AI in nuclear and particle physics

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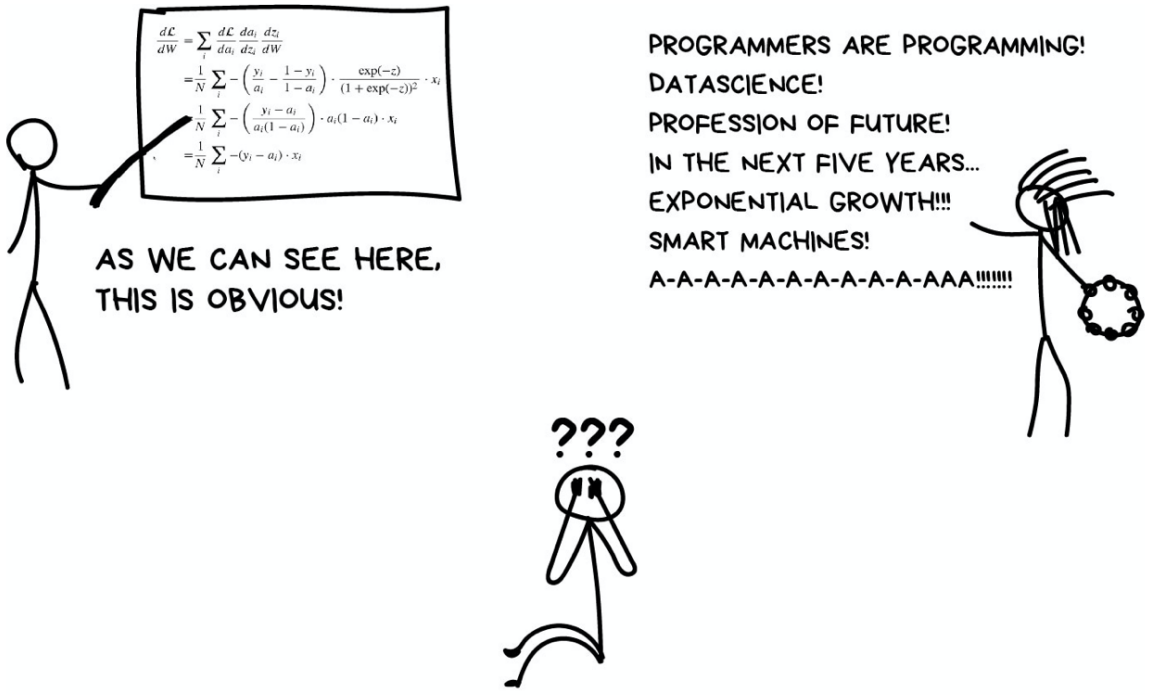
4 April 2022

This lecture



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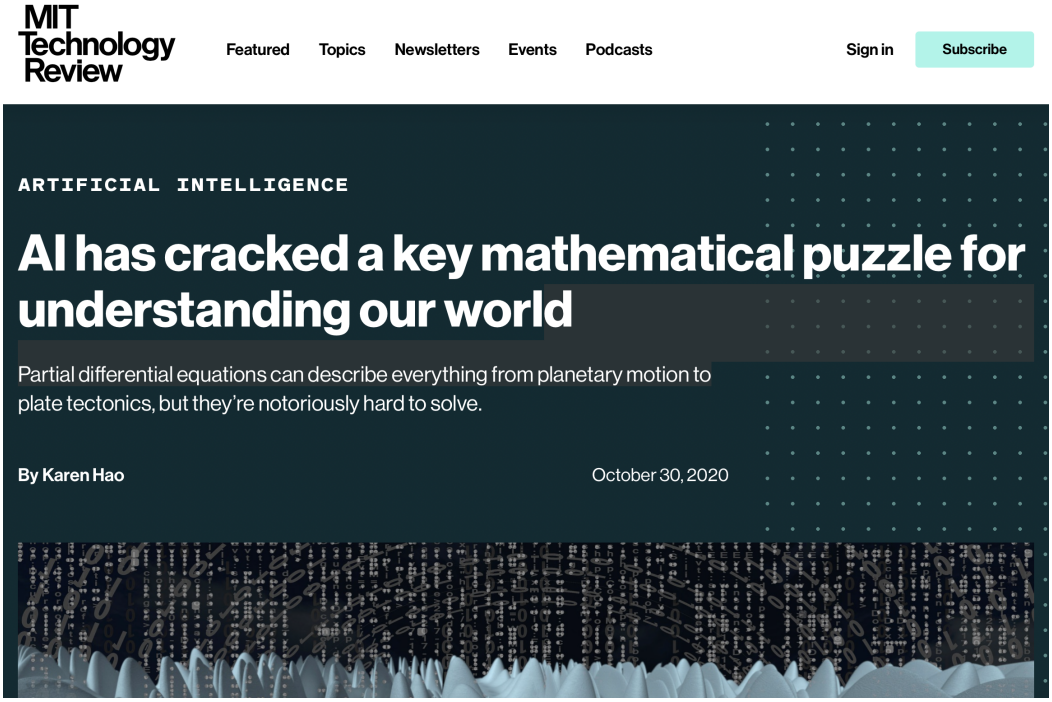
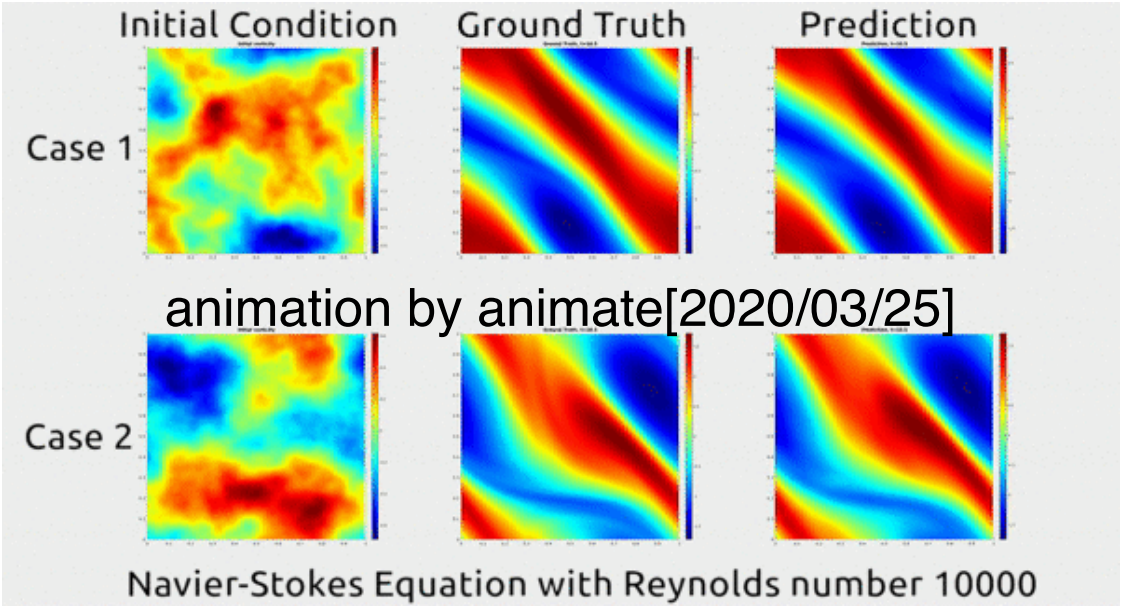
Not a systematic review, an attempt to understand the success

Example of bombarding news...



https://arxiv.org/pdf/2010.08895.pdf
https://www.technologyreview.com/2020/10/30/1011435/ai-fourier-neural-network-cracks-navier-stokes-and-partial-differential-equations/

Example of bombarding news...



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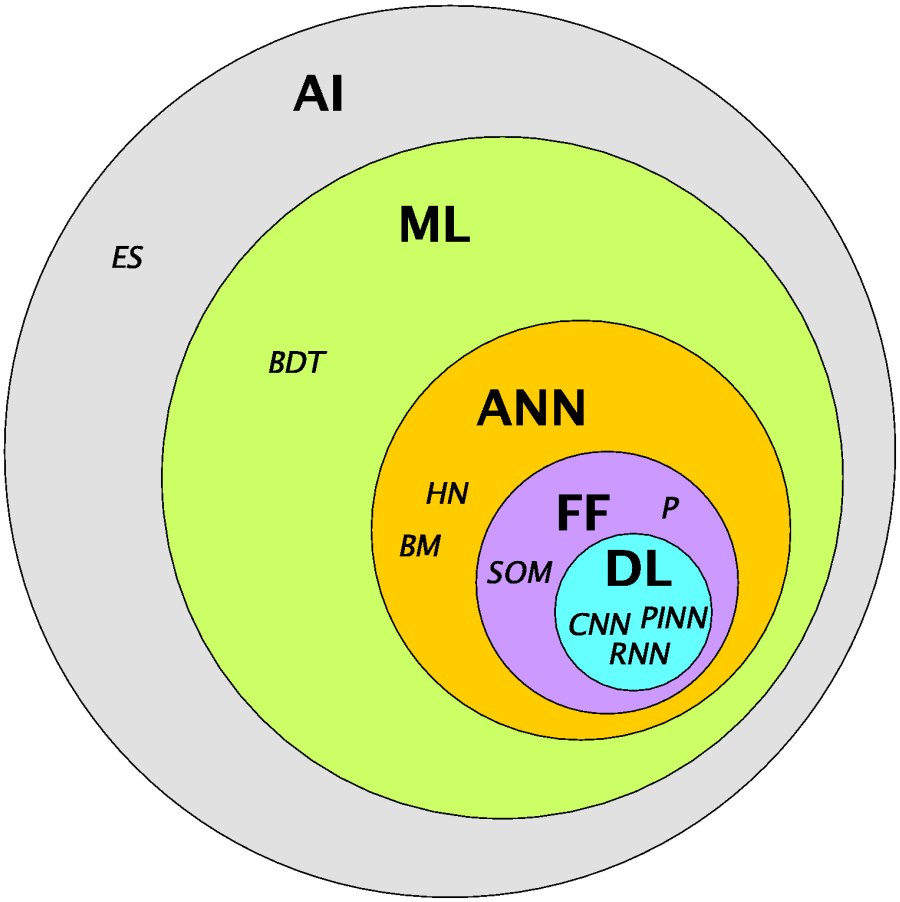
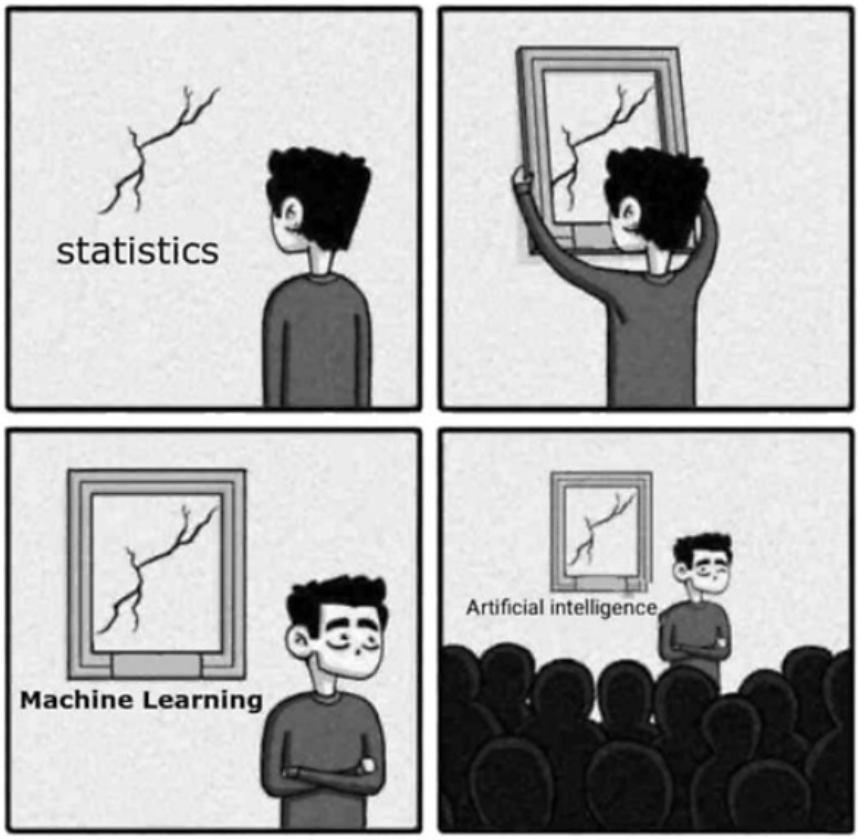
https://www.technologyreview.com/2020/10/30/1011435/ai-fourier-neural-network-cracks-navier-stokes-and-partial-differential-equations/

