

17-18 July 2019 | Bayer AG R&D, Berlin, Germany

an introduction to deep learning

Marco Chierici

Fondazione Bruno Kessler

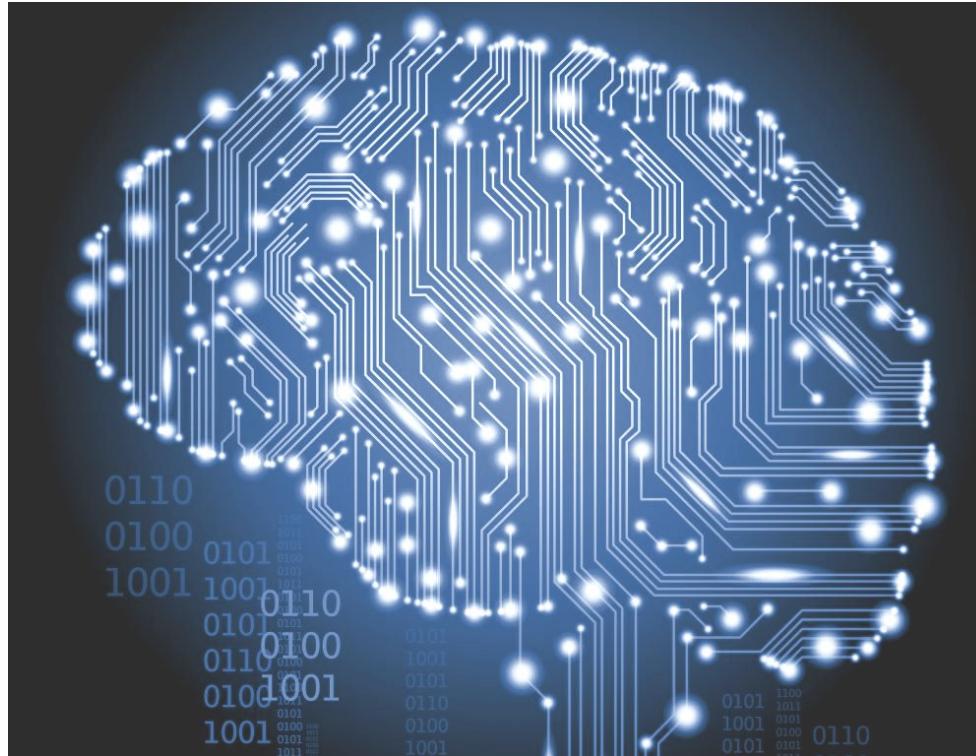
chierici@fbk.eu



machine learning

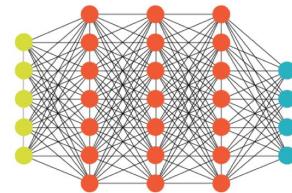
*The ability to learn making **predictions from data** without being explicitly programmed*

arthur samuel, 1959



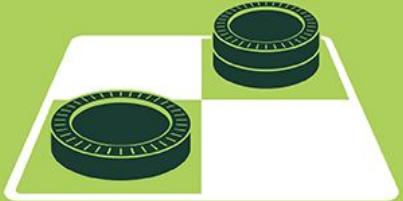
deep learning

*The ability to **learn representations** of data with multiple levels of **abstraction** through multiple processing **layers***



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MACHINE LEARNING

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DEEP LEARNING

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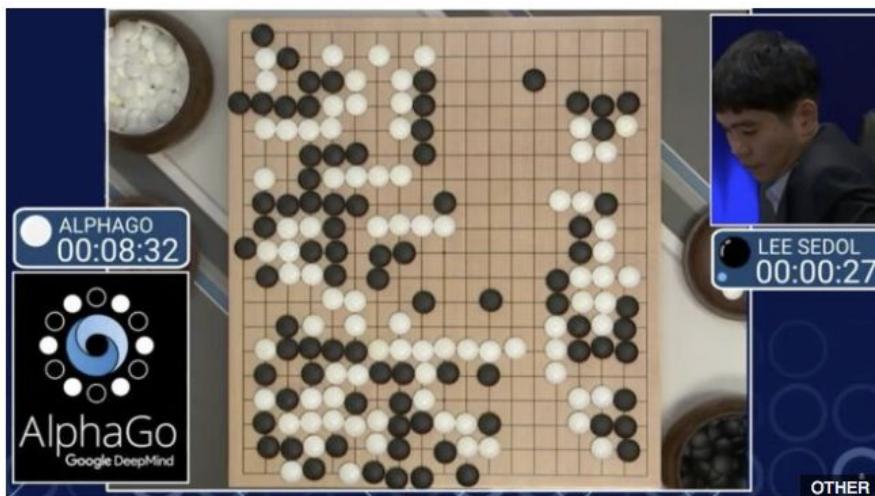
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Technology

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12 March 2016

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

DeepMind

hitting the headlines

The Telegraph

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AlphaZero in four hours

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AlphaGo Zero: Google DeepMind
supercomputer learns 3,000 years of
human knowledge in 40 days

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Article

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)

