Are Computers Better than Physicists at Physics?

Applications & Limitations of Deep Learning in Physics

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Agenda

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- Deep learning in physics
  - Data challenges in physics research
  - How deep learning has helped so far
  - Limitations of deep learning for scientific research

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- **Introduction to deep learning**
  - **What is deep learning? What are neural networks?**
  - **What can neural networks do? How?**
- Deep learning in physics
  - Data challenges in physics research
  - How deep learning has helped so far
  - Limitations of deep learning for scientific research

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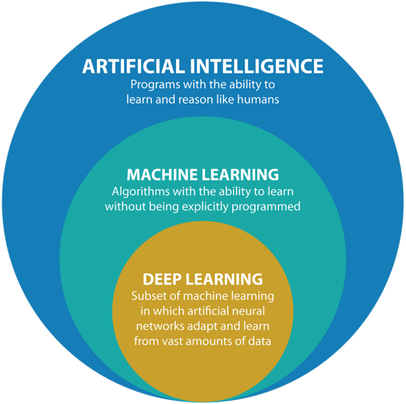
Definitions:

- AI: human-like, *intelligent* machines or programs
- ML: AI algorithms that *learn from data*

(This is still vague,
but don't worry! We will cover plenty examples later.)



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Deep learning (DL) is a specific set of ML algorithms that use artificial *neural networks* (NN's)

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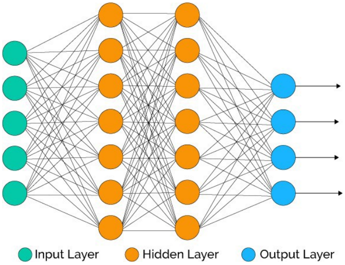
NN is a *function* whose computational graph mimics the structure of biological neural systems.

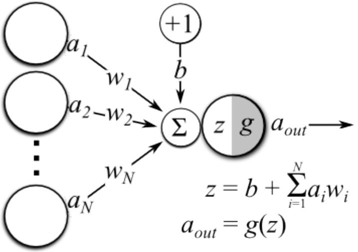
NN is defined by:

- Architecture (comp. graph)
- Parameters (connections)



Let us zoom into one hidden layer of a simple NN

M of



$$= M \text{ of } g\left(\sum_{i=1}^{N} w_i a_i + b\right)$$

$$= g\left(W\mathbf{a} + \mathbf{b}\right)$$

where $g : \mathbb{R} \to \mathbb{R}$ is called the *activation* function, W is the matrix of $M \times N$ *weights*, and $\mathbf{b}$ is the *bias*.

The activation function here is applied element-wise:

$$\mathbf{x} = [x_1, x_2, x_3, \ldots, x_N]$$
$$g(\mathbf{x}) = [g(x_1), g(x_2), g(x_3), \ldots, g(x_N)]$$

Universal Approximation Theorem

Sure... but so what? This is just a bunch of calculations.

Why are NN's so powerful?

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Universal Approximation Theorem

A single-hidden layer NN with sufficient nodes and a non-linear activation function can *approximate any function* with an arbitrary accuracy. NN's are *universal approximators*.

Caveats and details:

- A single-layer neural network defined by an activation function g and k hidden units $\mathcal{N}(g, k) : \mathbb{R}^{\text{in}} \rightarrow \mathbb{R}^{\text{out}}$ is dense in $L^p(\mu)$ for any finite measure μ
- The analytical details depend on properties of the activation function g
- Discussions & proofs mostly limited to continuous functions

Some references:

- *G. Cybenko*, "Approximation by Superpositions of a Sigmoidal Function" (1989) [1]
- *K. Hornik*, "Approximation Capabilities of Multilayer Feedforward Networks" (1991) [2]

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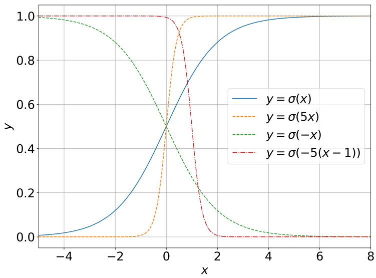
Visualizing Universal Approximation Theorem

Consider
a NN : $\mathbb{R} \to \mathbb{R}$ with the *sigmoid* activation: $\sigma(x) \equiv \frac{1}{1+e^{-x}}$.

