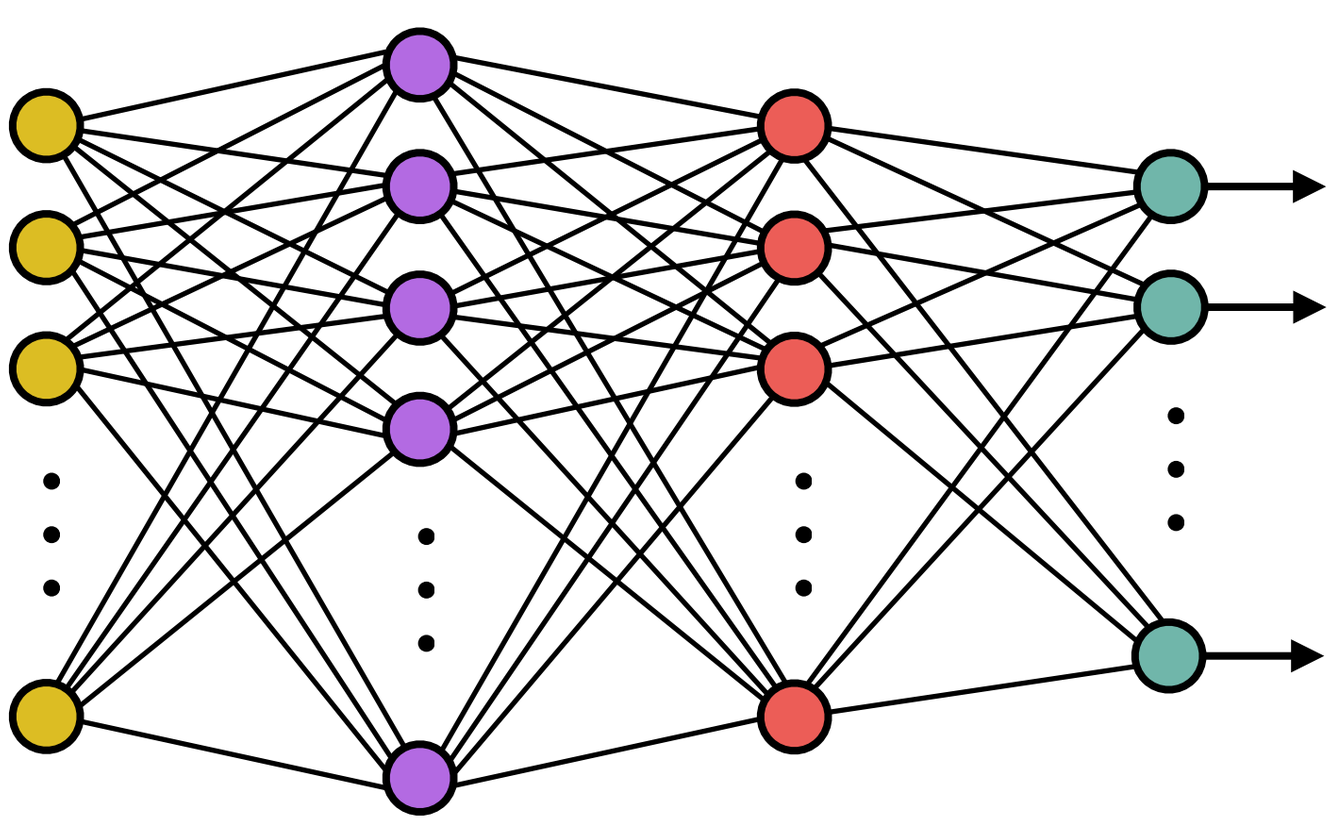
Introduction to Machine Learning

Lauren Hayward

October 29, 2019



Computational Tutorial Series

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Machine learning popularity

Interest over time

Google Trends

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What is machine learning?

“Machine learning is a field of computer science that uses statistical techniques to give computer systems the ability to "learn" (i.e., progressively improve performance on a specific task) with data, without being explicitly programmed.”

https://en.wikipedia.org

“[Machine learning] is about finding out regularities in data and making use of them for fun and profit.”

L.-G. Liu, S.-H. Li and L. Wang, http://wangleiphy.github.io

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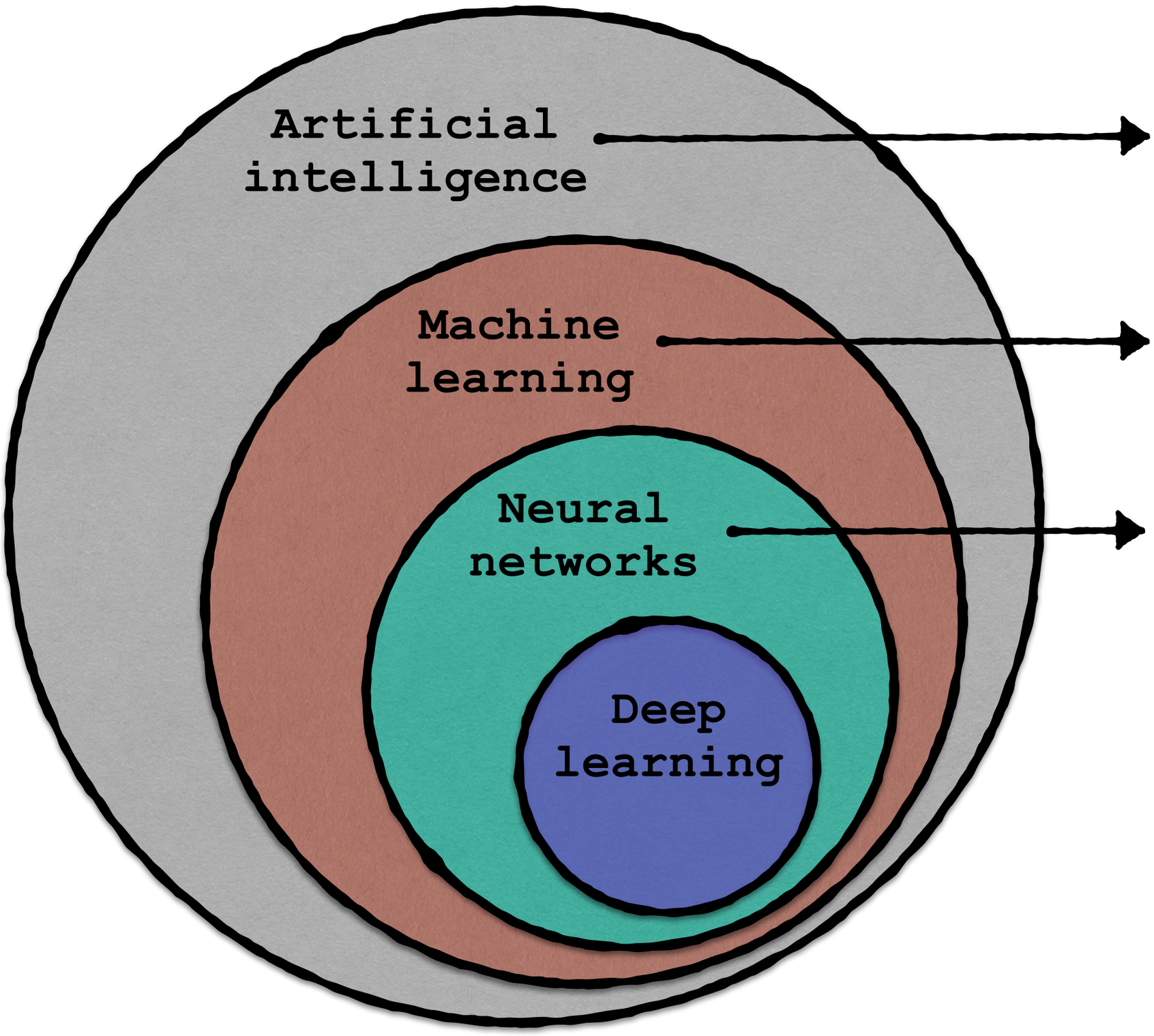
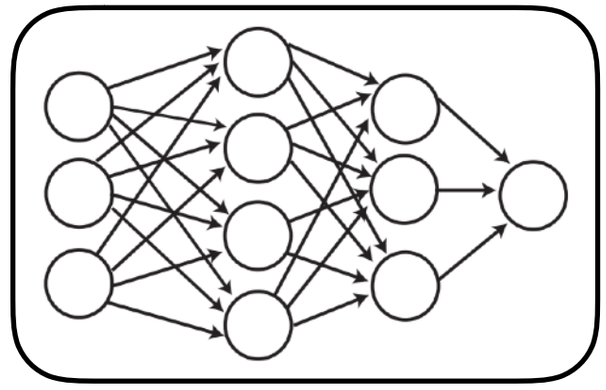


Computers that can mimic intelligent human behaviour

Computers that are programmed to learn (without being given explicit rules)



arXiv:1803.08823

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Image classification

ImageNet Classification with Deep Convolutional Neural Networks

Alex Krizhevsky
University of Toronto
kriz@cs.utoronto.ca

Ilya Sutskever
University of Toronto
ilya@cs.utoronto.ca

Geoffrey E. Hinton
University of Toronto
hinton@cs.utoronto.ca

Abstract

We trained a large, deep convolutional neural network to classify the 1.2 million high-resolution images in the ImageNet LSVRC-2010 contest into the 1000 different classes. On the test data, we achieved top-1 and top-5 error rates of 37.5% and 17.0% which is considerably better than the previous state-of-the-art. The neural network, which has 60 million parameters and 650,000 neurons, consists of five convolutional layers, some of which are followed by max-pooling layers, and three fully-connected layers with a final 1000-way softmax. To make training faster, we used non-saturating neurons and a very efficient GPU implementation of the convolution operation. To reduce overfitting in the fully-connected layers we employed a recently-developed regularization method called "dropout" that proved to be very effective. We also entered a variant of this model in the ILSVRC-2012 competition and achieved a winning top-5 test error rate of 15.3%, compared to 26.2% achieved by the second-best entry.