"Classification"



- Artificial Intelligence
  - Expert Systems
- Machine Learning
  - Boosted Decision Trees
- Artificial Neural Networks
  - Hopfield Network
  - Boltzmann Machine
- Feed Forward
  - Perceptron
  - Self-Organizing Maps
- Deep Learning
  - Convolutional NN
  - Recurrent NN
  - Physics-informed NN
- ...



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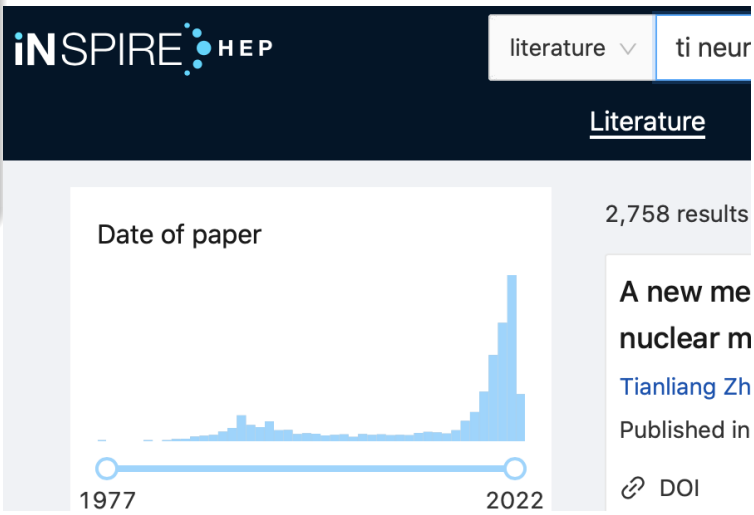
Outline

- Physics questions
- Mini-review of ANN
- Classification and regression
- Deep NN
- Physics-informed NN
- Outreach

Understanding the black box...

Revolution ∼2010:

- Abundance of data
- Huge computational power
- Novel NN architectures and algorithms



ML in nuclear/particle physics

Basic tasks

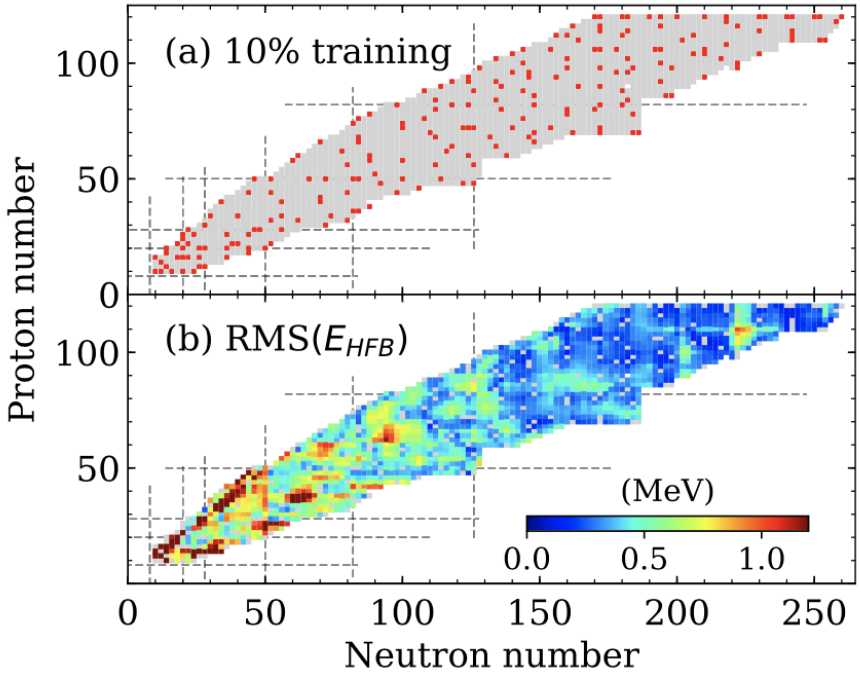
Reviews:
https://arxiv.org/abs/2112.02309
https://doi.org/10.1140/epja/s10050-020-00290-x

- Classification (data analysis, event identification, triggering, jets, dedicated searches, ...)
- Regression (efficient fitting of models, solving differential equations (!), inverse problems, ...)
- Clusterization (data analysis, efficient representation of data, ...)
- Generation (simulating events, data augmentation, detector physics, ...)
- ...

Teaching slow and expensive, using fast and cheap!

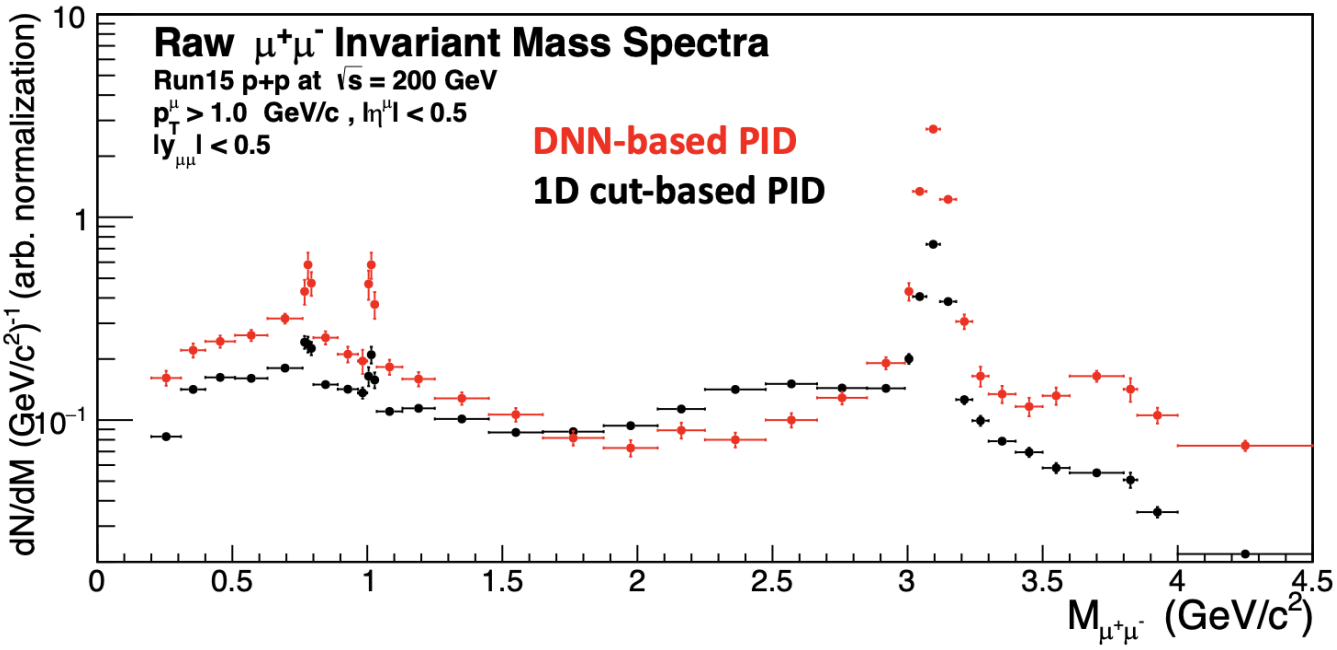
Example 1: Nuclear structure (Hatree-Fock-Bogolyubov)

https://doi.org/10.1103/PhysRevLett.124.162502: "deep neural networks is capable of predicting the ground-state and excited energies of more than 1800 atomic nuclei with an accuracy akin to the one achieved by state-of-the-art nuclear energy density functionals and with significantly less computational cost"