doi:10.1038/nature24270

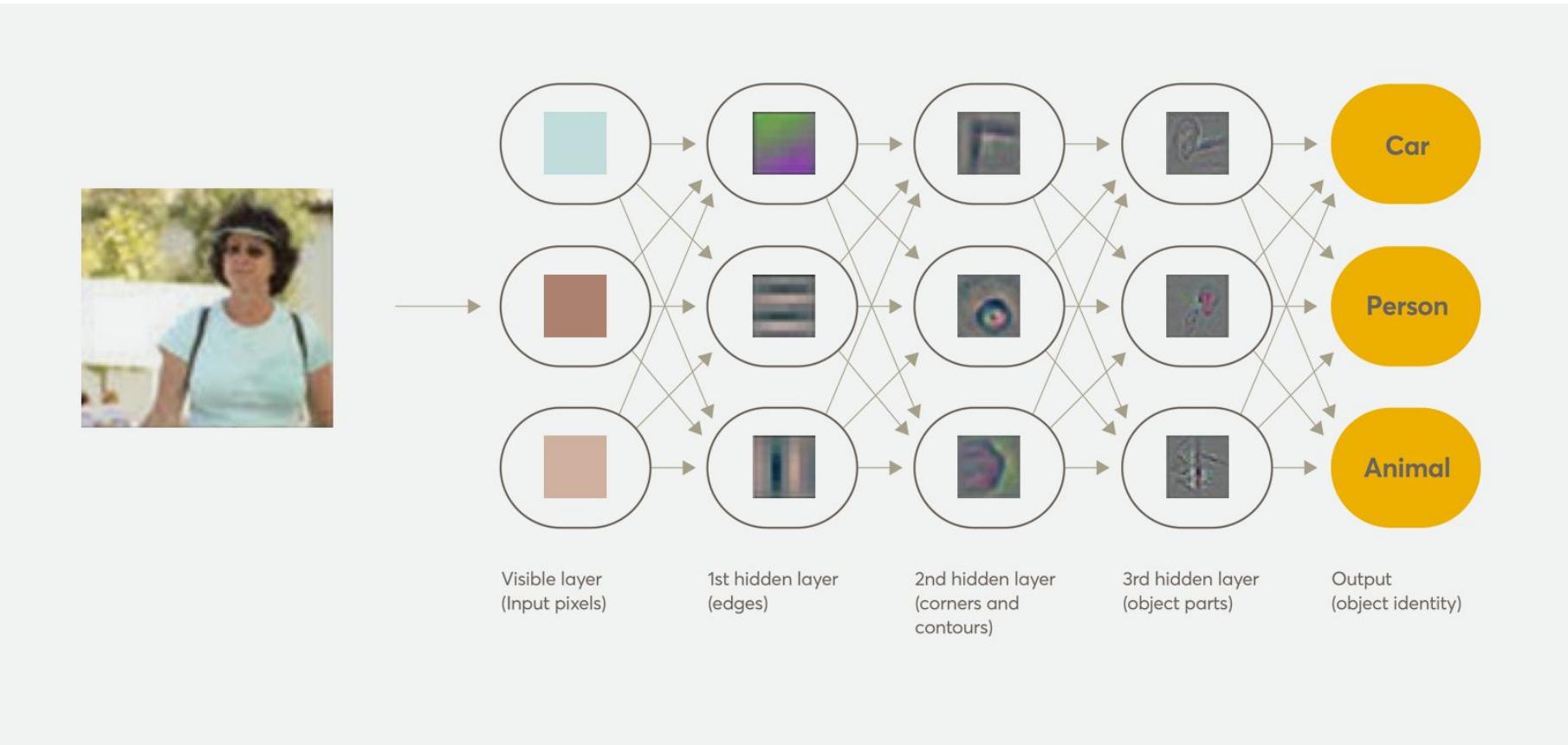
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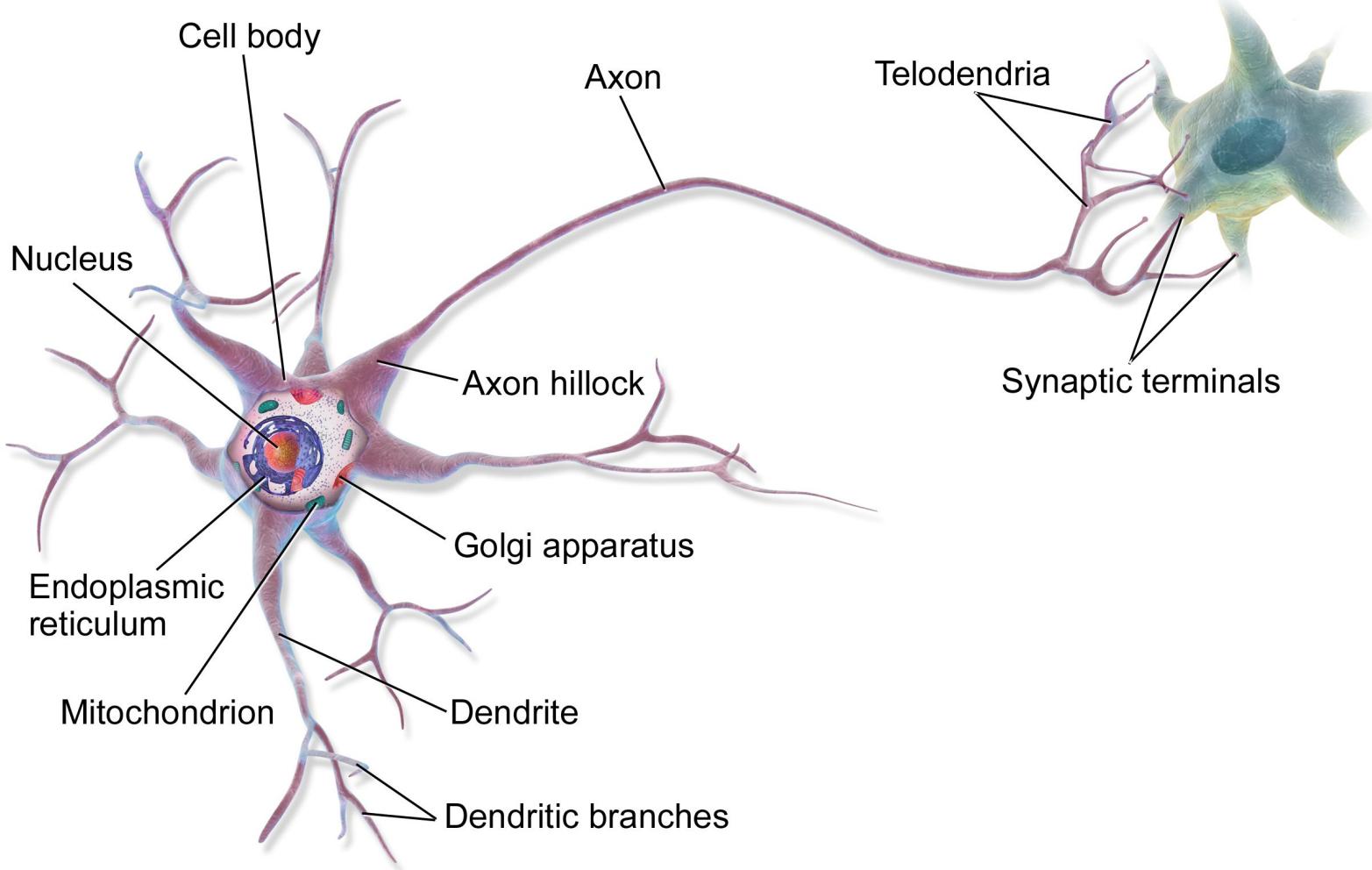
Accepted: 13 September 2017

