PDEs Meet Machine Learning: Integrating Numerics, Control, and Machine Learning

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Outline

The Nobel Prize in Chemistry 2024

They cracked the code for proteins' amazing structures

The Nobel Prize in Chemistry 2024 is about proteins, life's ingenious chemical tools. David Baker has succeeded with the almost impossible feat of building entirely new kinds of proteins. Demis Hassabis and John Jumper have developed an AI model to solve a 50-year-old problem: predicting proteins' complex structures. These discoveries hold enormous potential.

deepseek

ChatGPT

Geoffrey Hinton
Nobel Prize in Physics 2024

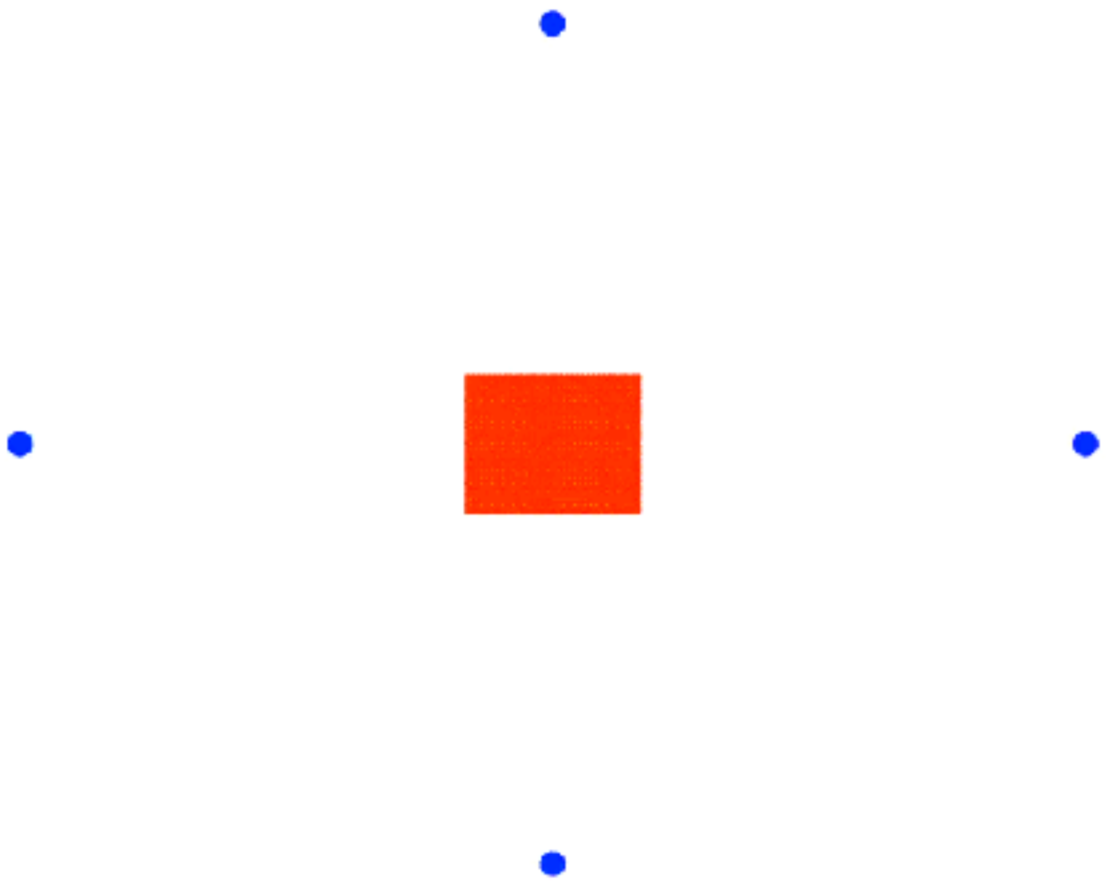
Born: 6 December 1947, London, United Kingdom

Affiliation at the time of the award: University of Toronto, Toronto, Canada

Prize motivation: "for foundational discoveries and inventions that enable machine learning with artificial neural networks"

