Physics-informed Neural Networks
Mixed Data-driven Model-based approach

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work conducted with J. Liu, M. Aguiar and K. H. Johansson

Introdution

Machine Learning

$$u^\star = \operatorname{argmin}_{\mathbf{u}} \quad \frac{1}{N}\sum_{i=1}^{N} L\left(\nu_i, y_i, \mathbf{u}\right)$$

Data-driven

Optimization problem

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Differential Equation

$$\begin{cases} \dfrac{\partial v}{\partial t}(t,x) + \mathcal{N}[v](t,x) = 0, & (t,x) \in [0,T) \times \Omega, \\ v(\cdot,x)|_{x\in\partial\Omega} = v_{\partial\Omega}, \\ v(0,\cdot) = v_0. \end{cases}$$

Initial condition

Boundary condition

PDE $\Rightarrow$ Model-based

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Examples

Weather forecast

Stock price prediction

...

Traffic jam forecast

Trajectory estimation

Machine learning to solve PDEs?

JOURNAL OF COMPUTATIONAL PHYSICS **91**, 110–131 (1990)

Neural Algorithm for Solving Differential Equations

HYUK LEE

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AND

IN SEOK KANG

Department of Chemical Engineering, California Institute of Technology, Pasadena, California 91125

Received August 17, 1988; revised October 6, 1989

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Artificial Neural Networks for Solving Ordinary and Partial Differential Equations

Isaac Elias Lagaris, Aristidis Likas, *Member, IEEE,* and Dimitrios I. Fotiadis

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of a feedforward neural network by replacing each spline with the sum of piecewise linear activation functions that correspond to the hidden units. This method considers local basis-functions and in general requires many splines (and consequently network parameters) in order to yield accurate solutions. Furthermore, it is not easy to extend these techniques to multidimensional domains.

In this article we view the problem from a different angle. We present a method for solving both ordinary differential equations (ODE's) and partial differential equations (PDE's) (defined on *orthogonal box* domains) that relies on the function approximation capabilities of feedforward neural networks and results in the construction of a solution written in a

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1) **infinitely differentiable closed analytic form;**
2) **superior interpolation properties as compared to well-established methods such as finite elements [1], [2];**
3) **small number of parameters;**
4) **suitability for efficient implementation on parallel computers;**

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DGM: A deep learning algorithm for solving partial differential equations ☆,☆☆

Justin Sirignano [a,*], Konstantinos Spiliopoulos [b]

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Solving Partial Differential Equations Using

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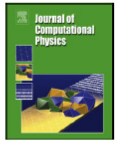

Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations

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Preliminaries on neural networks

A neural network unit:

$$H_{W,b}(\nu) = \phi(\underbrace{W}_{\in \mathbb{R}^{N_n \times ?}} \times \nu + \underbrace{b}_{\in \mathbb{R}^{N_n \times 1}})$$

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A multilayer neural network with linear output:

$$u_\theta(\nu) = W \times H_{\theta_{L-1}} \circ H_{\theta_{L-2}} \circ \cdots \circ H_{\theta_1}(\nu) + b$$

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Theorem: Universal approximation (K. Hornik)

A neural network can approximate any smooth function arbitrarily close provided a sufficient number of neurons N_n.

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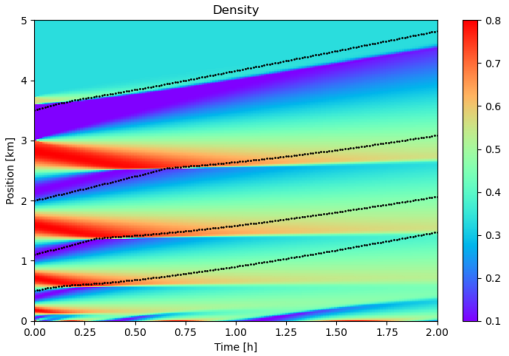
Proposition: Backpropagation (D. Rumelhart, G. Hinton & R. Williams)

Provided ϕ is differentiable, the backpropagation algorithm makes it possible to symbolically computes any derivative of u_θ and in particular, $\frac{\partial u}{\partial \nu}$.

