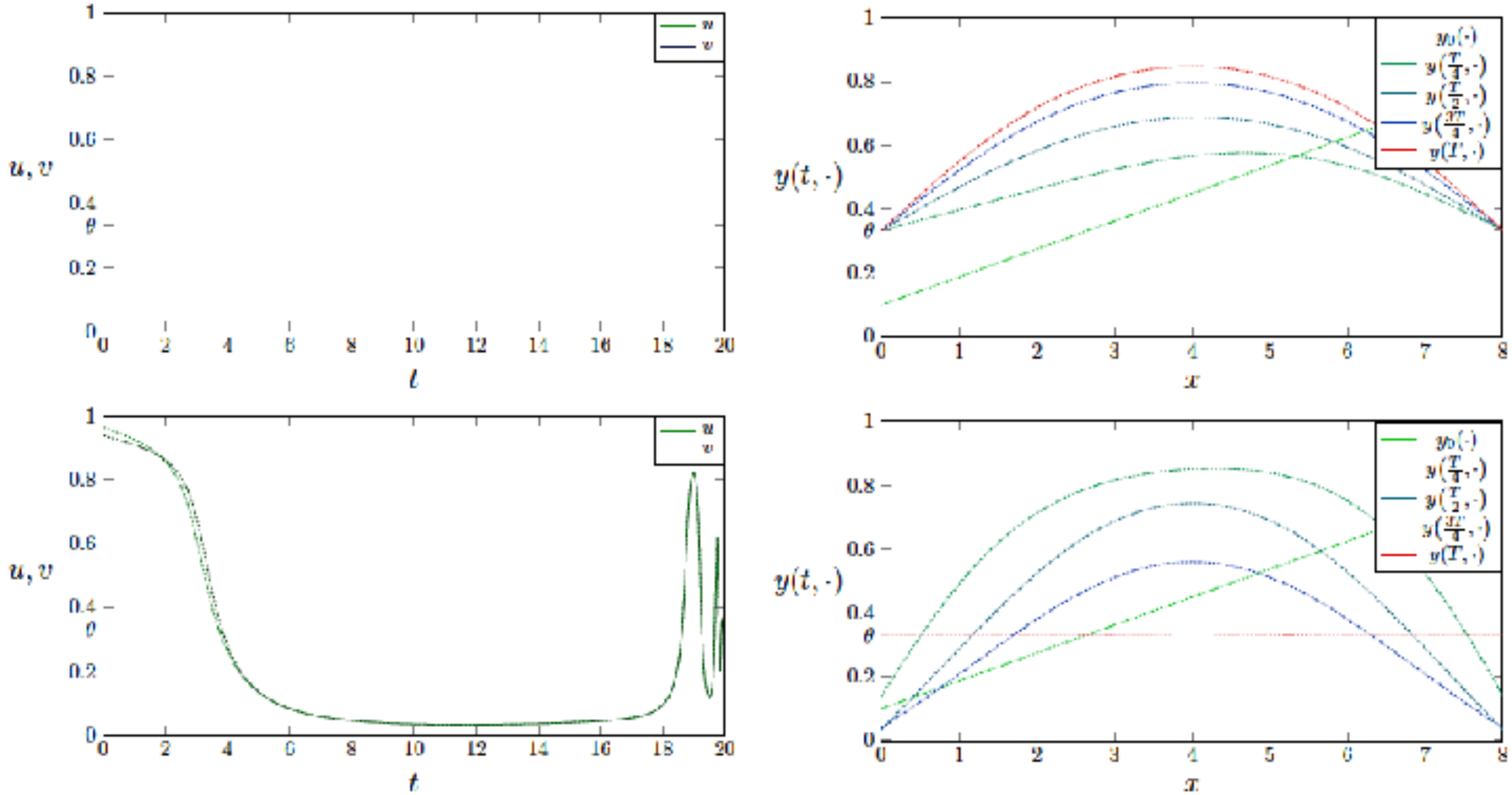


Construction of symmetric paths (Domenec Ruiz)