Published: 18 October 2017

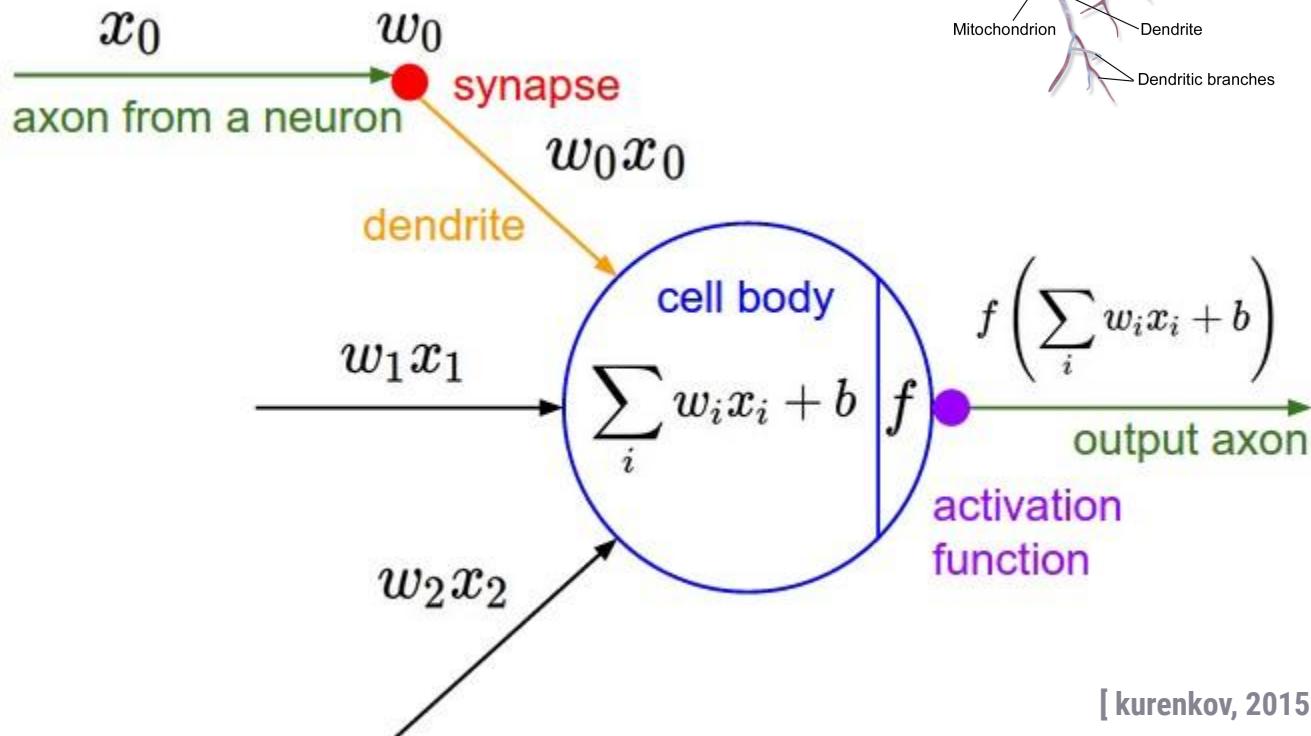
deep learning view



neurons



neuron model

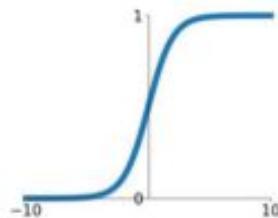


[kurenkov, 2015]

activation functions

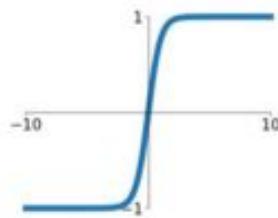
Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



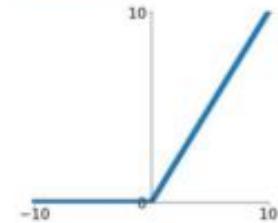
tanh

$$\tanh(x)$$



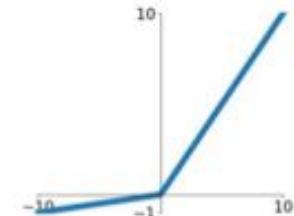
ReLU

$$\max(0, x)$$



Leaky ReLU

$$\max(0.1x, x)$$

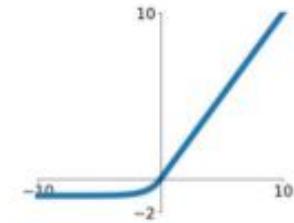


Maxout

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

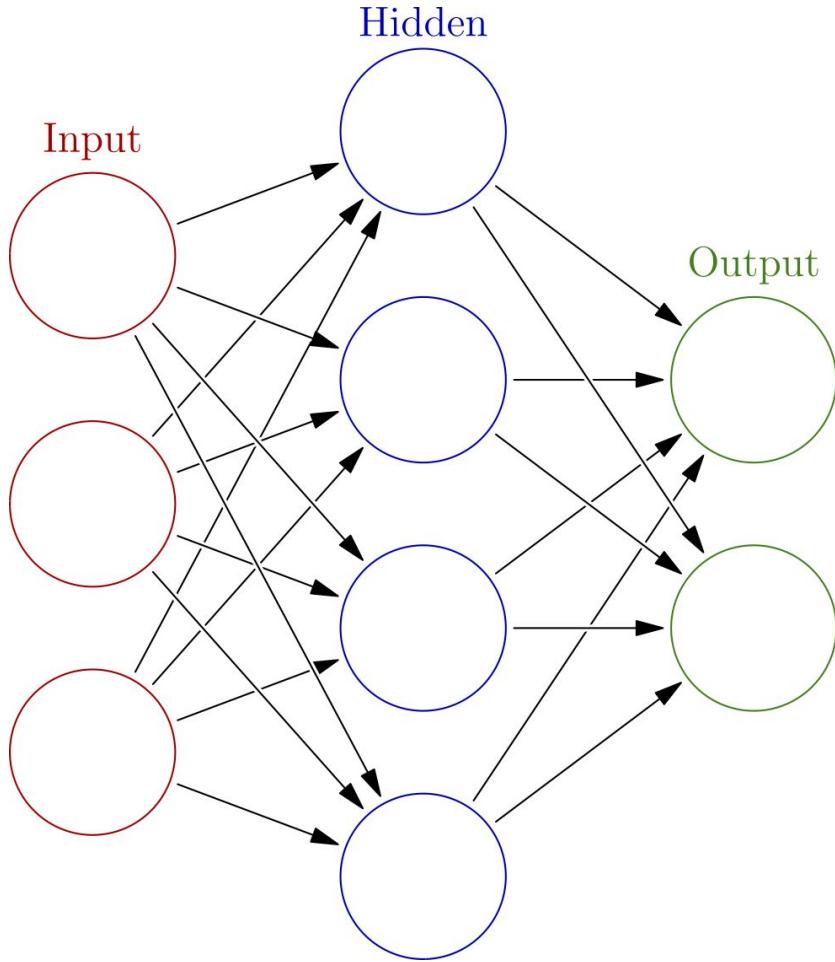
ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



[medium.com, 2017]