Bridges across Frontiers

Control & ML

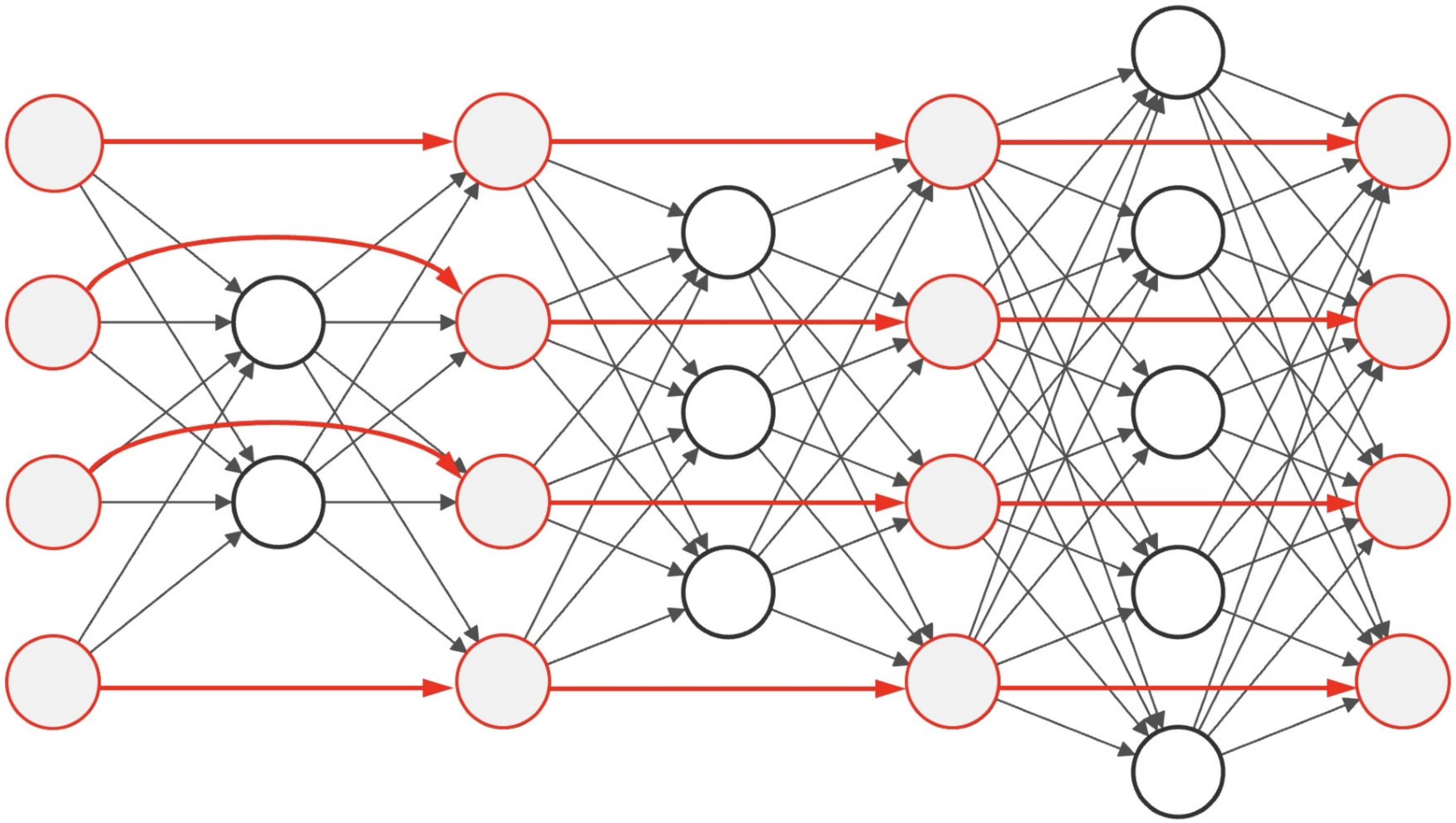


Control: Dogs-Sheep

Supervised Learning

How does it work? Computational practice

$$\underbrace{\frac{1}{N}\sum_{i=1}^{N}\text{loss}\left(x^i,\ell^i\right)}_{\text{empirical risk }:=E(x(\cdot))}+\alpha\sum_{j=1}^{K}\|(\mathbf{a_j},\mathbf{w_j},b_j)\|^2$$



Supervised Learning

From First Principles to Data: Opposing Paradigms

Partial Differential Equations

$$\Delta \phi = 0$$

Laplace Equation

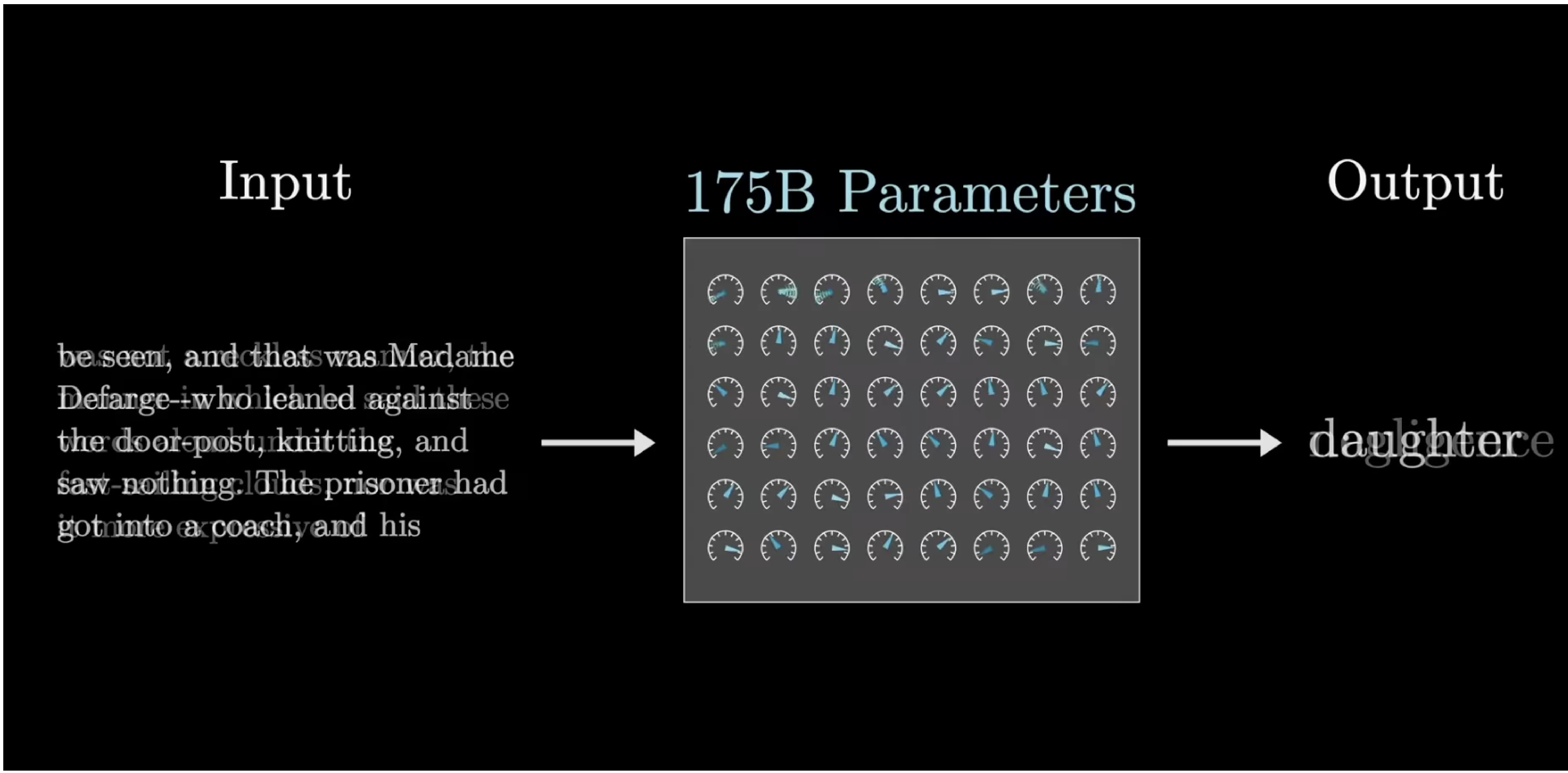
$$\frac{\partial T}{\partial t} = \Delta T$$

Heat Equation

$$\frac{\partial^2 u}{\partial t^2} = \Delta u$$

Wave Equation

Complexity: Curse of dimensionality
+ Devil of non-convexity



Some relevant questions

- **The Foundations of Machine Learning's Success**

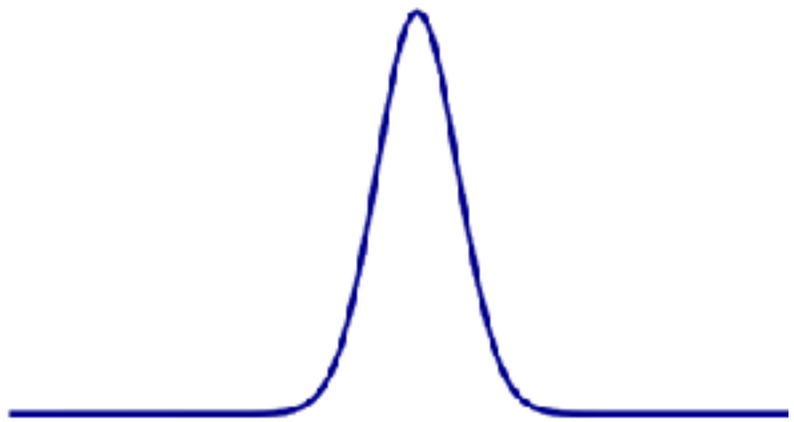
- **Machine Learning for PDE Approximation**

- **Rethinking Applied Mathematics in the Age of Machine Learning Merging: PDE+D(ata)**
  "Digital Twins: Where Data, Mathematics, Models and Decisions Collide"