$$\mathrm{NN}(x) = \sum_{i=1}^{k} w_i' \sigma(w_i x + b_i) + b'$$



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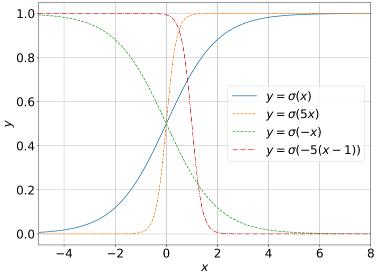
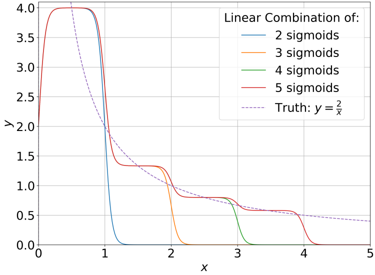
Each sigmoid (non-linearity) can approximate *a local change*

k sigmoids $\Rightarrow$
approximate at $\sim k$ points





To let the computers learn the right parameters to approximate a function, we use a set of *training dataset* and *loss function*

- Training dataset: $T = \{(x_i, y_i) | x_i \in X, y_i \in Y\}$
- Loss function: $\ell(\hat{y}, y)$ measures how *far* a prediction $\hat{y} = NN(x)$ is from the truth y

Backpropagation
How NN's learn

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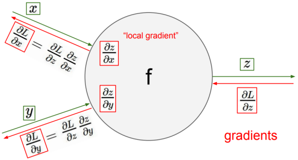
"Learning" is now an *optimization problem*; given T, find a set of NN params. that minimize $\ell_{\text{overall}} = \frac{1}{m} \sum_{i=1}^{m} \ell(\hat{y}_i, y_i)$.

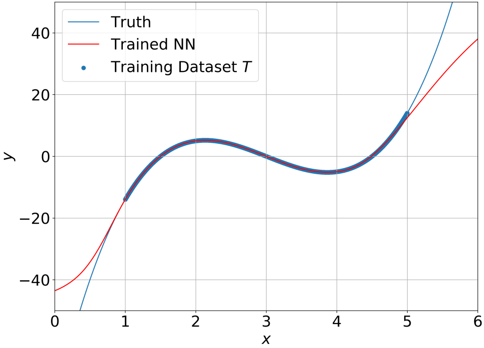


Use *chain rule of derivatives*:

$$\frac{\partial \ell_{\text{overall}}}{\partial h_j} = \frac{\partial \ell_{\text{overall}}}{\partial h_{j+1}} \times \frac{\partial h_{j+1}}{\partial h_j}$$

recursively backwards through the layers of NN

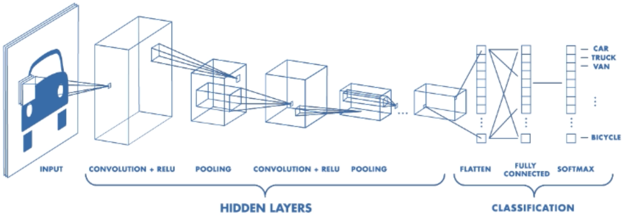
- NN: single hidden layer with $N_{\text{hidden}} = 100$ nodes, σ-activation
- $T = \{(x_i, y_i) | i = 1, \ldots, 50\text{k}, 1 \leq x_i \leq 5,$
$$y_i = 4x_i^3 - 36x_i^2 + 99x_i - 81\}$$
- Loss function: $\ell(\hat{y}, y) = |\hat{y} - y|$



Each edge in the computational graph is *not necessarily limited* to matrix multiplications

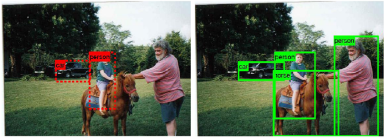
Convolutional Neural Network (CNN, ConvNet)

- Striding filters across different axes ($\sim$ convolution integral)
- Understands *positions / geometry*



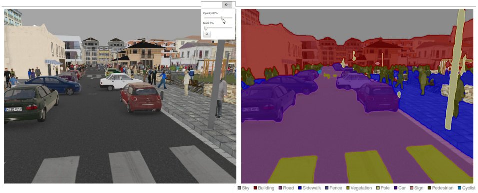
- Successes in image classification and other "vision" tasks

```
probability=0.569505, class=n02088364 beagle
probability=0.052795, class=n00452864 beagling
probability=0.039277, class=n02778669 ball
probability=0.017777, class=n02087122 hunting dog
probability=0.016321, class=n10611613 sleuth, sleuthhound
```