2012

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AlphaGo

nature
International journal of science

Article

Mastering the game of Go with deep neural networks and tree search

David Silver ✉, Aja Huang, Chris J. Maddison, Arthur Guez, Laurent Sifre, George van den Driessche, Julian Schrittwieser, Ioannis Antonoglou, Veda Panneershelvam, Marc Lanctot, Sander Dieleman, Dominik Grewe, John Nham, Nal Kalchbrenner, Ilya Sutskever, Timothy Lillicrap, Madeleine Leach, Koray Kavukcuoglu, Thore Graepel & Demis Hassabis ✉

Nature **529**, 484–489 (28 January 2016)
doi:10.1038/nature16961
Download Citation

Received: 11 November 2015
Accepted: 05 January 2016
Published: 27 January 2016

Abstract

The game of Go has long been viewed as the most challenging of classic games for artificial intelligence owing to its enormous search space and the difficulty of evaluating board positions and moves. Here we introduce a new approach to computer Go that uses 'value networks' to evaluate board positions and 'policy networks' to select moves. These deep neural networks are trained by a novel combination of supervised learning from human expert games, and reinforcement learning from games of self-play. Without any lookahead search, the neural networks play Go at the level of state-of-the-art Monte Carlo tree search programs that simulate thousands of random games of self-play. We also introduce a new search algorithm that combines Monte Carlo simulation with value and policy networks. Using this search algorithm, our program AlphaGo achieved a 99.8% winning rate against other Go programs, and defeated the human European Go champion by 5 games to 0. This is the first time that a computer program has defeated a human professional player in the full-sized game of Go, a feat previously thought to be at least a decade away.

AlphaGo seals 4-1 victory over Go grandmaster Lee Sedol

DeepMind's artificial intelligence astonishes fans to defeat human opponent and offers evidence computer software has mastered a major challenge

Steven Borowiec

Tue 15 Mar 2016 10.12 GMT

https://www.theguardian.com

2016

PERIMETER INSTITUTE

AlphaGo Zero

nature

Article | Published: 18 October 2017

Mastering the game of Go without human knowledge

David Silver ✉, Julian Schrittwieser, Karen Simonyan, Ioannis Antonoglou, Aja Huang, Arthur Guez, Thomas Hubert, Lucas Baker, Matthew Lai, Adrian Bolton, Yutian Chen, Timothy Lillicrap, Fan Hui, Laurent Sifre, George van den Driessche, Thore Graepel & Demis Hassabis

Nature **550**, 354–359 (19 October 2017)

Abstract

A long-standing goal of artificial intelligence is an algorithm that learns, *tabula rasa*, superhuman proficiency in challenging domains. Recently, AlphaGo became the first program to defeat a world champion in the game of Go. The tree search in AlphaGo evaluated positions and selected moves using deep neural networks. These neural networks were trained by supervised learning from human expert moves, and by reinforcement learning from self-play. Here we introduce an algorithm based solely on reinforcement learning, without human data, guidance or domain knowledge beyond game rules. AlphaGo becomes its own teacher: a neural network is trained to predict AlphaGo's own move selections and also the winner of AlphaGo's games. This neural network improves the strength of the tree search, resulting in higher quality move selection and stronger self-play in the next iteration. Starting ***tabula rasa***, our new program AlphaGo Zero achieved superhuman performance, winning 100–0 against the previously published, champion-defeating AlphaGo.

2017

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Self-driving cars

End to End Learning for Self-Driving Cars

Mariusz Bojarski
NVIDIA Corporation
Holmdel, NJ 07735

Davide Del Testa
NVIDIA Corporation
Holmdel, NJ 07735

Daniel Dworakowski
NVIDIA Corporation
Holmdel, NJ 07735

Bernhard Firner
NVIDIA Corporation
Holmdel, NJ 07735

Beat Flepp
NVIDIA Corporation
Holmdel, NJ 07735

Prasoon Goyal
NVIDIA Corporation
Holmdel, NJ 07735

Lawrence D. Jackel
NVIDIA Corporation
Holmdel, NJ 07735

Mathew Monfort
NVIDIA Corporation
Holmdel, NJ 07735

Urs Muller
NVIDIA Corporation
Holmdel, NJ 07735

Jiakai Zhang
NVIDIA Corporation
Holmdel, NJ 07735

Xin Zhang
NVIDIA Corporation
Holmdel, NJ 07735

Jake Zhao
NVIDIA Corporation
Holmdel, NJ 07735

Karol Zieba
NVIDIA Corporation
Holmdel, NJ 07735

Abstract

We trained a convolutional neural network (CNN) to map raw pixels from a single front-facing camera directly to steering commands. This end-to-end approach proved surprisingly powerful. With minimum training data from humans the system learns to drive in traffic on local roads with or without lane markings and on highways. It also operates in areas with unclear visual guidance such as in parking lots and on unpaved roads.

The system automatically learns internal representations of the necessary processing steps such as detecting useful road features with only the human steering angle as the training signal. We never explicitly trained it to detect, for example, the outline of roads.

Compared to explicit decomposition of the problem, such as lane marking detection, path planning, and control, our end-to-end system optimizes all processing steps simultaneously. We argue that this will eventually lead to better performance and smaller systems. Better performance will result because the internal components self-optimize to maximize overall system performance, instead of optimizing human-selected intermediate criteria, e. g., lane detection. Such criteria understandably are selected for ease of human interpretation which doesn't automatically guarantee maximum system performance. Smaller networks are possible because the system learns to solve the problem with the minimal number of processing steps.

We used an NVIDIA DevBox and Torch 7 for training and an NVIDIA DRIVE™ PX self-driving car computer also running Torch 7 for determining where to drive. The system operates at 30 frames per second (FPS).

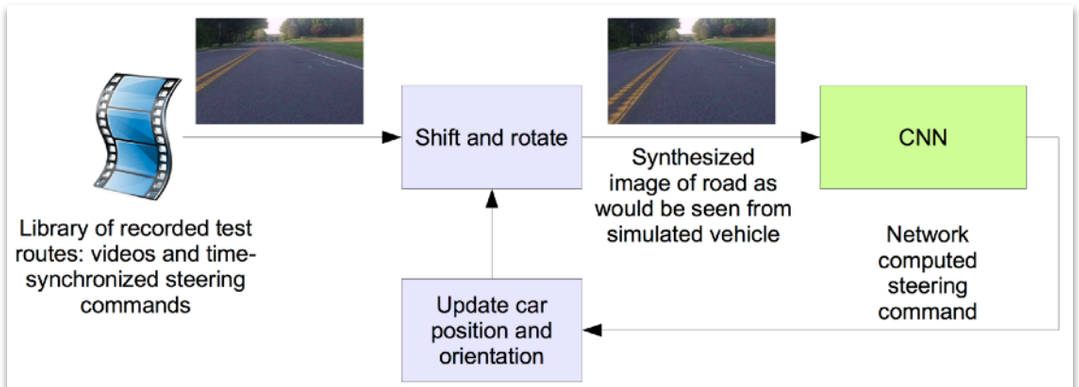

Figure 5: Block-diagram of the drive simulator.