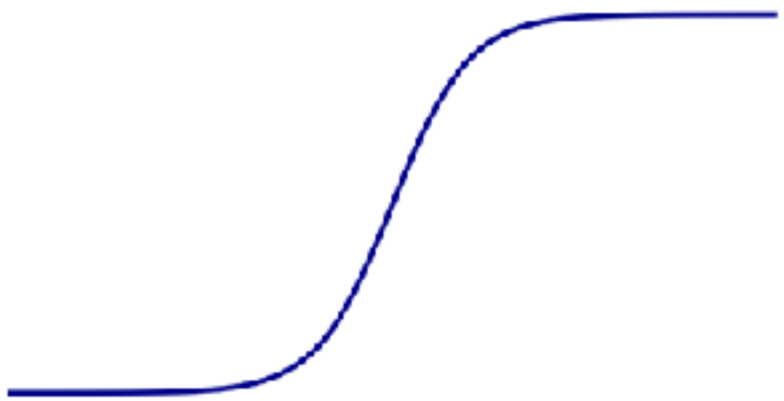
Outline

Why does it work? Universal Approximation

N. Wiener, Tauberian Theorems,
Annals of Mathematics, 33 (1) (**1932**), 1-100.



$$f(x) \sim \sum_{j=1}^{K} w_j G(x + \mathbf{b}_j)$$



G. Cybenko, Approximation by superpositions of a sigmoidal function,
Mathematics of Control, Signals and Systems, (**1989**), 2: 303-314.

$\lim_{x\to-\infty} \sigma(x) = 0, \quad \lim_{x\to+\infty} \sigma(x) = 1$

$$f(x) \sim \sum_{j=1}^{K} w_j \sigma(\mathbf{a}_j \cdot x + b_j)$$

The linear finite d-dimensional system

$$x'(t) = Ax(t) + Bu(t)$$

with $m << d$ controls.
$A \in M_{d\times d}$, $B \in M_{d\times m}$ and $x^0 \in \mathbb{R}^n$; $x : [0, T] \longrightarrow \mathbb{R}^d$ represents the *state* and $u : [0, T] \longrightarrow \mathbb{R}^m$ the *control*.

Can we control d states with only m controls, even if $n \gg m$?

Theorem

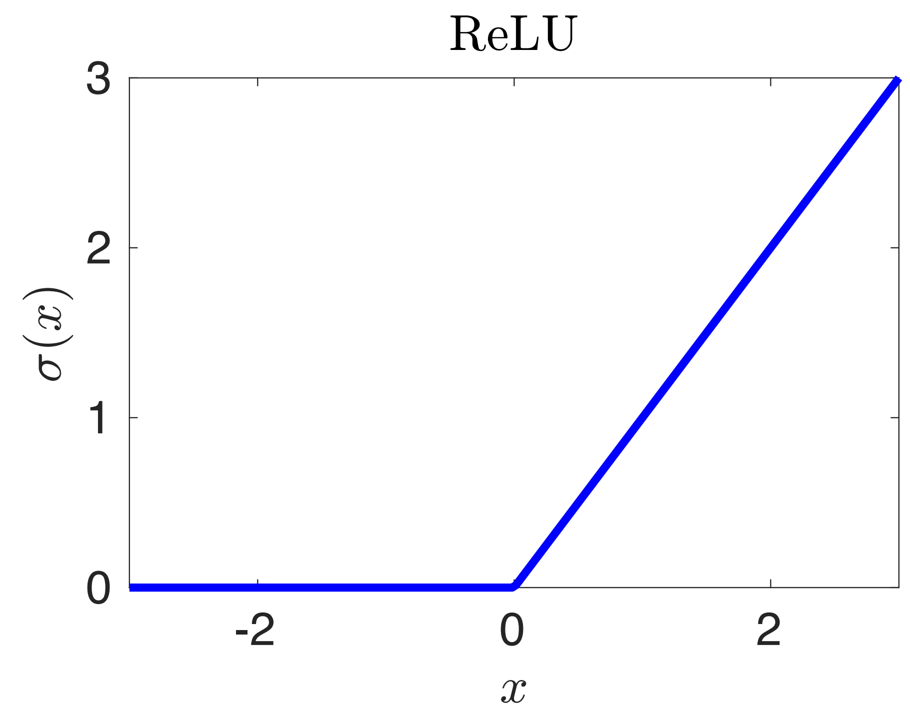
(1958, Rudolf E. Kálmán) System (1) *is controllable iff*

$$\mathrm{rank}\,[B, AB, \cdots, A^{d-1}B] = d.$$

DeepMind breaks 50-year math record using AI; new record falls a week later

AlphaTensor discovers better algorithms for matrix math, inspiring another improvement from afar.

$$f(x) \sim \sum_{j=1}^{K} \mathbf{w}_j \sigma(\mathbf{a}_j \cdot x + b_j)$$

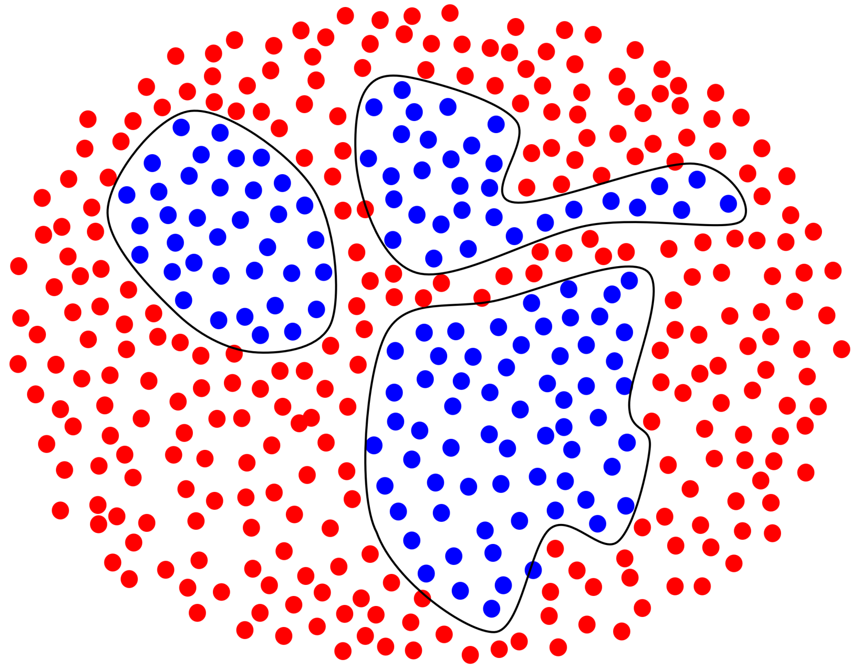


$$\Updownarrow$$

$$\mathbf{x}^{k+1} = \mathbf{x}^k + h\, \mathbf{w}^k \sigma(\mathbf{a}^k \cdot \mathbf{x}^k + b^k)$$

$$\Updownarrow$$

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{w}(t)\, \sigma(\mathbf{a}(t) \cdot \mathbf{x}(t) + b(t))$$



ResNets / Neural ODEs in action

$$\dot{\mathbf{x}}(t) = \mathbf{w}(t)\,\sigma(\mathbf{a}(t)\cdot\mathbf{x}(t) + b(t))$$

[1] [1] K. He, X. Zhang, S. Ren, J. Sun, 2016: Deep residual learning for image recognition. [2] E. Weinan, 2017: A proposal on machine learning via dynamical systems. [3] R. Chen, Y. Rubanova, J. Bettencourt, D. Duvenaud, 2018. [4] E. Sontag, H. Sussmann, 1997.