Detection
(classification + localization)

probability=0.692314, class=n02122948 kitten, kitty
probability=0.043846, class=n01323155 kit
probability=0.030001, class=n01318894 pet
probability=0.029692, class=n02122878 tabby, queen
probability=0.026972, class=n01322221 baby

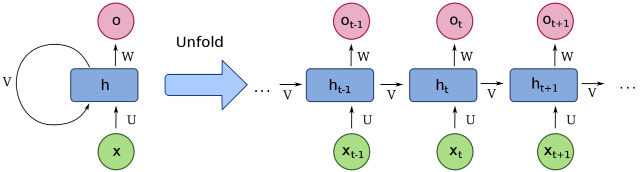


Segmentation (pixel-wise labeling)

Computational graphs *need not be one-directional*

Recurrent Neural Network (RNN)

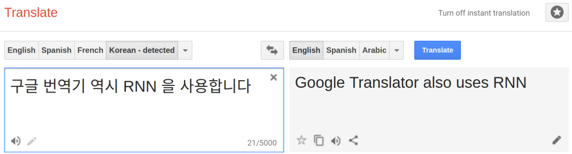
- Previous outputs are re-entered as inputs
- Can deal with sequences of variable lengths
- Understands *order and context* (has memory)

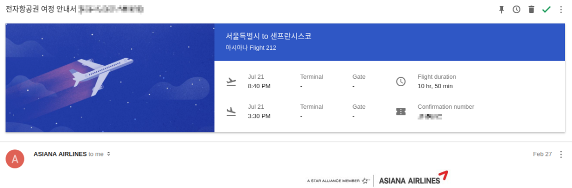


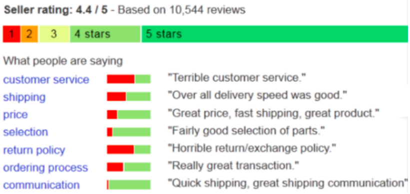
- Successes in natural language tasks (translation, semantic understanding) and time-sequential data (future prediction)

RNN: Successful Examples

Natural language processing, time-sequences



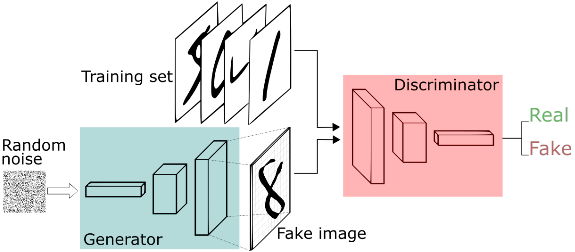




We can *combine multiple NN's* for more complicated tasks

Generative Adversarial Network (GAN)

- Two NN's, generator $\mathcal{G}$ and discriminator $\mathcal{D}$, compete



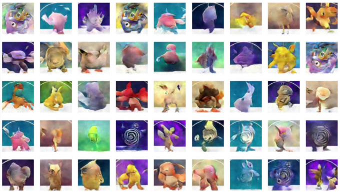
- $\mathcal{G}$ fools $\mathcal{D}$, $\mathcal{D}$ distinguishes real data v.s. generated data

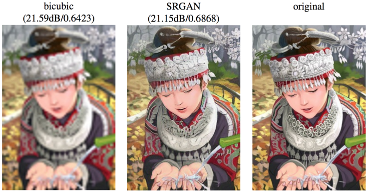
$$\min_{\mathcal{G}} \max_{\mathcal{D}} \mathbb{E}_{x \sim p_{\text{data}}(x)} \log \mathcal{D}(x) + \mathbb{E}_{z \sim p_z(z)} \log(1 - \mathcal{D}(\mathcal{G}(z)))$$

- Eventually, $\mathcal{G}$ becomes good at *generating realistic data*

GAN: Successful Examples

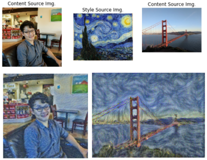
Generating ‘realistic‘ images





Grayscale, original, GAN-colored

a clock tower in the middle of a city
a brown horse standing on top of a dirt field
a brown horse standing in a field of grass
a group of people riding horses on a dirt road



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    - **How deep learning has helped so far**
    - **Limitations of deep learning for scientific research**

