

Deep learning for biologists

A practical and theoretical introduction

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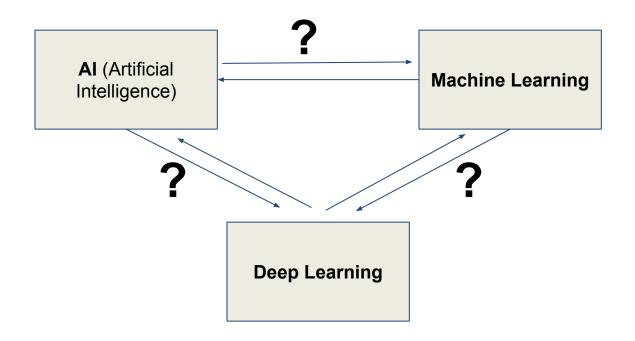






What is deep learning?











What is deep learning?

AI >> ML >> DL

Source:

https://en.wikipedia.org/wiki/Deep_learning#/media/File:Al-ML-DL.png

Artificial Intelligence:

Mimicking the intelligence or behavioural pattern of humans or any other living entity.

Machine Learning:

A technique by which a computer can "learn" from data, without using a complex set of different rules. This approach is mainly based on training a model from datasets.

Deep Learning:

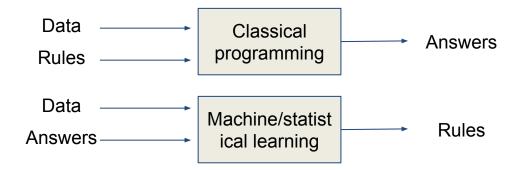
A technique to perform machine learning inspired by our brain's own network of neurons.





What is (deep) learning?





- (machine; statistical) learning
 - tune a mathematical model using some training data to make predictions on unknown, new data
 - a machine/statistical learning model is trained rather than explicitly programmed







What is (deep) learning?



(machine; statistical) learning

- 1. <u>Input data</u> (e.g. sound recordings, images)
- 2. Output examples (e.g. sound transcripts, image-tags)
- Performance measure: how well is the algorithm working → adjustment steps → learning







You can do (statistical) learning in your head!

- The first edition of this course gets 10 students
- The second edition gets 20 students
- The third edition gets 40 students
- The fourth edition gets 80 students
- How many students in the sixth edition?







You can do (statistical) learning in your head!

TRAINING DATA

- The first edition of this course gets 10 students
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- The third edition gets 40 students
- The fourth edition gets 80 students
- How many students in the sixth edition?

NEW, UNKNOWN DATA

STUDENTS IN SIXTH EDITION = 320

 $STUD = 10 \times 2 \exp(YEAR - 1)$

PREDICTION







What is <u>deep</u> learning?



- (machine; statistical) learning
 - tune a mathematical model using some training data to make predictions on unknown, new data
 - «If you make a bunch of random changes to your program until it sort-of works, that's "hacky" and "bad coding practice". But if you do it really fast, it's "machine learning"» [Steve Maine, Software Engineer]
- Deep learning
 - Neural networks, a mathematical model "inspired" by biology
 - Artificial Neural Networks have been around for ~80 years ...
 - ... but became "deep" in the last ten years







Why "deep"?



What do you think?

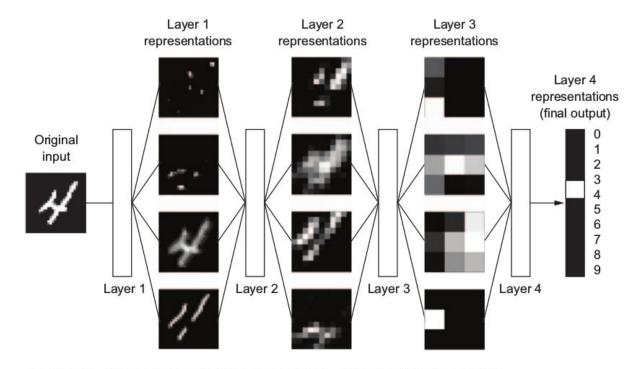






Why "deep"?





deep neural networks (i.e. with many layers)

Figure 1.6 Deep representations learned by a digit-classification model







A brief history of DL



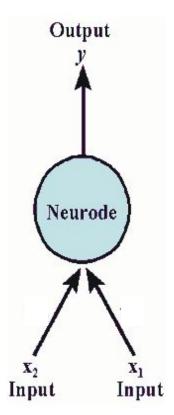




How it all began



- 1943, McCulloch & Pitts:
 - first mathematical model of a neural network
 - only binary input and output (0/1),
 - only used the threshold step activation function
 - did not incorporate weighting the different inputs
- 1950s: pioneers started asking whether computers could be made to "think" → (A.I.)





