



Andreas Holzinger
185.A83 Machine Learning for Health Informatics
2017S, VU, 2.0 h, 3.0 ECTS
Lecture 13 - Week 25 – 20.06.2017



Deep Learning Medical Towards Deep Transfer Learning

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<http://hci-kdd.org/machine-learning-for-health-informatics-course>



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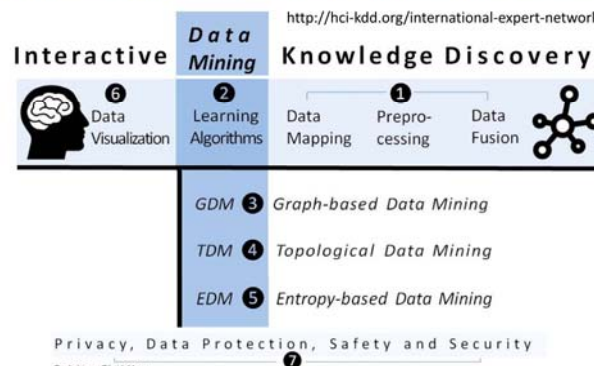
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01 Fundamentals: from Neural Networks to Deep Learning

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Holzinger, A. 2014. Trends in Interactive Knowledge Discovery for Personalized Medicine: Cognitive Science meets Machine Learning. IEEE Intelligent Informatics Bulletin, 15, (1), 6-14.

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NOTION	BIOLOGICAL UNIVERSE	COMPUTATIONAL UNIVERSE
Chromosome		
Fitness		
Gene		
Generation		
Individual		
Population		

Holzinger, K., Palade, V., Rabadan, R. & Holzinger, A. 2014. Darwin or Lamarck? Future Challenges in Evolutionary Algorithms for Knowledge Discovery and Data Mining. In: LNCS 8401. Heidelberg, Berlin: Springer, pp. 35-56.

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- Deep Learning := ML method based on learning representations of data. An observation (e.g., an image) can be represented in many ways such as a vector of intensity values per pixel, or in a more abstract way as a set of edges, regions of particular shape, etc.
- Feature:= specific measurable property of a phenomenon being observed.
- Feature engineering:= using domain knowledge to create features useful for ML. ("Applied ML is basically feature engineering. Andrew Ng").
- Feature learning:= transformation of raw data input to a representation, which can be effectively exploited in ML.

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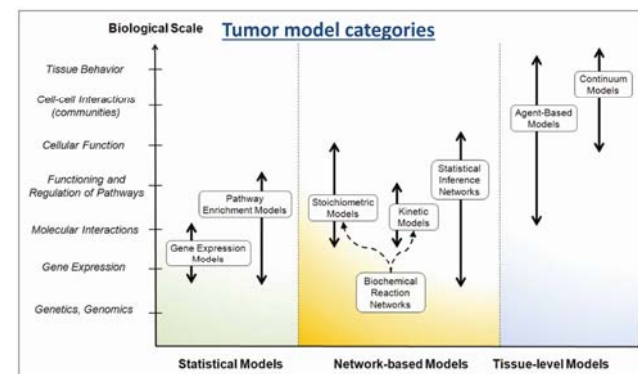
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- 00 Reflection
- 01 Fundamentals: From NN to Deep Learning
- 02 Representing and dealing with uncertainty
- 03 From Bayesian NN to Gaussian Processes
- 04 Stochastic Gradient Descent
- 05 Deep Autoencoders
- 06 Applications: Biomedical Examples
- 07 Future Challenges and Extravaganza Topics

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Edelman, L. B., Eddy, J. A. & Price, N. D. 2010. In silico models of cancer. Wiley Interdisciplinary Reviews: Systems Biology and Medicine, 2, (4), 438-459, doi:10.1002/wsbm.75.

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- High variety of data in the life sciences –
- a key to deal with high variety is data integration;
- What levels in deep learning architectures are appropriate for feature fusion with heterogeneous data [1]?

[1] Xue-Wen, C. & Xiaotong, L. 2014. Big Data Deep Learning: Challenges and Perspectives. Access, IEEE, 2, 514-525.

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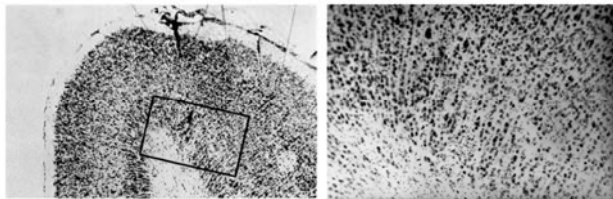
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Le, Q. V. Building high-level features using large scale unsupervised learning. IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), 2013. IEEE, 8595-8598.

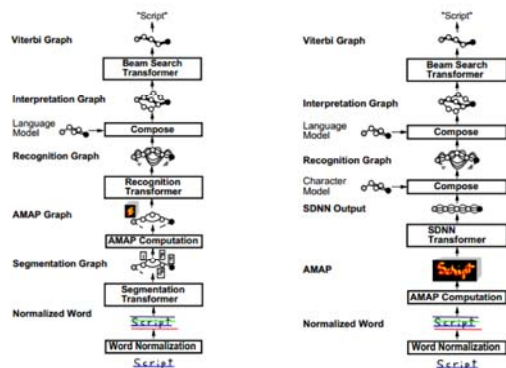
Cerebral cortex interconnections Hubel & Wiesel (1962)



106
J. Physiol. (1962), 168, pp. 106-154
With 5 plates and 20 text-figures
Printed in Great Britain
RECEPTIVE FIELDS, BINOCULAR INTERACTION AND FUNCTIONAL ARCHITECTURE IN THE CAT'S VISUAL CORTEX
By D. H. HUBEL AND T. N. WIESEL
From the Neurophysiology Laboratory, Department of Pharmacology
Harvard Medical School, Boston, Massachusetts, U.S.A.
(Received 31 July 1961)

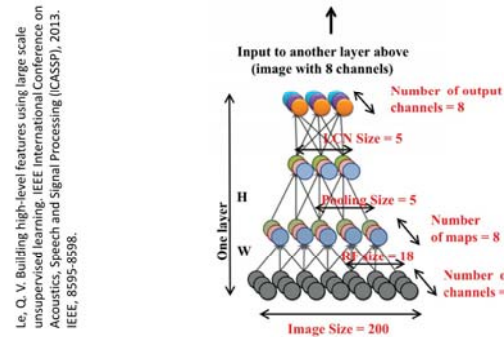
Hubel, D. H. & Wiesel, T. N. 1962. Receptive fields, binocular interaction and functional architecture in the cat's visual cortex. The Journal of physiology, 160, (1), 106-154.