2016

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Language translation

Google's Neural Machine Translation System: Bridging the Gap between Human and Machine Translation

Yonghui Wu, Mike Schuster, Zhifeng Chen, Quoc V. Le, Mohammad Norouzi
yonghui,schuster,zhifengc,qvl,mnorouzi@google.com

Wolfgang Macherey, Maxim Krikun, Yuan Cao, Qin Gao, Klaus Macherey, Jeff Klingner, Apurva Shah, Melvin Johnson, Xiaobing Liu, Łukasz Kaiser, Stephan Gouws, Yoshikiyo Kato, Taku Kudo, Hideto Kazawa, Keith Stevens, George Kurian, Nishant Patil, Wei Wang, Cliff Young, Jason Smith, Jason Riesa, Alex Rudnick, Oriol Vinyals, Greg Corrado, Macduff Hughes, Jeffrey Dean

Abstract

Neural Machine Translation (NMT) is an end-to-end learning approach for automated translation, with the potential to overcome many of the weaknesses of conventional phrase-based translation systems. Unfortunately, NMT systems are known to be computationally expensive both in training and in translation inference – sometimes prohibitively so in the case of very large data sets and large models. Several authors have also charged that NMT systems lack robustness, particularly when input sentences contain rare words. These issues have hindered NMT's use in practical deployments and services, where both accuracy and speed are essential. In this work, we present GNMT, Google's Neural Machine Translation system, which attempts to address many of these issues. Our model consists of a deep LSTM network with 8 encoder and 8 decoder layers using residual connections as well as attention connections from the decoder network to the encoder. To improve parallelism and therefore decrease training time, our attention mechanism connects the bottom layer of the decoder to the top layer of the encoder. To accelerate the final translation speed, we employ low-precision arithmetic during inference computations. To improve handling of rare words, we divide words into a limited set of common sub-word units ("wordpieces") for both input and output. This method provides a good balance between the flexibility of "character"-delimited models and the efficiency of "word"-delimited models, naturally handles translation of rare words, and ultimately improves the overall accuracy of the system. Our beam search technique employs a length-normalization procedure and uses a coverage penalty, which encourages generation of an output sentence that is most likely to cover all the words in the source sentence. To directly optimize the translation BLEU scores, we consider refining the models by using reinforcement learning, but we found that the improvement in the BLEU scores did not reflect in the human evaluation. On the WMT'14 English-to-French and English-to-German benchmarks, GNMT achieves competitive results to state-of-the-art. Using a human side-by-side evaluation on a set of isolated simple sentences, it reduces translation errors by an average of 60% compared to Google's phrase-based production system.

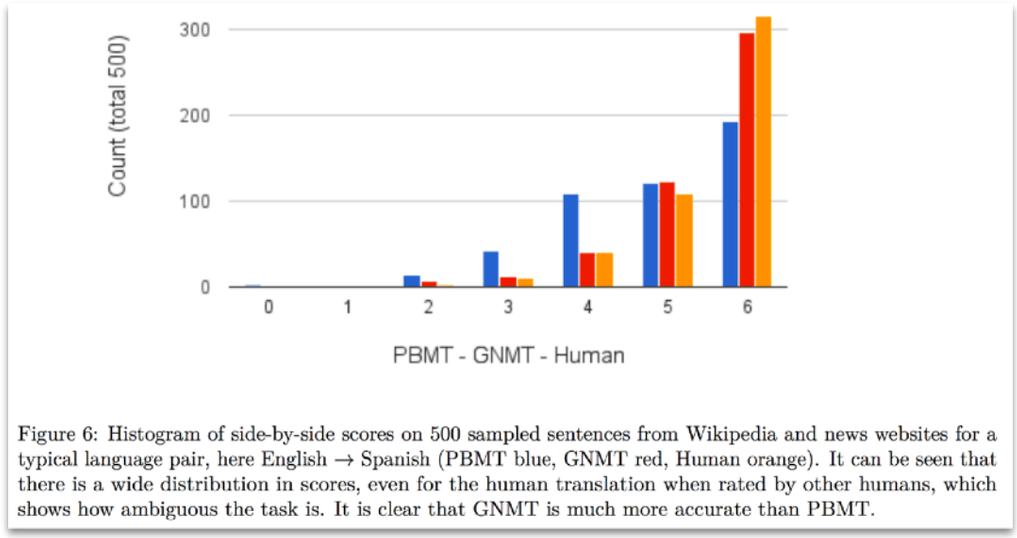

Figure 6: Histogram of side-by-side scores on 500 sampled sentences from Wikipedia and news websites for a typical language pair, here English → Spanish (PBMT blue, GNMT red, Human orange). It can be seen that there is a wide distribution in scores, even for the human translation when rated by other humans, which shows how ambiguous the task is. It is clear that GNMT is much more accurate than PBMT.

2016

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Generating art

https://deepart.io/

Step 1: Upload photo

Step 2: Choose style

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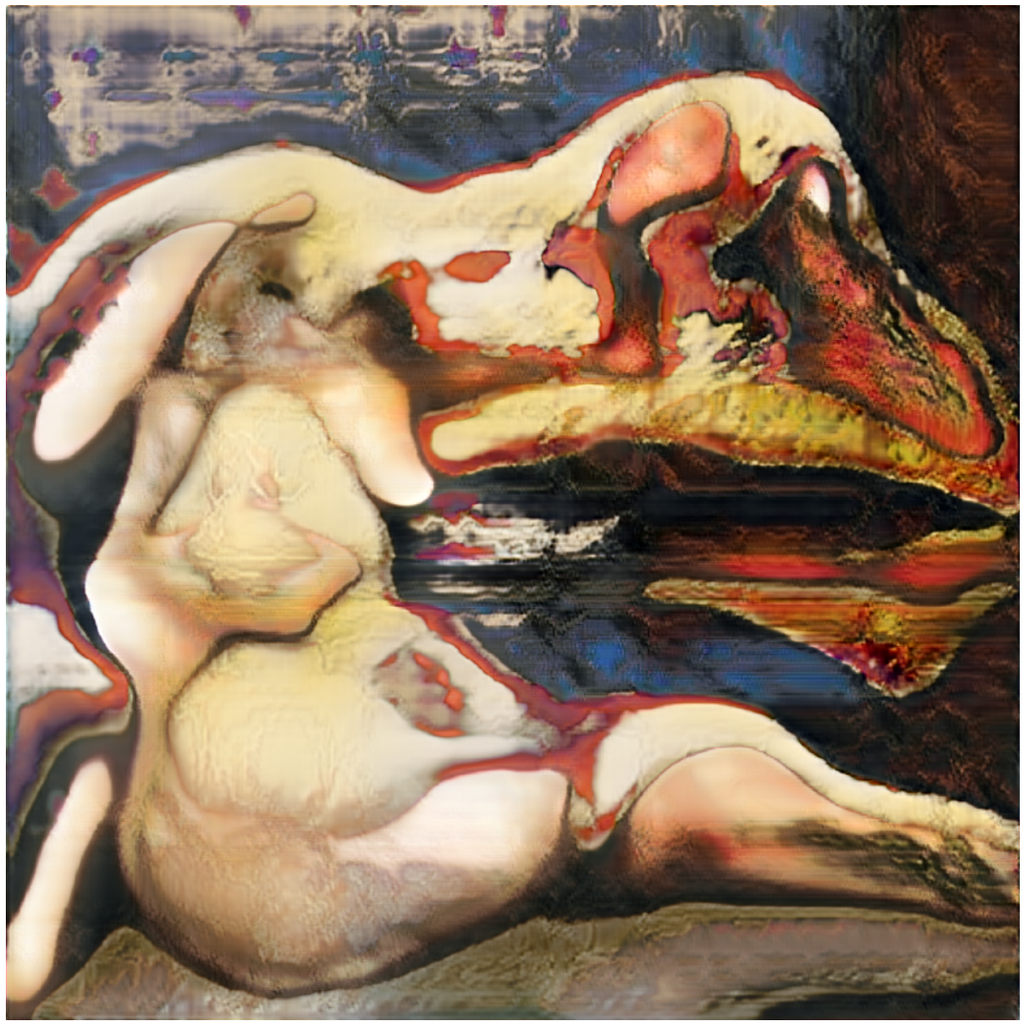
Generating art

Robbie Barrat
https://robbiebarrat.github.io



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Computer-generated people

https://thispersondoesnotexist.com






2018

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Medical diagnosis

CheXNet: Radiologist-Level Pneumonia Detection on Chest X-Rays with Deep Learning

Pranav Rajpurkar [*1] **Jeremy Irvin** [*1] **Kaylie Zhu** [1] **Brandon Yang** [1] **Hershel Mehta** [1]
Tony Duan [1] **Daisy Ding** [1] **Aarti Bagul** [1] **Robyn L. Ball** [2] **Curtis Langlotz** [3] **Katie Shpanskaya** [3]
Matthew P. Lungren [3] **Andrew Y. Ng** [1]

Abstract

We develop an algorithm that can detect pneumonia from chest X-rays at a level exceeding practicing radiologists. Our algorithm, CheXNet, is a 121-layer convolutional neural network trained on ChestX-ray14, currently the largest publicly available chest X-ray dataset, containing over 100,000 frontal-view X-ray images with 14 diseases. Four practicing academic radiologists annotate a test set, on which we compare the performance of CheXNet to that of radiologists. We find that CheXNet exceeds average radiologist performance on the F1 metric. We extend CheXNet to detect all 14 diseases in ChestX-ray14 and achieve state of the art results on all 14 diseases.