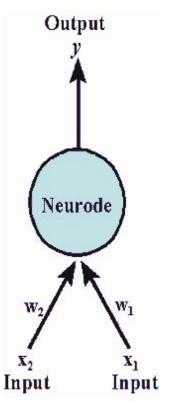




How it all began



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- 1957, Rosenblatt: introducing the perceptron:
 - weighting inputs
 - additional activation functions (e.g. sigmoid)









From symbolic AI to ML



- this was all no learning Al
 - e.g. early chess programs based on hardcoded rules crafted by programmers
 - experts believed that human-level A.I. could be achieved by handcrafting a sufficiently large set of explicit rules → symbolic AI
- dominant paradigm from the 1950s to the late 1980s
- **expert systems boom** of the 1980s
- symbolic Al suitable to solve well-defined, logical problems (like chess); impossible to figure out explicit rules for solving more complex, fuzzy problems like image classification, speech recognition etc.
- enter learning: ML emerged to take the place of symbolic Al
 - the missing piece was an efficient way to train large neural networks
 - → enter the backpropagation algorithm!
 - 1989, Yann LeCun: first application of NN to the recognition of handwritten digits







Beware of the hype!



too high expectations (hype)		disappointment		< research investment (stop progress)
------------------------------	--	----------------	--	---------------------------------------

This happened <u>twice</u> in the past:

1. symbolic Al in the 1960s:

- a. expectations: 1967, Marvin **Minsky**: "the problem of creating 'artificial intelligence' will be solved soon"; Minsky, 1970: "in three to eight years we will have a machine with the general intelligence of an average human being";
- b. failure: researchers and funds turned away from the field \rightarrow **first Al winter**

2. 1980s, expert systems:

- a. initial success stories attracted investment, companies developed expert systems
- b. expert systems were expensive to maintain, difficult to scale, limited in scope: interest declined
 → second Al winter







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What now? Third cycle of AI hype and disappointment? In spite of possibly unrealistic short-term expectations, the long-term picture is bright: **no short-term hype** → **long-term vision instead!**

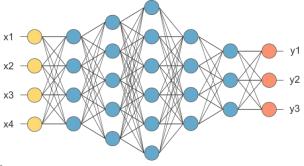






Rationing NN through winter, before summer!

- 1990s: SVM (Vladimir Vapnik, 1995)
- 2000s: Random Forest, Gradient Boosting (tree-based methods)
- deep NN (DL at last!):
 - 2011, Dan Ciresan: **GPU-trained deep neural networks** for image classification
 - 2012, Alex Krizhevsky & Geoffrey Hinton: deep convolutional neural network → 83.6% accuracy at image classification
 - DL automates feature extraction and engineering



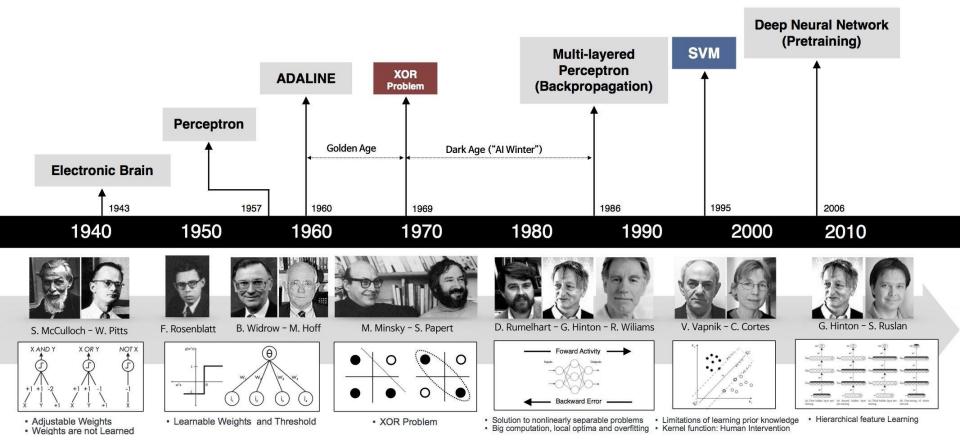






A little timeline of Neural Networks



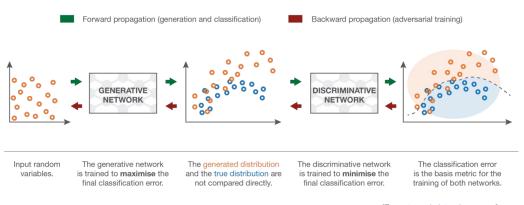


Credits: Andrew Beam, Department of Biomedical Informatics @ Harvard Medical School

Latest developments - what in the 2010/20s?