Data-driven versus Model-based

Example: Traffic density estimation



Real density - Simulation

- 2-D map (spatiotemporal diagram)
- colormap = density
- Black dots are measurements (sparse)

Data-driven versus Model-based

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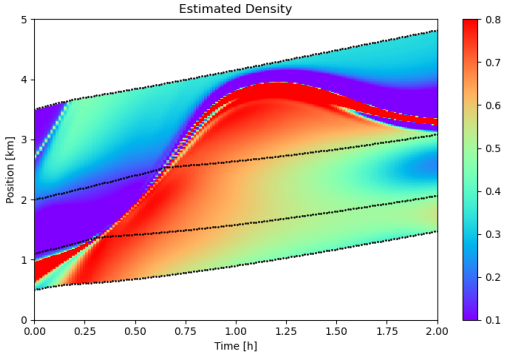

Estimated density - Data

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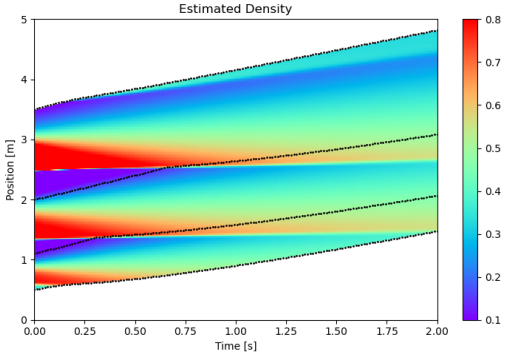

Estimated density - Model

- 2-D map (spatiotemporal diagram)
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- Model for traffic

$$\frac{\partial u}{\partial t} + V_f(1-2u)\frac{\partial u}{\partial x} = 0$$

Data-driven versus Model-based

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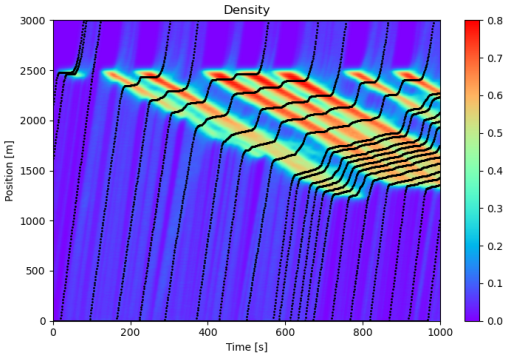

Real density - Road

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Data-driven versus Model-based

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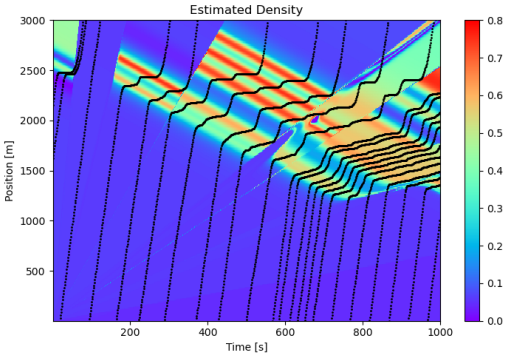

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Data-driven

- ⊕ Good estimation if large dataset
- ⊕ Robust to noise and disturbances
- ⊕ No curse of dimensionality
- ⊕ Can infer hidden pattern
- ⊖ Large computational time
- ⊖ No convergence proof
- ⊖ Require a large dataset

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Model-based

- ⊕ No measurements needed
- ⊕ Fast to compute
- ⊕ Error bounds on the solution
- ⊖ Sometimes not robust to noise
- ⊖ Require a precise model
- ⊖ Subject to curse of dimensionality

Can we use both Data-driven and Model-based simulation tools?