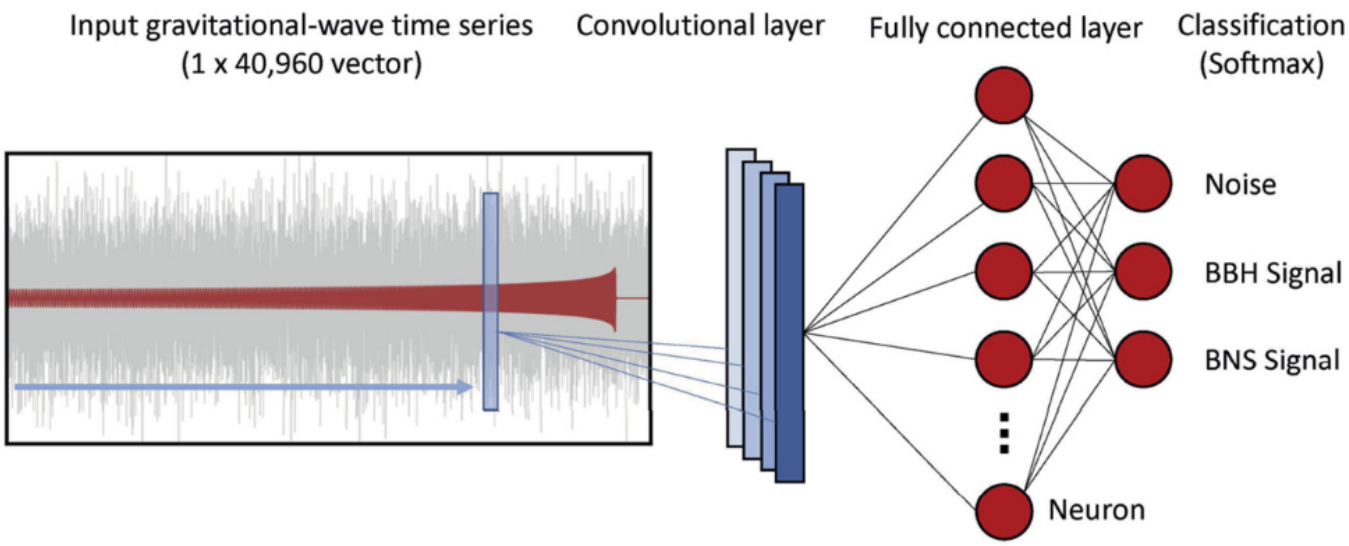
Example 2: Muon identification at STAR

Muon identification with deep NN with the STAR muon telescope detector
QM2019: 10.1016/j.nuclphysa.2018.10.036



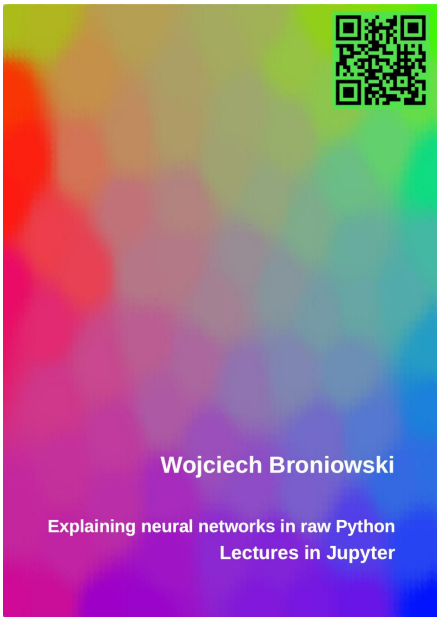
Example 3: Gravitational waves from binary merger

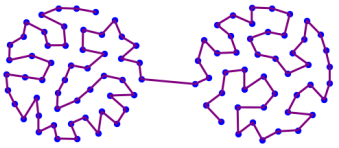
https://doi.org/10.1016/j.physletb.2020.135330



Mini-review of ANN

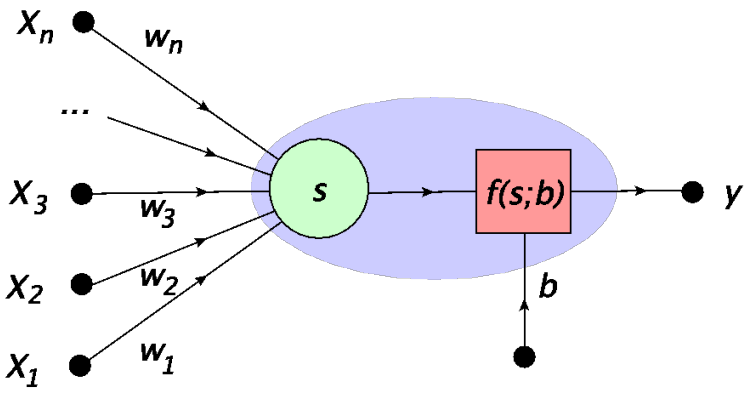
Simplest Pythonic introduction ever!





Executable Jupyter Book

McCulloch-Pitts neuron (MCP), 1943

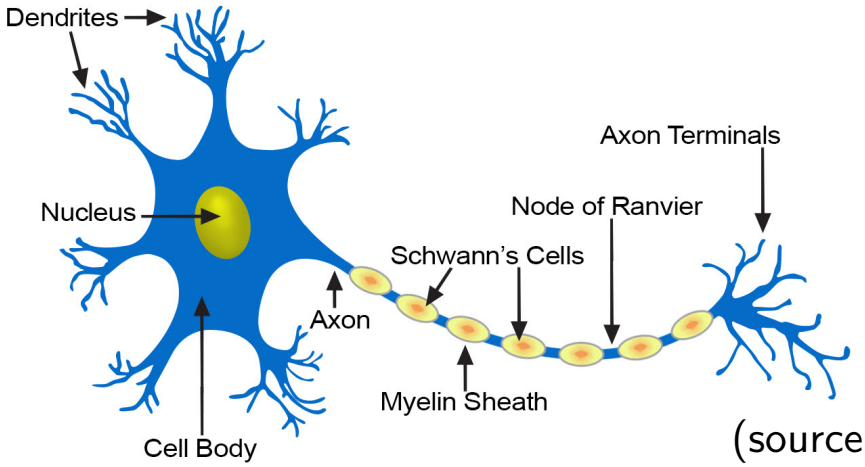


$$s = \sum_i x_i w_i$$

x_i – inputs
w_i – weights (hyperparameters)
s – signal (weighed sum of inputs)
f – activation function
b – bias (threshold)
y – output

- Fires, if the signal is sufficiently strong, $s > b$
- Mimics (approximately) the biological neuron

Structure of a Typical Neuron



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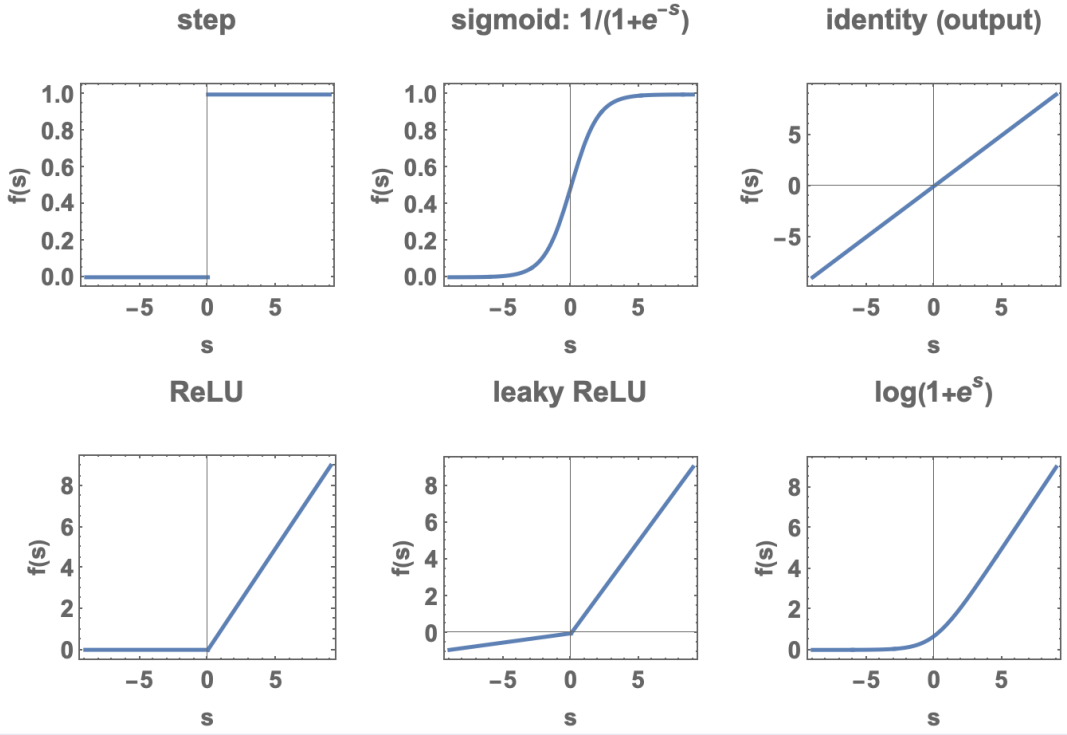
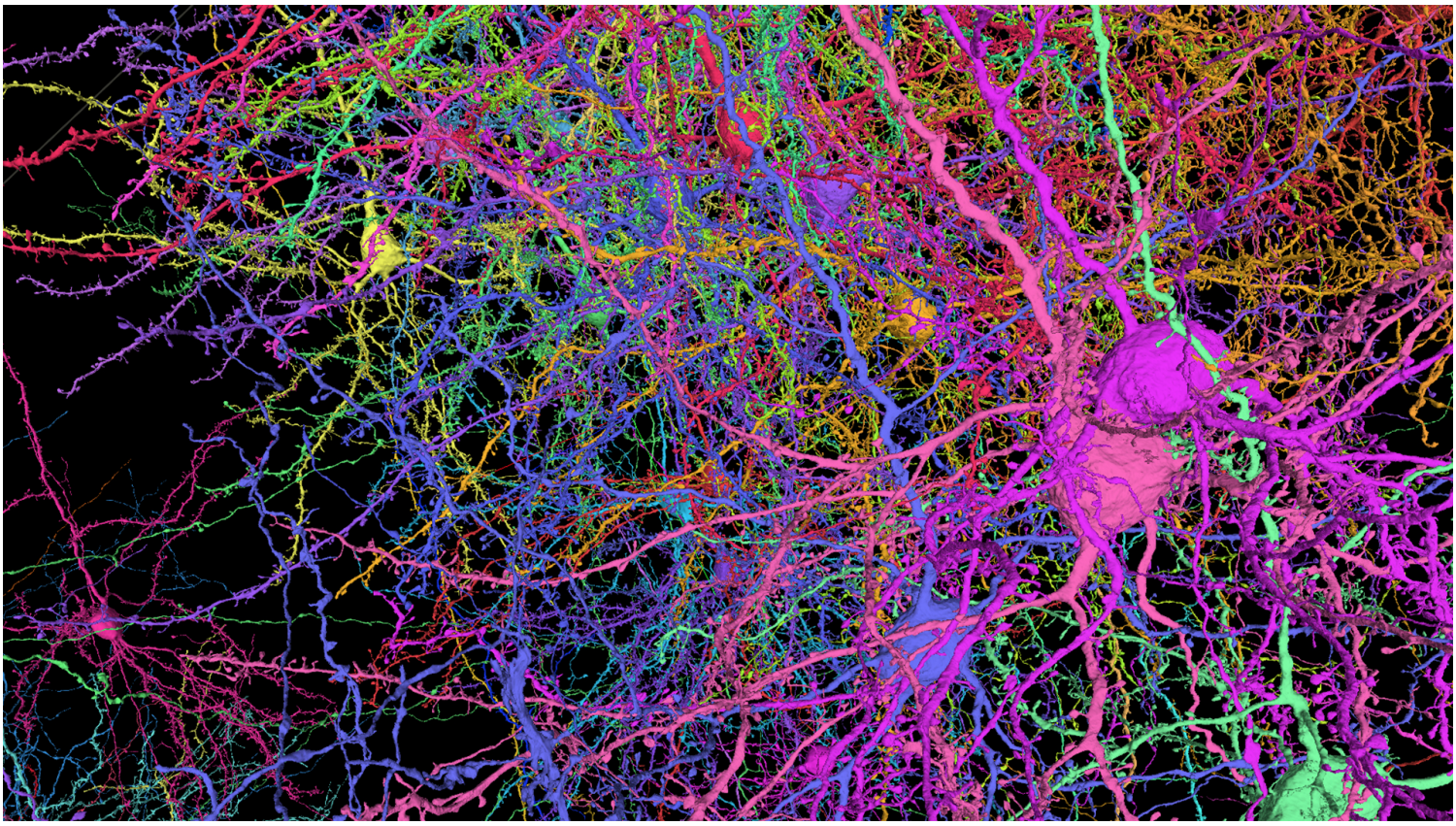
Activation functions



Nonlinearity absolutely essential!