Physicia Courses

- DL and gradient boosting **dominate Kaggle competitions** since 2012
- unsupervised / semi-supervised learning → Google Brain, the cat experiment (2012, Arxiv)
- Generative Adversarial Networks (GANs): <u>lan Goodfellow et al.</u>, 2014: generative models trained "indirectly" by trying to fool another network that is trained at the same time to distinguish "generated" data from "true" data
- **GRU** (gated-recurrent units): Cho et al., 2014: breakthrough for RNN
- LLMs: large language models (more on this later)



[From: towardsdatascience.com]







[REF] History of deep learning



- McCulloch and Pitts, A logical calculus of the ideas immanent in nervous activity, 1943.
 https://link.springer.com/article/10.1007/BF02478259
- Wang and Raj, On the Origin of Deep Learning, 2017 https://arxiv.org/pdf/1702.07800.pdf
- Andrew Beam, Deep Learning 101 Part 1: History and Background, 2017
 https://beamandrew.github.io/deeplearning/2017/02/23/deep_learning_101_part1.html
- Chung et al., 2014. Empirical Evaluation of Gated Recurrent Neural Networks on Sequence Modeling → GRU layers https://arxiv.org/abs/1412.3555
- Hochreiter & Schmidhuber 1997. Long short-term memory → LSTM layers https://ieeexplore.ieee.org/abstract/document/6795963









Innovations in:

- Hardware
- Big Data
- Algorithms
- Infrastructure









Innovations in:

- Hardware:
 - CPUs now 5,000 times faster than 25 years ago
 - GPUs (thanks to videogames!)
 - TPUs (Tensor Processing Units: designed specifically for deep learning)
 - Active R&D on specialised A.I. processors/accelerators: e.g. <u>Google's</u>
 <u>TPU</u>, <u>Intel's Loihi</u>, <u>IBM's TrueNorth</u>



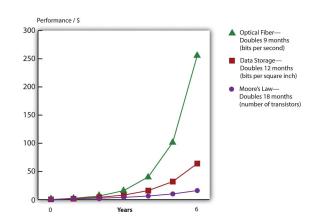






Innovations in:

- Big Data:
 - Internet: search engines, social media, image datasets etc.
 - IoT: sensors, interconnected devices
 - Data storage (Moore's law)
 - GPT-3 was trained on 570 GB of text data (september 2021)
 - Google Search index: 1e+8 GB



https://2012 books.lard bucket.org/books/getting-the-most-out-of-information-systems-v1.2/s09-moore-s-law-fast-cheap-computi.html.









Innovations in:

- Algorithms:
 - backpropagation/gradient propagation (efficient ways to solve deep learning models)
 - better activation functions (e.g. ReLU)
 - better optimizers (e.g. RMSProp and ADAM)
 - specialized layers (e.g. GRU, LSTM)









Innovations in:

- Infrastructure:
 - scaling-up of computation frameworks (e.g. cloud computing)
 - distributed computing (and storage)
 - programming frameworks







Deep learning is a matter of



Scale

- Available hardware (GPU: thanks gamers)
- Available big data (e.g. massive databases of <u>labeled</u> images)
- Available infrastructure
- Available pre-trained model (transfer learning)

Theoretical breakthrough

- ReLU activation functions
- Back propagation
- Gradient descent and other solvers/optimizers









State of the art: nerd stuff







Image generation

 \rightarrow



DALL·E 2 can create original, realistic images and art from a text description. It can combine concepts, attributes, and styles.