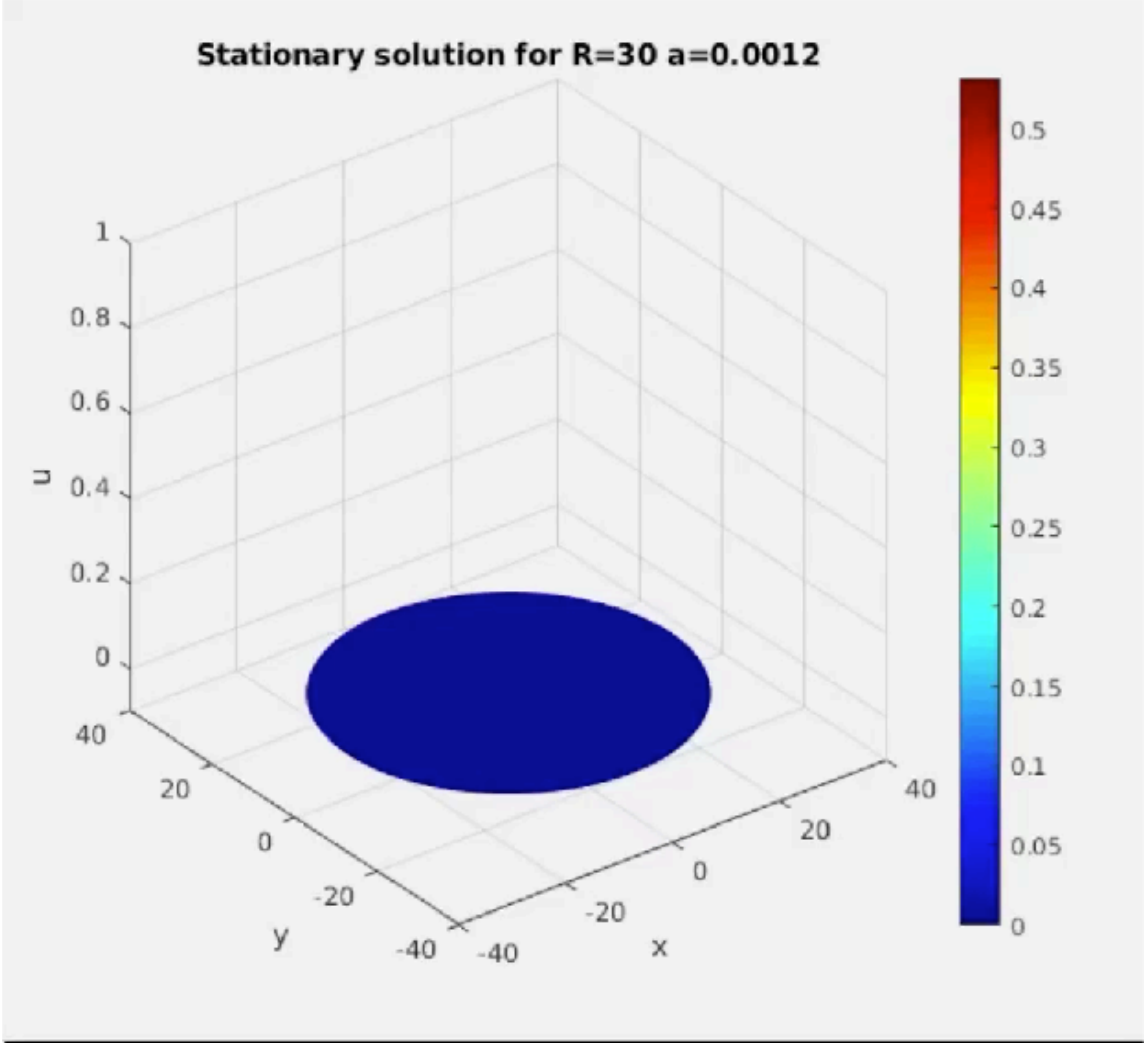
Numerical experiment: Minimal time control (IPOPT)



Conclusion

- The optimal control strategies are not necessarily simple or intuitive.
- The landscape of the set of steady states can be complex.
- There might be unexpected bridges indicating the path to follow for control.