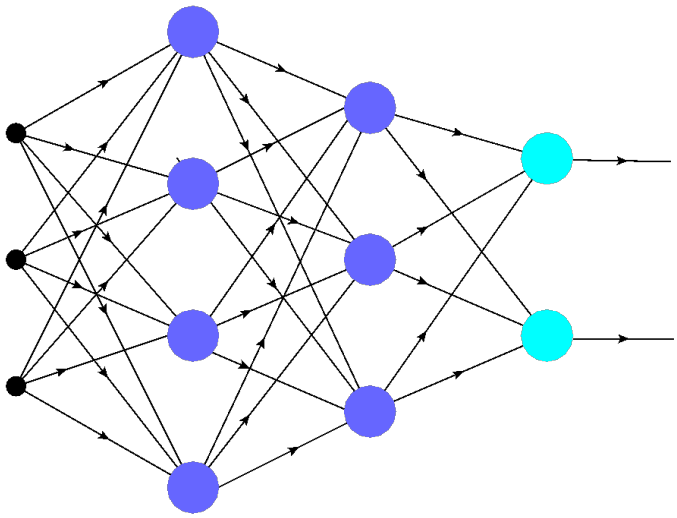
Without nonlinearity just matrix multiplication! Nonlinearity → dissipative characteristics, attractor-based dynamics, allows NN to better catch non-trivial correlations

1mm^3 of the mouse brain



(MICrONS)

Artificial neural network (ANN)



input output neuron layer

intermediate neuron layers (≥ 0)

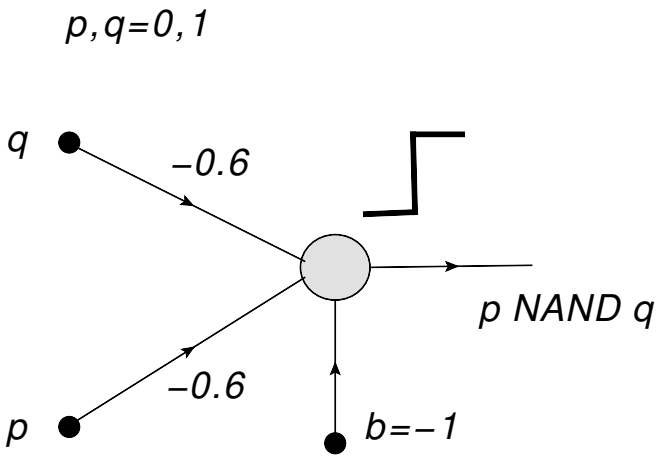
here:

- feed-forward network
- fully connected
- 2 intermediate neuron layers

- Edges carry weights w_{ij} (many hyperparameters)

Logical networks

With proper selection of weights, the MCP neuron becomes a logical gate



- Completeness of NAND (or NOR) gates: any logical network (boolean function) can be constructed as a feed-forward (multilayer) ANN
- → Completeness of ANN in the Church-Turing sense: any computation possible
- Fuzzy logic with smooth step functions

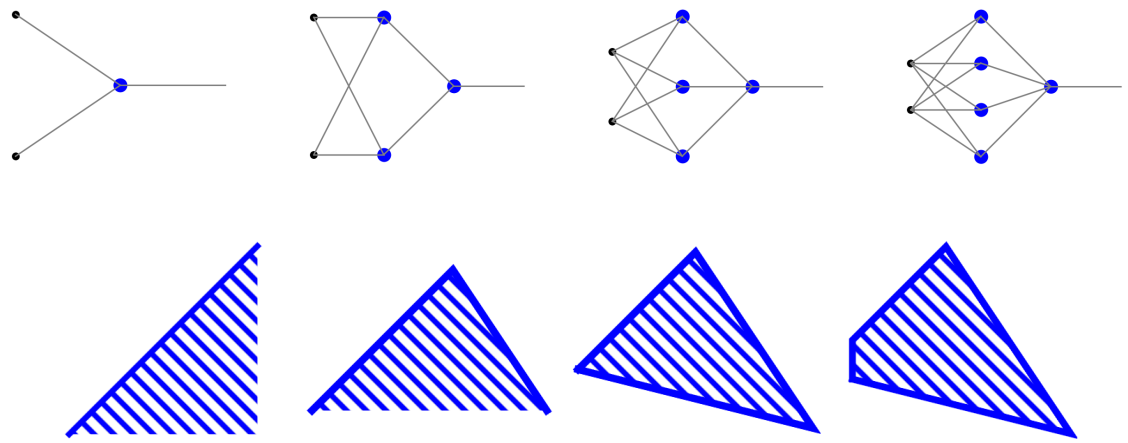
Inequality conditions from MCP neurons

Example in 2 dimensions: (Binary classifier)

$x_1 w_1 + x_2 w_2 > b$ – half-plane condition (in more dim. hyper half-space)

linearly separable sets

first neuron layer – half-plane conditions, second (output) – multiple conjunction



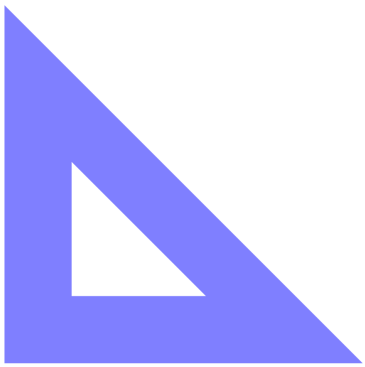
Any convex polytope region can be classified with a 2-neuron layer ANN

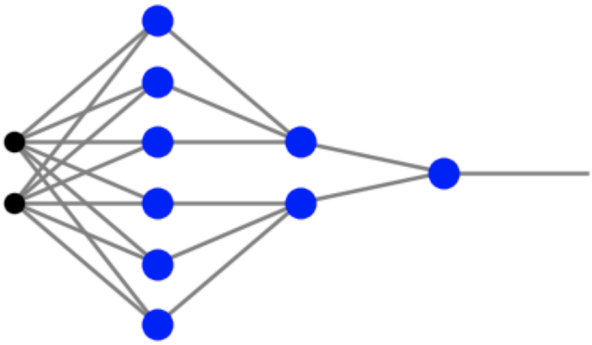
More layers

half-plane conditions

p – in big triangle
q – in small triangle

$$p \wedge \sim q$$





Any polytope region in any number of dimensions can be classified with an at least 3-neuron layer ANN. The number of needed neurons reflects the complexity of the region

Setting hyperparameters by hand

In our example one can easily (from geometry) infer the weights and biases *a priori*. The geometric conditions $\rightarrow$ the first neuron layer:

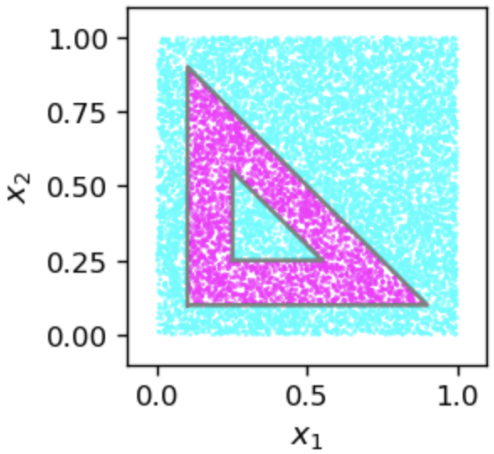
α	inequality condition	b^1_α	$w^1_{1\alpha}$	$w^1_{2\alpha}$	
1	$x_1 > 0.1$	0.1	1	0	
2	$x_2 > 0.1$	0.1	0	1	big triangle
3	$x_1 + x_2 < 1$	-1	-1	-1	
4	$x_1 > 0.25$	0.25	1	0	
5	$x_2 > 0.25$	0.25	0	1	small triangle
6	$x_1 + x_2 < 0.8$	-0.8	-1	-1	

Conjunctions in the second neuron layer:

α	b^2_α	$w^2_{1\alpha}$	$w^2_{2\alpha}$	$w^2_{3\alpha}$	$w^2_{4\alpha}$	$w^2_{5\alpha}$	$w^2_{6\alpha}$
1	1	0.4	0.4	0.4	0	0	0
2	1	0	0	0	0.4	0.4	0.4

Finally, in the output layer we need the $p \wedge \sim q$ gate:

α	b^3_α	$w^3_{1\alpha}$	$w^3_{2\alpha}$
1	1	1.2	-0.6



This is not what we want to do in ML!

Concept of learning

Learning

A suitable algorithm sets the hyperparameters based on the data alone, "automatically", without a direct programers interference!