artificial neural networks



layer

all neurons at the same depth

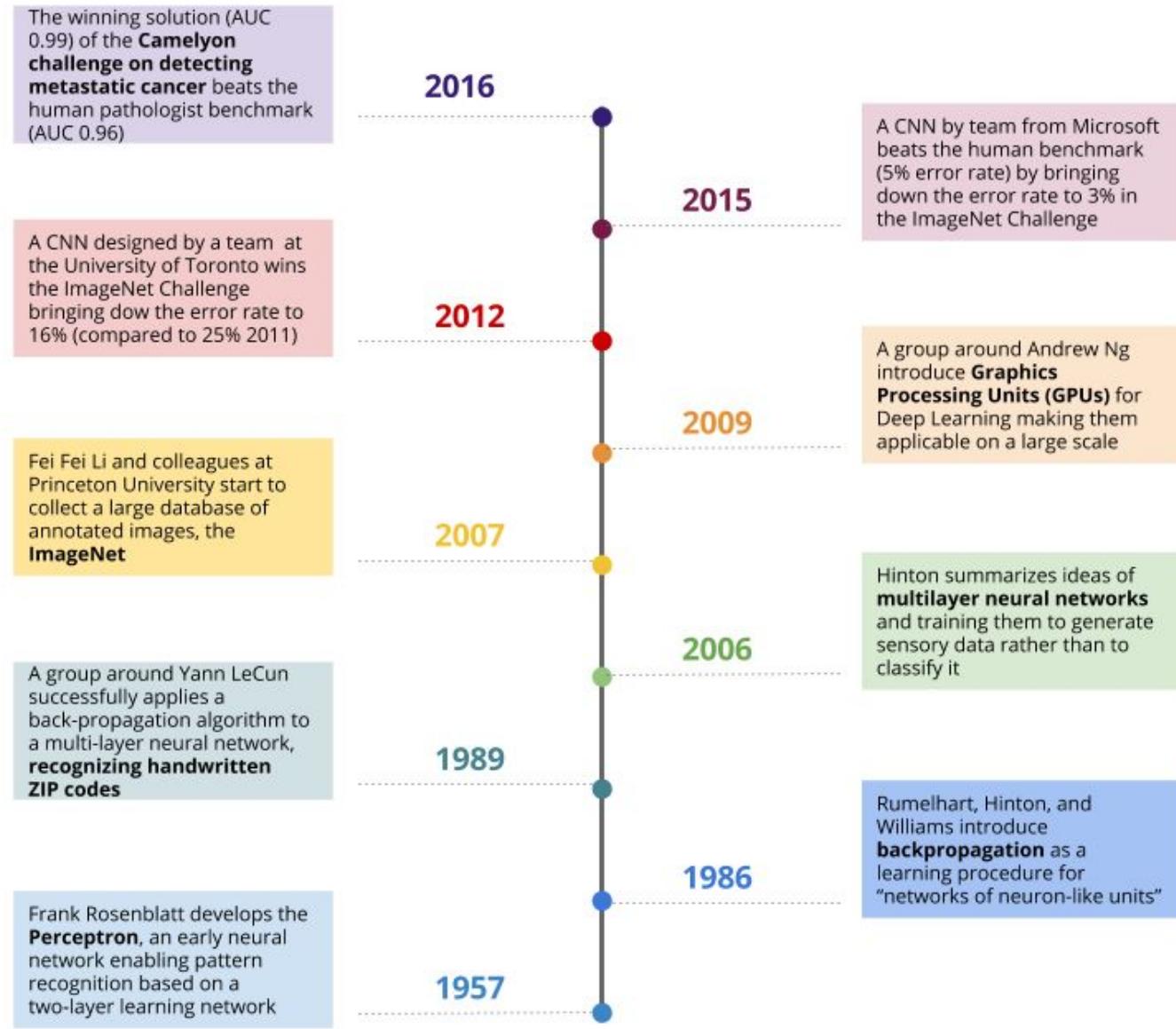
hidden layer

any layer but the input or output layer

deep learning

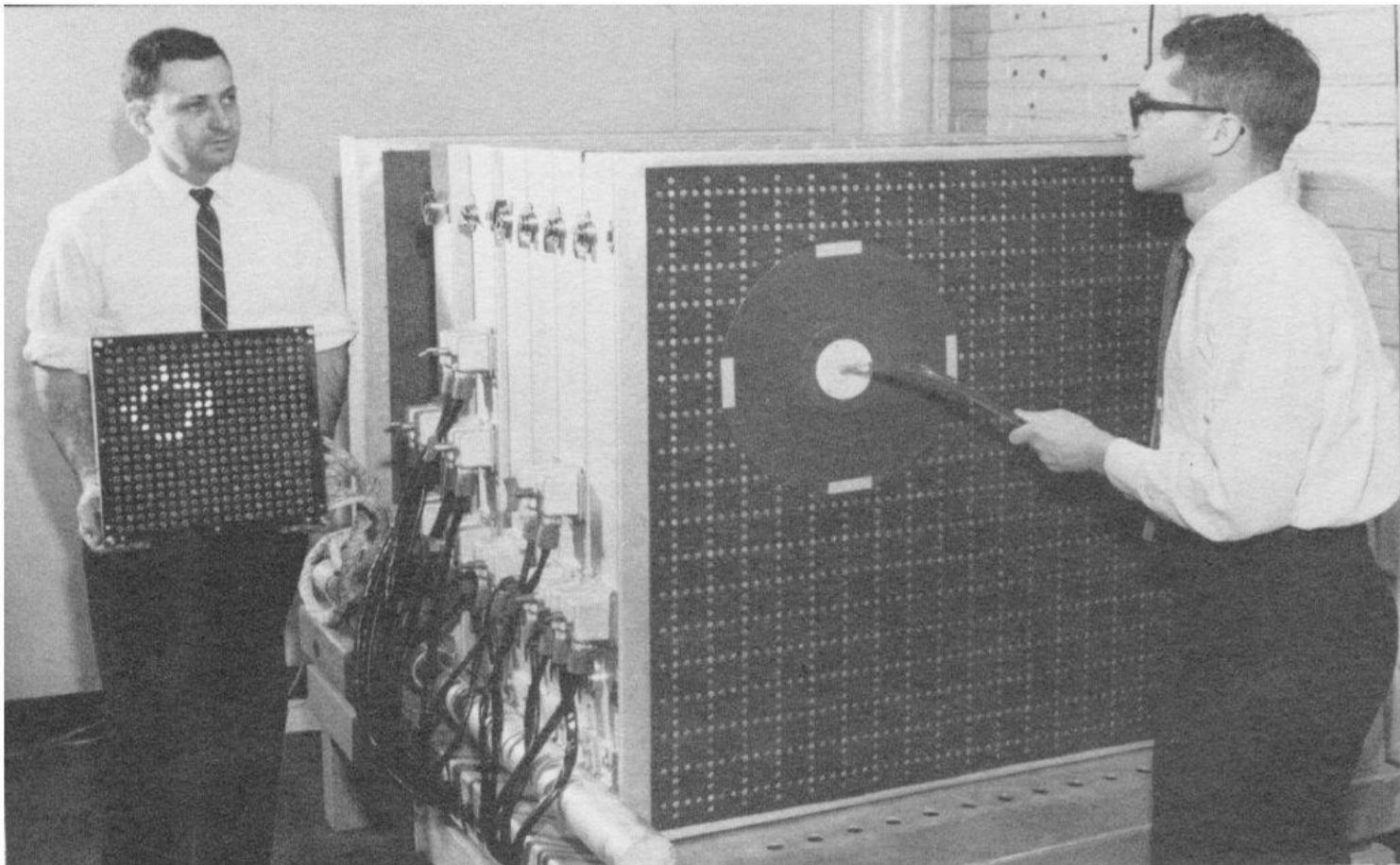
many hidden layers (> 3)