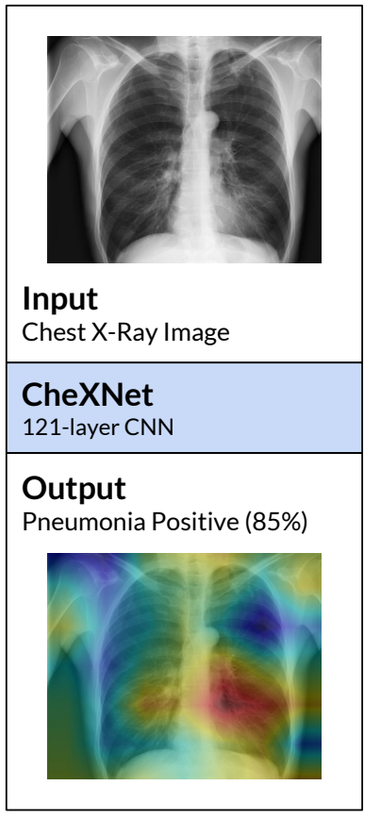


Figure 1. CheXNet is a 121-layer convolutional neural network that takes a chest X-ray image as input, and outputs the probability of a pathology. On this example, CheXnet correctly detects pneumonia and also localizes areas in the image most indicative of the pathology.

2017

Machine Learning for Physics

nature communications

Article | Published: 02 July 2014

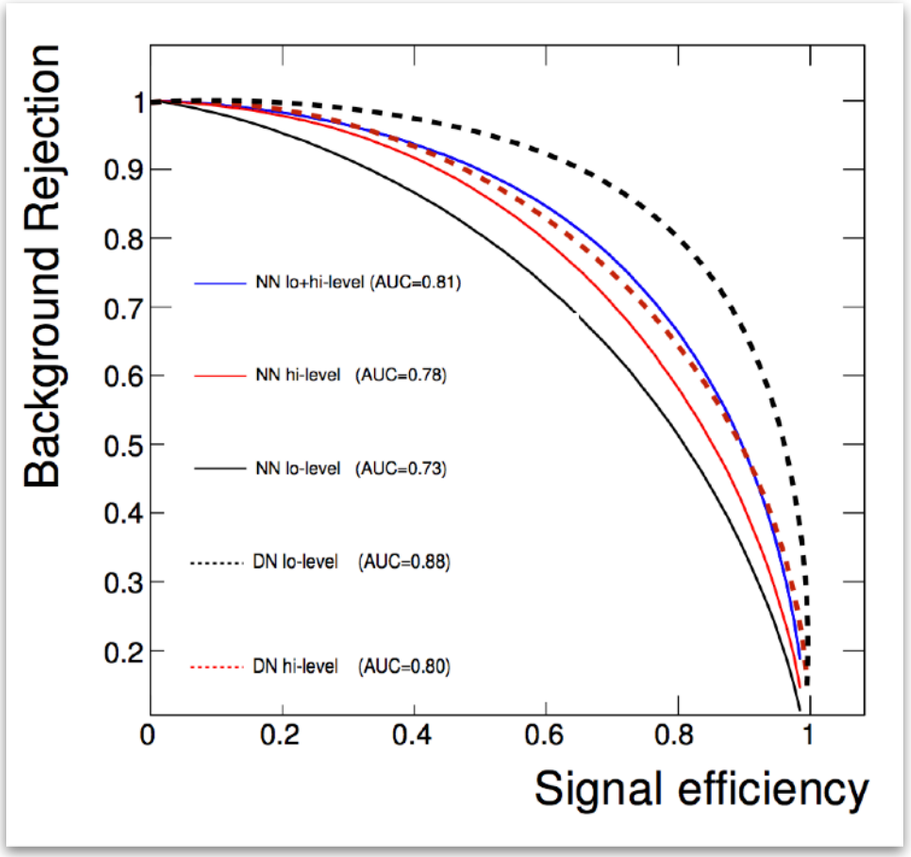
Searching for exotic particles in high-energy physics with deep learning

P. Baldi, P. Sadowski & D. Whiteson

Nature Communications **5**, Article number: 4308 (2014)

Abstract

Collisions at high-energy particle colliders are a traditionally fruitful source of exotic particle discoveries. Finding these rare particles requires solving difficult signal-versus-background classification problems, hence machine-learning approaches are often used. Standard approaches have relied on 'shallow' machine-learning models that have a limited capacity to learn complex nonlinear functions of the inputs, and rely on a painstaking search through manually constructed nonlinear features. Progress on this problem has slowed, as a variety of techniques have shown equivalent performance. Recent advances in the field of deep learning make it possible to learn more complex functions and better discriminate between signal and background classes. Here, using benchmark data sets, we show that deep-learning methods need no manually constructed inputs and yet improve the classification metric by as much as 8% over the best current approaches. This demonstrates that deep-learning approaches can improve the power of collider searches for exotic particles.



arXiv:1806.11484

2014

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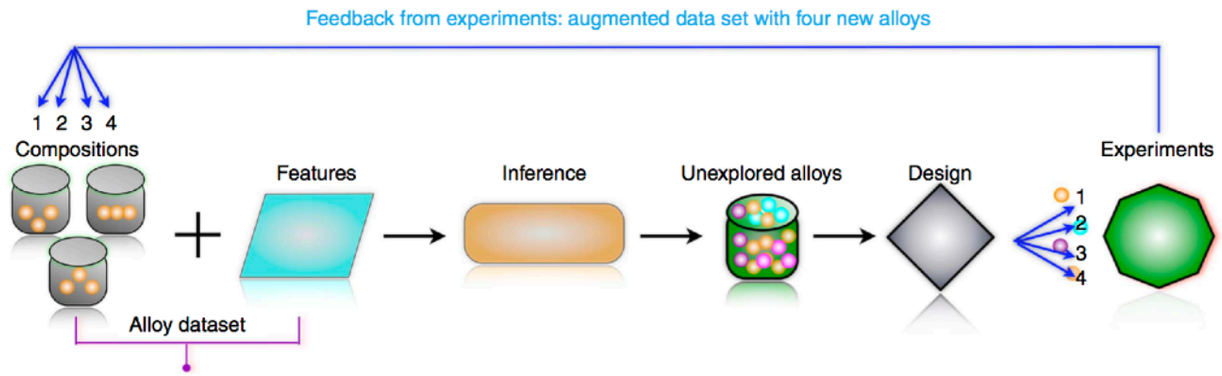
Machine Learning for Physics

nature COMMUNICATIONS

Accelerated search for materials with targeted properties by adaptive design

Dezhen Xue[1,2], Prasanna V. Balachandran[1], John Hogden[3], James Theiler[4], Deqing Xue[2] & Turab Lookman[1]

Finding new materials with targeted properties has traditionally been guided by intuition, and trial and error. With increasing chemical complexity, the combinatorial possibilities are too large for an Edisonian approach to be practical. Here we show how an adaptive design strategy, tightly coupled with experiments, can accelerate the discovery process by sequentially identifying the next experiments or calculations, to effectively navigate the complex search space. Our strategy uses inference and global optimization to balance the trade-off between exploitation and exploration of the search space. We demonstrate this by finding very low thermal hysteresis (ΔT) NiTi-based shape memory alloys, with $Ti_{50.0}Ni_{46.7}Cu_{0.8}Fe_{2.3}Pd_{0.2}$ possessing the smallest ΔT (1.84 K). We synthesize and characterize 36 predicted compositions (9 feedback loops) from a potential space of ~800,000 compositions. Of these, 14 had smaller ΔT than any of the 22 in the original data set.