- Supervised learning:
  Data points have features and labels
  Example: features – coordinates, labels – belongs to an area,
  i.e., has a property (1) or not (0)
  Training and test data samples, loss function
- Unsupervised learning:
  No labels, looking for correlations/clusterization in the data
- Semi-supervised, online, ...
- Reinforcement learning (not covered):
  Agent actions to maximize reward, interaction with the environment
  (robotics)

Back-propagation [Bryson, Ho, 1969]

Goal: minimize the loss function between (feed-forward) NN answers and labels

Notation: $x_0^j = 1$, $w_{0m}^j = -b_m^j$, $p \in$ training sample

$$E(\{w\}) = \sum_p \sum_{\alpha_l=1}^{n_l} \left[y_{o,\alpha_l}(\{w\}) - y_{t,\alpha_l} \right]^2 = \sum_p \sum_{\alpha_l=1}^{n_l}$$

$$\left[f\left(\sum_{\alpha_{l-1}=1}^{n_{l-1}} f\left(\dots f\left(\sum_{\alpha_0=0}^{n_0} x_{\alpha_0}^0 w_{\alpha_0\alpha_1}^1 \right) w_{\alpha_1\alpha_2}^2 + x_0^1 w_{0\alpha_2}^2 \dots \right) w_{\alpha_{l-1}\alpha_l}^l + x_0^{l-1} w_{0\alpha_l}^l \right) - y_{t,\alpha_l} \right]^2$$

Chain rule, steepest gradient (differentiability of f) $\rightarrow$

Backprop

$$D_{\alpha_l}^l = 2(y_{o,\alpha_l} - y_{t,\alpha_l})\, f'(s_{\alpha_l}^l)$$

$$D_{\alpha_j}^j = \sum_{\alpha_{j+1}} D_{\alpha_{j+1}}^{j+1}\, w_{\alpha_j\alpha_{j+1}}^{j+1}\, f'(s_{\alpha_j}^j), \qquad j = l-1, l-2, \dots, 1$$

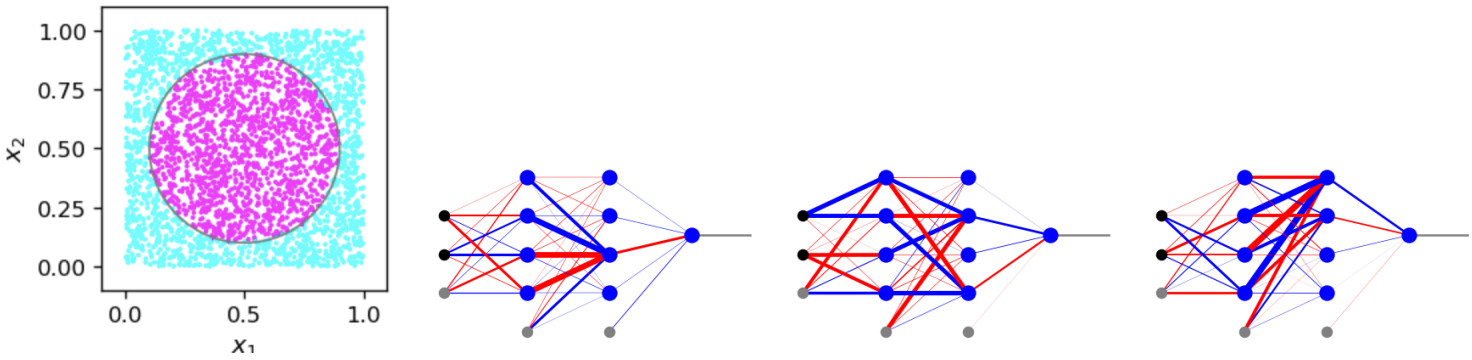
$$w_{\alpha_{j-1}\alpha_j}^j \rightarrow w_{\alpha_{j-1}\alpha_j}^j - \varepsilon x_{\alpha_{j-1}}^{j-1} D_{\alpha_j}^j$$

(recursion goes backwards)

Example, local minima

- Methodology: the program "writes itself" by finding the parameters via minimization of the loss function
- Black box - different paradigm, works, many local minima are fine!

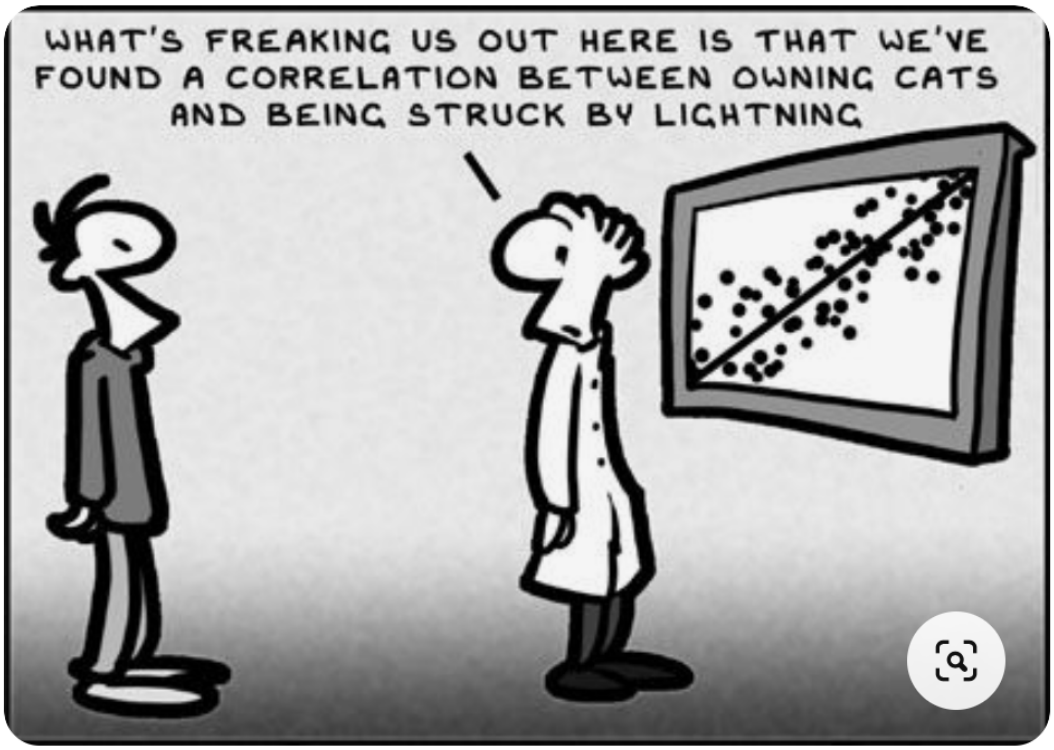
Example:



ANN does not have any idea about geometry!

Learn on mistakes!

Regression


WHAT'S FREAKING US OUT HERE IS THAT WE'VE FOUND A CORRELATION BETWEEN OWNING CATS AND BEING STRUCK BY LIGHTNING

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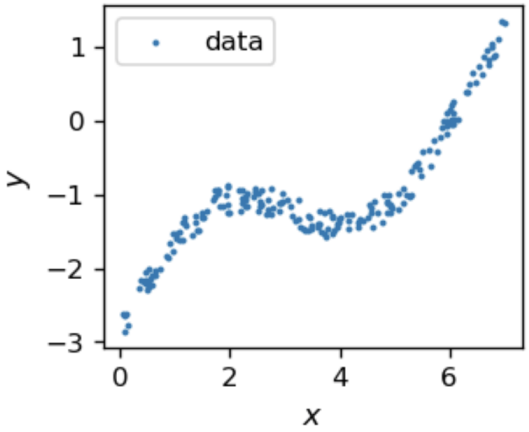
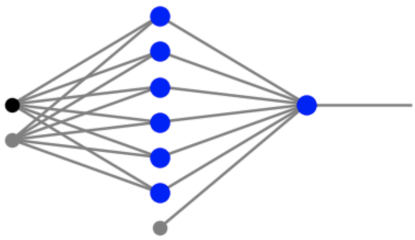
Regression

We want to represent (interpolate) some noisy experimental data



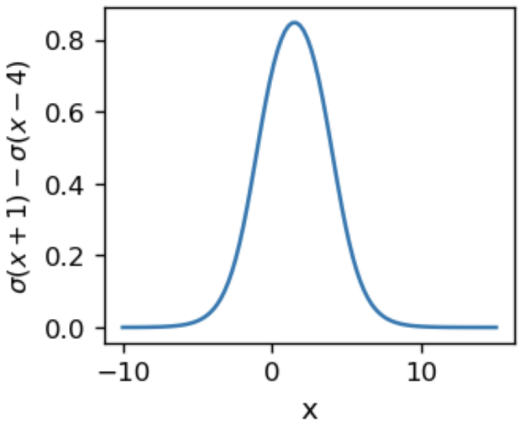


Instead of using a specific function (e.g. polynomial) we use ANN. The intermediate layer has sigmoid activation functions, but the last layer has an identity activation to cover the values range

x - feature, y - label

Sigmoid basis

To see that a basis of sigmoid can be used to represent a function, consider a difference of two sigmoids with different thresholds:



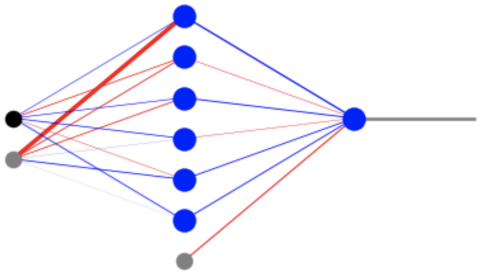
We can "fill" any function with such bell-shaped functions, or more generally with (sufficiently many) sigmoids

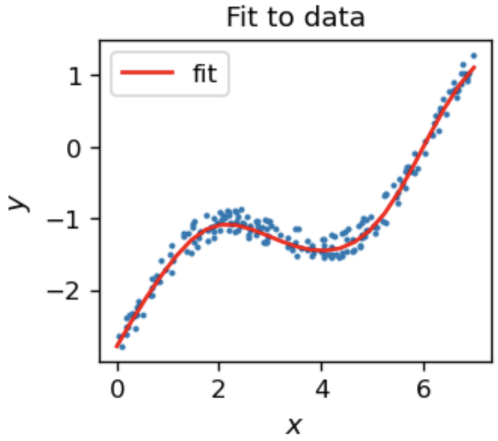
The first neuron layer forms the basis, the second provides "amplitudes"

The loss function = least squares, or other choices

Training regression

Use backprop to train (19 parameters!)

