Physics informed machine learning

With a focus on PINN

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Disclaimer

I do not work in this field.

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What is Machine Learning?

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Roughly speaking algorithms that can analyze data to identify patterns and/or make predictions.

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Very closely related to optimization, curve fitting, model selection, classification etc..

Success of Neural Networks

Neural Networks became popular in the last decade.
Best performing algorithms in fields related to speech, NLP(Natural Language Processing), image analysis, recommender systems etc..

Reasons behind the success of Neural Networks

- Fast and efficient hardware.
- Large amount of data.
- Easy to use software*.

Hardware Lottery [1]

"when a research idea wins because it is suited to the available software and hardware and not because the idea is universally superior to alternative research directions"

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[1] https://hardwarelottery.github.io/

Nivdia H100 specs https://www.nvidia.com/en-us/data-center/h100/

Form Factor	H100 SXM
FP64	30 teraFLOPS
FP64 Tensor Core	60 teraFLOPS
FP32	60 teraFLOPS
TF32 Tensor Core	1,000 teraFLOPS* | 500 teraFLOPS
BFLOAT16 Tensor Core	2,000 teraFLOPS* | 1,000 teraFLOPS
FP16 Tensor Core	2,000 teraFLOPS* | 1,000 teraFLOPS
FP8 Tensor Core	4,000 teraFLOPS* | 2,000 teraFLOPS
INT8 Tensor Core	4,000 TOPS* | 2,000 TOPS

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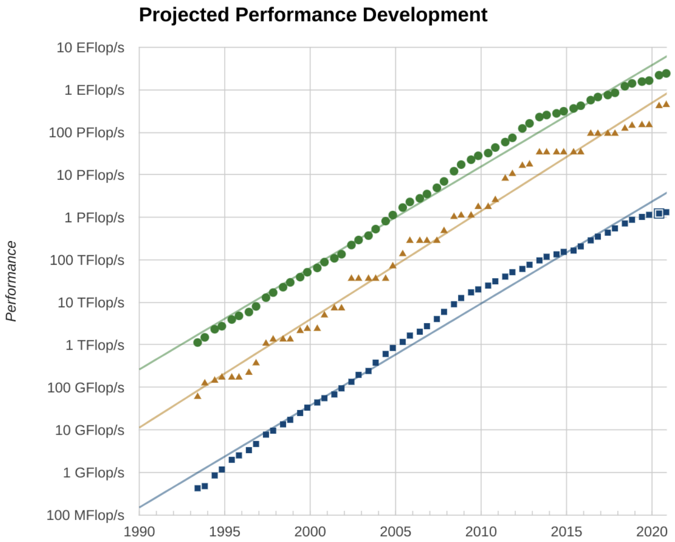
Top 500 supercomputers https://www.top500.org/statistics/perfdevel/



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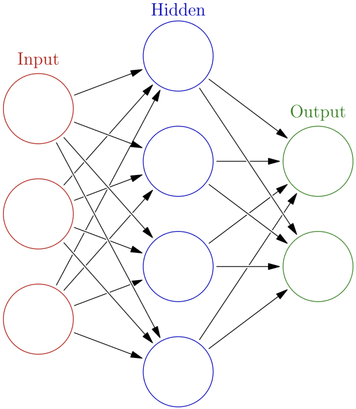

Figure: A simple feed forward neural network (By Glosser.ca - Own work, Derivative of File:Artificial neural network.svg, CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=24913461)

The arrows have numeric values associated with them called weights w^l_{jk}.

The circles are called nodes and their value(a^l_j) is calculated using

$$a^l_j = \sum_k w^l_{jk} a^{l-1}_k + b^l_j \quad .$$

An appropriate cost function that tells us how close are we to the desired result.

l: layer number; j,k: node numbers; : activation function

Training a Neural Network

Find the values of w and b that give the desired output. Basically, a optimization problem which can be solved very efficiently on GPUs.

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Crux of the story

Not enough to throw data at a NN and hope for the best. Most of the successful use cases of NN depend on these specialized architectures.

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Using Machine learning in Physics

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For data analysis. Classification clustering type stuff.

Solving differential equations.

System identification, Reduced order modeling.

Why do we want to use NNs for solving differential equations? [4]

Noisy data can not be easily incorporated in the current algorithms.

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[4] Ref: Physics-informed machine learning, `https://doi.org/10.1038/s42254-021-00314-5`

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No complicated mesh generation required!

NNs can overcome the curse of dimensionality.

Once trained NN can be very fast in making predictions.

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How to solve differential equations using a NN a.k.a. PINN.[5]

We want to solve Burgers equations with appropriate boundary conditions.

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}$$

Rough idea is that we want to approximate $u(t, x)$ using a NN with a loss functions that forces the solution to satisfy the differential equation and boundary conditions.

$$L = w_{\text{data}}\, L_{\text{data}} + w_{\mathrm{PDE}} L_{\mathrm{PDE}},$$

where

$$L_{\text{data}} = \frac{1}{N_{\text{data}}} \sum_{i=1}^{N_{\text{data}}} \left(u\left(x_i, t_i\right) - u_i\right)^2 \quad \text{and}$$

$$L_{\mathrm{PDE}} = \frac{1}{N_{\mathrm{PDE}}} \sum_{j=1}^{N_{\mathrm{PDE}}} \left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} \right)^2_{(x_j, t_j)}$$

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How to solve differential equations using a NN a.k.a. PINN.[6]