Bridge of steady states linking 0 and θ, multi-d



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The model

Consider a distribution of population $N > 0$. Consider that the population is divided between two traits. We model the evolution of the proportion of one trait by[7]:

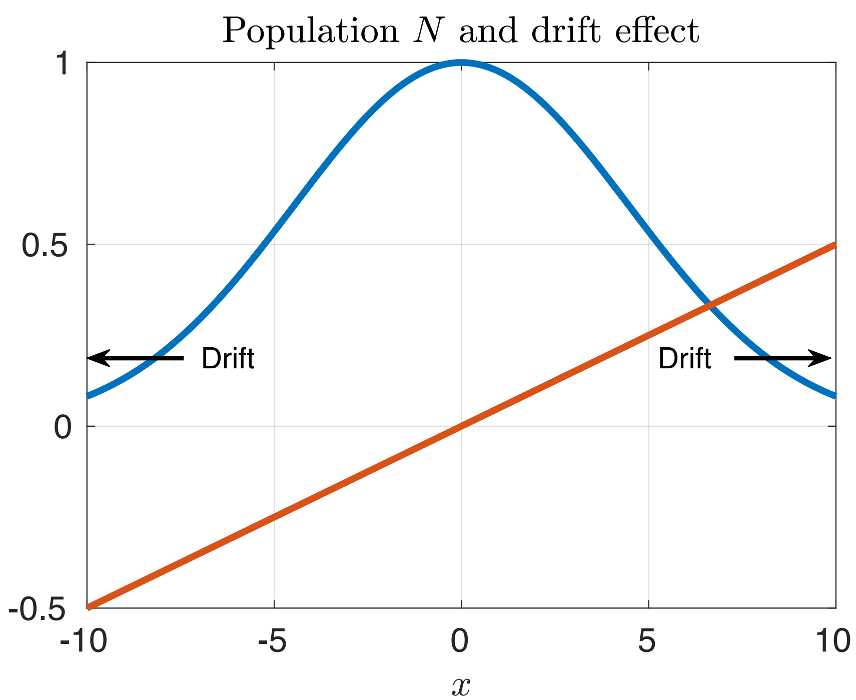
$$\begin{cases} u_t - \Delta u - \frac{\nabla N(x)}{N(x)} \nabla u = f(u) & (x,t) \in \Omega \times (0,T) \\ u = a(x,t) & (x,t) \in \partial\Omega \times (0,T) \\ 0 \leq u(x,0) \leq 1 \end{cases}$$