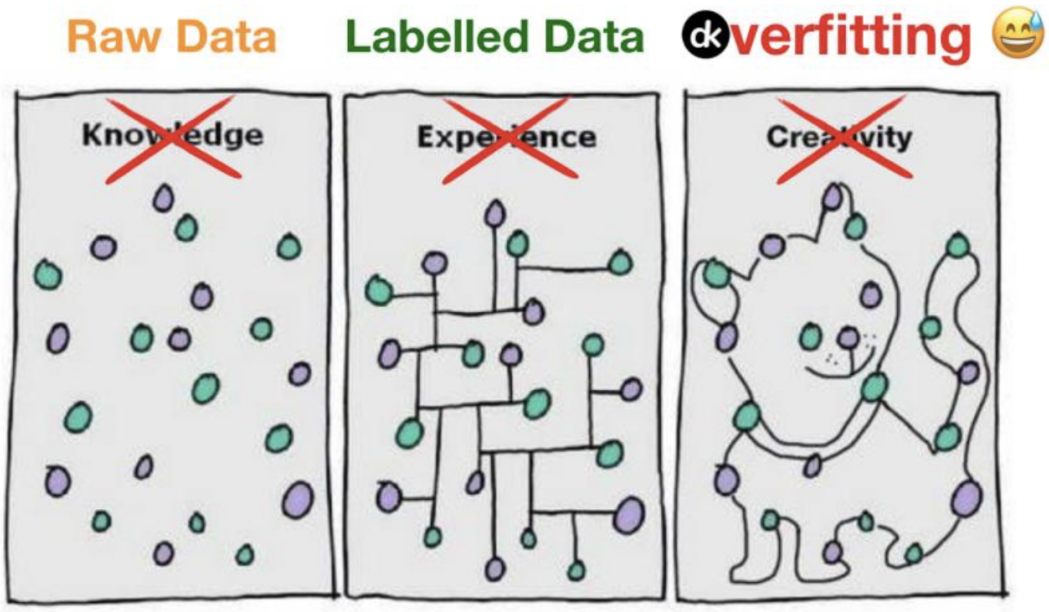




- $\Delta E_{test} \geq \Delta E_{train}$, possible overfitting problem (regularization), optimum number of neurons
- Adaptiveness

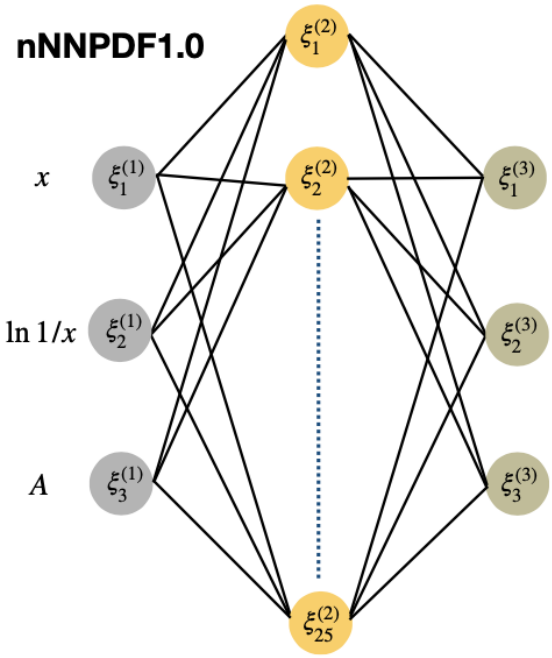
To interpolate in 2 or more dim. one needs ANNs with at least 3 neuron layers

A pair of neurons in the first neuron layer can form a hump in x_1, another pair – in x_2, and so on for the remaining x_i. Conjunction of these humps in the second neuron layer yields a "basis" function focused in a region around a certain point in the n-dimensional input space. The last layer provides amplitudes. [cf. Müller, Reinhardt, Strickland]


Raw Data
Labelled Data
verfitting
Knowledge
Experience
Creativity

(source)

Example: NNPDF



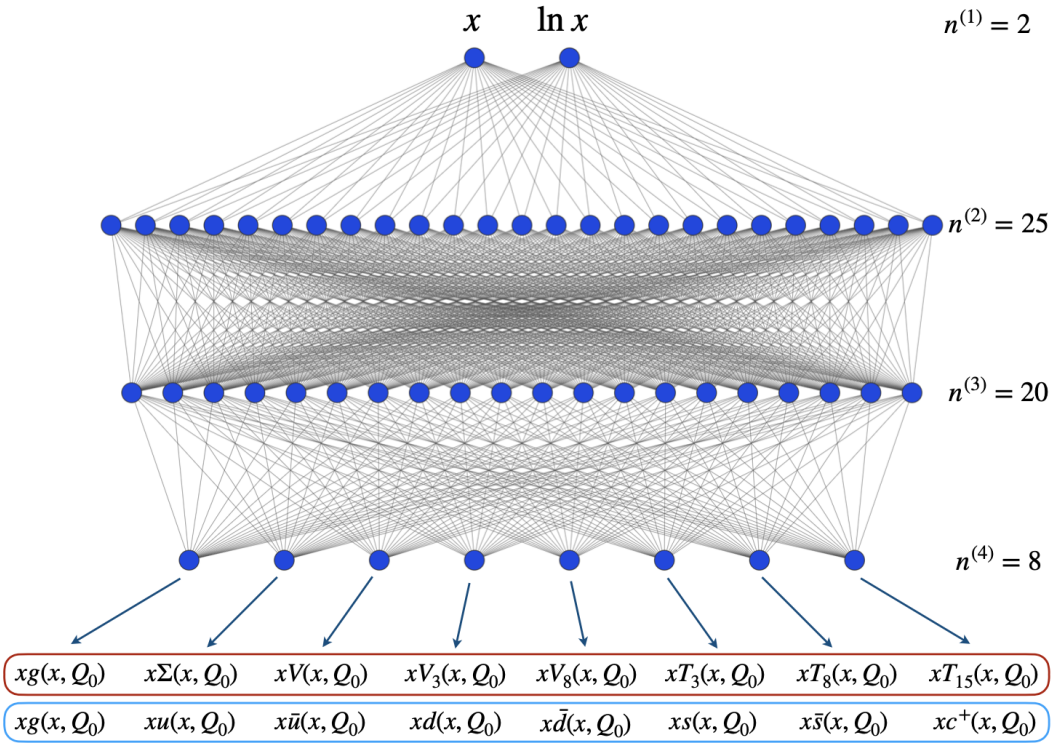
$$g(x, Q_0, A) = B_g x^{-\alpha_g}(1-x)^{\beta_g}\,\xi_1^{(3)}$$

$$\Sigma(x, Q_0, A) = x^{-\alpha_\Sigma}(1-x)^{\beta_\Sigma}\,\xi_2^{(3)}$$

$$T_8(x, Q_0, A) = x^{-\alpha_{T_8}}(1-x)^{\beta_{T_8}}\,\xi_3^{(3)}$$

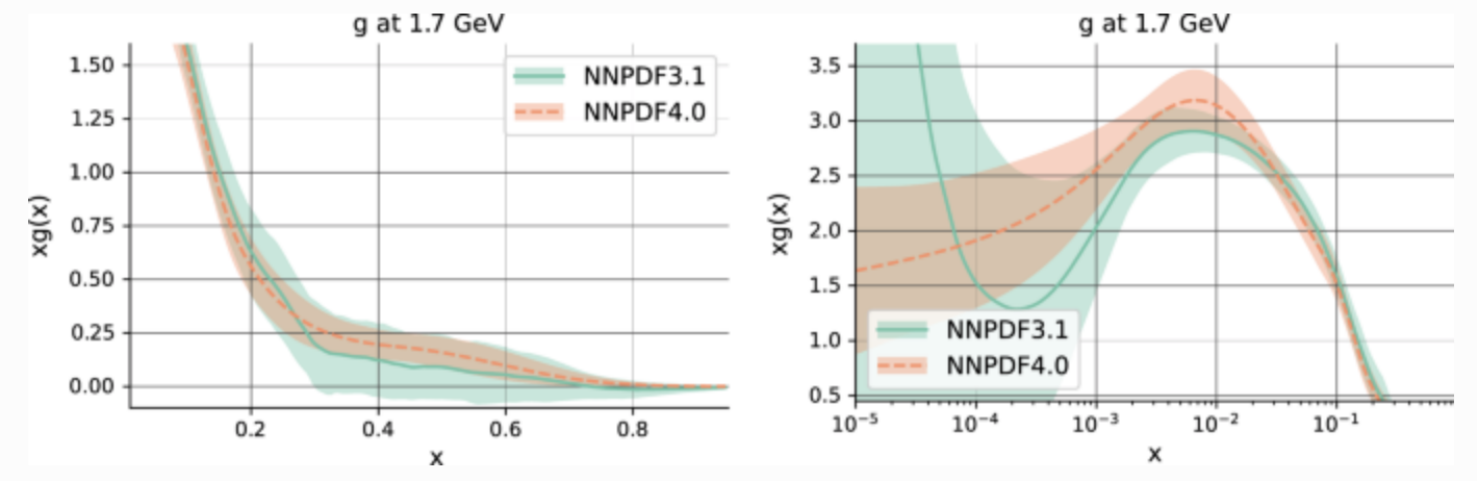
[NNPDF Collaboration, Eur. Phys. J. C (2019) 79:471]

NNPDF 4



[arXiv:2109.02653]