2016

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Machine Learning for Physics

nature physics

Letter | Published: 13 February 2017

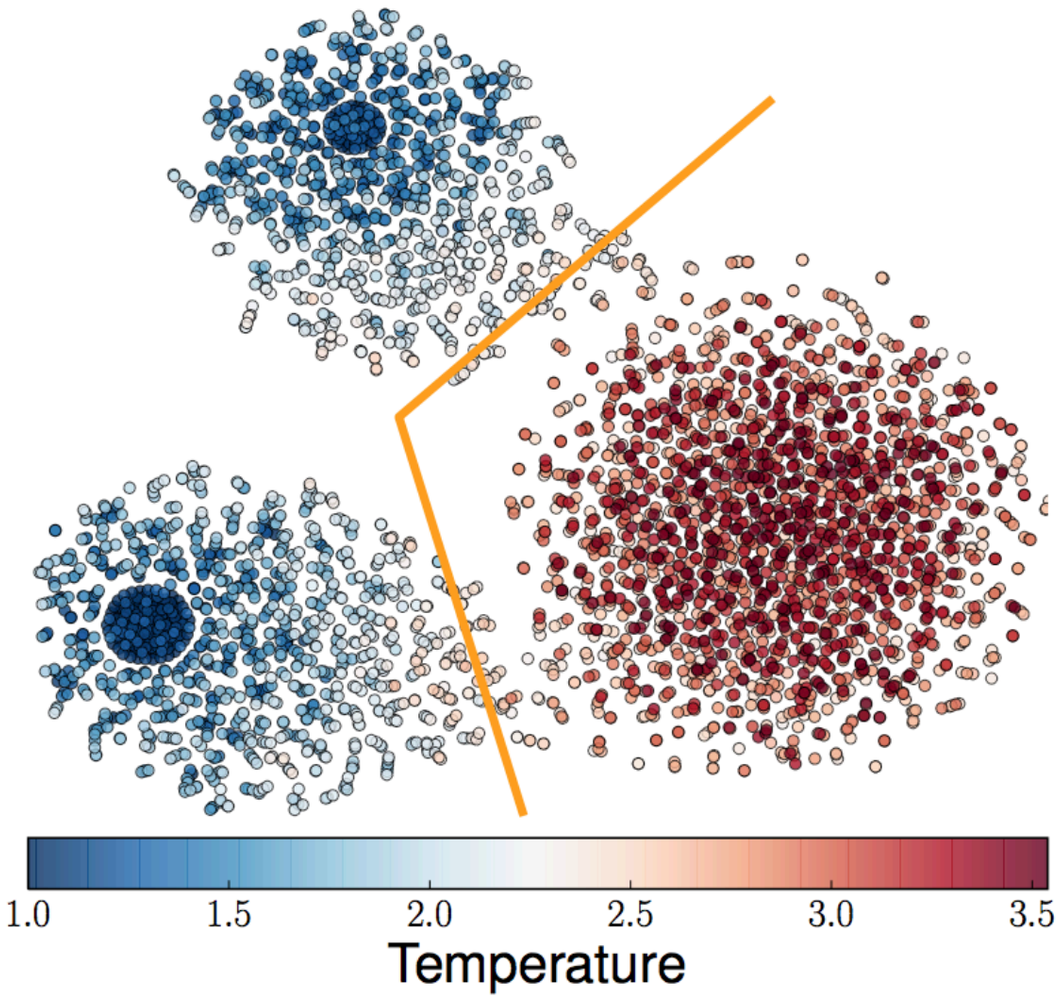
Machine learning phases of matter

Juan Carrasquilla ✉ & Roger G. Melko

Nature Physics **13**, 431–434 (2017)

Abstract

Condensed-matter physics is the study of the collective behaviour of infinitely complex assemblies of electrons, nuclei, magnetic moments, atoms or qubits[1]. This complexity is reflected in the size of the state space, which grows exponentially with the number of particles, reminiscent of the 'curse of dimensionality' commonly encountered in machine learning[2]. Despite this curse, the machine learning community has developed techniques with remarkable abilities to recognize, classify, and characterize complex sets of data. Here, we show that modern machine learning architectures, such as fully connected and convolutional neural networks[3], can identify phases and phase transitions in a variety of condensed-matter Hamiltonians. Readily programmable through modern software libraries[4,5], neural networks can be trained to detect multiple types of order parameter, as well as highly non-trivial states with no conventional order, directly from raw state configurations sampled with Monte Carlo[6,7].



2016

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Machine Learning for Physics

QuCumber: wavefunction reconstruction with neural networks

Matthew J. S. Beach[1,2], Isaac De Vlugt[2], Anna Golubeva[1,2], Patrick Huembeli[1,3], Bohdan Kulchytskyy[1,2], Xiuzhe Luo[2], Roger G. Melko[1,2*], Ejaaz Merali[2], Giacomo Torlai[1,2,4]

1 Perimeter Institute for Theoretical Physics, Waterloo, Ontario N2L 2Y5, Canada
2 Department of Physics and Astronomy, University of Waterloo, Ontario N2L 3G1, Canada
3 ICFO-Institut de Ciencies Fotoniques, Barcelona Institute of Science and Technology, 08860 Castelldefels (Barcelona), Spain
4 Center for Computational Quantum Physics, Flatiron Institute, 162 5th Avenue, New York, NY 10010, USA
* rgmelko@uwaterloo.ca

December 27, 2018

Abstract

As we enter a new era of quantum technology, it is increasingly important to develop methods to aid in the accurate preparation of quantum states for a variety of materials, matter, and devices. Computational techniques can be used to reconstruct a state from data, however the growing number of qubits demands ongoing algorithmic advances in order to keep pace with experiments. In this paper, we present an open-source software package called QuCumber that uses machine learning to reconstruct a quantum state consistent with a set of projective measurements. QuCumber uses a restricted Boltzmann machine to efficiently represent the quantum wavefunction for a large number of qubits. New measurements can be generated from the machine to obtain physical observables not easily accessible from the original data.

2018

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Machine Learning for Physics: Resources

- Michael Nielsen, “Neural networks and deep learning”, **neuralnetworksanddeeplearning.com**
- Goodfellow, Bengio and Courville, “Deep learning”, MIT Press (2016), **deeplearningbook.org**
- Liu, Li and Wang, “Lecture note on deep learning and quantum many-body computation”, **http://wangleiphy.github.io/lectures/DL.pdf**
- Mehta, Bukov, Wang, Day, Richardson, Fisher, and Schwab, “A high-bias, low-variance introduction to machine learning for physicists”, **arXiv:1803.08823**
- Carleo, Cirac, Cranmer, Daudet, Schuld, Tishby, Vogt-Maranto, and Zdeborová, “Machine learning and the physical sciences”, **arXiv:1903.10563**
- Guest, Cranmer, and Whiteson, “Deep learning and its application to LHC physics”, **arXiv:1806.11484**
- Torlai and Melko, “Machine learning quantum states in the NISQ era”, **arXiv:1905.04312**
- **physicsml.github.io**

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Machine Learning (ML)

ML: Training computers to detect and characterize features from data

Categories of algorithms:

1. **Supervised learning (SL)**

   Given a dataset $\mathscr{D} = \{\vec{x}, \vec{y}\}$ of data points $\vec{x}$ and labels $\vec{y}$, fit a function $\vec{f}(\vec{x})$ to $\vec{y}$.

2. **Unsupervised learning (UL)**

   Given an unlabelled dataset $\mathscr{D} = \{\vec{x}\}$, efficiently represent the data's underlying probability distribution $p(\vec{x})$.

3. **Reinforcement learning (RL)**

   Given an environment, take an action such that the resulting reward will be maximized.

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Machine Learning (ML)

ML: Training computers to detect and characterize features from data

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TODAY: SL using neural networks

2. **Unsupervised learning (UL)**

   Given an unlabelled dataset $\mathscr{D} = \{\vec{x}\}$, efficiently represent the data's underlying probability distribution $p(\vec{x})$.

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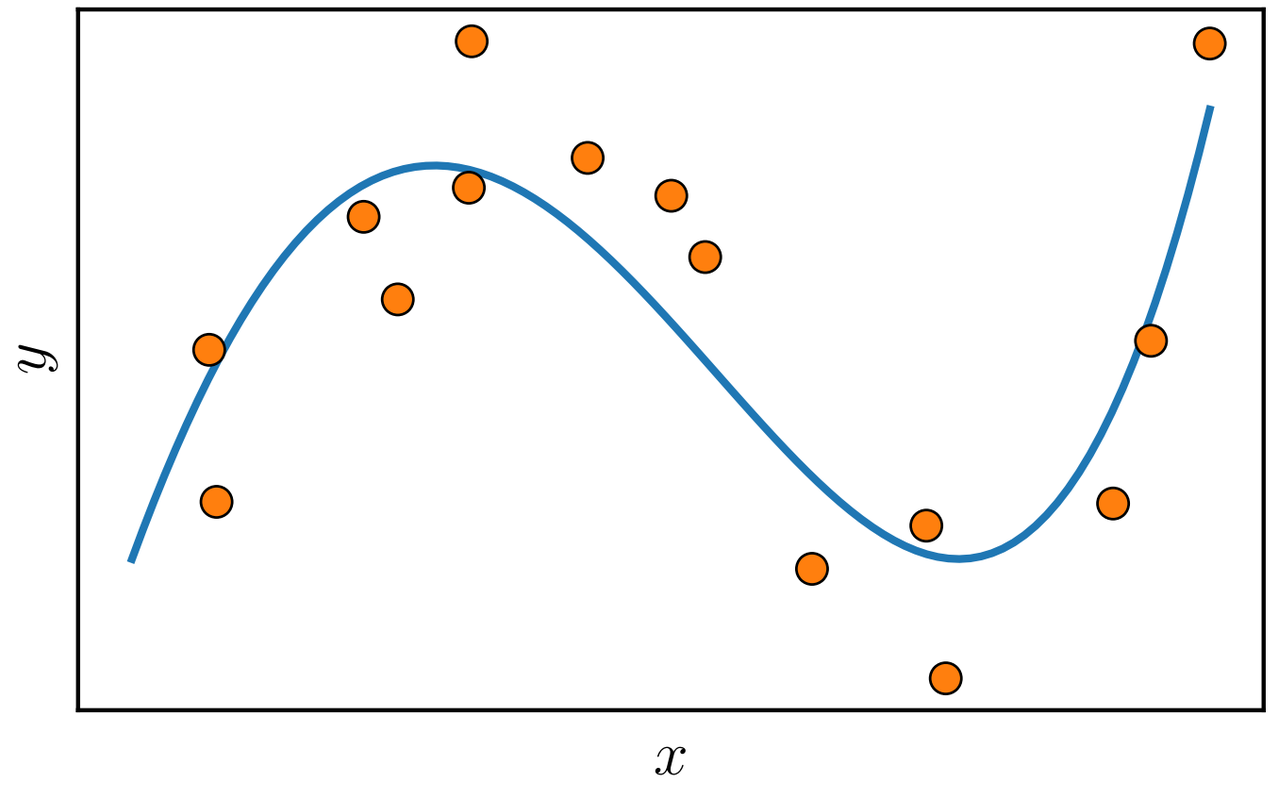
Supervised Learning Example: 1D Regression