TEXT DESCRIPTION

An astronaut Teddy bears A bowl of soup

mixing sparkling chemicals as mad scientists shopping for groceries working

in the style of ukiyo-e as a one-line drawing in ancient Egypt



Credits: Dall-E 2 https://openai.com/dall-e-2/

Zero-Shot Text-to-Image Generation

Aditya Ramesh ¹ Mikhail Pavlov ¹ Gabriel Goh ¹ Scott Gray ¹ Chelsea Voss ¹ Alec Radford ¹ Mark Chen ¹ Ilya Sutskever ¹

Abstract

Text-to-image generation has traditionally focused on finding better modeling assumptions for training on a fixed dataset. These assumptions might involve complex architectures, auxiliary losses, or side information such as object part labels or segmentation masks supplied during training. We describe a simple approach for this task based on a transformer that autoregressively mod-



Play with the small version: Dall-E Mini (then train your own on Colab)

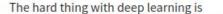
- https://dallemini.com/
- https://www.craiyon.com/
- https://github.com/borisdayma/dalle-mini
- https://colab.research.google.com/github/borisdayma/dalle-mini/blob/main/tools/inference/inference_nineline_invnb

Natural Language Processing (NLP)

2 - Supervised training on a specific task with a

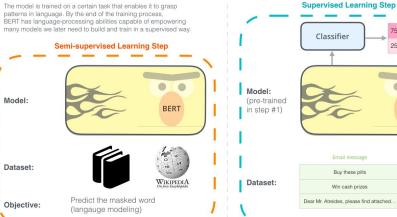
labeled dataset.





Spam

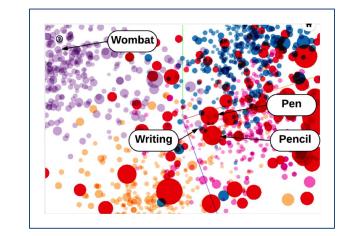
1 - Semi-supervised training on large amounts of text (books, wikipedia..etc). The model is trained on a certain task that enables it to grasp patterns in language. By the end of the training process. BERT has language-processing abilities capable of empowering many models we later need to build and train in a supervised way.



having the chance to make something happen.

to learn the system.

having an open mind.

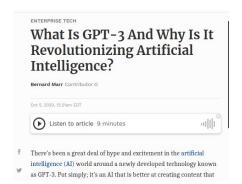


Credits:

https://mc.ai/whats-new-in-deep-learning-research-facebook-meta-embeddings-allow-nlp-models-to-choose-their/ http://ialammar.github.io/illustrated-bert/

Text generation: GPT2, 3, 3.5, 4...





What is GPT-3 Al and How Can it Help









https://doi.org/10.48550/arXiv.2005.14165

Submission history

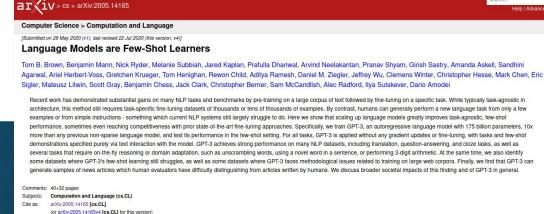
From: Tom B Brown [view email]
[v1] Thu, 28 May 2020 17:29:03 UTC (6,995 KB)
[v2] Mon, 1 Jun 2020 17:08:53 UTC (6,997 KB)
[v3] Fri, 5 Jun 2020 02:52:35 UTC (6,998 KB)
[v4] Wed, 22 Jul 2020 19:47:17 UTC (6,998 KB)



F FACEBOOK

in LINKEDIN

What Is GPT-3: How It Works and Why You Should Care



GPT3/4 → **ChatGPT**

- Has anybody <u>not</u> heard of ChatGPT?
- Hype of the moment: here to stay?
- → https://openai.com/blog/chatgpt/
- → https://chat.openai.com/auth/login

RTutor

- http://rtutor.ai
- uses OpenAl's powerful text-davinci-003 language model to translate natural language into R code

Microsoft Bing

- https://www.bing.com → chat
- Microsoft has beaten the competitors and started a partnership with OpenAI

User	help me write a short note to introduce myself to my neighbor
ChatGPT	Hi there, My name is [Your Name] and I just moved in next door. I wanted to reach out and introduce myself. I'm looking forward to getting to know you and the neighborhood. If you ever need anything or just want to chat, please don't hesitate to stop by or give me a call. Best, [Your Name]
User	can you make it more formal?
ChatGPT	Dear Neighbor, I am writing to introduce myself. My name is [Your Name] and I have recently moved in next door. I wanted to take a moment to reach out and say hello. I am looking forward to getting to know you and the neighborhood. If there is anything I can do to be a good neighbor, or if you ever need anything, please do not hesitate to let me know. I am happy to help in any way that I can. Sincerely, [Your Name]
User	can you send it for me?
ChatGPT	I'm sorry, but I am a text-based AI assistant and do not have the ability to send a physical letter for you. I can only provide suggestions and advice on what to write. It is up to you to take that advice and send the letter yourself.