Sample result: glue from NNPDF

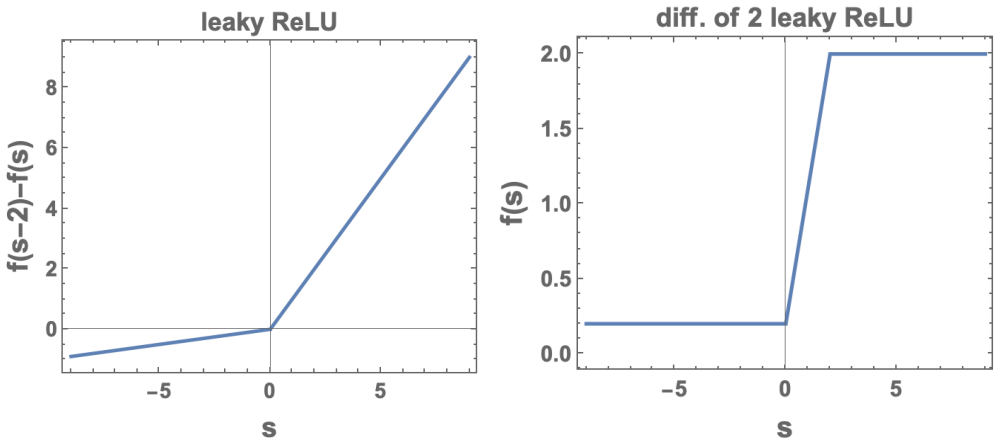


https://doi.org/10.1140/epjc/s10052-021-09863-6

Going deep

Better activation functions, limited connections

Rectification: ReLU, leaky ReLU ... – also form a basis

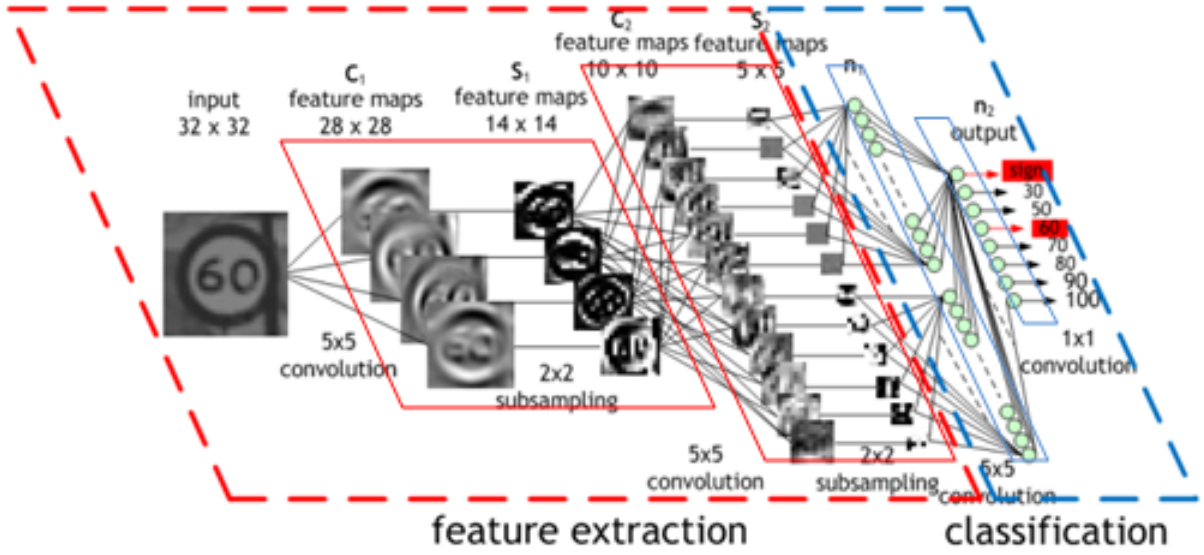


Especially needed for deep ANN – no dead neuron problem

Less connections limit the dimensionality curse

Convolutional NN (CNN)

Limited (local) connectiveness (as in our biological vision system), action of various filters producing feature maps, run on GPU



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Composing ANNs as "Lego blocks", backprop, partially-trained networks

Local features are extracted and correlated, longer and longer range

CNN for gravitational waves classifier from intro

Table 1
Architecture of the deep neural network. The architecture of the deep one-dimensional convolutional network consist of input layer, followed by 19 hidden layers, and output *softmax* layer. The size of the network is about 83 MB.

	Layer	Array Type	Size
	Input	Vector	40960
1	Reshape	Matrix	1×40960
2	Convolution (1D)	Matrix	32×40945
3	Pooling	Matrix	32×10236
4	ReLU	Matrix	32×10236
5	Convolution (1D)	Matrix	64×10229
6	Pooling	Matrix	64×2557
7	ReLU	Matrix	64×2557
8	Convolution (1D)	Matrix	128×2550
9	Pooling	Matrix	128×637
10	ReLU	Matrix	128×637
11	Convolution (1D)	Matrix	256×623
12	Pooling	Matrix	256×155
13	ReLU	Matrix	256×155
14	Flatten	Vector	39680
15	Dense Layer	Vector	128
16	ReLU	Vector	128
17	Dense Layer	Vector	64
18	ReLU	Vector	64
19	Dense Layer	Vector	3
	Output (Softmax)	Vector	3

(taught on 100000 augmented data)

Modern ML

Some thoughts from a review by Matthiew D. Schwartz (Harvard)

https://arxiv.org/abs/2103.12226

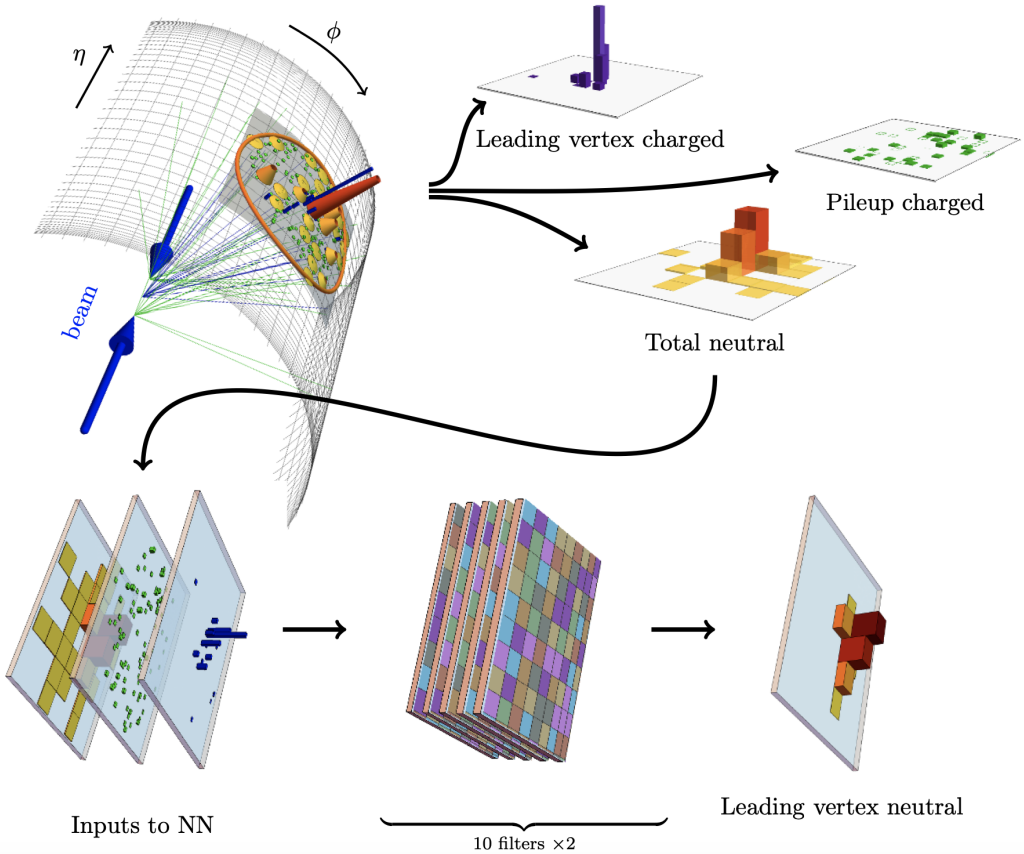
The modern approach is to feed raw, minimally-processed data, rather than high-level physically-motivated variables, into a deep neural network. The network is then free to find what it thinks is most valuable in the data

In the past, physicists ... would devote their efforts to understanding signatures of particular particles or processes from first-principles: why should a stream of pions coming from a W boson decay look different than a stream coming from an energetic gluon? Now we simply simulate the events, and let neural network learn to tell the two samples apart. Even a relatively simple dense network with 10 lines of python code can blow the traditional discriminants out of the water. Progress ... has come from taking algorithms masterly engineered for other applications, like convolutional neural networks, and shoehorning the collider data into a format that these algorithms can process. Unfortunately doing so can inhibit the extraction of any kind of physical understanding from the network itself

While it is easy to train an algorithm to reproduce the majority of a model's output, it is much harder to train it to reproduce every nuance of the model

Example: pile-up mitigation

Pile-up mitigation with machine learning (PUMML) at the LHC (Pythia)
https://doi.org/10.1007/JHEP12(2017)051



Other developments

Detector simulation with Generative Adversarial NN (GAN)

GAN uses one NN to generate (noisy) data samples, and a second *adversary* NN (trained on a training sample) to assess if the generated data are OK

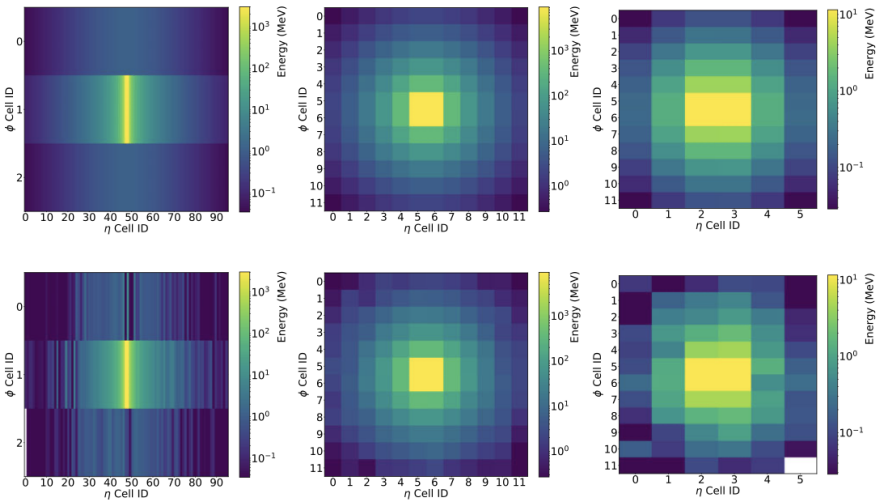


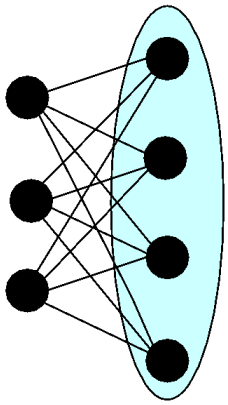
FIG. 6. Average e^+ GEANT4 shower (top), and average e^+ CALOGAN shower (bottom), with progressive calorimeter depth (left to right).

Orders of magnitude faster!