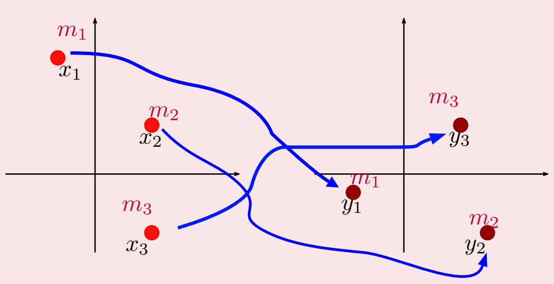
Classification by simultaneous or ensemble control of Neural ODEs

Theorem (Classification, Domènec Ruiz-Balet & EZ, SIREV, 2023)

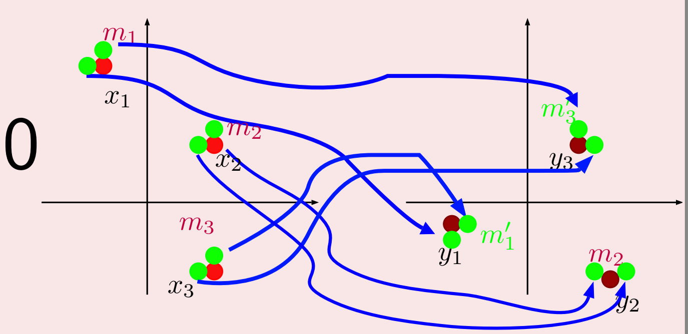
In dimension $d \geq 2$, in any time horizon $[0, T]$, a finite number of arbitrary items can be driven to pre-assigned open subsets of the Euclidean space, corresponding to its labels, by piece-wise constant controls.

Generative Neural Transport

Neural ODEs $\dot{\mathbf{x}}(t) = \mathbf{w}(t)\,\sigma(\mathbf{a}(t)\cdot\mathbf{x}(t)+b(t))$, interpreted as the characteristics of the transport equation:



$$\partial_t \rho + \mathrm{div}_x\big[\underbrace{\big(\mathbf{w}(t)\,\sigma(\mathbf{a}(t)\cdot x + b(t))\big)}_{V(x,t)}\,\rho\big] = 0$$



allow transporting atomic measures and constitute a tool for generative transport.

2

[2]Related results for smooth sigmoids using Lie brackets: A. Agrachev and A. Sarychev, arXiv:2008.12702, (2020); Li, Q., Lin, T., & Shen, Z. (2022), JEMS.

$$\dot{\mathbf{x}}(t) = \mathbf{w}(t)\,\sigma(\mathbf{a}(t)\cdot\mathbf{x}(t) + b(t))$$

Control functions $(\mathbf{w}, \mathbf{a}, \mathbf{b}) \longrightarrow$ Piecewise constant.
Each time discontinuity $\sim$ change of layer.

- $\mathbf{a}(t), b(t)$ define a hyperplane $H(\mathbf{x}) = \mathbf{a}(t)\cdot\mathbf{x}(t) + b(t) = 0$ in $\mathbb{R}^d$.
- $\sigma(z) = \max\{z, 0\}$ "activates" the halfspace $H(\mathbf{x}) > 0$ and "freezes" $H(\mathbf{x}) \leq 0$.
- $\mathbf{w}(t)$ determines the direction of the field in the active halfspace.

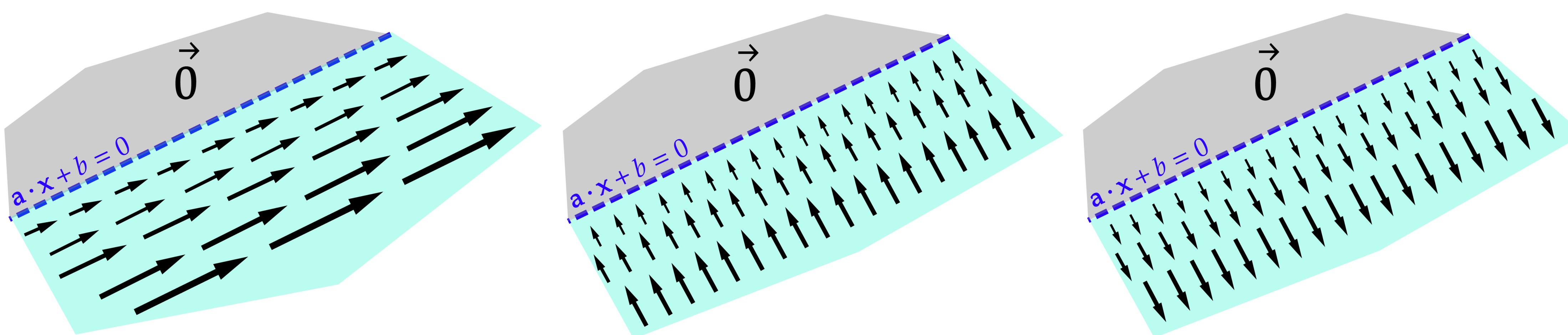
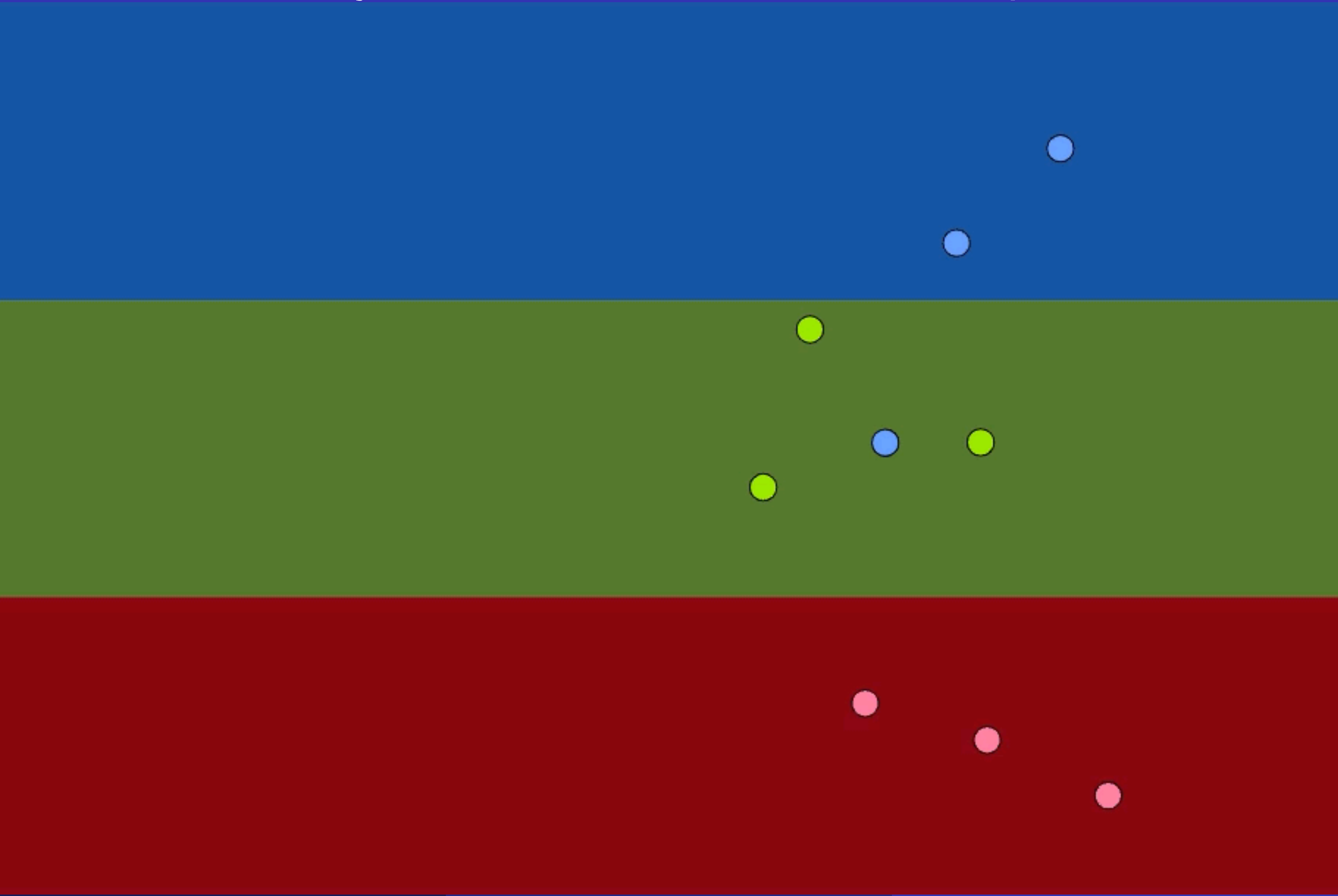