The data points x and labels y are both 1D coordinates. The goal is to find a function $f(x)$ (such as the blue curve) that describes the data.

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Supervised Learning Example: Classifying handwritten digits

$\vec{x}_1 =$  $y_1 = 5$

$\vec{x}_2 =$  $y_2 = 0$

$\vec{x}_3 =$  $y_3 = 4$

$\vec{x}_4 =$  $y_4 = 9$

Data points taken from the MNIST database

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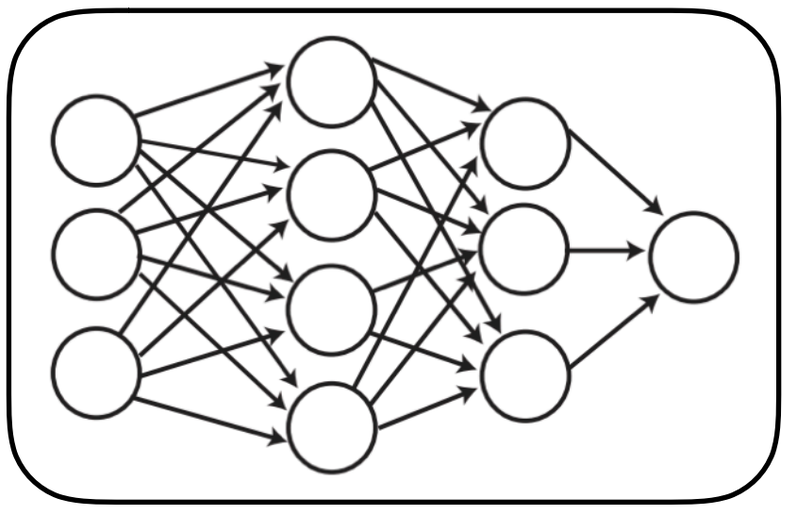
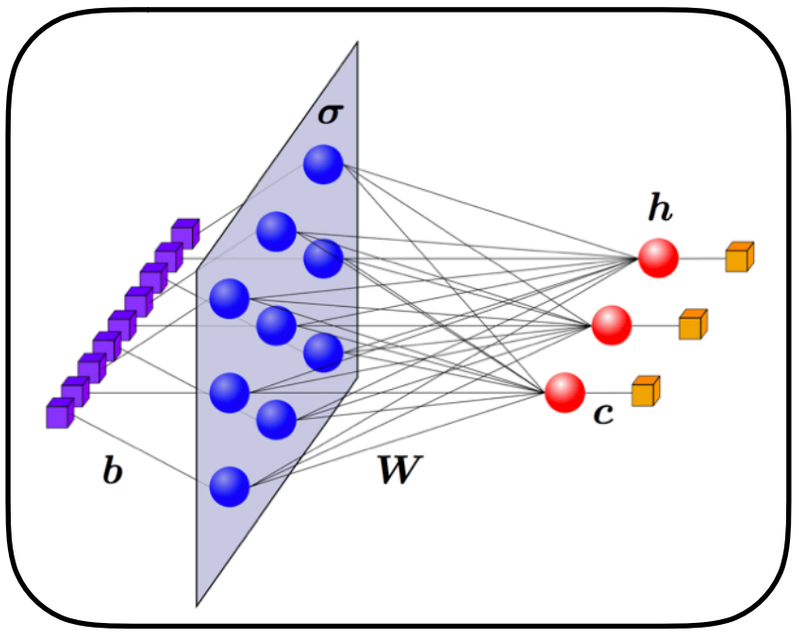
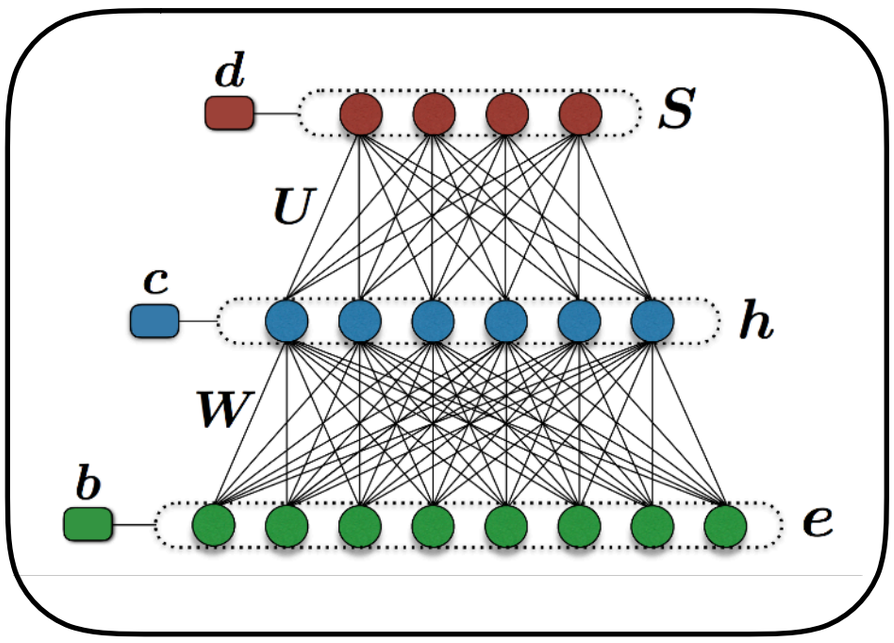
Artificial neural networks