Deep Learning 1998



Le Cun, Y., Bottou, L., Bengio, Y. & Haffner, P. 1998. Gradient-based learning applied to document recognition. Proceedings of the IEEE, 86, (11), 2278-2324.

Perform a num. optimization to find optimal stimuli



$$x^* = \arg \min_x f(x; W, H), \text{ subject to } \|x\|_2 = 1.$$

Principles of human information processing ...

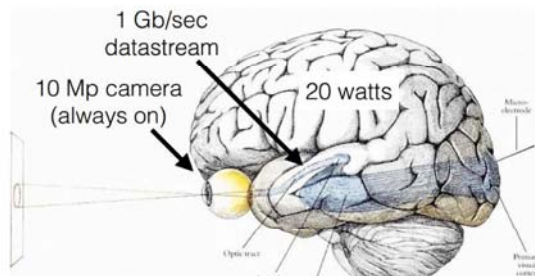
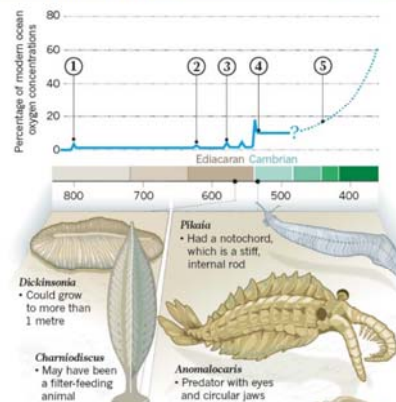


Image credit to Bruno Olshausen, Redwood Center for Theoretical Neuroscience, UC Berkeley
Olshausen BA (2014) Perception as an inference problem.
In: The Cognitive Neurosciences V,M. Gazzaniga, R. Mangun, Eds. MIT Press.

15 years later ... a kind of Cambrian explosion



<http://www.nature.com/news/what-sparked-the-cambrian-explosion-1.19379>

Historical Issues of Deep Learning



Gauss, C. F. (1809). Theoria motus corporum coelestium in sectionibus conicis solem ambientium.

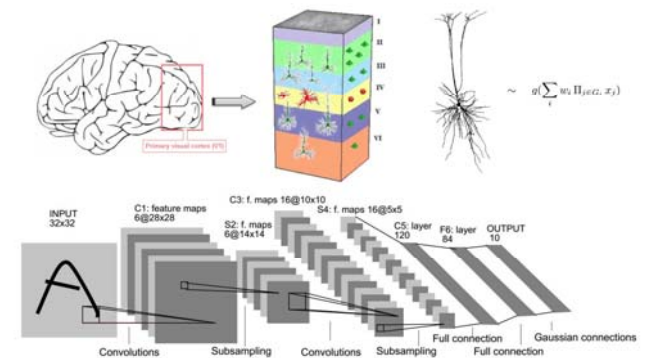
Gauss, C. F. (1821). Theoria combinationis observationum erroribus minimis obnoxiae (Theory of the combination of observations least subject to error)

Hebb, D. O. 1949. The organization of behavior: A neuropsychological approach, John Wiley & Sons.

Rosenblatt, F. 1958. The perceptron: a probabilistic model for information storage and organization in the brain. Psychological review, 65, (6), 386.

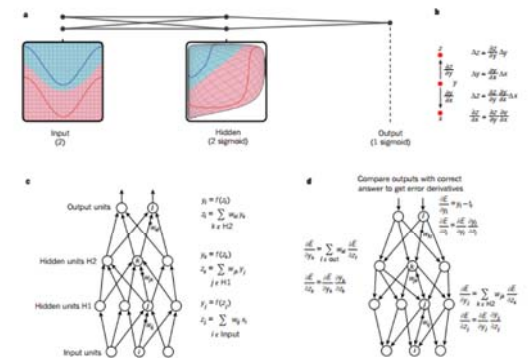
Excellent Review Paper: Schmidhuber, J. 2015. Deep learning in neural networks: An overview. Neural Networks, 61, 85-117.

From Deep Neural Learning to Deep Learning



Le Cun, Y., Bottou, L., Bengio, Y. & Haffner, P. 1998. Gradient-based learning applied to document recognition. Proceedings of the IEEE, 86, (11), 2278-2324.

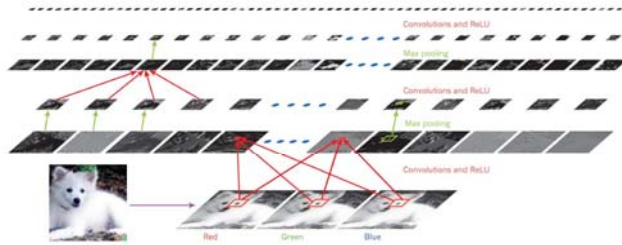
2015 ...



Le Cun, Y., Bengio, Y. & Hinton, G. 2015. Deep learning. Nature, 521, (7553), 436-444.

$$U(f) = (C_{W(K)} \dots \circ C_{W(2)} \circ C_{W(1)})(f)$$

Samoyed (3.6); Papillon (5.7); Pomeranian (2.7); Arctic fox (1.0); Eskimo dog (3.0); white wolf (3.0); Siberian husky (3.0)



Le Cun, Y., Bengio, Y. & Hinton, G. 2015. Deep learning. Nature, 521, (7553), 436-444.

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Limitations of Deep Learning approaches

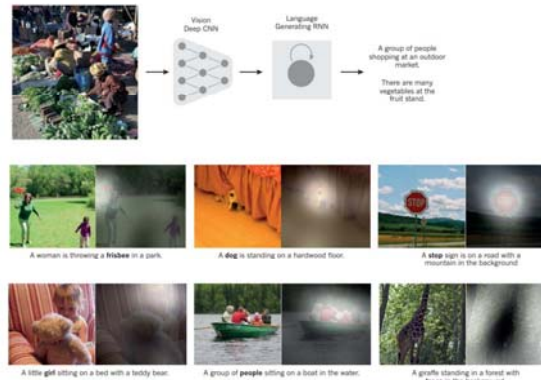


- Computational resource intensive (supercomps, cloud CPUs, **federated learning**, ...)
- Data intensive (needs often millions of training samples – “**big data**” is necessary!)
- Black-Box approaches – lack **transparency**, do not foster trust and acceptance among end-user, however, legal aspects make it difficult!
- Non-convex**: difficult to set up, to train, to optimize, needs a lot of expertise, error prone
- Most of all: bad in dealing with **uncertainty** ...