Figure: Parallel (left); Contraction (center); Expansion (right).

Classification by Control of ResNets: One step + Induction



Outline

NN version of variational PDEs

Warning: Lack of convexity!

$$\begin{cases} -\Delta u = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

$$u \in H_0^1(\Omega) : \int_\Omega \nabla u \cdot \nabla \varphi dx = \int_\Omega f \varphi dx \quad \forall \varphi \in H_0^1(\Omega)$$

$$u \in H_0^1(\Omega) : min_{v \in H_0^1(\Omega)} \left[\frac{1}{2} \int_\Omega |\nabla v|^2 dx - \int_\Omega fv dx \right]$$

FEM approximation (Galerkin): Replace the search and test infinite-dimensional space $H_0^1(\Omega)$ by a FEM finite-dimensional one V_h

$$u_h \in V_h : min_{v \in V_h} \left[\frac{1}{2} \int_\Omega |\nabla v|^2 dx - \int_\Omega fv dx \right]$$

$$||u - u_h||_{H_0^1(\Omega)} \leq Ch||f||_{L^2(\Omega)}$$

The NN version

What can NN do?
Replace V_h by a NN finite-dimensional manifold $\mathcal{M}_K$:

$$\mathcal{M}_K = \left\{ v(x) = \sum_{j=1}^{K} w_j \sigma(\mathbf{a}_j \cdot x + b_j) \right\}$$

$$dim(\mathcal{M}_K) = K(d+2), \quad d = dim(\Omega)$$

Then

$$u_K \in \mathcal{M}_K : min_{v \in \mathcal{M}_K} \left[\frac{1}{2} \int_\Omega |\nabla v|^2 dx - \int_\Omega fv dx \right]$$

And letting $K \to \infty$... one can develop a Γ-convergence like theory. [3]

But the problem of minimising Dirichlet's energy in $\mathcal{M}_K$ is non-convex!

[3] (1) W. E & B. Yu, (2017). The Deep Ritz method: A deep learning-based numerical algorithm for solving variational problems.
(2) Luo, T. & Yang, H., (2020). Two-layer neural networks for partial differential equations: Optimization and generalization theory.

Mean-field relaxation Back to ∞-dimensions...

Mean-field relaxation is commonly employed in shallow NNs. [4]

Shallow NN

The original Shallow NN writes:

$$\sum_{j=1}^{K} w_j \sigma(\mathbf{a}_j \cdot x + b_j),$$

where $(w_j, \mathbf{a}_j, b_j) \in \mathbb{R} \times \mathbb{R}^d \times \mathbb{R}$ for all j.

As the number of neurons K tends to infinity, the ansatz evolves into its relaxed version.

Mean-field shallow NN

The mean-field shallow NN writes:

$$v_\mu(x) = \int_{\mathbb{R}^{d+1}} \sigma(\mathbf{a} \cdot x + b) d\mu(a, b),$$

where $\mu \in \mathcal{M}(\mathbb{R}^{d+1})$.
The outcome is linear with respect to μ!

This leads to the minimisation problem

$$\min_{\mu \in \mathscr{M}} \left[\frac{1}{2} \int_\Omega |\nabla v_\mu|^2 dx - \int_\Omega f v_\mu dx \right].$$