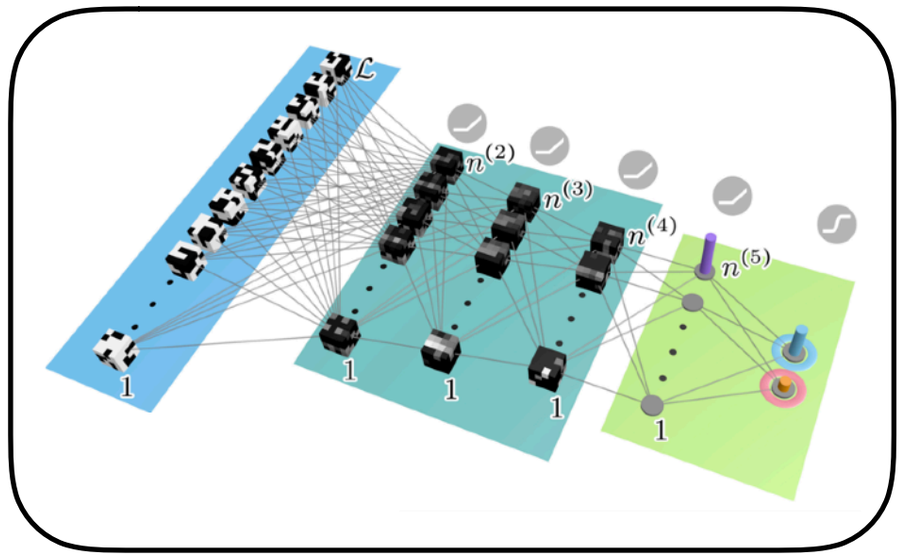
arXiv:1803.08823



arXiv:1606.02718



arXiv:1610.04238



arXiv:1609.02552

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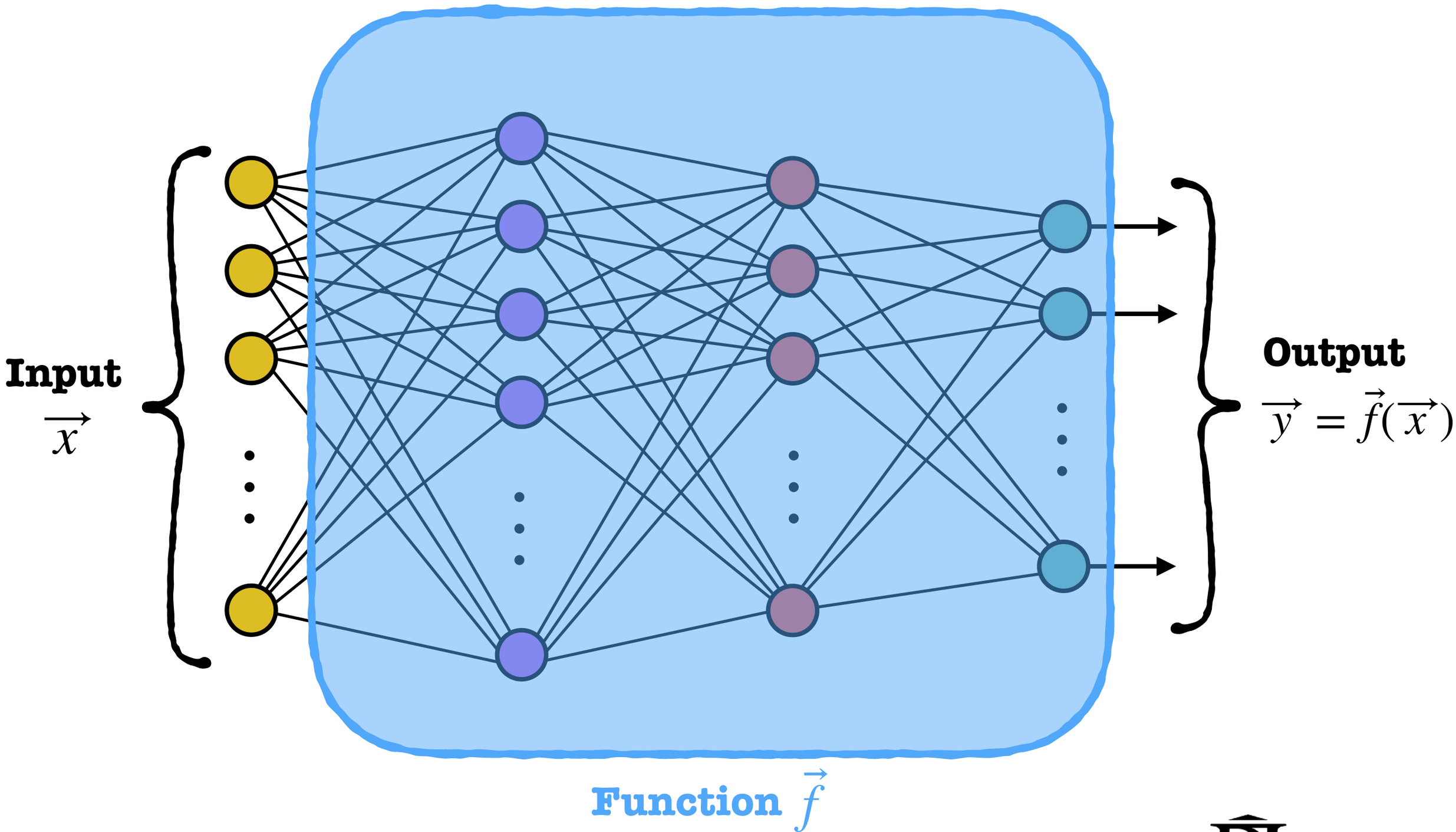
Feedforward neural networks



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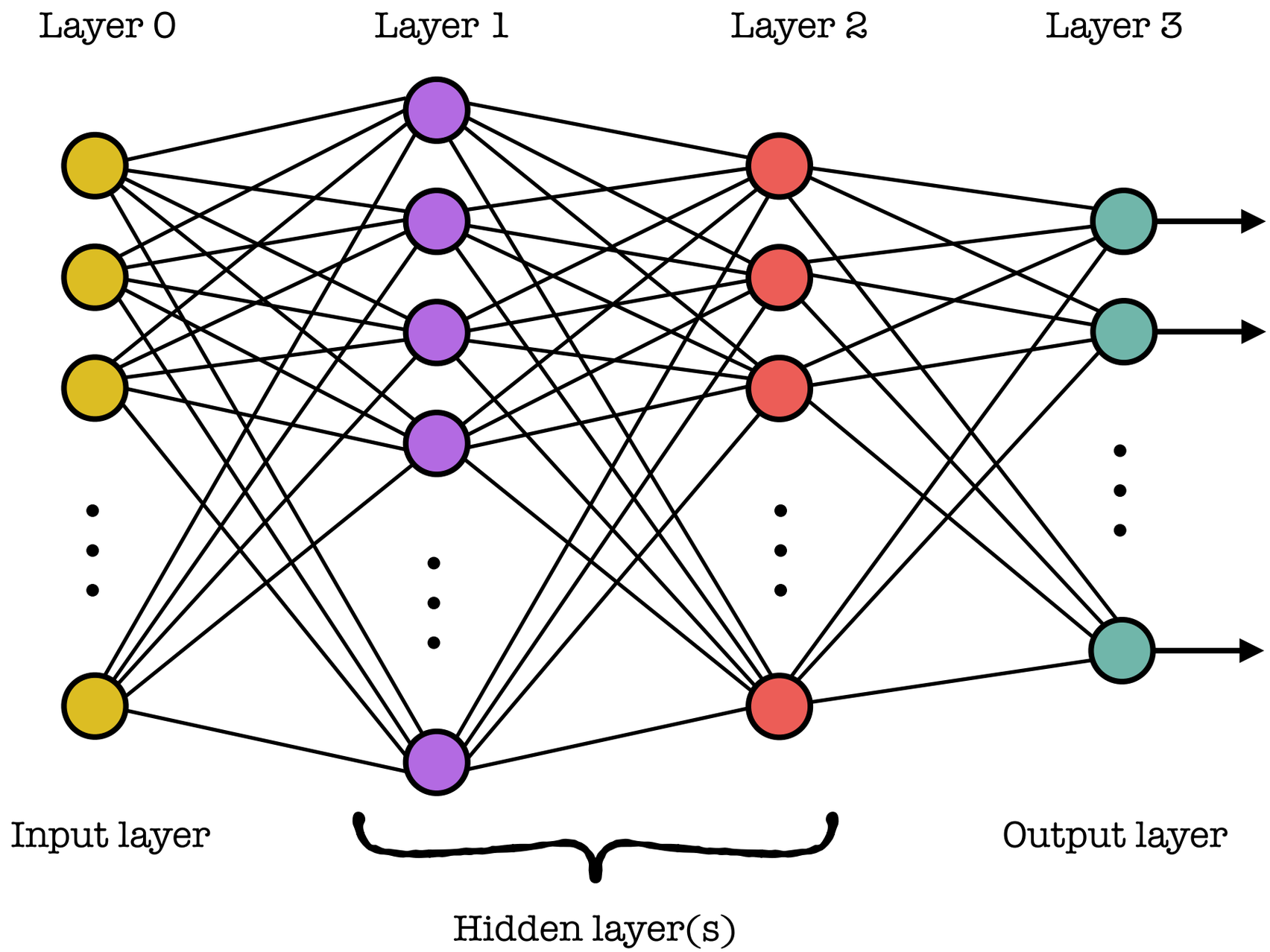
Feedforward neural networks