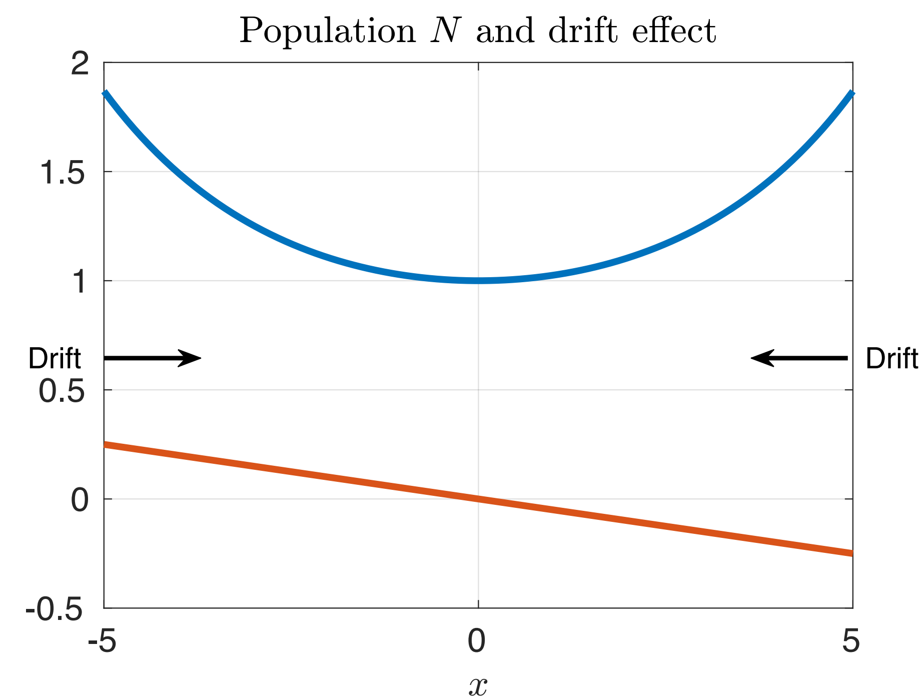
we will also use the notation $\nabla b(x) = \frac{\nabla N(x)}{N(x)}$

[7] I. Mazari, D. Ruiz-Balet, and E. Zuazua, Constrained control of bistable reaction-diffusion equations: Gene- flow and spatially heterogeneous models, Preprint (2019)

Two examples

- For $N(x) = e^{-\frac{x^2}{\sigma}}$, $$u_t - u_{xx} + \frac{2x}{\sigma} u_x = f(u)$$
- For $N(x) = e^{\frac{x^2}{\sigma}}$, $$u_t - u_{xx} - \frac{2x}{\sigma} u_x = f(u)$$