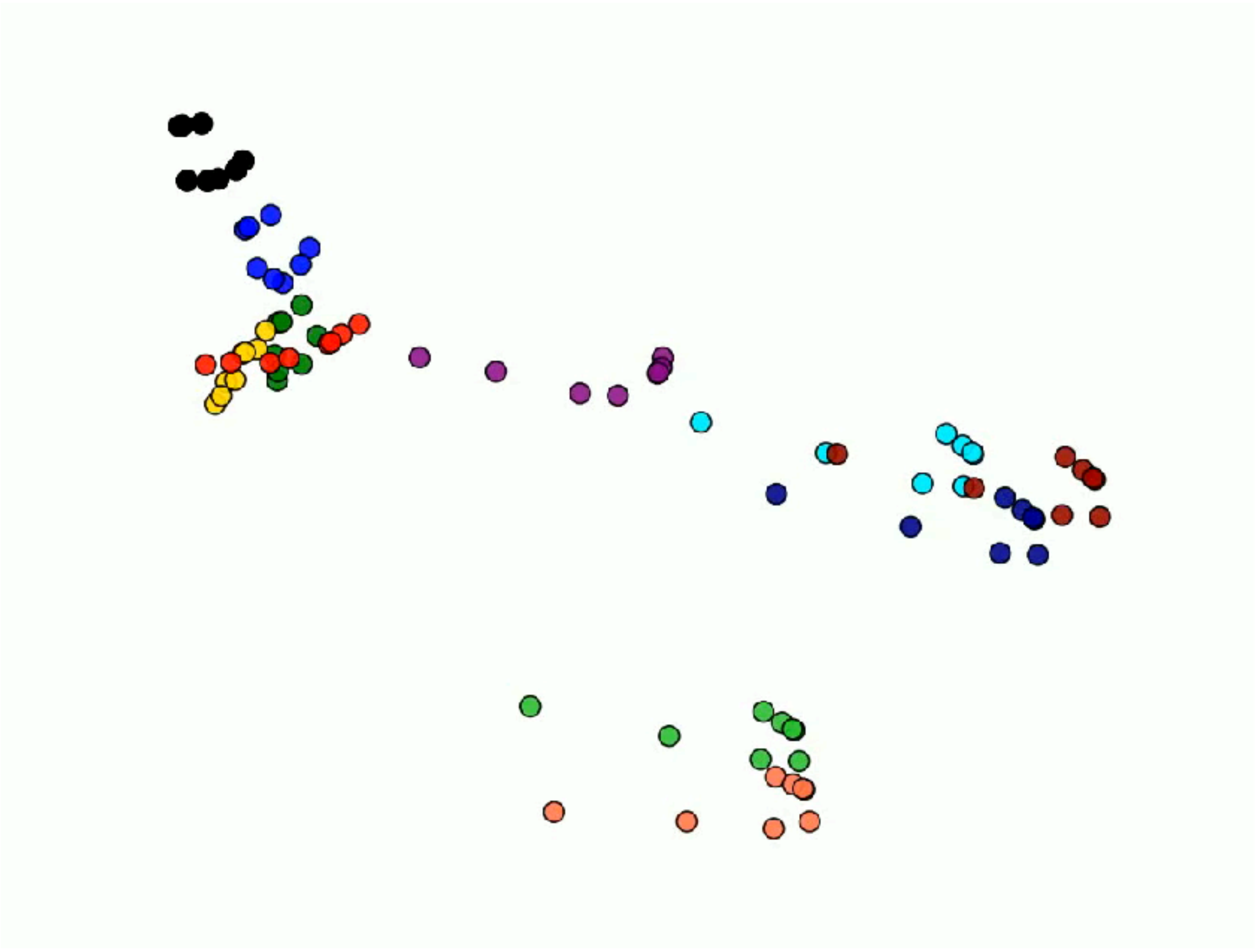
Is it well-posed? Does the minimiser exist? Does it coincide with the weak solution of the Dirichlet problem?

[4] [Mei-Montanari-Nguyen, 2018], [Chizat-Bach, 2018], [K. Liu & E. Zuazua, Representation and regression problems in NN: Relaxation, Generalisation and Numerics, M3AS, 2025.]

Outline

Tracking dynamic data

Joint work with K. Liu, L. Liverani and Z. Li



Semi-autonomous NODEs

Joint with Kang Liu, Lorenzo Liverani and Ziqian Li

- The structure is motivated by the Universal Approximation property of ReLU activation functions (Pinkus, 1999)

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t), t) \rightarrow \mathbf{f}(\mathbf{x}, t) \sim \sum_{j=1}^{K} \mathbf{w}_j \, \sigma(\mathbf{a}_j^1 \cdot \mathbf{x} + a_j^2 t + b_j)$$

- Complexity reduction
- Anticipate future evolution of trajectories.

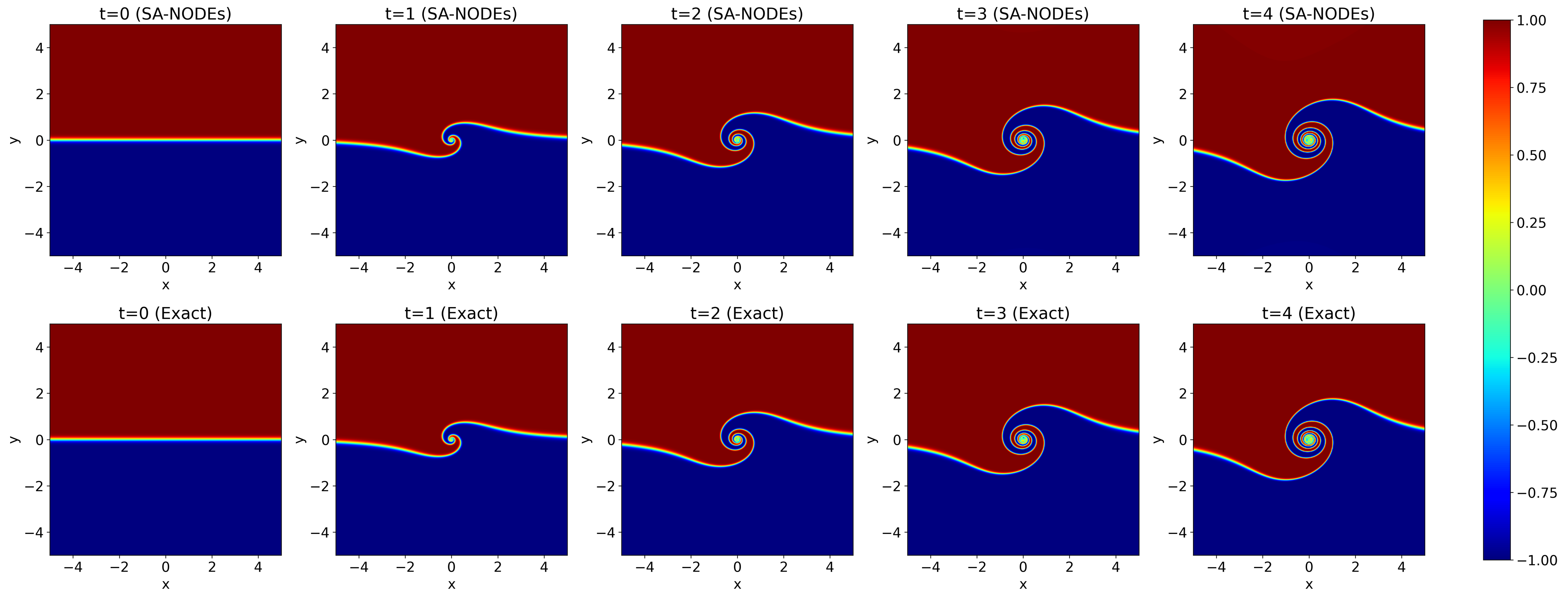
A time-independent choice of the parameters leads to a non-autonomous dynamics, but with a trivial time-dependence,

$$\dot{\mathbf{x}}(t) = \sum_{j=1}^{K} \mathbf{w}_j \, \sigma(\mathbf{a}_j^1 \cdot \mathbf{x}(t) + a_j^2 t + b_j)$$

To be complemented with Model Predictive Control (MPC)

Doswell Frontogenesis

Joint work with Ziqian Li, Weiwei Hu, Yubiao Zhang on optimal fluid mixing



SA-NODEs and exact solution of the transport equation modeling Doswell frontogenesis

$$\partial_t \rho(x, y, t) + \mathrm{div}\left(\rho(x, y, t)\left(-yg(r), xg(r)\right)\right) = 0,$$