OpenAl models are directly available (if you pay)



```
response = openai.Completion.create(
model="text-davinci-003",
  prompt="Tell me a joke about AI",
  temperature=0.6
)
```

- Models: https://platform.openai.com/docs/models/overview
- Cost is token-dependent, see https://platform.openai.com/tokenizer
- For actual application you'll need fine tuning: https://platform.openai.com/docs/guides/fine-tuning
- [QUESTION] A course for a deeper dive?







Alternatives to ChatGPT



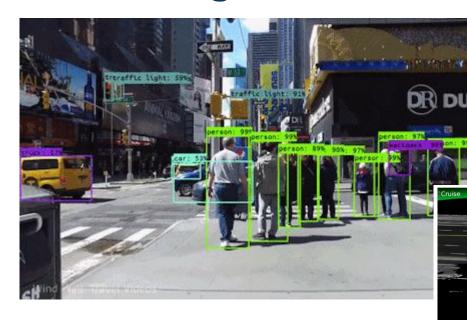
- Google's Bard:
 - https://bard.google.com/
 - More updated to recent world event
 - Less capable of complex tasks
- Meta's blenderbot
 - https://blenderbot.ai
 - Available to US only
 - Seems lagging a bit behind...
- Phind
 - https://www.phind.com/
 - Supports you for writing code
 - Not a chatbot







Self driving cars

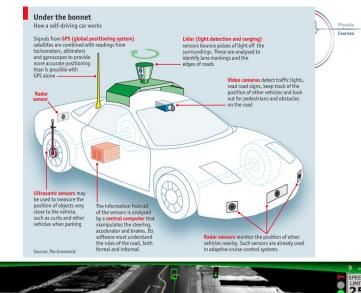




https://medium.com/@feiqi9047/the-data-science-behind-self-driving-cars-eb7d0579c80b





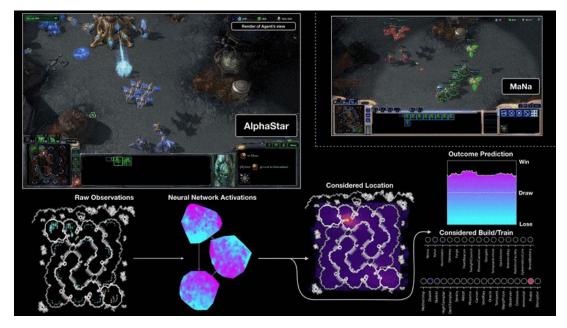


Games & Videogames











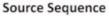




Generating believable videos (deepfake)









Our Reenactment (Full Head)



Averbuch-Elor et al. 2017



Living portraits









Credits:

https://www.gizmodo.co.uk/2018/06/deepfake-videos-are-getting-impossibly-good/

https://www.sciencealert.com/samsung-s-ai-can-now-generate-talking-heads-from-a-single-image

YouTube @ birbfakes

And many, many more...



- News Aggregation and Fraud News Detection
- <u>Virtual Assistants</u>
- Entertainment
- Visual Recognition
- Fraud Detection
- Healthcare
- Personalisations
- Detecting Developmental Delay in Children
- Colourisation of Black and White images
- Adding sounds to silent movies
- Automatic Machine Translation
- Automatic Handwriting Generation
- Language Translations
- Pixel Restoration
- Photo Descriptions
- Demographic and Election Predictions
- Deep Dreaming







[REF] Deep learning applications



- State of the art for self driving cars: https://neurohive.io/en/state-of-the-art/self-driving-cars/ and https://www.bloomberg.com/features/2020-self-driving-car-race/
- Waymo blog on their autonomous vehicles: https://blog.waymo.com/
- Updated repository of NPL state of the art https://github.com/sebastianruder/NLP-progress
- NPL transformers: https://github.com/huggingface/transformers
- NPL BERT
 https://medium.com/analytics-vidhya/text-classification-with-bert-using-transformers-for-long-text-inputs-f54833994df
 https://medium.com/analytics-vidhya/text-classification-with-bert-using-transformers-for-long-text-inputs-f54833994df
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 https://medium.com/analytics-vidhya/text-classification-with-bert-using-text-inputs-f54833994df
 https://medium.com/analytics-vidhya/text-classification-with-bert-using-text-us
- Deepmind Agent on mastering Atari Games
 https://deepmind.com/blog/article/Agent57-Outperforming-the-human-Atari-benchmark
- Deepmind AlphaGO on mastering the game of game of GO https://deepmind.com/research/case-studies/alphago-the-story-so-far
- Deepming Alphastar on mastering Real Time Strategy videogame Starcraft II
 https://deepmind.com/blog/article/alphastar-mastering-real-time-strategy-game-starcraft-ii
- Generating living portraits from few shots https://arxiv.org/abs/1905.08233
- Deep video portraits original paper ACM TOG 2018 conference https://dl.acm.org/doi/abs/10.1145/3197517.3201283