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Le Cun, Y., Bengio, Y. & Hinton, G. 2015. Deep learning. Nature, 521, (7553), 436-444.

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Features!



Image courtesy of Leon Bottou (2010)

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- Initial features**
 - Bio data -> DNA, RNA, Biomarker, Sequences, Genes, etc.
 - Images -> pixels, contours, textures, etc.
 - Time series data -> trends, reversals, anomalies, ticks, etc.
 - Signal data -> spectrograms, samples, etc.
 - Text data -> words, grammar classes, relations, etc.
- Combined features**
 - Combinations that linear system cannot represent, e.g.:
 - polynomial combinations, logical conjunctions, dec. trees.
 - Total number of features then grows **very quickly**.
- Solutions**
 - Kernels
 - Feature selection

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Book Recommendations



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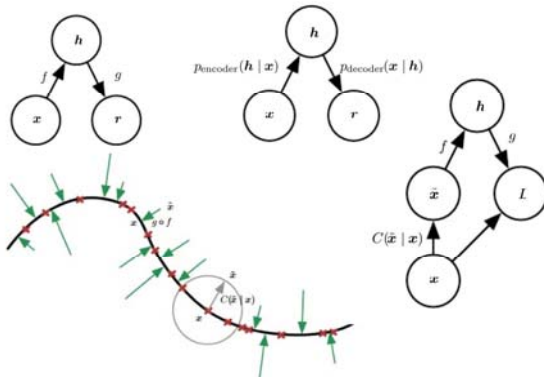
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02 Representing and Dealing with Uncertainty

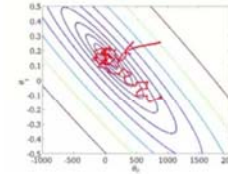
03 From Bayesian Networks to Gaussian Processes

04 Stochastic Gradient Descent



$$f(\theta) = \mathbb{E}[f(\theta, z)] \quad \bar{\theta}_k = \frac{1}{k} \sum_{t=1}^k \theta_t$$

Nemirovskii, A. & Yudin, D. 1978. Cesaro convergence of gradient method approximation of saddle points for convex-concave functions. Doklady Akademii Nauk SSSR, 239, 1056-1059.

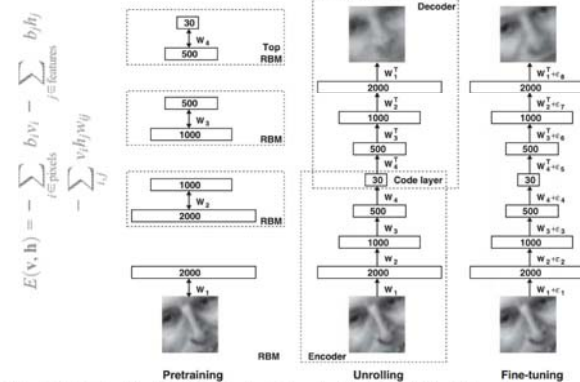


Algorithm 8.3: Stochastic gradient descent

```

1 Initialize  $\theta, \eta$ ;
2 repeat
3   Randomly permute data;
4   for  $i = 1 : N$  do
5      $g = \nabla f(\theta, z_i)$ ;
6      $\theta \leftarrow \text{proj}_{\Theta}(\theta - \eta g)$ ;
7   Update  $\eta$ ;
8 until converged;
```

Murphy, K. P. 2012. Machine learning: a probabilistic perspective, Cambridge (MA), MIT press; Chapter 8.5.2



05 Deep Autoencoders (unsupervised NN)

- Encoder: Det. mapping f_{θ} that transforms an input vector x into a representation y
- Decoder: Resulting hidden representation y is then mapped back to a reconstructed d -dimensional vector z in input space, $z = g \circ \theta'(y)$. This mapping $g \circ \theta'$ is called the decoder

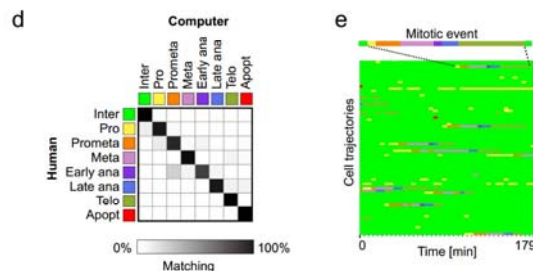
$$f_{\theta}(x) = s(Wx + b)$$

$$g_{\theta'}(y) = s(W'y + b')$$

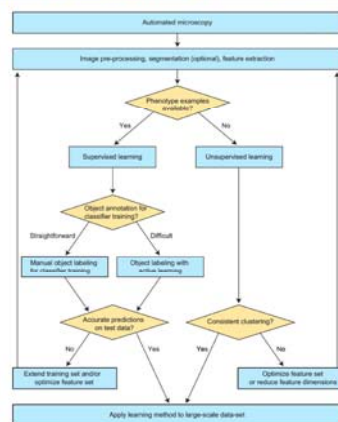
Vincent, P., Larochelle, H., Lajoie, I., Bengio, Y. & Manzagol, P.-A. 2010. Stacked denoising autoencoders: Learning useful representations in a deep network with a local denoising criterion. The Journal of Machine Learning Research, 11, 3371-3408.

06 Deep Learning Applications in Biomedicine

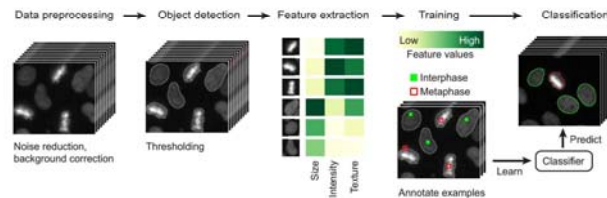
<http://www.nature.com/nmeth/journal/v7/n9/extref/nmeth.1486-S3.mov>



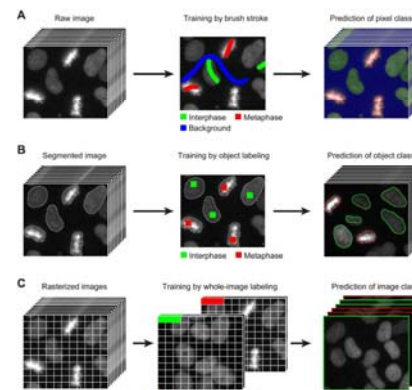
Held, M., Schmitz, M. H., Fischer, B., Walter, T., Neumann, B., Olma, M. H., Peter, M., Ellenberg, J. & Gerlich, D. W. 2010. CellCognition: time-resolved phenotype annotation in high-throughput live cell imaging. Nature methods, 7, (9), 747-754.



