



Friedrich-Alexander-Universität Research Center for Mathematics of Data | MoD



Control and Machine Learning

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Alexander von Humboldt Stiftung/Foundation



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RESEARCH LABORATORY

ALB FORCE



CONTROL FOR DEEP AND FEDERATED LEARNING

1 Context: Applied Mathematics + Machine Learning

2 Why does it work?

3 NN for PDE approximation

4 PDE+D

Nowadays AI: small and big

First demonstration of predictive control of fusion plasma by digital twin

by National Institutes of Natural Sciences



Image of digital twin control, in which real plasma is controlled by virtual plasm...





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.

How does it work? Computational practice



Complexity: Curse of dimensionality + Devil of non-convexity



Input

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• Why does it work?

Can traditional applied mathematics contribute to explain the theoretical foundations of this success?

• Use NN for PDE approximation

Replace the classical linear ansätze (finite differences, spectral, FEM) by a NN nonlinear one.

(Devil of non-convexity!)

What can Applied Maths learn from these new tools? Merging: PDE+D(ata)

"Digital Twins: Where Data, Mathematics, Models and Decisions Collide"

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Why does it work? Universal Approximation

Math. Control Signals Systems (1989) 2: 303-314

Mathematics of Control, Signals, and Systems © 1989 Springer-Verlag New York Inc.



Approximation by Superpositions of a Sigmoidal Function*

G. Cybenko†

$$\sum_{j=1}^{N} \alpha_{j} \sigma(y_{j}^{\mathsf{T}} x + \theta_{j}),$$

where $y_j \in \mathbb{R}^n$ and $\alpha_j, \theta \in \mathbb{R}$ are fixed. (y^T is the transpose of y so that $y^T x$ is the inner product of y and x.) Here the univariate function σ depends heavily on the context of the application. Our major concern is with so-called sigmoidal σ 's:

$$\sigma(t) \to \begin{cases} 1 & \text{as } t \to +\infty, \\ 0 & \text{as } t \to -\infty. \end{cases}$$

Tauberian Theorems Author(s): Norbert Wiener Source: Annals of Mathematics, Vol. 33, No. 1 (Jan., 1932), pp. 1-100



(1)

CoML

Why does it work so well? Control \leftrightarrow ML



Control: Dogs-Sheep

Supervised Learning

Nature inspires



Border Collies segregate ducks

CoML

Cybernetics, Norbert Wiener, 1948

The science of control and communication in animals and machines

Let $d, m \in \mathbb{N}^*$ and T > 0 and the linear finite *d*-dimensional system

$$x'(t) = Ax(t) + Bu(t), \quad t \in (0, T); \quad x(0) = x^{0}$$
 (1)

A is a $d \times d$ real matrix, B is $d \times m$ (m controls) and $x^0 \in \mathbb{R}^d$. The function $x : [0, T] \longrightarrow \mathbb{R}^d$ represents the *state* and $u : [0, T] \longrightarrow \mathbb{R}^m$ the *control*.

Can we control d states with only m controls, even if d >> m?

Theorem





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



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

An example: Nelson's car.



Two controls suffice to control a four-dimensional dynamical system.¹

¹E. Sontag, *Mathematical control theory*, 2nd ed., Springer-Verlag, NewYork, 1998.

Enrique Zuazua

NN Modelling



2

Supervised learning by control

Goal: Find an approximation of a function $f_{\rho} : \mathbb{R}^d \to \mathbb{R}^n$ from a dataset

 $\{\vec{x}_i, \vec{y}_i\}_{i=1}^N \subset \mathbb{R}^d \times \mathbb{R}^n$

drawn from an unknown probability measure ρ on $\mathbb{R}^d \times \mathbb{R}^n$.

Classification: match points (images) to respective labels (cat, dog).



This is typically done by training a neural network. We will do it through the simultaneous or ensemble control of Neural ODEs.

ResNets / Neural ODEs in action (Borjan Geshkovski)

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



[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 $d \ge 2$, 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 $\dot{\mathbf{x}}(t) = \mathbf{w}(t) \sigma(\mathbf{a}(t) \cdot \mathbf{x}(t) + \mathbf{b}(t))$, interpreted as the characteristics of the transport equation:

$$\frac{\int_{x_1}^{m_1} \int_{y_2}^{m_2} \int_{y_3}^{m_3} \int_{y_1}^{m_3} \int_{y_2}^{m_3} \partial_t \rho + \operatorname{div}_x \left[\underbrace{(\mathbf{w}(t) \, \sigma(\mathbf{a}(t) \cdot x + b(t))}_{V(x,t)} \rho \right] = 0 \xrightarrow[x_1]{(w_1 + b(t))}_{y_3} \int_{y_3}^{m_3} \int_{y_3}^{m_3} \int_{y_4}^{m_3} \int_{y_4}^{m_3} \int_{y_4}^{m_3} \int_{y_4}^{m_3} \int_{y_4}^{m_3} \int_{y_4}^{m_4} \int_{y_4}^{m_3} \int_{y_4}^{m_4} \int_{y_4}^{m_5} \int_{y_4}^{$$

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

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

What is the ResNet doing? Basic control actions

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

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

a(t), b(t) define a hyperplane H(x) = a(t) ⋅ x(t) + b(t) = 0 in ℝ^d.
σ(z) = max{z,0} "activates" the halfspace H(x) > 0 and "freezes" H(x) ≤ 0.
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





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NN version of variational PDEs

Warning: Lack of convexity!

$$\begin{cases} -\Delta u = f & \text{in } \Omega\\ u = 0 & \text{on } \partial\Omega \end{cases}$$
$$u \in H_0^1(\Omega) : \int_{\Omega} \nabla u \cdot \nabla \varphi dx = \int_{\Omega} f \varphi dx \quad \forall \varphi \in H_0^1(\Omega)$$
$$u \in H_0^1(\Omega) : \min_{v \in H_0^1(\Omega)} \left[\frac{1}{2} \int_{\Omega} |\nabla v|^2 dx - \int_{\Omega} f v dx \right]$$

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

$$egin{aligned} u_h \in V_h : \min_{v \in V_h} \left[rac{1}{2} \int_{\Omega} |
abla v|^2 dx - \int_{\Omega} fv dx
ight] \ & ||u - u_h||_{H^1_0(\Omega)} \leq Ch||f||_{L^2(\Omega)} \end{aligned}$$

The NN version

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

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

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

Then

$$u_{\mathcal{K}} \in \mathcal{M}_{\mathcal{K}} : \min_{v \in \mathcal{M}_{\mathcal{K}}} \left[\frac{1}{2} \int_{\Omega} |\nabla v|^2 dx - \int_{\Omega} f v dx \right]$$

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 is commonly employed in shallow NNs. ⁴

Shallow NN

The original Shallow NN writes:

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

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

As the number of neurons K tends to infinity and densifies 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

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

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, (2024). Representation and regression problems in NN: Relaxation, Generalisation and Numerics.]

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Tracking dynamic data

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



Semi-autonomous NODEs

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

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

- 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,

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

To be complemented with Modelm Predictive Control (MPC)?

Doswell Frontogenesis

Ongoing work with Weiwei Hu (Atlanta) on optimal fluid mixing



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

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

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

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

The exact solution:

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

Trajectory



t = 0.00

PDE+D

Hybrid Methodology: Data Driven + PDE modelling + Collapse



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.

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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.

Conclusions and Perspectives

Fantastic horizon for mathematical research

• 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