State of the art/2: wet stuff

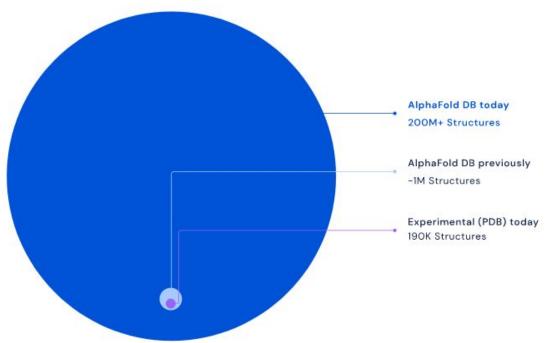






Protein folding + public DB

Number of Protein Structures



Images credit: AlphaFold reveals the structure of the protein universe https://www.deepmind.com/blog/alphafold-reveals-the-structure-of-the-protein-universe



nature

Explore content v About the journal v Publish with us v nature > articles > article Article Open Access | Published: 15 July 2021 Highly accurate protein structure prediction with **AlphaFold** John Jumper ☑, Richard Evans, ... Demis Hassabis ☑ + Show authors Nature 596, 583-589 (2021) | Cite this article

Abstract

Proteins are essential to life, and understanding their structure can facilitate a mechanistic understanding of their function. Through an enormous experimental effort 1.2.3.4, the structures of around 100,000 unique proteins have been determined but this represents a



pubs.acs.org/JPCB

<u>™</u> (9) (\$)

Al in Structural Biology

AlphaFold, Artificial Intelligence (AI), and Allostery

745k Accesses 2740 Citations 3148 Altmetric Metrics

Published as part of The Journal of Physical Chemistry virtual special issue "Protein Folding and Dynamic An Overview on the Occasion of Harold Scheraga's 100th Birthday".

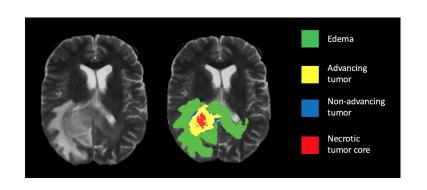
Ruth Nussinov,* Mingzhen Zhang, Yonglan Liu, and Hyunbum Jang



intelligence (AI). AlphaFold has appended projects and research directions.

Brain Tumor Segmentation







RANK	METHOD	DICE	EXTRA TRAINING DATA	PAPER	CODE	RESULT	YEAR
1	OM-Net + CGAp	87%	×	One-pass Multi-task Networks with Cross-task Guided Attention for Brain Tumor Segmentation	0	Ð	2019
2	CNN + 3D filters	85%	~	CNN-based Segmentation of Medical Imaging Data		∌	2017

Images credit: Brain Tumor Segmentation with Deep Neural Networks https://github.com/naldeborgh7575/brain_segmentation

Classification of medical images



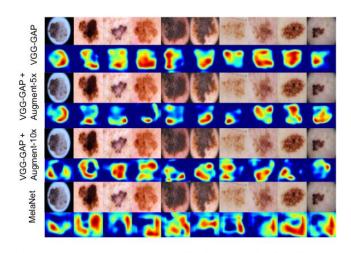


Figure 8: Grad-CAM heat maps for the correctly classified malignant cases by MelaNet and baseline methods.

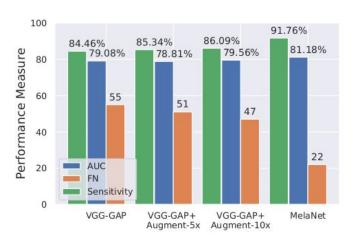


Figure 5: Classification performance of MelaNet and the baseline methods using AUC, FN and Sensitivity as evaluation metrics on the ISIC-2016 test set.

Source: Zunair and Hamza, 2020. Melanoma Detection using Adversarial Training and Deep Transfer Learning.