timeline

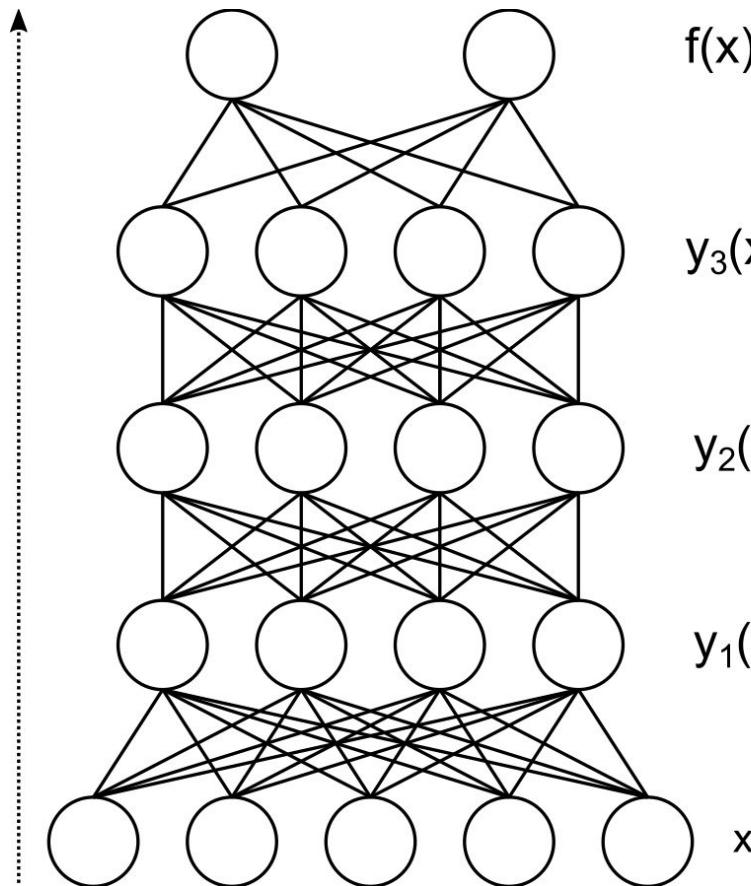


[Wahrmann, 2017]

| 1957 Rosenblatt perceptron



multilayer perceptron



$$f(x) = \varphi_4(W_4 y_3(x))$$

$$y_3(x) = \varphi_3(W_3 y_2(x)) = \varphi_3(W_3 \varphi_2(W_2 \varphi_1(W_1 x)))$$

$$y_2(x) = \varphi_2(W_2 y_1(x)) = \varphi_2(W_2 \varphi_1(W_1 x))$$

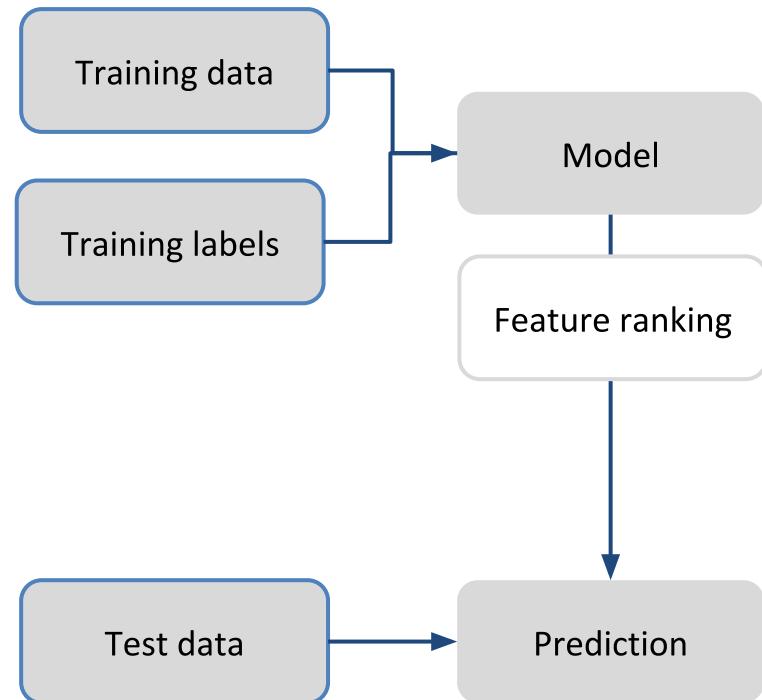
$$y_1(x) = \varphi_1(W_1(x))$$

multilayer perceptron in scikit-learn

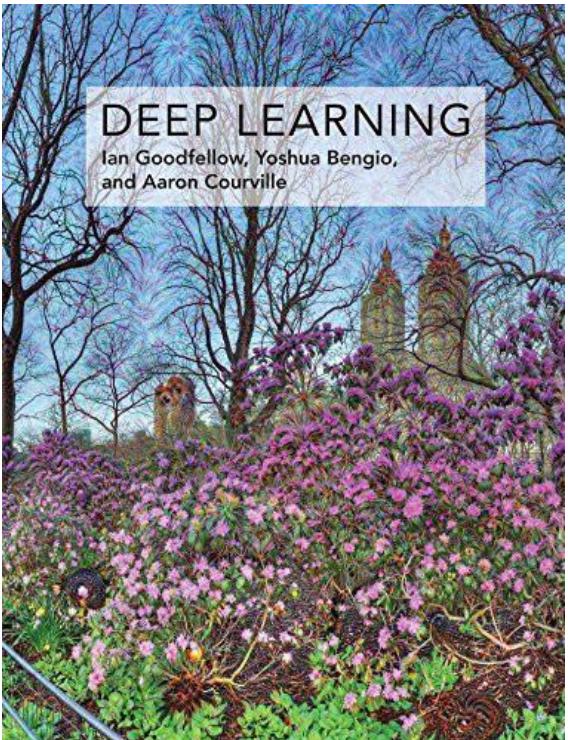
```
from sklearn.neural_network import MLPClassifier  
  
clf = SVC(solver='sgd', hidden_layer_sizes=(100, 50, 25, 2))
```

```
clf.fit(x_tr, y_tr)
```