10.1103/PhysRevD.97.014021

Other architectures

- Recurrent NN (RNN) – long chains of data (jet classification)
- Auto-encoders (simulating data)
- Hopfield, Boltzmann, Helmholtz networks, restricted Boltzmann machine



RBM: visible nodes – two-way communication – hidden nodes

memory

Physics-informed NN (PINN)

Include physics information in the architecture and/or loss function (symmetries, constraints, physics laws)

$\rightarrow$ learn (partial) differential equations with boundary/initial conditions

DeepXDE

Lu, Meng, Mao, Karniadakis https://epubs.siam.org/doi/pdf/10.1137/19M1274067

Karniadakis et al. https://www.nature.com/articles/s42254-021-00314-5

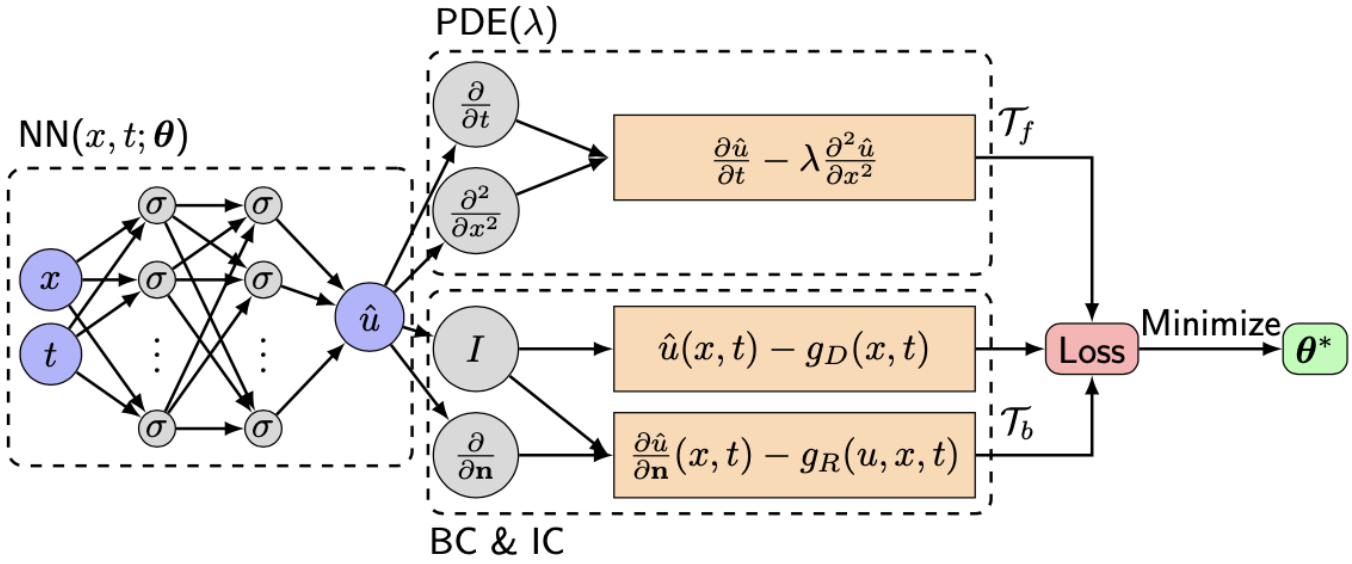


FIG. 1. *Schematic of a PINN for solving the diffusion equation* $\frac{\partial u}{\partial t} = \lambda \frac{\partial^2 u}{\partial x^2}$ *with mixed boundary conditions (BC)* $u(x,t) = g_D(x,t)$ *on* $\Gamma_D \subset \partial\Omega$ *and* $\frac{\partial u}{\partial \mathbf{n}}(x,t) = g_R(u,x,t)$ *on* $\Gamma_R \subset \partial\Omega$. *The initial condition (IC) is treated as a special type of boundary conditions.* $\mathcal{T}_f$ *and* $\mathcal{T}_b$ *denote the two sets of residual points for the equation and BC/IC.*

DeepXDE

Lu, Meng, Mao, Karniadakis https://epubs.siam.org/doi/pdf/10.1137/19M1274067
Karniadakis et al. https://www.nature.com/articles/s42254-021-00314-5

Laplace eqn.

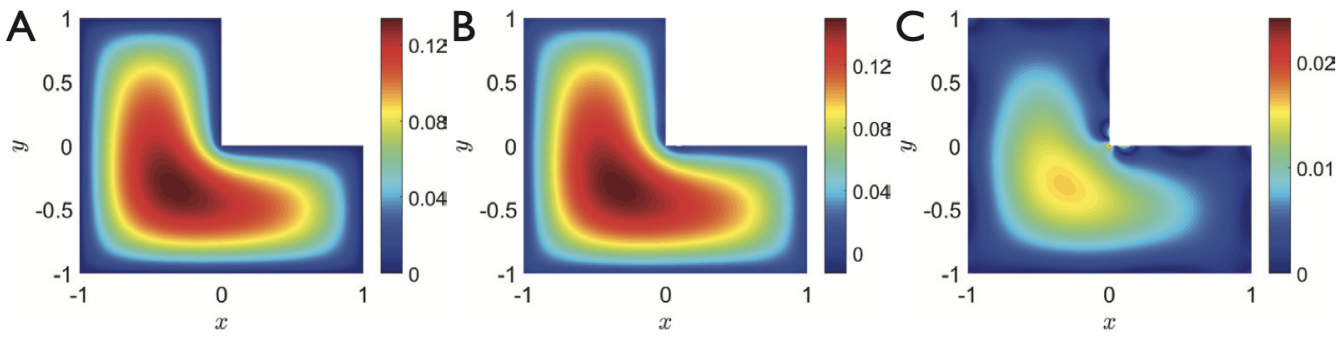


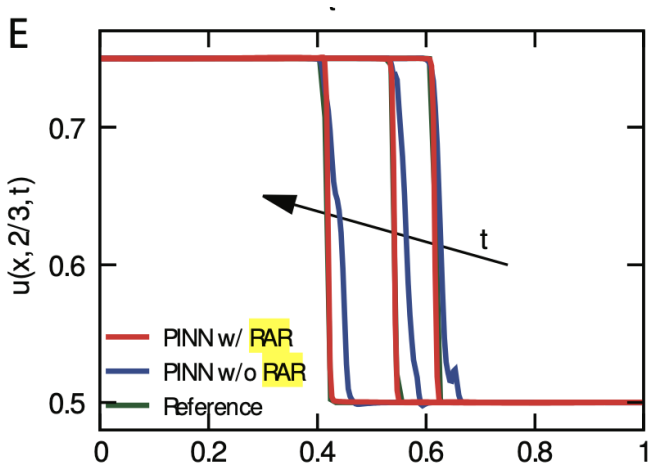
Fig. 7 *Example in subsection 4.1. Comparison of the PINN solution with the solution obtained by using the spectral element method (SEM).* (A) *The SEM solution* u_{SEM}, (B) *the PINN solution* u_{NN}, (C) *the absolute error* $|u_{SEM} - u_{NN}|$.

(SEM – conventional Spectral Element Method)

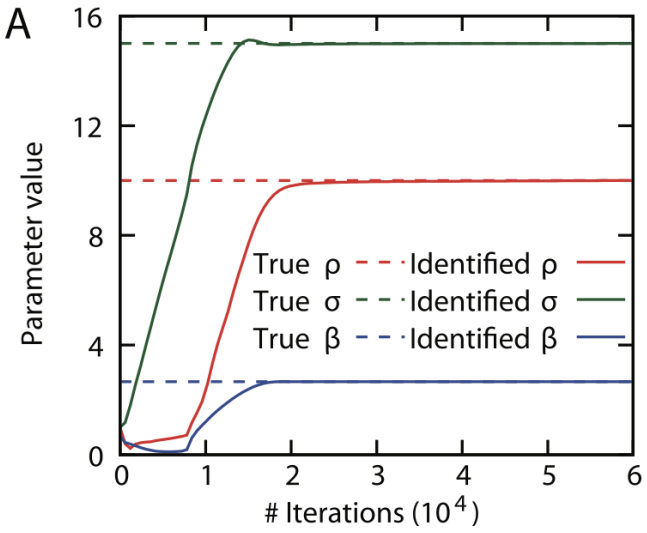
DeepXDE

Lu, Meng, Mao, Karniadakis https://epubs.siam.org/doi/pdf/10.1137/19M1274067
Karniadakis et al. https://www.nature.com/articles/s42254-021-00314-5

Burgers eqn. (shock waves)



Inverse problem of the Lorentz system



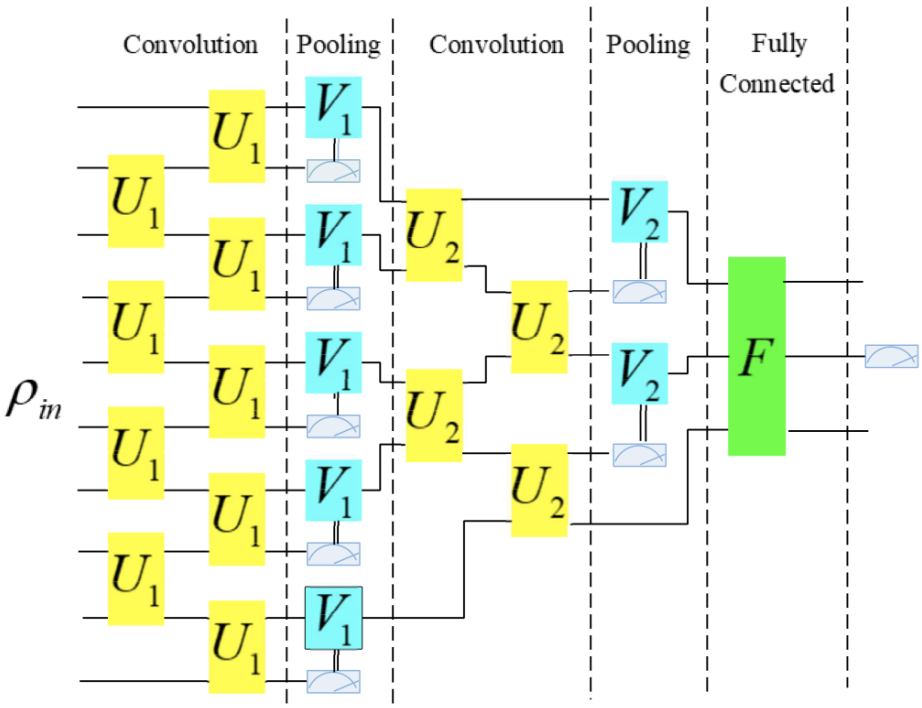
(RAR – adaptive improvement)

Further horizon: Quantum NN

(see the following lecture on Quantum technologies by Artur Ekert)

Stage of building algorithms

Review: https://arxiv.org/abs/2109.01840



convolutional, QCNN

Conclusions

Status of ML in physics

- Not long ago: novelty, curiosity, fashion $\rightarrow$ absolute standard (as Simpson's method, least squares, MC, ... before)
- In physics, ideas and methods largely transplanted from other fields
- Continuous improvements
- Active on-going development: architecture, Hopfield, Boltzmann... – interesting mathematically
- Sea of practical applications, "production phase" of simple to use libraries and dedicated codes
- Libraries and platforms: PyTorch, Keras/TensorFlow (Google), fastai (DL in Python), AutoML (Google cloud), Watson (IBM), SageMaker (Amazon), ...

We need to HL (human-learn) this stuff!

https://cerncourier.com/a/designing-an-ai-physicist

Jesse Thaler (MIT):

... We have gained trust in AI decisions through careful studies of "control regions" and painstaking numerical simulations. As our physics ambitions grow, however, we are using "deeper" networks with more layers and more complicated architectures, which are difficult to validate in the traditional way. And to mitigate 10 to 100-fold increases in computing costs, we are planning to fully integrate AI into data collection, simulation and analysis at the high-luminosity LHC ...

To build trust in AI, I believe we need to teach it to think like a physicist ...

If we don't exploit the full power of AI, we will not maximize the discovery potential of the LHC and other experiments

Thanks!