Applying All of These to Physics Research

Some data challenges we covered so far:

- Fitting a curve to points
- Dog or cat?
- Locating humans within image data
- Contextual understanding of a word within a sentence
- Generating and coloring realistic images

Applying All of These to Physics Research

Some data challenges we covered so far:
In physics research, these are:

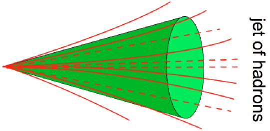
- Fitting a curve to points
  $\longmapsto$ *regression and parameter estimation*
- Dog or cat?
  $\longmapsto$ *Signal or noise? What kind of signal?*
- Locating humans within image data
  $\longmapsto$ *Finding signals within the detector*
- Contextual understanding of a word within a sentence
  $\longmapsto$ *Understanding time- (and other-) sequential data*
- Generating and coloring realistic images
  $\longmapsto$ *Simulating realistic physical processes*

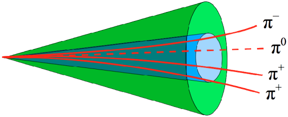
Data Challenges in Particle Physics

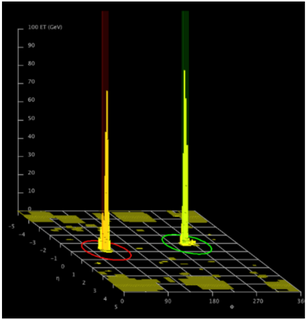
Some common data challenges
in *experimental particle physics*:

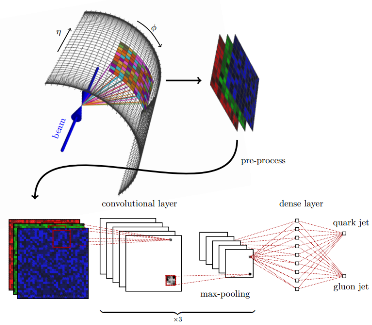
- Classification: identify the original particle from its decay product
- De-noising: remove noises from our detector responses
- Simulation: mimic collision events @ LHC

In particular, I will mainly
talk about *jet physics* today.









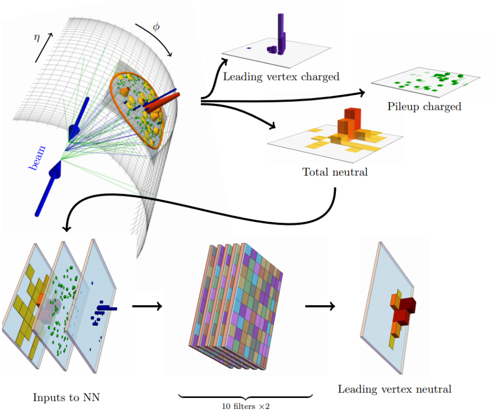
"Deep Learning in Color: towards Automated Quark/Gluon Jet Discrimination" (2017)

"Unroll" cylindrical detector (e.g. ATLAS, CMS) to form *jet images*

- Each pixel: direction of particle flight
- Color channel: features like energy

Use CNN's to *classify* these images.

Quark v.s. gluon, flavor-tagging, $W^{\pm}$ jets, merged objects



"Pileup Mitigation with Machine Learning (PUMML)" (2017)

Similar technique is used (by similar people) to *clean up* jet images and *only leave important variables*

Jet Simulation with GAN's

Monte Carlo simulation of jets @ LHC is *extremely* slow

$$\text{Theory} \to \text{Collision} \to \text{Decay (hadronization)}$$
$$\to \text{Detector simulation, electronics} \to \ldots \text{ and more}$$

... but GAN's could *accelerate* this!

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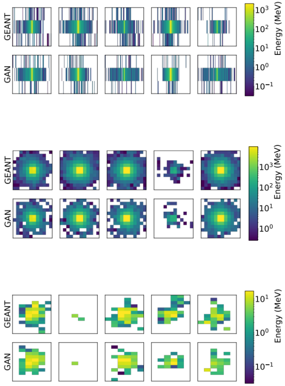
CaloGAN: Calorimeter GAN

- Generate full simulations of different physics processes
- Use energy deposits in 3 layers of calorimeters as "jet images"
- Train GAN's that generates similar jet images