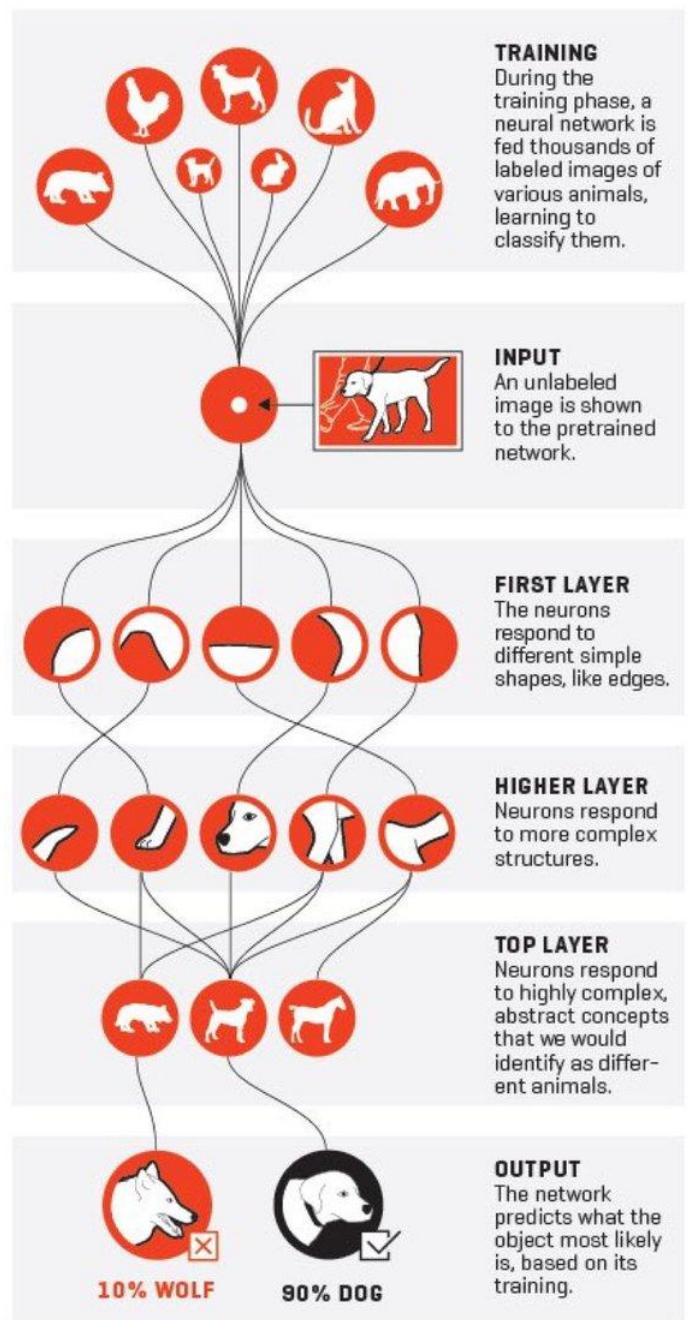
```
y_pred = clf.predict(x_ts)
```



take-home message



HOW NEURAL NETWORKS RECOGNIZE A DOG IN A PHOTO



challenges



@teenybiscuit (Karen Zack)



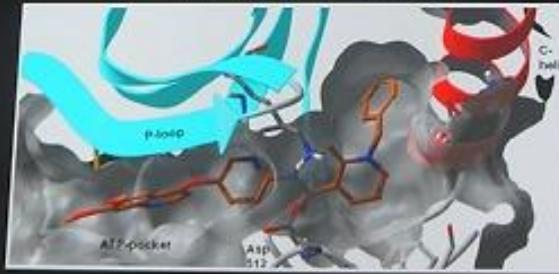
deep learning in biology.

DEEP LEARNING REVOLUTIONIZING MEDICAL RESEARCH

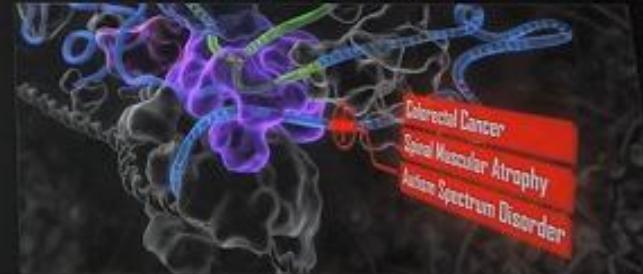
Detecting Mitosis in Breast Cancer Cells
— IDSIA



Predicting the Toxicity of New Drugs
— Johannes Kepler University

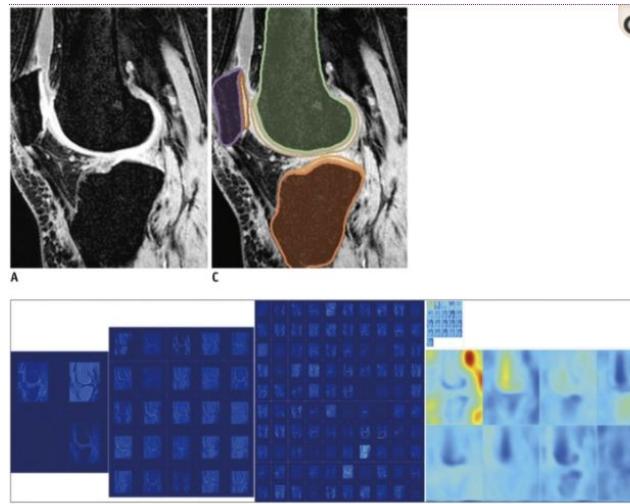


Understanding Gene Mutation to Prevent Disease
— University of Toronto

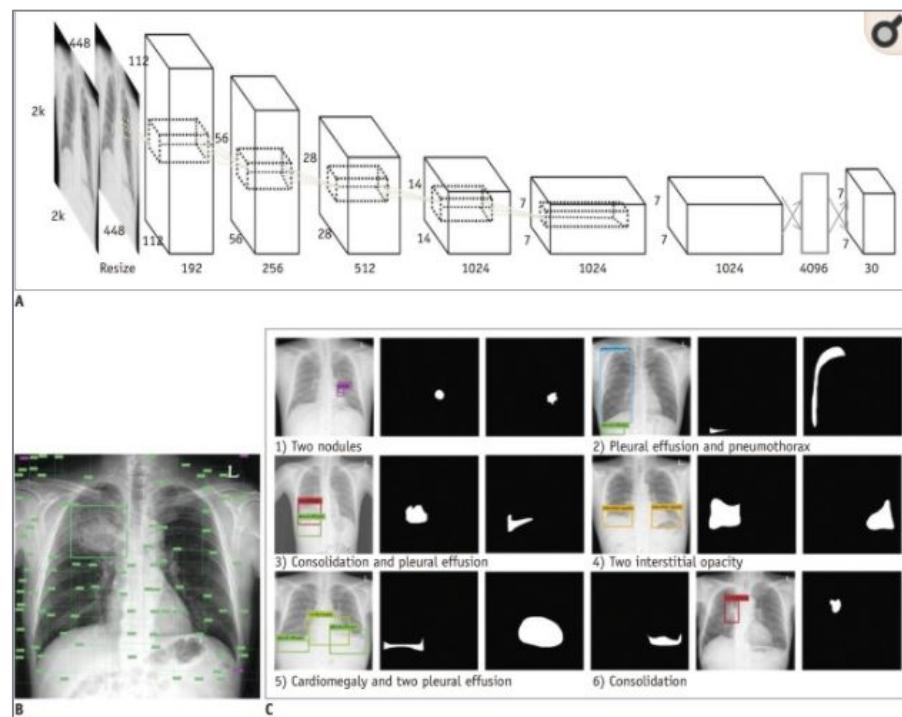


[nvidia, 2018]

imaging classification



[lee et al, 2017]



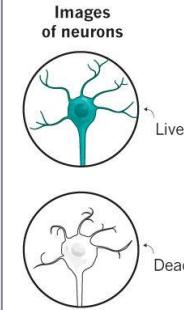
FONDAZIONE
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DEEP THOUGHTS

Deep-learning algorithms take many forms. Steve Finkbeiner's lab used a convolutional neural network (CNN) such as this one to identify, with high accuracy, dead neurons in a population of live and dead cells.