Sommer, C. & Gerlich, D. W. 2013. Machine learning in cell biology—teaching computers to recognize phenotypes. Journal of Cell Science, 126, (24), 5529-5539.

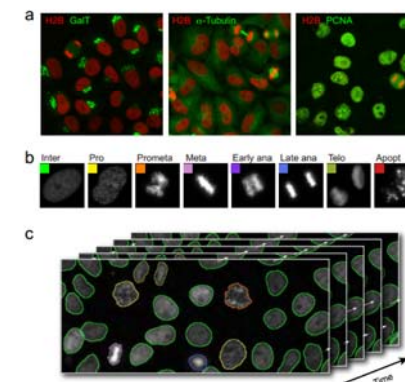


Sommer, C. & Gerlich, D. W. 2013. Machine learning in cell biology—teaching computers to recognize phenotypes. Journal of Cell Science, 126, (24), 5529-5539.

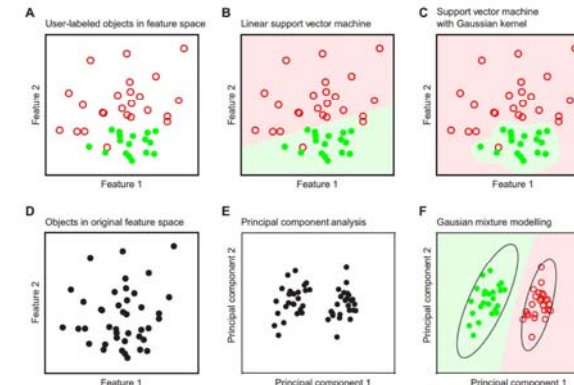


Sommer, C. & Gerlich, D. W. 2013. Machine learning in cell biology—teaching computers to recognize phenotypes. Journal of Cell Science, 126, (24), 5529-5539.

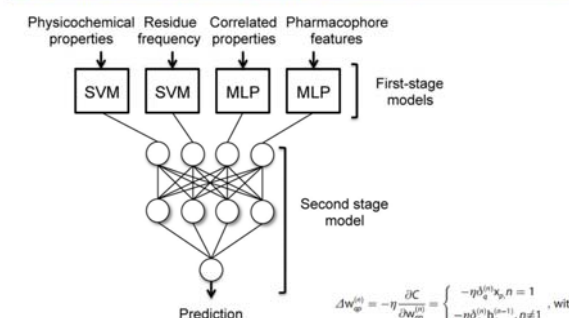
- Cell Profiler and Cell Profiler Analyst (Carpenter et al., 2006; Jones et al., 2008; Kamentsky et al., 2011) (<http://www.cellprofiler.org>).
 - Incl. modular workflow design, which enables rapid development of analysis assays. It provides a multi-class active learning interface based on boosting. CellProfiler runs on all major operating systems and supports computing on clusters for large-scale screening.
- Cell Cognition (Held et al., 2010) (<http://www.cellcognition.org/>)
 - has been optimized for time-resolved imaging applications. It comprises a complete machine-learning pipeline from cell segmentation and feature extraction to supervised and unsupervised learning. Cell Cognition runs on all major operating systems and supports computing on clusters for large-scale screening.
- ilastik (Sommer et al., 2011) (<http://www.ilastik.org>)
 - is an interactive segmentation tool based on pixel classification, which facilitates more complex image-segmentation tasks and provides real-time feedback.
- Bioconductor image HTS and EBIImage (Gentleman et al., 2004; Pau et al., 2010; Pau et al., 2013) (<http://www.bioconductor.org>)
 - provides a versatile toolbox for statistical data analysis and image processing in the programming language R.



Held, M., Schmitz, M. H., Fischer, B., Walter, T., Neumann, B., Olma, M. H., Peter, M., Ellenberg, J. & Gerlich, D. W. 2010. CellCognition: time-resolved phenotype annotation in high-throughput live cell imaging. Nature methods, 7, (9), 747-754.



Sommer, C. & Gerlich, D. W. 2013. Machine learning in cell biology—teaching computers to recognize phenotypes. Journal of Cell Science, 126, (24), 5529-5539.

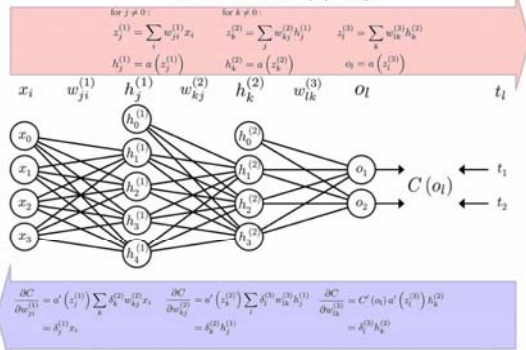


$$\Delta w_{\phi}^{(n)} = -\eta \frac{\partial C}{\partial w_{\phi}^{(n)}} = \begin{cases} -\eta \delta^{(n)} x_n, n=1 \\ -\eta \delta^{(n)} h_{\phi}^{(n-1)}, n \neq 1 \end{cases}, \text{ with}$$

$$\delta^{(n)} = \frac{\partial C}{\partial z_{\phi}^{(n)}} = \begin{cases} E(\phi) \delta^{(n)}, n=N \\ \delta^{(n)} \left(z_{\phi}^{(n+1)} \right) \sum_{i=1}^N \delta_i^{(n+1)} w_{\phi}^{(n+1)}, n \neq N \end{cases}$$

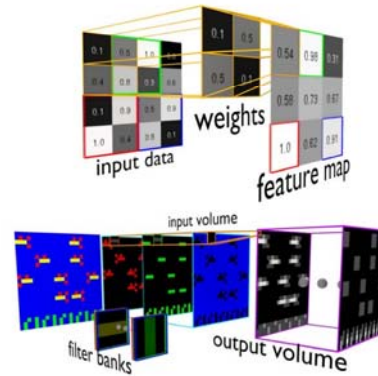
Gawehn, E., Hiss, J. A. & Schneider, G. 2016. Deep Learning in Drug Discovery. Molecular Informatics, 35, 3-14.