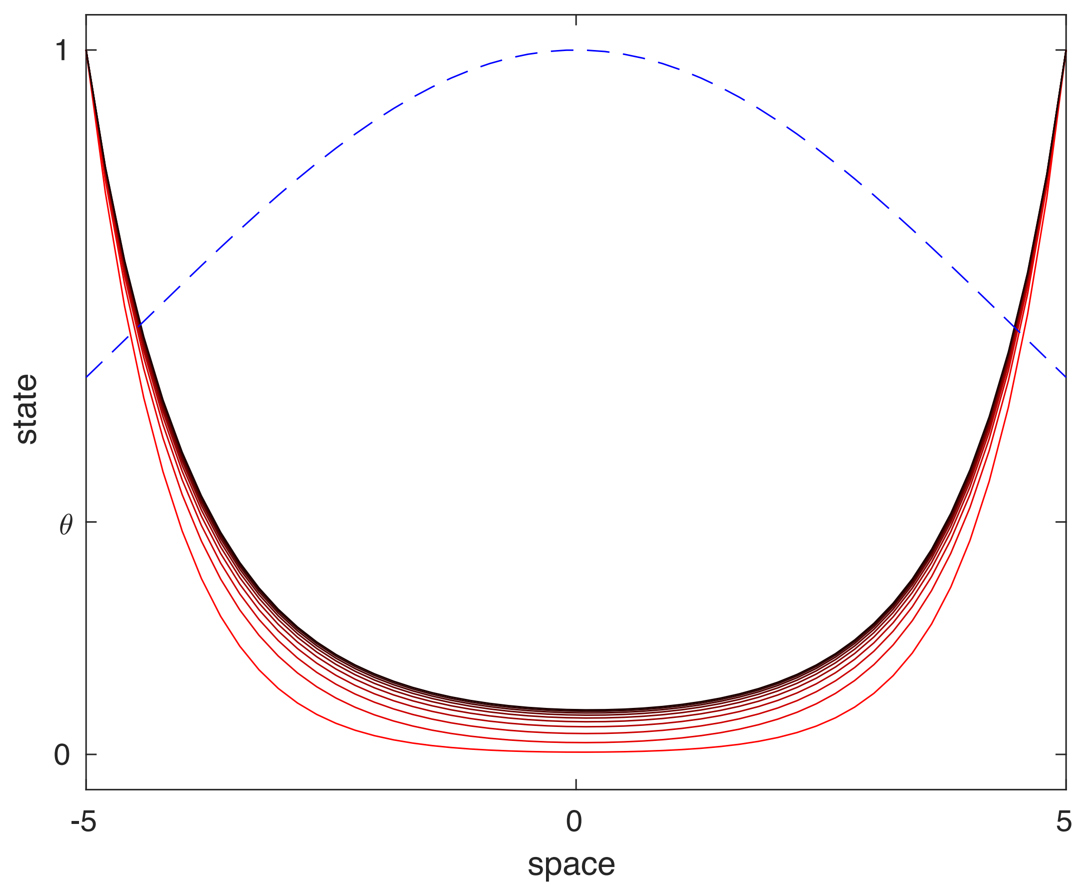




New Upper Barriers

Take $N(x) = e^{-\frac{x^2}{\sigma}}$. We observe that new barriers can exist.

$$\begin{cases} -u_{xx} + 2\frac{x}{\sigma}u_x = f(u) \\ u(-L) = u(L) = 1 \end{cases} \tag{3}$$



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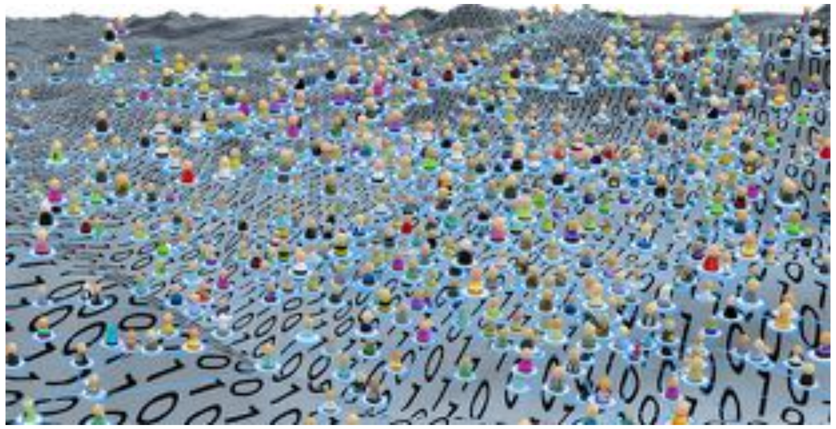
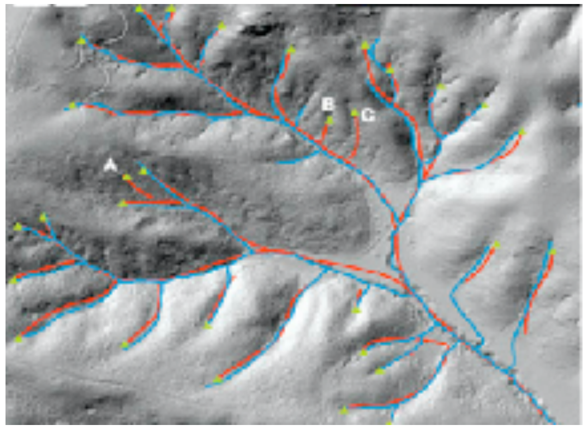
Perspectives

- Significant work to be done from a modeling perspective, to get closer to real social or biological issues.
- Plenty still to be done to gain understanding of these models from a control perspective.
- Extensions to multi-d[8] and to systems (gene-flow[9]) raises interesting new questions about the nature of set of steady state solutions, their stability, etc.
- **The great challenge**: Making our analysis to be, not only qualitatively sound, but quantitatively efficient.





[8] Work in progress with Domenec Ruiz
[9] Work in progress with Idriss Mazari and Domenec Ruiz