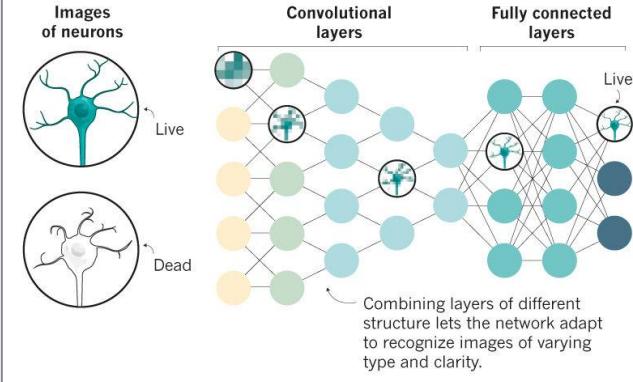
INPUT

The network is trained using several hundred thousand annotated images of live and dead cells.



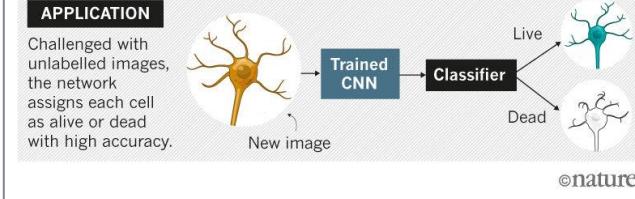
TRAINING AI

Over multiple iterations, the network discovers patterns in the data that can distinguish live from dead cells. Convolutional layers identify structural features of the images, which are integrated in fully connected layers.



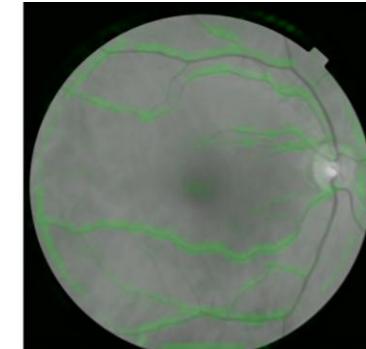
APPLICATION

Challenged with unlabelled images, the network assigns each cell as alive or dead with high accuracy.

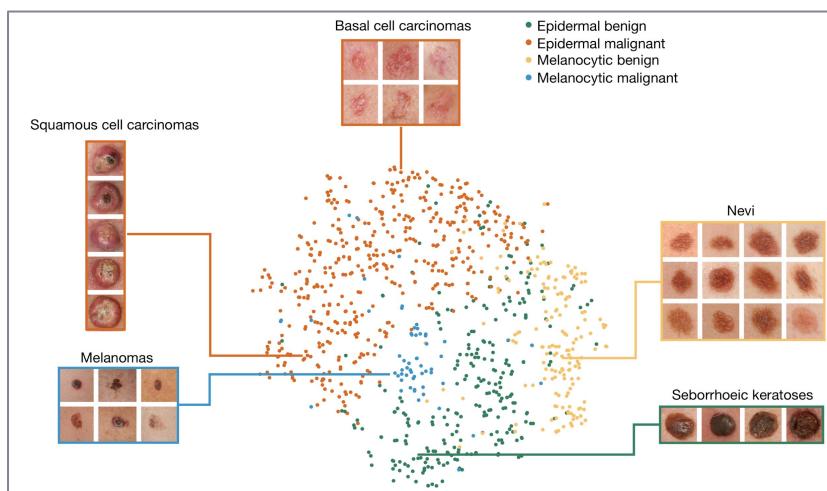


[finkbeiner, 2018]

[google & stanford, 2018]



breakthrough



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International journal of science

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Letter

Dermatologist-level classification of skin cancer with deep neural networks

Andre Esteva ✉, Brett Kuprel ✉, Roberto A. Novoa ✉, Justin Ko, Susan M. Swetter, Helen M. Blau & Sebastian Thrun ✉

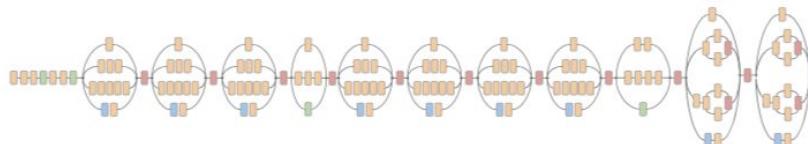
Nature 542, 115–118 (02 February 2017)
doi:10.1038/nature21056
Received: 28 June 2016
Accepted: 14 December 2016
Published: 25 January 2017
Download Citation
Diagnosis | Machine learning | Skin cancer
Corrigendum: 28 June 2017

129,450 images, 2,032 diseases: DL \sim 21 board-certified dermatologists

Skin lesion image



Deep convolutional neural network (Inception v3)



- Convolution
- AvgPool
- MaxPool
- Concat
- Dropout
- Fully connected
- Softmax

Training classes (757)

- Acral-lentiginous melanoma
- Amelanotic melanoma
- Lentigo melanoma
- ...
- Blue nevus
- Halo nevus
- Mongolian spot
- ...
- ...
- ...

Inference classes (varies by task)

- 92% malignant melanocytic lesion
- 8% benign melanocytic lesion

other clinical apps



Predicting cancer outcomes from histology and genomics using convolutional networks

Pooya Mobadersany^a, Safoora Yousefi^a, Mohamed Amgad^a, David A. Gutman^b, Jill S. Barnholtz-Sloan^c, José E. Velázquez Vega^d, Daniel J. Brat^e, and Lee A. D. Cooper^{a,f,g,1}

^aDepartment of Biomedical Informatics, Emory University School of Medicine, Atlanta, GA 30322; ^bDepartment of Neurology, Emory University School of Medicine, Atlanta, GA 30322; ^cCase Comprehensive Cancer Center, Case Western Reserve University School of Medicine, Cleveland, OH 44106; ^dDepartment of Pathology and Laboratory Medicine, Emory University School of Medicine, Atlanta, GA 30322; ^eDepartment of Pathology, Northwestern University Feinberg School of Medicine, Chicago, IL 60611; ^fWinship Cancer Institute, Emory University, Atlanta, GA 30322; and ^gDepartment of Biomedical Engineering, Emory University and Georgia Institute of Technology, Atlanta, GA 30322

EXPERT REVIEW OF PRECISION MEDICINE AND DRUG DEVELOPMENT, 2017

VOL. 2, NO. 5, 239–241

<https://doi.org/10.1080/23808993.2017.1380516>

EDITORIAL

The role of artificial intelligence in precision medicine

Bertalan Mesko

The Medical Futurist Institute; Department of Behavioral Sciences, Semmelweis University, Budapest, Hungary

SCIENTIFIC REPORTS

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Article | OPEN

Predicting clinical outcomes from large scale cancer genomic profiles with deep survival models

Safoora Yousefi, Fatemeh Amrollahi, Mohamed Amgad, Chengliang Dong, Joshua E. Lewis, Congzheng Song, David A. Gutman, Sameer H. Halani, Jose Enrique Velazquez Vega, Daniel J. Brat & Lee A. D. Cooper

Scientific Reports 7, Article number: 11707

(2017)

[doi:10.1038/s41598-017-11817-6](https://doi.org/10.1038/s41598-017-11817-6)

Received: 23 May 2017

Accepted: 30 August 2017

Published online: 15 September 2017

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Artificial intelligence in health care: enabling informed care