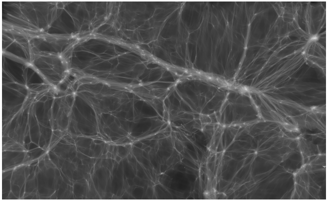


"CaloGAN" (2017)

Data Challenges in Cosmology

Common data challenges in *observational cosmology*:

- Parameter estimation: estimate physical parameters like Ω_m and Ω_Λ from cosmic mass distribution
- Simulation: cosmic-scale general-relativistic fluid dynamics simulation
- Image processing: extract core info. from telescope images



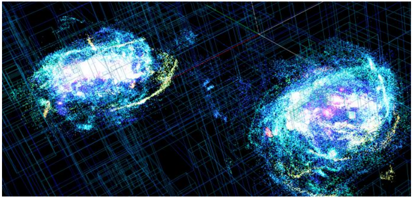
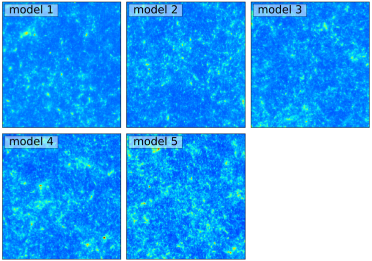


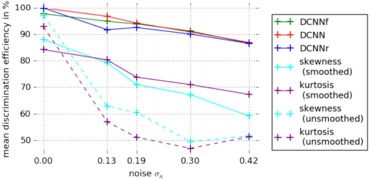
Image credit: Stanford/SLAC KIPAC
Computational Astrophysics & Dark Energy Groups

Some cosmological parameters are *degenerate*; different pair of params. give very *similar distributions* in the universe.

- Run full cosmo. simulations with a set of params
- Train CNN's on the simulated images

This approach can be generalized into a regression problem; predict the true parameters *hypothesis-free*

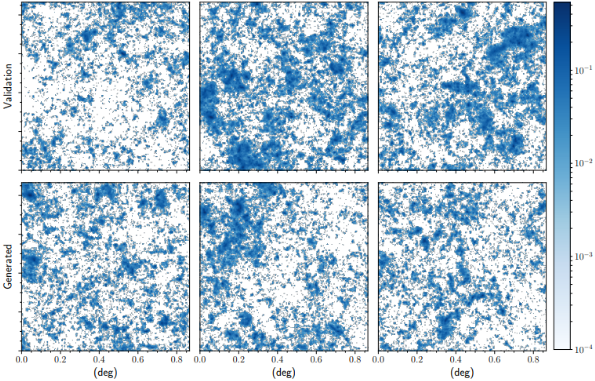




"Cosmological Model Discrimination with Deep Learning" (2017)

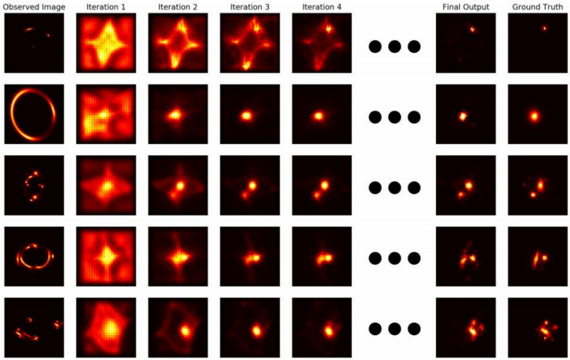
Cosmic-scale general-relativistic fluid dynamics simulation

... that already sounds intimidating, but we have GAN's!



"Creating Virtual Universes Using Generative Adversarial Networks" (2017)

Gravitational lenses distort images of galaxies and other astronomical objects, and inverting distortions is *extremely difficult*.



"MagNet: Deep Machine Vision for the Cosmic Dawn" (2018)

Limitations of Deep Learning in Scientific Research

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Deep learning algorithms seem amazing so far, but:

- Difficult to quantify their *uncertainties*
  - No clear rule for error propagation
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- They don't *understand* physics
  - In examples seen so far, they *hint at* previously unknown physics, at best
  - Physicists have not only data-driven, but also *subjective* measures of "good physics"

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  - In examples seen so far, they *hint at* previously unknown physics, at best
  - Physicists have not only data-driven, but also *subjective* measures of "good physics"
- There are *unquantifiable* physics problems to solve
  - Hierarchy problem, naturalness problem
  - Looking for "elegant" theories

Thank you for your attention!

and I'm happy to take any questions now or later :)

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