Forward mapping

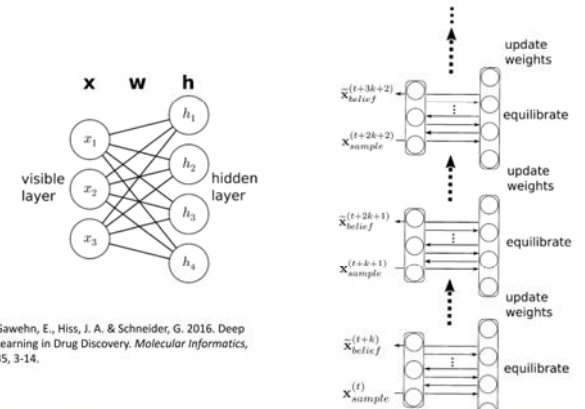


Error back-propagation

Gawehn, E., Hiss, J. A. & Schneider, G. 2016. Deep Learning in Drug Discovery. *Molecular Informatics*, 35, 3-14.
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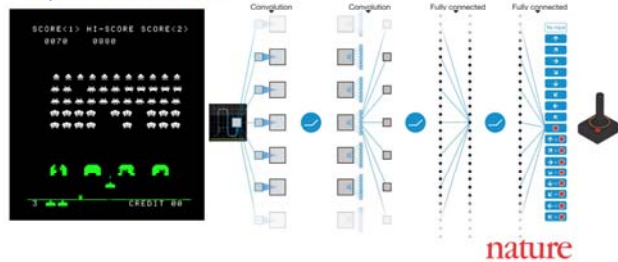


Gawehn, E., Hiss, J. A. & Schneider, G. 2016. Deep Learning in Drug Discovery. *Molecular Informatics*, 35, 3-14.
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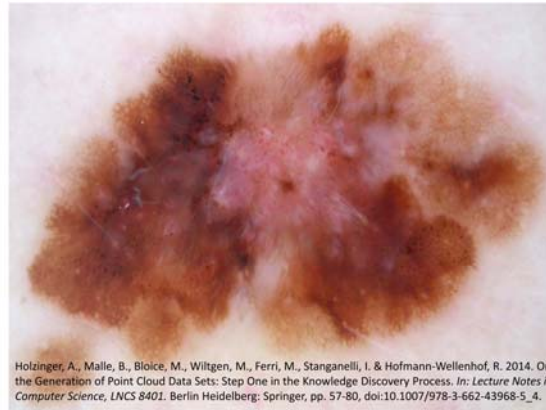
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Deep Q-networks (Q-Learning is a model-free RL approach) have successfully played Atari 2600 games at expert human levels

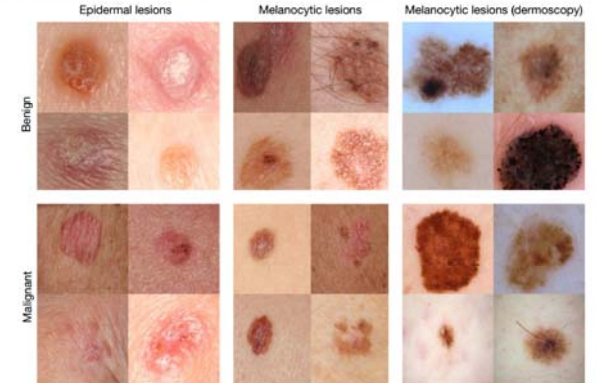


Mnih, V., Kavukcuoglu, K., Silver, D., Rusu, A. A., Veness, J., Bellemare, M. G., Graves, A., Riedmiller, M., Fidjeland, A. K., Ostrovski, G., Petersen, S., Beattie, C., Sadik, A., Antonoglou, I., King, H., Kumaran, D., Wierstra, D., Legg, S. & Hassabis, D. 2015. Human-level control through deep reinforcement learning. *Nature*, 518, (7540), 529-533, doi:10.1038/nature14236

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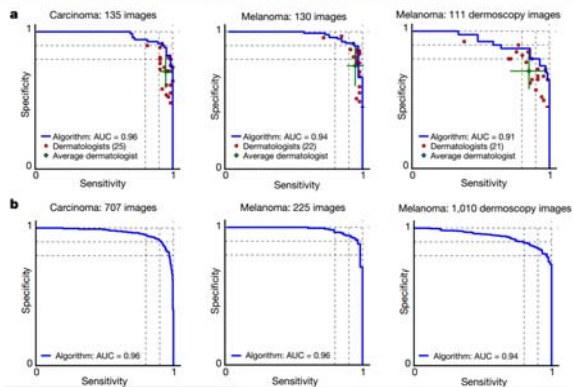


Holzinger, A., Malle, B., Bloice, M., Wiltgen, M., Ferri, M., Stanganeli, I. & Hofmann-Wellenhof, R. 2014. On the Generation of Point Cloud Data Sets: Step One in the Knowledge Discovery Process. In: *Lecture Notes in Computer Science, LNCS 8401*. Berlin Heidelberg: Springer, pp. 57-80, doi:10.1007/978-3-662-43968-5_4.



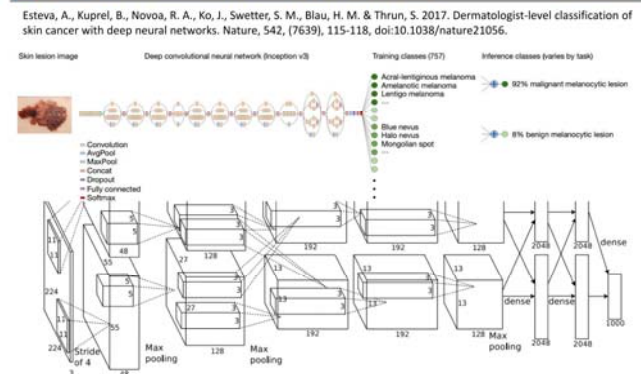
Esteva, A., Kuprel, B., Novoa, R. A., Ko, J., Swetter, S. M., Blau, H. M. & Thrun, S. 2017. Dermatologist-level classification of skin cancer with deep neural networks. *Nature*, 542, (7639), 115-118, doi:10.1038/nature21056.

Skin cancer classification performance: Human vs. CNN



Esteva, A., Kuprel, B., Novoa, R. A., Ko, J., Swetter, S. M., Blau, H. M. & Thrun, S. 2017. Dermatologist-level classification of skin cancer with deep neural networks. *Nature*, 542, (7639), 115-118, doi:10.1038/nature21056.