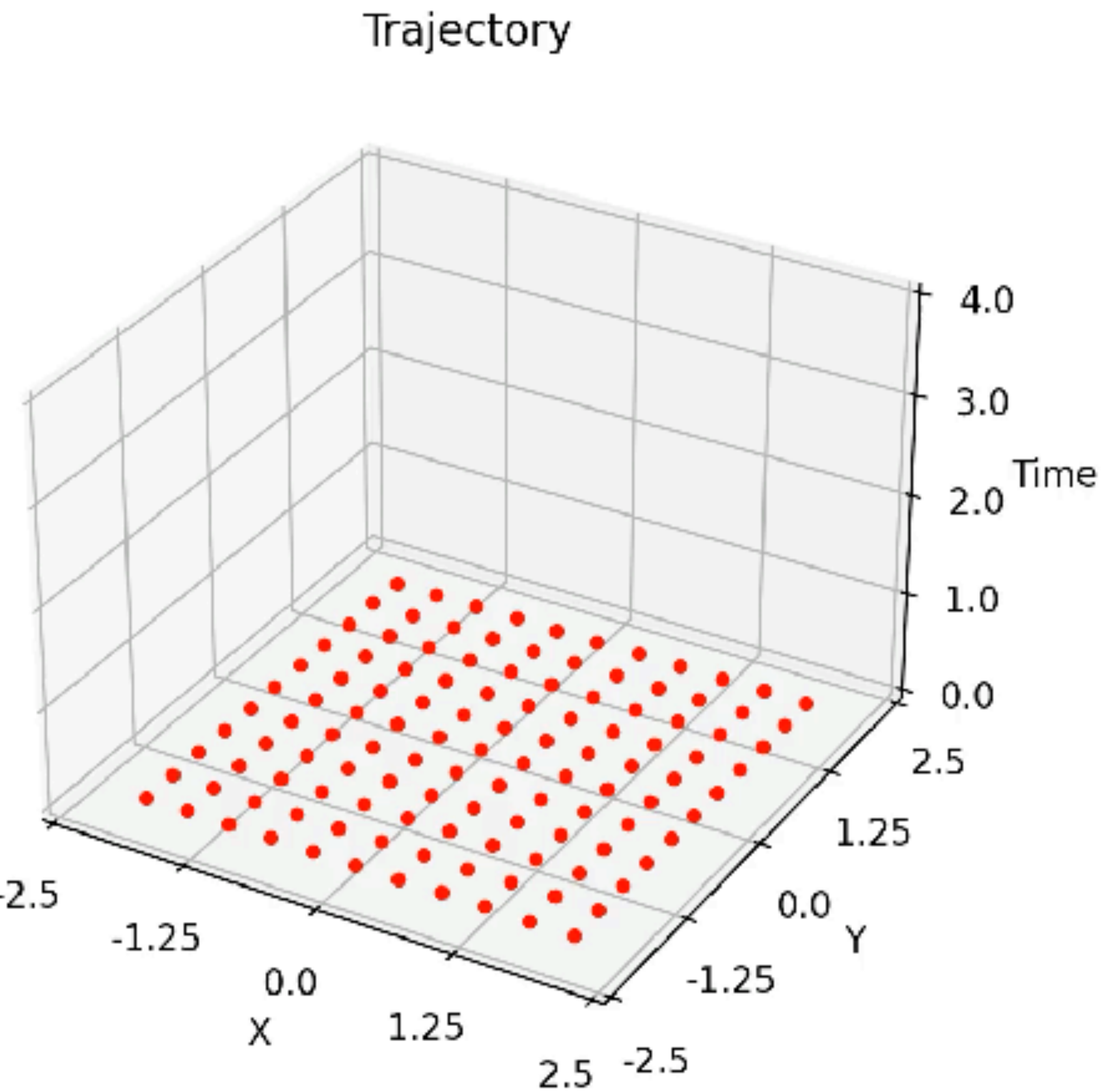
where $(x, y, t) \in \mathbb{R}^2 \times [0, T]$ and,

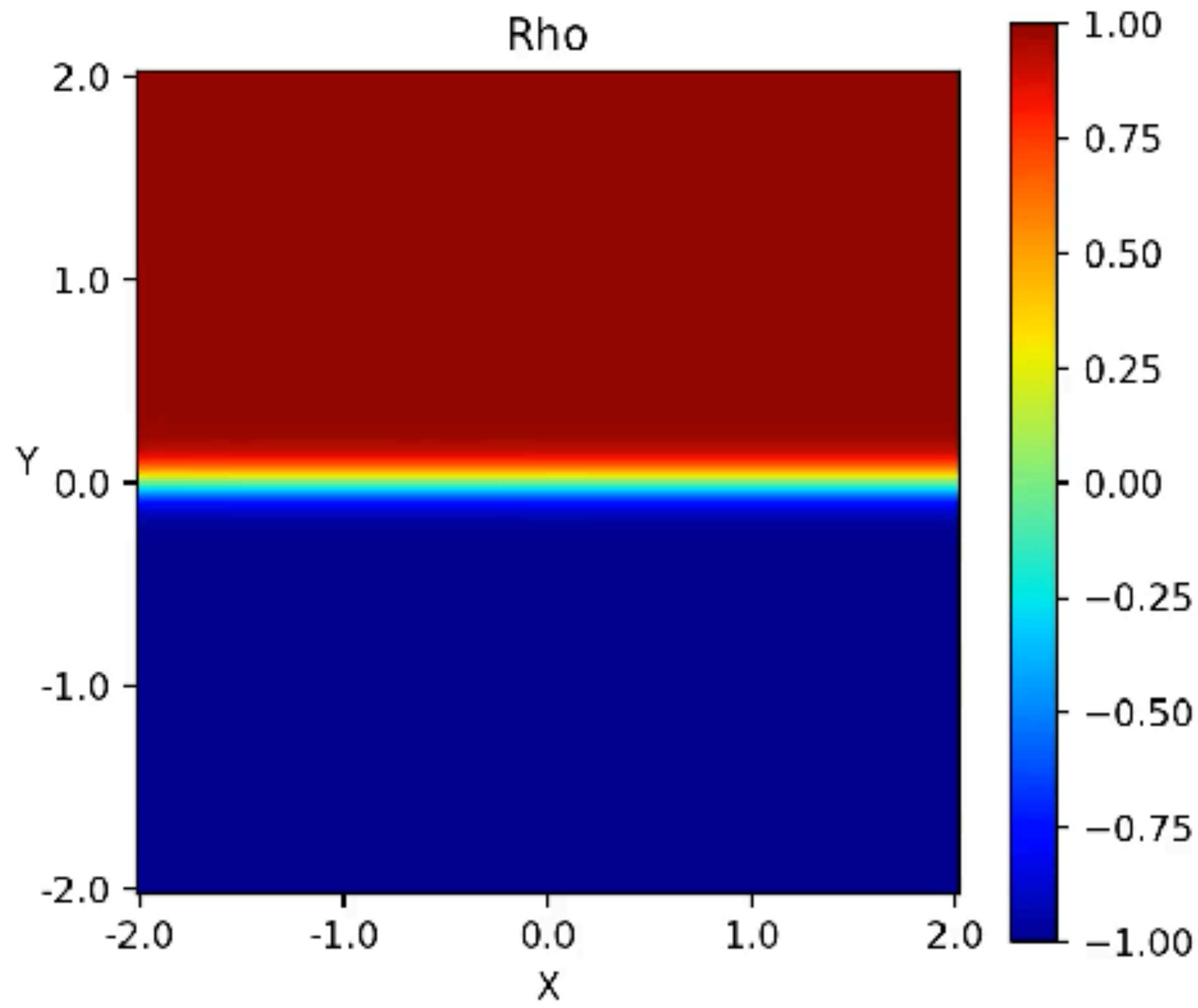
$$g(r) = c\, r^{-1}\, \mathrm{sech}^2 r \tanh r, \quad \rho_0(x, y) = \tanh\left(y/\delta\right).$$