Lionel Tarassenko, Peter Watkinson

Published: 31 March 2018

SCIENTIFIC REPORTS

Altmetric: 909 Citations: 30

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Article | OPEN

Deep Patient: An Unsupervised Representation to Predict the Future of Patients from the Electronic Health Records

Riccardo Miotto, Li Li, Brian A. Kidd & Joel T. Dudley

Scientific Reports 6, Article number: 26094

(2016)

[doi:10.1038/srep26094](https://doi.org/10.1038/srep26094)

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Received: 28 January 2016

Accepted: 27 April 2016

Published: 17 May 2016

other clinical apps

New Results

Opportunities And Obstacles For Deep Learning In Biology And Medicine

Travers Ching, Daniel S. Himmelstein, Brett K. Beaulieu-Jones, Alexandr A. Kalinin, Brian T. Do, Gregory P. Way, Enrico Ferrero, Paul-Michael Agapow, Wei Xie, Gail L. Rosen, Benjamin J. Lengerich, Johnny Israeli, Jack Lanchantin, Stephen Woloszyn, Anne E. Carpenter, Avanti Shrikumar, Jinbo Xu, Evan M. Cofer, David J. Harris, Dave DeCaprio, Yanjun Qi, Anshul Kundaje, Yifan Peng, Laura K. Wiley, Marwin H. S. Segler, Anthony Gitter, Casey S. Greene

doi: <https://doi.org/10.1101/142760>

Previous



Posted May 28, 2017

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Conclusions

Deep learning-based methods now match or surpass the previous state of the art in a diverse array of tasks in patient and disease categorization, fundamental biological study, genomics, and treatment development. Returning to our central question: given this rapid progress, has deep learning transformed the study of human disease? Though the answer is highly



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Deep learning in bioinformatics

Seonwoo Min, Byunghan Lee, Sungroh Yoon

Brief Bioinform bbw068. DOI: <https://doi.org/10.1093/bib/bbw068>

Published: 25 July 2016 Article history ▾

Although deep learning holds promise, it is not a silver bullet and cannot provide great results in ad hoc bioinformatics applications. There remain many potential challenges, including limited or imbalanced data, interpretation of deep learning results, and selection of an appropriate architecture and hyperparameters. Furthermore, to fully exploit the capabilities of

608

IEEE TRANSACTIONS ON NANOBIOSCIENCE, VOL. 14, NO. 6, SEPTEMBER 2015

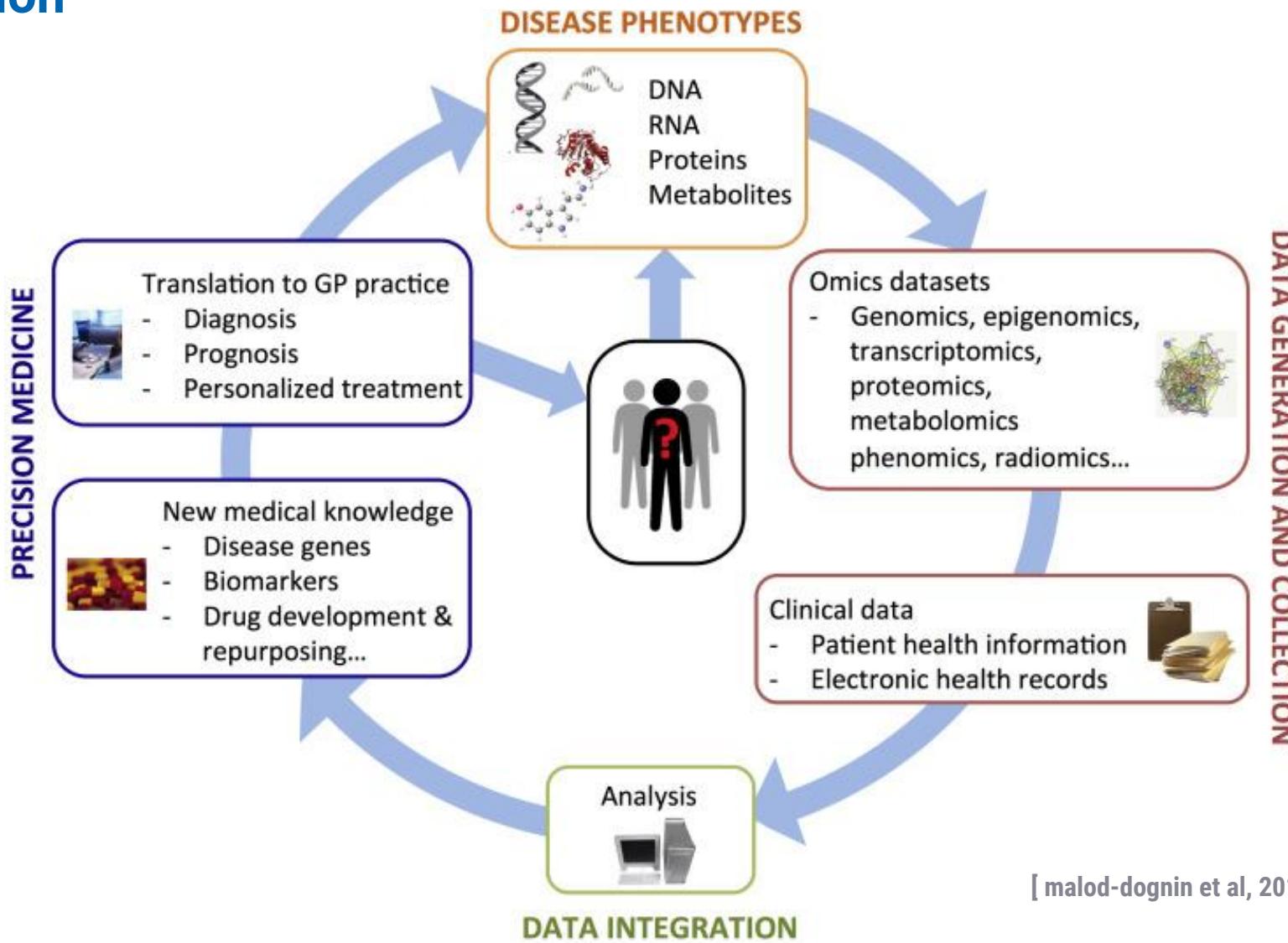
Multi-Layer and Recursive Neural Networks for Metagenomic Classification

Gregory Ditzler*, Member, IEEE, Robi Polikar, Senior Member, IEEE, and Gail Rosen, Senior Member, IEEE

V. DISCUSSION

The experiments discussed in the previous section demonstrated that: i) the deep learning approaches are not superior, at least on the data sets we evaluated, and ii) traditional MLPNNs are quite competitive with the RFCs, and in general perform better. However, none of the classifiers—deep or shallow—uniformly performs better than the RFCs across different experiments. The performance of the deep learning approaches may be improved upon with data sets that are much larger. It appears that—at least based on accuracy alone—the deep learning approaches may not be suitable for metagenomic applications. Accuracy, however, is not the only figure of merit.





thank you / danke / grazie !



Acks

Giuseppe Jurman
Margherita Francescato
Cesare Furlanello