TU Deep Convolutional Neural Network Pipeline

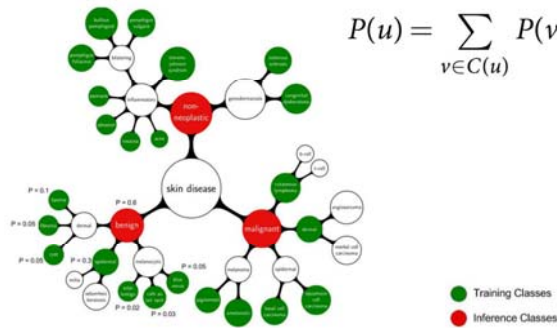


Krizhevsky, A., Sutskever, I. & Hinton, G. E. Imagenet classification with deep convolutional neural networks. In: Pereira, F., Burges, C. J. C., Bottou, L. & Weinberger, K. Q., eds. *Advances in neural information processing systems* (NIPS 2012), 2012 Lake Tahoe. 1097-1105.

TU Tree-structured taxonomy of skin cancer

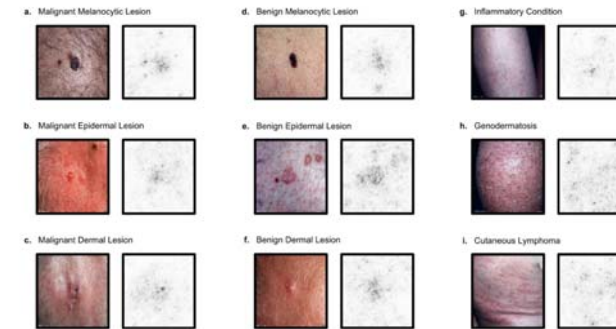


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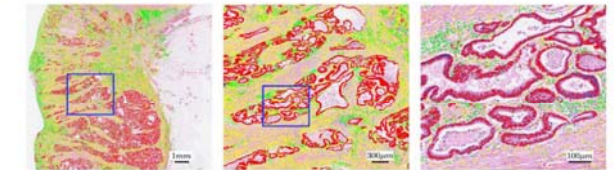
Esteve, A., Kuprel, B., Novoa, R. A., Ko, J., Swetter, S. M., Blau, H. M. & Thrun, S. 2017. Dermatologist-level classification of skin cancer with deep neural networks. Nature, 542, (7639), 115-118, doi:10.1038/nature21056.

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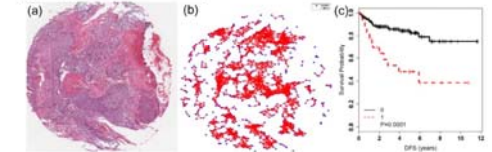


Esteve, A., Kuprel, B., Novoa, R. A., Ko, J., Swetter, S. M., Blau, H. M. & Thrun, S. 2017. Dermatologist-level classification of skin cancer with deep neural networks. Nature, 542, (7639), 115-118, doi:10.1038/nature21056.

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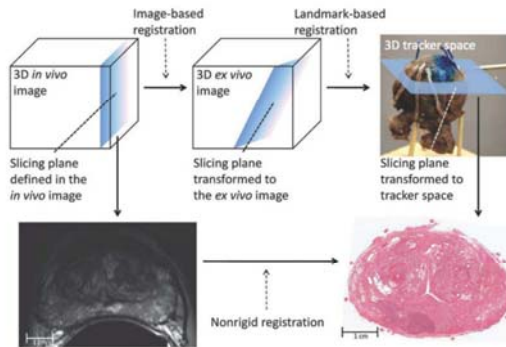


Sirinukunwattana, K., Raza, S. E. A., Tsang, Y. W., Snead, D. R. J., Cree, I. A. & Rajpoot, N. M. 2016. Locality Sensitive Deep Learning for Detection and Classification of Nuclei in Routine Colon Cancer Histology Images. IEEE Transactions on Medical Imaging, 35, (5), 1196-1206, doi:10.1109/TMI.2016.2525803.



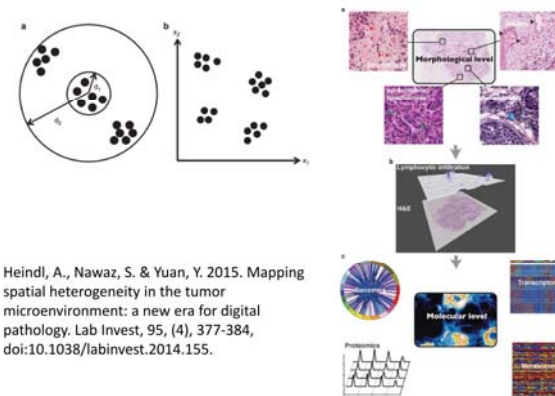
Madabhushi, A. & Lee, G. 2016. Image analysis and machine learning in digital pathology: Challenges and opportunities. Medical Image Analysis, 33, 170-175, doi:10.1016/j.media.2016.06.037.

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Ward, A. D., Crukley, C., McKenzie, C. A., Montreuil, J., Gibson, E., Romagnoli, C., Gomez, J. A., Moussa, M., Chin, J., Bauman, G. & Fenster, A. 2012. Prostate: Registration of Digital Histopathologic Images to in Vivo MR Images Acquired by Using Endorectal Receive Coil. Radiology, 263, (3), 856-864, doi:10.1148/radiol.12102294.

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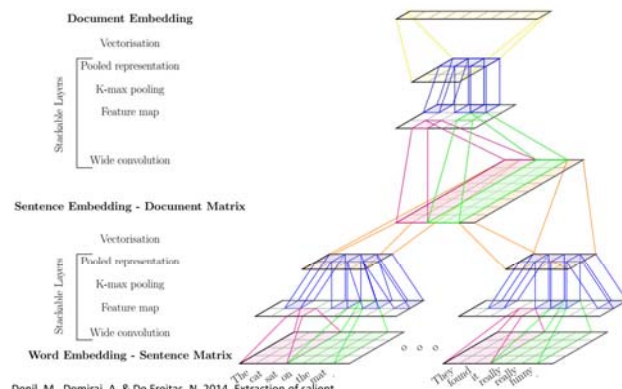
Heindl, A., Nawaz, S. & Yuan, Y. 2015. Mapping spatial heterogeneity in the tumor microenvironment: a new era for digital pathology. Lab Invest, 95, (4), 377-384, doi:10.1038/labinvest.2014.155.

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07 Future Challenges and Extravaganza *) Topics

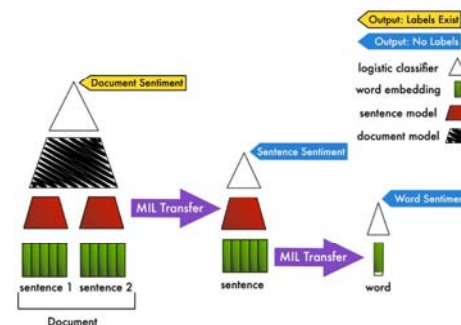
*) Holzinger, A. 2014. Extravaganza Tutorial on Hot Ideas for Interactive Knowledge Discovery and Data Mining in Biomedical Informatics. In: Slezak, D., Tan, A.-H., Peters, J. F. & Schwabe, L. (eds.) Brain Informatics and Health, BIH 2014, Lecture Notes in Artificial Intelligence, LNAI 8609. Heidelberg, Berlin: Springer, pp. 502-515, doi:10.1007/978-3-319-09891-3_46.