The exact solution:

$$\rho(x, y, t) = \tanh\left(\frac{y\cos(gt) - x sin(gt)}{\delta}\right).$$

Tornado Emergence

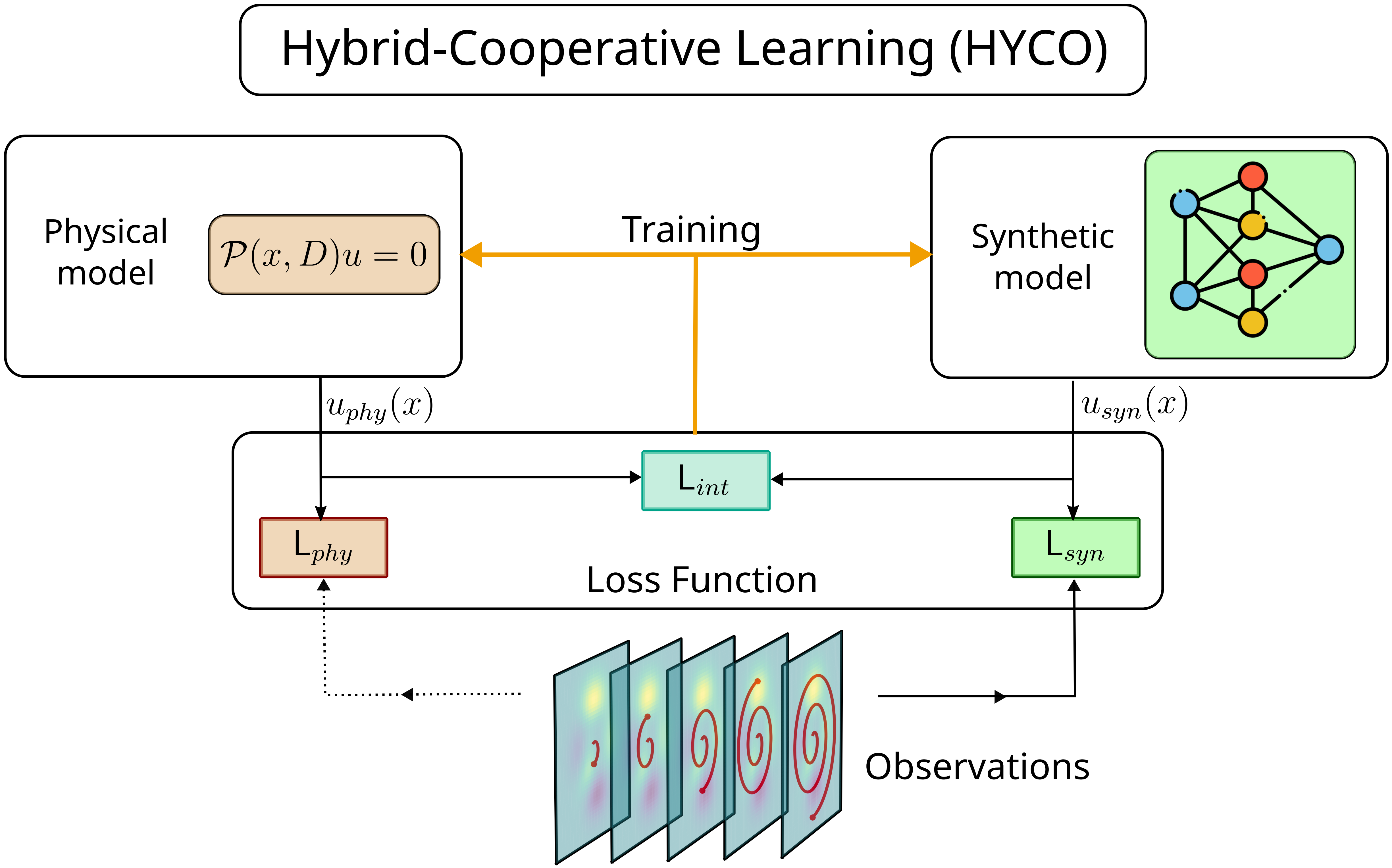




t = 0.00

HYCO: A Hybrid-Cooperative Strategy for Data-Driven PDE Model Learning

joint work with Lorenzo Liverani and Thys Steynberg



Conclusions and Perspectives

The Future of Mathematics in the Age of AI

- **Maths for Learning**
  - Gradient descent dynamics
  - Generalization
  - Generation
  - Width/Depth... Architectures
  - Dimensionality and probabilities
  - Attention mechanisms
  - Federated Learning
  - .... Curse of dimensionality + Devil of non-convexity.
- **Digital Twins Methodologies** pose specific challenges
  - Scalability / Adaptivity / Personalised / Goal oriented (Model Predictive Control?)
  - Control of control for DT modelling
  - Reliability / generalisation / synthetic data
  - Merging with Physics and Mechanics
  - Applications: Personalised Medicine, Environment, Climate, Energy,...

Thank you for the invitation and attention

Our recent contributions

E. Zuazua, *Control and Machine Learning*, SIAM News, October 2022

D. Ruiz-Balet, E. Zuazua, *Neural ODE control for classification, approximation and transport*, SIAM Review, 65 (3)3 (2023), 735-773.

A. Alcalde, G. Fantuzzi, E. Zuazua, *Clustering in pure-attention hardmax transformers*, arXiv:2407.01602 (2024)

Z. Li, K. Liu, L. Liverani, E. Zuazua,*Universal approximation of dynamical systems by semi-autonomous ODEs and applications*, arXiv:2407.17092 (2024)

B. Geshkovski, E. Zuazua, *Turnpike in optimal control of PDEs, ResNets, and beyond*, Acta Numer., 31 (2022), 135–263

And more...

D. Ruiz-Balet, E. Zuazua, *Control of neural transport for normalizing flows, Journal de mathématiques pures et appliquées*, 181 (2024), 58-90.

Z. Wang, Y. Song, E. Zuazua, *Approximate and Weighted Data Reconstruction Attack in Federated Learning*, arXiv:2308.06822 (2023)

A. Álvarez-López, R. Orive-Illera, E. Zuazua, *Optimized classification with neural ODEs via separability*, arXiv:2312.13807 (2023)

A. Álvarez-López, A. H. Slimane, E. Zuazua, *Interplay between depth and width for interpolation in neural ODEs*, NEUNET, 180 (2024), 106640.

M. Hernández, E. Zuazua, *Deep neural networks: multi-classification and universal approximation*, arXiv preprint arXiv:2409.06555.