Drug discovery/optimization



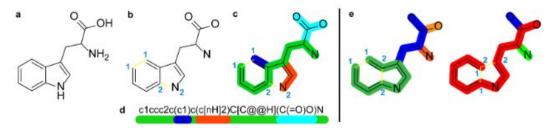
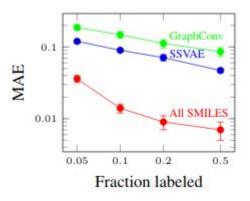


Figure 1: The molecular graph of the amino acid Tryptophan (a). To construct a SMILES string, all cycles are broken, forming a spanning tree (b); a depth-first traversal is selected (c); and this traversal is flattened (d). The beginning and end of intermediate branches in the traversal are denoted by (and) respective. The ends of broken cycles are indicated with matching digits. The full grammar is listed in Appendix D. A small set of SMILES strings can cover all paths through a molecule (e).



Source: Alperstein et al, 2019. All SMILES Variational Autoencoder

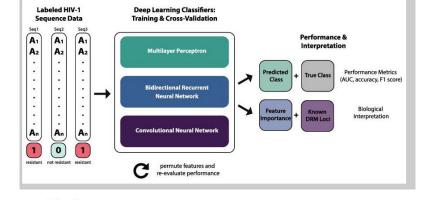






Drug resistance prediction





Viruses. 2020 May; 12(5): 560.

Published online 2020 May 19. doi: 10.3390/v12050560

Drug Resistance Prediction Using Deep Learning Techniques on HIV-1 Sequence Data

Margaret C. Steiner, 1,* Keylie M. Gibson, 1 and Keith A. Crandall 1,2

▶ Author information ▶ Article notes ▶ Copyright and License information <u>Disclaimer</u>

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7290575/



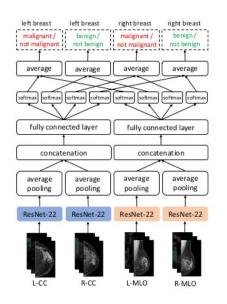


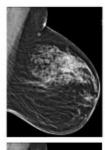


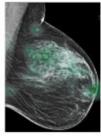
And the slack channel (thanks Pleuni!)

Breast Cancer detection









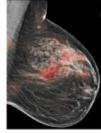
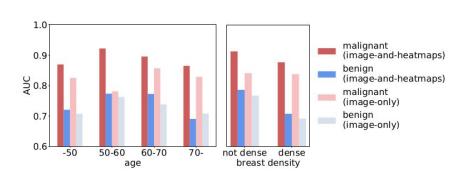


Fig. 5. The original image, the 'malignant' heatmap over the image and the 'benign' heatmap over the image.



Source: Wu et al, 2019. Deep Neural Networks Improve Radiologists' Performance in Breast Cancer Screening

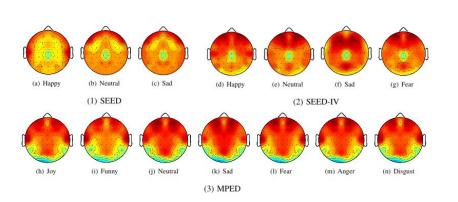






EEG interpretation/analysis





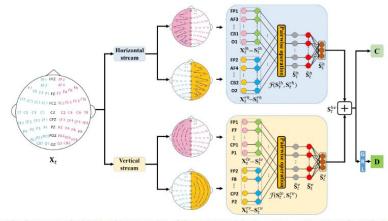


Fig. 1: The framework of BiHDM. BiHDM consists of four RNN modules to capture each hemispheric EEG electrodes' information from horizontal and vertical streams. Then all the electrodes' data representations interact and construct the final vector for the classifier and discriminator.

Source: Li et al., 2019. A Novel Bi-hemispheric Discrepancy Model for EEG Emotion Recognition

[REF] Deep learning state of the art



- Continuously updated applications of DL, divided by topic (Computer Vision, NPL, medical...)
 https://paperswithcode.com/sota
- MIT Deep learning state of the art 2020 seminar and course https://deeplearning.mit.edu/
- Deep Learning Papers Reading Roadmap
 https://github.com/floodsung/Deep-Learning-Papers-Reading-Roadmap







[REF] Conferences



- Deep Learning World is the premier conference covering the commercial deployment of deep learning https://www.deeplearningworld.com/
- Machine Learning Week Europe Berlin October 5-6, 2022 https://machinelearningweek.eu/







Keywords



- Classification
- Regression
- Data representation
- Model/Method/Algorithm/Software
- Data regularization
- Accuracy, error, correlation
- Overfitting
- Training set, test set









Can deep learning predict it all?







Difficult or easy?



 "Prediction is very difficult, especially about the future" (Niels Bohr)

Or not? (with deep learning)

- spam filters accuracy: 99.9% (1 out of 1000 emails escapes) [here]
- OCR (optical character recognition) accuracy: 99% [here]
- retinal disease diagnosis accuracy: 94.5% [here]
- LLMs, Chat-GPT etc.