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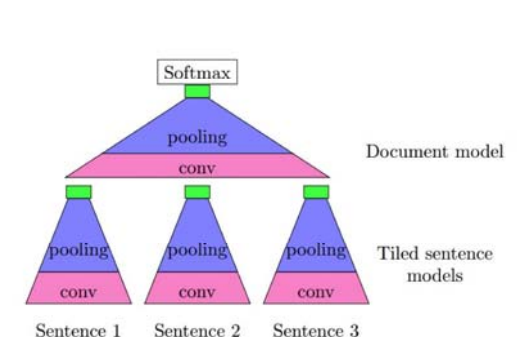
Denil, M., Demiraj, A. & De Freitas, N. 2014. Extraction of salient sentences from labelled documents. arXiv preprint arXiv:1412.6815.

Holzinger Group, hci-kdd.org 61 Machine Learning Health 13



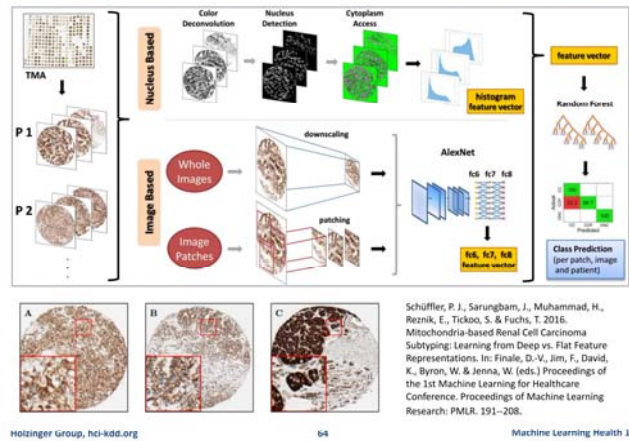
Kotzias, D., Denil, M., Blunsom, P. & De Freitas, N. 2014. Deep multi-instance transfer learning. arXiv preprint arXiv:1411.3128.

Holzinger Group, hci-kdd.org 62 Machine Learning Health 13



Kotzias, D., Denil, M., Blunsom, P. & De Freitas, N. 2014. Deep multi-instance transfer learning. arXiv preprint arXiv:1411.3128.

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Overcoming catastrophic forgetting in neural networks

James Kirkpatrick¹, Razvan Pascanu¹, Neil Rabinowitz¹, Joel Veness¹, Guillaume Desjardins¹, Andrei A. Rusu¹, Kieran Milan¹, John Quan¹, Tiago Ramalho¹, Agnieszka Grabska-Barwinska¹, Demis Hassabis¹, Claudia Clopath¹, Dharshan Kumaran¹, and Raia Hadsell¹

¹DeepMind, London EC4 3TW, United Kingdom; and ²Engineering department, Imperial College London, SW7 2AZ, London, United Kingdom

Edited by James L. McClelland, Stanford University, Stanford, CA, and approved February 13, 2017 (received for review July 19, 2016)

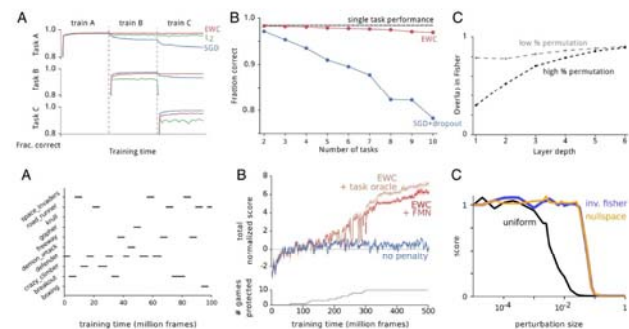
The ability to learn tasks in a sequential fashion is crucial to the development of artificial intelligence. Until now neural networks have not been capable of this and it has been widely thought that catastrophic forgetting is an inevitable feature of connectionist models. We show that it is possible to overcome this limitation and train networks that can maintain expertise on tasks that they have not experienced for a long time. Our approach remembers old tasks by selectively slowing down learning on the weights important for those tasks. We demonstrate our approach is scalable and effective by solving a set of classification tasks based on a hand-written digit dataset and by learning several Atari 2600 games sequentially.

synaptic consolidation | artificial intelligence | stability plasticity | continual learning | deep learning

Overcoming catastrophic forgetting in neural networks
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Abstract: The ability to learn tasks in a sequential fashion is crucial to the development of artificial intelligence. Until now neural networks have not been capable of this and it has been widely thought that catastrophic forgetting is an inevitable feature of connectionist models. We show that it is possible to overcome this limitation and train networks that can maintain expertise on tasks that they have not experienced for a long time. Our approach remembers old tasks by selectively slowing down learning on the weights important for those tasks. We demonstrate our approach is scalable and effective by solving a set of classification tasks based on a hand-written digit dataset and by learning several Atari 2600 games sequentially.

PNAS | March 28, 2017 | vol. 114 | no. 13 | 3521–3526

22 citations as of 20.06.2017



Kirkpatrick, J., Pascanu, R., Rabinowitz, N., Veness, J., Desjardins, G., Rusu, A. A., Milan, K., Quan, J., Ramalho, T., Grabska-Barwinska, A., Hassabis, D., Clopath, C., Kumaran, D. & Hadsell, R. 2017. Overcoming catastrophic forgetting in neural networks. Proceedings of the National Academy of Sciences, 114, (13), 3521–3526, doi:10.1073/pnas.1611835114.

- “How do humans generalize from very few examples?”
- They transfer knowledge from previous learning:
 - Representation learning (features!)
 - Explanatory factors
 - Previous learning from unlabeled data and labels for other tasks
- Prior: shared underlying explanatory factors, in particular between $P(x)$ and $P(Y|X)$, with a causal link between $Y \rightarrow X$

Bengio, Y., Courville, A. & Vincent, P. 2013. Representation learning: A review and new perspectives. IEEE transactions on pattern analysis and machine intelligence, 35, (8), 1798–1828, doi:10.1109/TPAMI.2013.50.