Physics-Informed Neural Network (PINN)

Machine Learning

$$u^\star = \operatorname{argmin}_{\mathbf{u}} \quad \frac{1}{N}\sum_{i=1}^{N} L\left(\nu_i, y_i, \mathbf{u}\right)$$

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Physics-Informed Neural Networks

Optimization

$$\theta^\star = \operatorname{argmin}_{\boldsymbol{\theta}} \quad \frac{1}{N}\sum_{i=1}^{N} \left(u_{\boldsymbol{\theta}}(t_i,x_i) - y_i\right)^2$$

Measurement error

Constraint

$$\text{s. t.} \quad \frac{\partial u_{\boldsymbol{\theta}}}{\partial t}(t,x) + \mathcal{N}[u_{\boldsymbol{\theta}}](t,x) = 0, \quad (t,x) \in [0,T) \times \Omega.$$

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$\Rightarrow$ Learning under constraint problem

Optimize a PINN

$$\theta^\star = \text{argmin}_{\boldsymbol{\theta}} \quad \sum_{i=1}^{N} \frac{\left(u_{\boldsymbol{\theta}}(t_i, x_i) - y_i\right)^2}{N}$$

$$\text{s. t.} \qquad \frac{\partial u_{\boldsymbol{\theta}}}{\partial t}(t,x) + \mathcal{N}[u_{\boldsymbol{\theta}}](t,x) = 0, \quad (t,x) \in [0,T) \times \Omega.$$

Optimize a PINN

$$\theta^\star = \text{argmin}_{\boldsymbol{\theta}} \quad \sum_{i=1}^{N} \frac{(u_{\boldsymbol{\theta}}(t_i, x_i) - y_i)^2}{N}$$

$$\text{s. t.} \quad \iint_{[0,T]\times\Omega} \left(\frac{\partial u_{\boldsymbol{\theta}}}{\partial t}(t,x) + \mathcal{N}[u_{\boldsymbol{\theta}}](t,x) \right)^2 dtdx = 0.$$

Optimize a PINN

$$\theta^\star = \text{argmin}_{\boldsymbol{\theta}} \max_{\lambda \geq 0} \sum_{i=1}^{N} \frac{\left(u_{\boldsymbol{\theta}}(t_i, x_i) - y_i\right)^2}{N} + \lambda \underbrace{\iint_{[0,T]\times\Omega} \left(\frac{\partial u_{\boldsymbol{\theta}}}{\partial t}(t,x) + \mathcal{N}[u_{\boldsymbol{\theta}}](t,x) \right)^2 dtdx}_{\text{Physics cost}}$$

Optimize a PINN

$$\theta^\star = \text{argmin}_{\boldsymbol{\theta}} \max_{\lambda \geq 0} \sum_{i=1}^{N} \frac{\left(u_{\boldsymbol{\theta}}(t_i, x_i) - y_i\right)^2}{N} + \lambda \frac{1}{N_{\text{phy}}} \sum_{j=1}^{N_{\text{phy}}} \left(\frac{\partial u_{\boldsymbol{\theta}}}{\partial t}(t_i^p, x_i^p) + \mathcal{N}[u_{\boldsymbol{\theta}}](t_i^p, x_i^p) \right)^2$$

$$= \text{argmin}_{\boldsymbol{\theta}} \max_{\lambda \geq 0} \mathcal{L}_\lambda(\theta)$$

Optimize a PINN

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- Primal-dual optimization can solve the previous problem:

$$\theta \leftarrow \theta - \alpha_\theta \nabla_\theta \mathcal{L}_\lambda(\theta) \qquad \lambda \leftarrow \theta + \alpha_\lambda \nabla_\lambda \mathcal{L}_\lambda(\theta)$$

Optimize a PINN

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$$= \text{argmin}_{\boldsymbol{\theta}} \max_{\lambda \geq 0} \mathcal{L}_\lambda(\theta)$$

- Primal-dual optimization can solve the previous problem;
- About the number of physics points N_{phy}:

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- Primal-dual optimization can solve the previous problem;
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  - New dataset: $N + N_{\text{phy}}$;

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- Primal-dual optimization can solve the previous problem;
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  - New dataset: $N + N_{\text{phy}}$;
  - The confidence in the model relates to the number of physics points;