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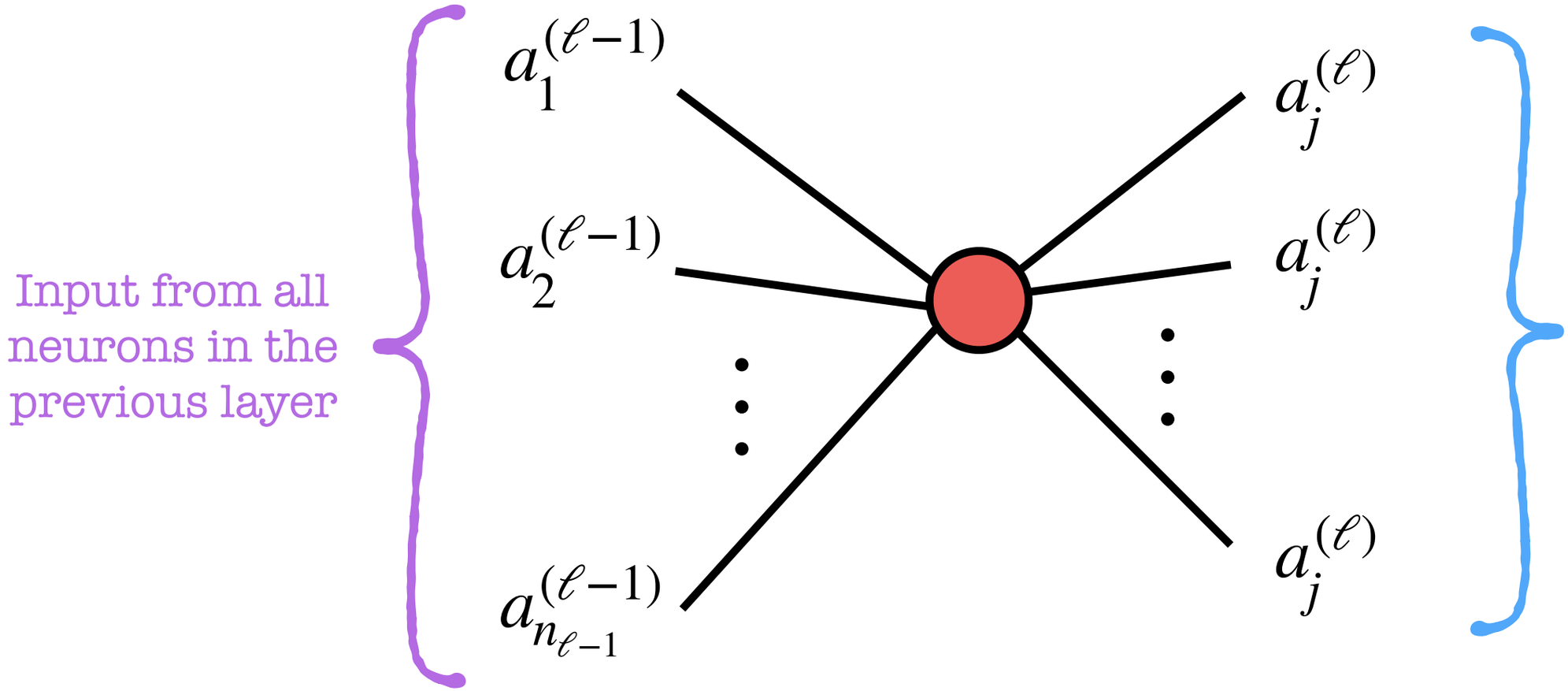
Neuron output

Let's zoom in on the j^{th} neuron in layer $\ell > 0$



$n_\ell \equiv$ number of neurons in layer ℓ

$L \equiv$ total number of layers

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Neuron output

$$a_j^{(\ell)} = g_\ell\left(\underbrace{\sum_{i=1}^{n_{\ell-1}} a_i^{(\ell-1)} W_{ij}^{\ell} + b_j^{\ell}}_{\equiv\, z_j^{(\ell)}}\right)$$

non-linear **activation function**

weight for each link

bias for each neuron

The weights and biases are adjusted as the network **learns**.

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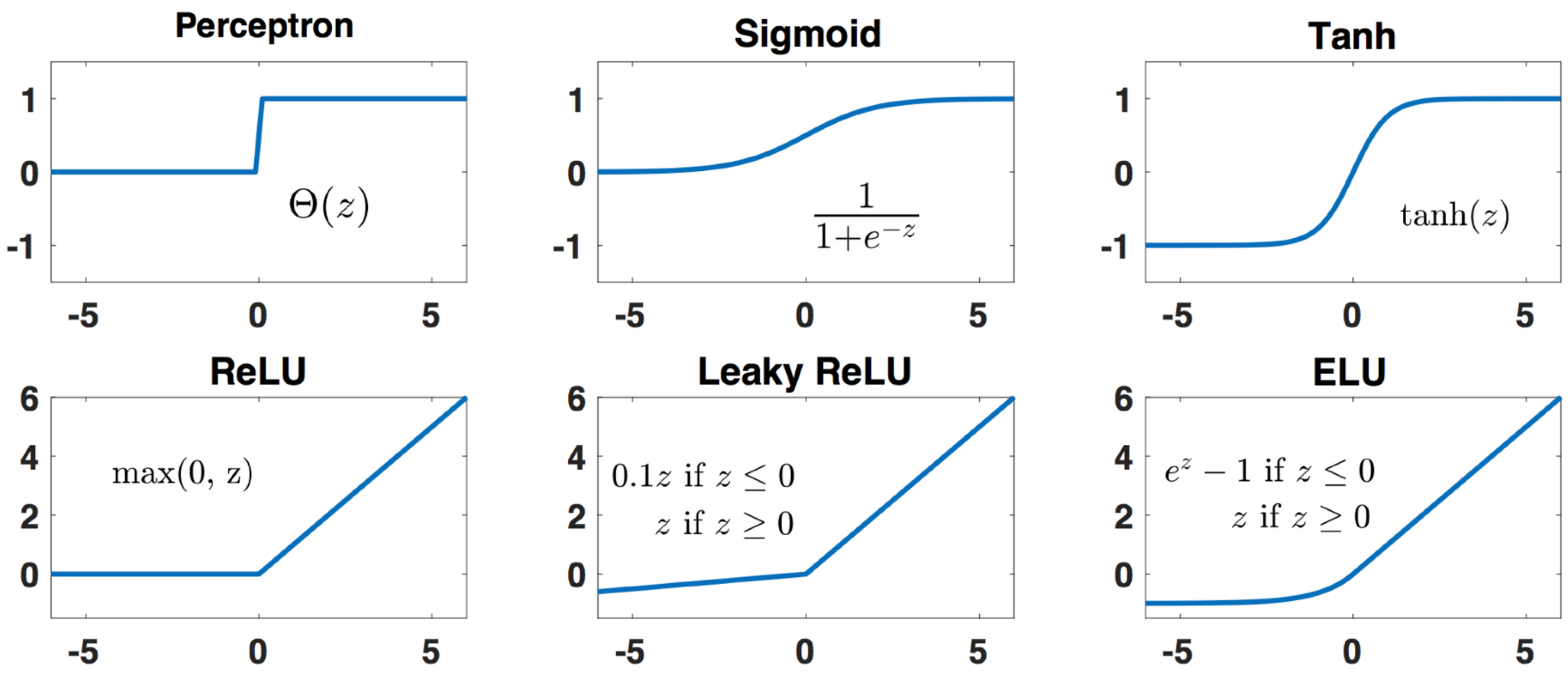
Activation functions

We can choose various non-linear activation functions g_ℓ, such as:



arXiv:1803.08823

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Cost functions

Our goal is to find weights and biases such that when $\vec{x}$ is the input, the network's output $\vec{a}^{(L)}(\vec{x}) = \vec{f}(\vec{x})$ is close to the label $\vec{y}$.

We use a **cost function** to measure how well the neural network is approximating the labels.

Possible cost functions include:

- **Mean-squared error:** $$C_{\text{MSE}} = \frac{1}{2|\mathcal{D}|} \sum_{\vec{x} \in \mathcal{D}} \sum_{i=1}^{n_L} \left[a_i^{(L)}(\vec{x}) - y_i(\vec{x}) \right]^2$$

- **Cross entropy:** $$C_{\text{CE}} = -\frac{1}{|\mathcal{D}|} \sum_{\vec{x} \in \mathcal{D}} \sum_{i=1}^{n_L} \left[y_i(\vec{x}) \log a_i^{(L)}(\vec{x}) + (1 - y_i(\vec{x})) \log(1 - a_i^{(L)}(\vec{x})) \right]$$

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Cost functions

We would like to minimize the cost function over all possible weights and biases in each layer such that

$$\left.\begin{aligned} \frac{\partial C}{\partial W_{ij}^{(\ell)}} &= 0 \\ \frac{\partial C}{\partial b_j^{(\ell)}} &= 0 \end{aligned}\right\} \text{For all } i, j, \ell$$

Learning algorithms

- **Gradient descent:**

$$W_{ij}^{(\ell)} \rightarrow W_{ij}^{(\ell)} - \eta \frac{\partial C}{\partial W_{ij}^{(\ell)}}$$

$$b_{j}^{(\ell)} \rightarrow b_{j}^{(\ell)} - \eta \frac{\partial C}{\partial b_{j}^{(\ell)}}$$

η : **Learning rate**

- **Stochastic gradient descent**

- **RMSProp**

- **Adam optimizer**

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Feedforward Neural Networks in TensorFlow

Go to:

https://drive.google.com/file/d/17CihZKb04U2TRwDXQwwmMDYODFXMfbCf/view?usp=sharing

- Open with Google Colaboratory
- Choose ‘Open in Playground’
- Choose the option ‘Copy to Drive’