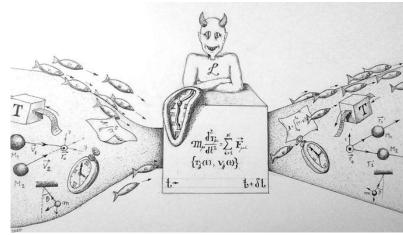






It has the ability to know the exact position and state of motion of **every particle in the universe**, and it fully understands the laws of physics that describe how they interact with each other.

In a **deterministic universe**, this all-knowing demon could work out how the universe will evolve over time and predict its state in the future.

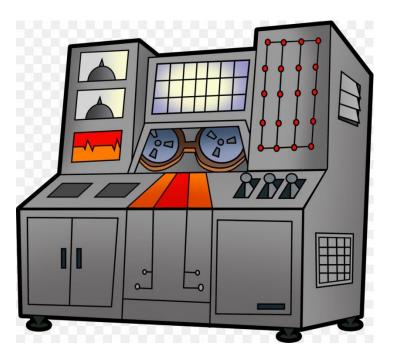


source

« Une intelligence qui, à un instant donné, connaîtrait toutes les forces dont la nature est animée et la situation respective des êtres qui la composent, si d'ailleurs elle était suffisamment vaste pour soumettre ces données à l'analyse, embrasserait dans la même formule les mouvements des plus grands corps de l'univers et ceux du plus léger atome ; rien ne serait incertain pour elle, et l'avenir, comme le passé, serait présent à ses yeux. »







source



Laplace's really believed in the deterministic universe and that his demon could predict everything.

But is this true?

We can think of Laplace's demon as a **supercomputer** that contains all the information of the universe, and is able to compute precisely how the future will unfold

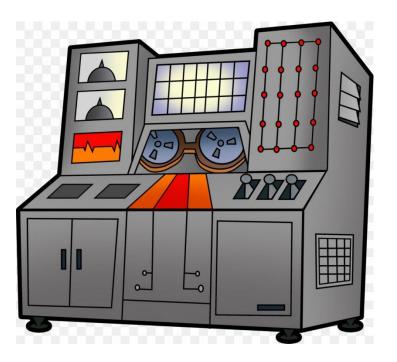
But then it could decide to use this information to change the course of events compared to its earlier prediction, thus making the prediction wrong (or a short-circuit may alter the course of events)

So can it or can it not predict everything?









source









Let's examine what it means for the supercomputer to have knowledge about its own decisions (or short-circuits)

To predict its own actions (voluntary or not) the supercomputer would need to include in the calculations also every details of its inner structure and functioning (the state and motion of every atom and every electron it is made of)

But this information would need to be stored in memory disks which are themselves made of atoms and particles arranged in a special way, which would be other pieces of information to be stored, and so on in an infinite recursion

The demon can't therefore include itself in its calculations, hence its knowledge of the universe is incomplete and its predictions imperfect





We conclude that this omniscient supercomputer can predict everything about the universe outside it, but not what happens inside it

Max theoretical accuracy is not 1, but maybe 0.99999

source







But is the universe deterministic?



Isaac Newton and the clockwork universe → determinism.

- The probabilistic nature of the quantum world:
 - The behaviour of single particles is unpredictable (e.g. radioactive decay)
 - The average behaviour of many particles is predictable







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Max theoretical accuracy further down, from 0.99999 to say 0.99988







And is the universe predictable?



- Konrad Lorenz and the butterfly effect: tiny changes in the initial conditions lead to huge differences in the end results:
 - e.g. weather, or tossing a coin in the exact same manner
 - to make 100% accurate predictions we would need to know the initial conditions to infinite accuracy (which is not possible)
- Chaos theory and nonlinear dynamics:
 - simple cause → complex effect (non linear) (e.g. turbulent fluids)
 - determinism can generate randomness: a complex system obeys the laws of physics, but can become disordered and unpredictable
 - but also: from a chaotic system order and structure may emerge (e.g. A.I.)







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More reasons to reduce the max theoretical accuracy from 0.99999 to say 0.99988







To sum up



- part of the universe may be inherently random / probabilistic
- even if our universe is deterministic:
 - Laplace's demon can never know it all
 - sensitivity to the initial conditions and chaos theory lead to unpredictability

 "Prediction is still very difficult, not only about the future" (Niels Bohr)