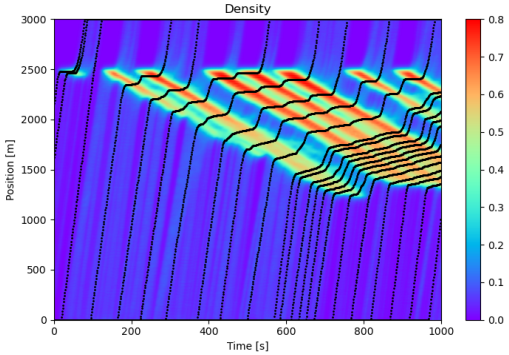
Optimize a PINN

$$\theta^\star = \text{argmin}_{\boldsymbol{\theta},\mu} \max_{\lambda \geq 0} \sum_{i=1}^{N} \frac{(u_{\boldsymbol{\theta}}(t_i, x_i) - y_i)^2}{N} + \lambda \frac{1}{N_{\text{phy}}} \sum_{j=1}^{N_{\text{phy}}} \left(\frac{\partial u_{\boldsymbol{\theta}}}{\partial t}(t_i^p, x_i^p) + \mathcal{N}_\mu[u_{\boldsymbol{\theta}}](t_i^p, x_i^p) \right)^2$$

$$= \text{argmin}_{\boldsymbol{\theta},\mu} \max_{\lambda \geq 0} \mathcal{L}_\lambda(\theta)$$

- Primal-dual optimization can solve the previous problem;
- About the number of physics points N_{phy}:
  - New dataset: $N + N_{\text{phy}}$;
  - The confidence in the model relates to the number of physics points;
- The operator $\mathcal{N}_\mu$ can be defined with uncertain parameters μ $\Rightarrow$ identification.

PINN example: Traffic density estimation



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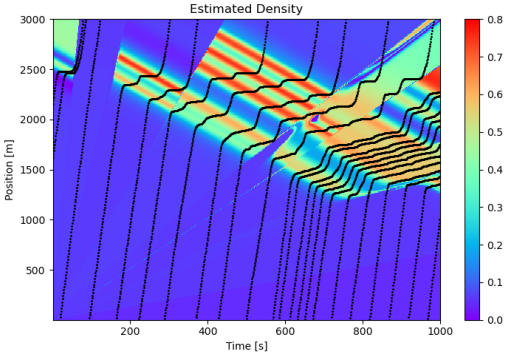

Estimated density - Model

- 2-D map (spatiotemporal diagram)
- colormap = density
- Black dots are measurements (sparse)
- Model for traffic

$$\frac{\partial u}{\partial t} + V_f(1-2u)\frac{\partial u}{\partial x} = 0$$

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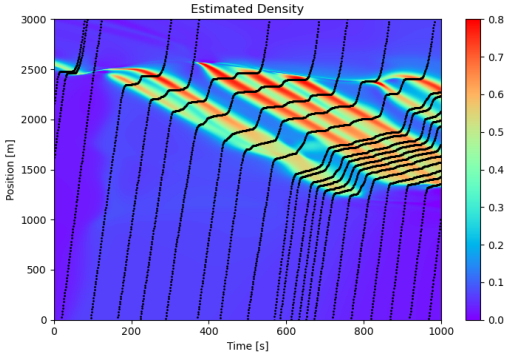

Estimated density - PINN

- 2-D map (spatiotemporal diagram)
- colormap = density
- Black dots are measurements (sparse)
- Model for traffic

$$\frac{\partial u}{\partial t} + \left(\sum_{k=0}^{N_k} \mu_k u^k \right) \frac{\partial u}{\partial x} = 0$$

Advantages and drawbacks of PINN

PINN summary

- ⊕ Good estimation with small/large dataset
- ⊕ Robust to noise and disturbances
- ⊕ No curse of dimensionality
- ⊕ Can infer hidden pattern
- ⊕ Model tuning
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Challenges

- Improve the convergence
  - Less stochastic output (robust w.r.t. training)
  - Fastest convergence
  - Conditions for convergence
- Prove approximation capacity for a broader class of operators $\mathcal{N}$
- Solve strongly coupled systems (multiple PDEs)

Perspectives for PINN

General perspectives:

- Investigate other neural network architectures (LSTM, Convolutional network ...);
- Change the training procedure (primal-dual update, ...)
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Broader perspectives:

- Use the PINN methodology in other domains (fluid mechanics, signal processing, astrology...)
- Increment the framework for use in different contexts (?)

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Thanks!