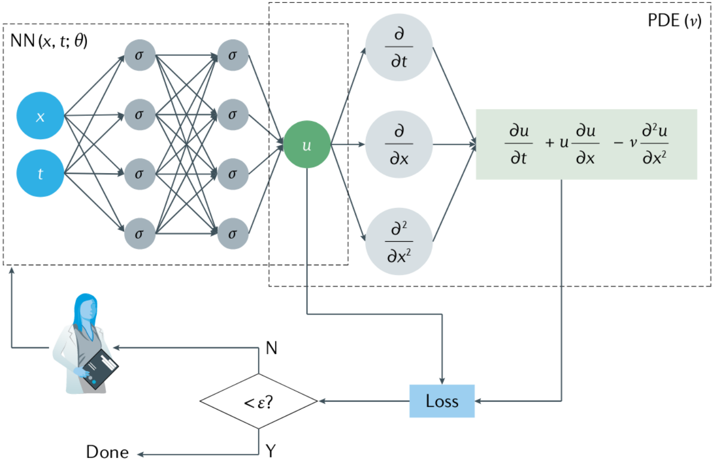

Figure: Physics Informed Neural Network(PINN)

PINNs in action

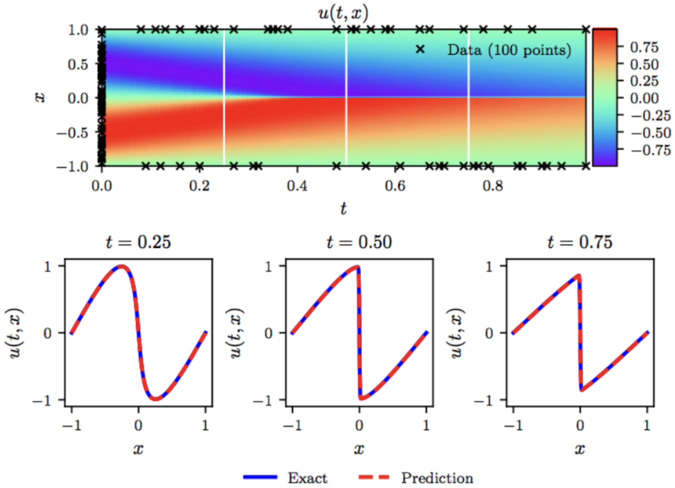

Figure: Solution of burgers equation using PINN https://maziarraissi.github.io/PINNs/

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PINNs in action

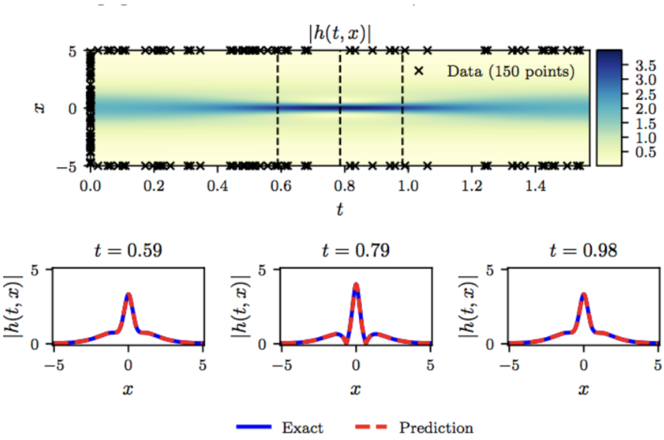

Figure: Solution of Shrödinger equation using PINN https://maziarraissi.github.io/PINNs/

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Three ways we can make machines learn physics[7]

Making the training of NNs simpler.

- Learning bias, already saw an example.
- Observational bias
- Inductive bias

In practice a combination of these is used.

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[7]Ref: Physics-informed machine learning, `https://doi.org/10.1038/s42254-021-00314-5`

Observational bias

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Augment your data with symmetries about what to learn.

New auxiliary variables.

$f(x; y) = x^y + x$, then make x^y a new variable and provide as input.

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Scale, rotate, translate etc. in a way that reflects the underlying physics, instead of making the NN learn these.

Take Fourier transform if your data is periodic.

Inductive bias

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Embed physics in your NN architecture, so that the whole NN exactly satisfies the desired physical laws.

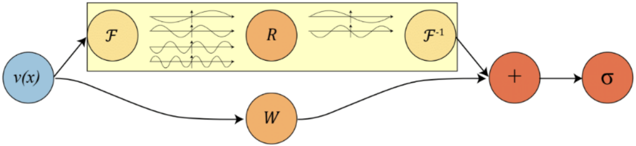

Figure: Fourier Layer `https://zongyi-li.github.io/blog/2020/fourier-pde/`

Need to do on per problem basis. Hard to design architecture that satisfy non-trivial laws.
May not be possible to design architectures that scale well!

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Most of the time a complete black box.

Hype Hype Hype?

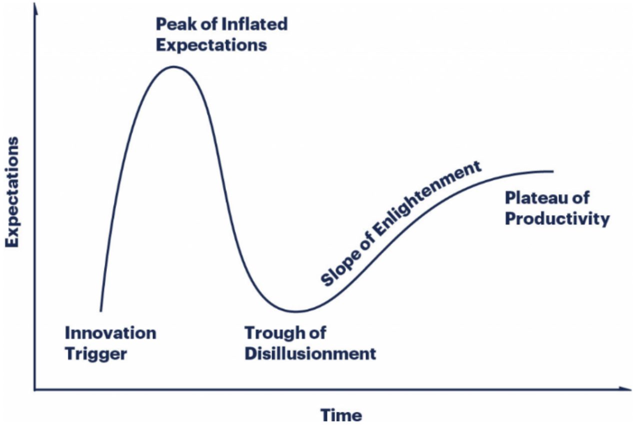

Figure: Gartner Hype Cycle [8]

[8] https://www.bmc.com/blogs/gartner-hype-cycle/

Thanks