- Kirkpatrick et al. (2017) demonstrate that task-specific synaptic consolidation offers a unique solution to the continual-learning problem for artificial intelligence.
- Developed an algorithm analogous to synaptic consolidation for artificial neural networks,
- Elastic Weight Consolidation (EWC).
- This algorithm slows down learning on certain weights based on how important they are to previously seen tasks.
- They show how EWC can be used in supervised learning and reinforcement learning problems to train several tasks sequentially without forgetting older ones, in marked contrast to previous deep-learning techniques.

Kirkpatrick, J., Pascanu, R., Rabinowitz, N., Veness, J., Desjardins, G., Rusu, A. A., Milan, K., Quan, J., Ramalho, T., Grabska-Barwinska, A., Hassabis, D., Clopath, C., Kumaran, D. & Hadsell, R. 2017. Overcoming catastrophic forgetting in neural networks. Proceedings of the National Academy of Sciences, 114, (13), 3521–3526, doi:10.1073/pnas.1611835114.

Trends in Cognitive Sciences

Volume 21, Issue 6, June 2017, Pages 407–408

Spotlight Avoiding Catastrophic Forgetting

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Available online 23 April 2017

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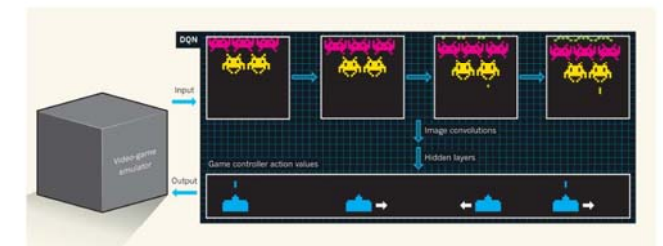
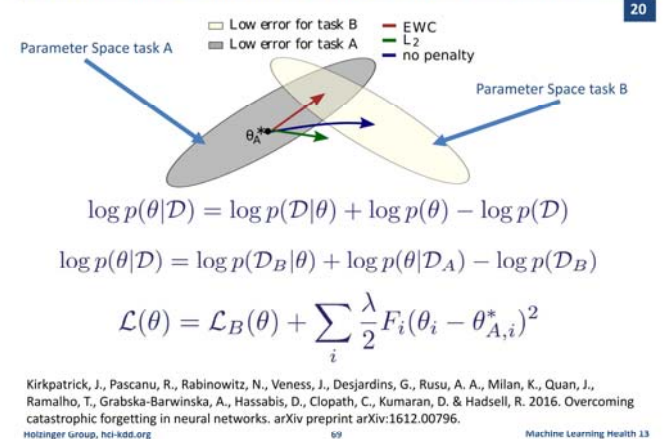
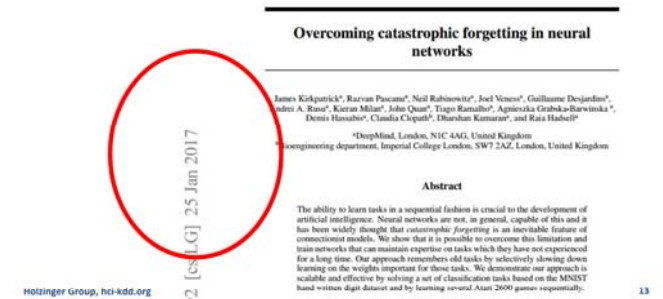
https://doi.org/10.1016/j.tics.2017.04.001

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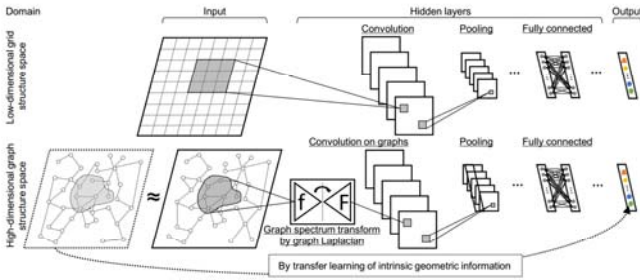
Humans regularly perform new learning without losing memory for previous information, but neural network models suffer from the phenomenon of catastrophic forgetting in which new learning impairs prior function. A recent article presents an algorithm that spares learning at synapses important for previously learned function, reducing catastrophic forgetting.

Hasselmo, M. E. 2017. Avoiding Catastrophic Forgetting. Trends in Cognitive Sciences, 21, (6), 407–408.

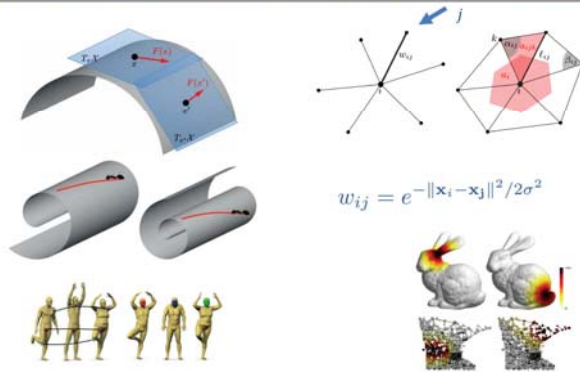
- When trained on one task, then trained on a 2nd task, many machine learning models (“deep learning”) forget how to perform the first task.



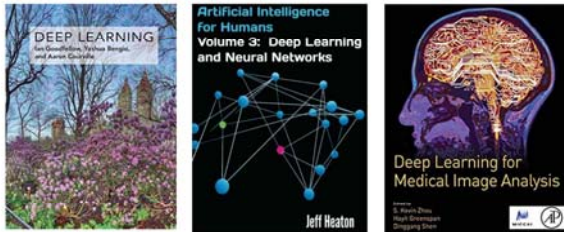
Mnih, V., Kavukcuoglu, K., Silver, D., Rusu, A. A., Veness, J., Bellemare, M. G., Graves, A., Riedmiller, M., Fiedelnd, A. K., Ostrovski, G., Petersen, S., Beattie, C., Sadik, A., Antonoglou, I., King, H., Kumaran, D., Wierstra, D., Legg, S. & Hassabis, D. 2015. Human-level control through deep reinforcement learning. Nature, 518, (7540), 529–533, doi:10.1038/nature14236



Lee, J., Kim, H., Lee, J. & Yoon, S. 2016. Intrinsic Geometric Information Transfer Learning on Multiple Graph-Structured Datasets. arXiv:1611.04687.



Bronstein, M. M., Bruna, J., Lecun, Y., Szlam, A. & Vandergheynst, P. 2016. Geometric deep learning: going beyond Euclidean data. arXiv preprint arXiv:1611.08097.



Goodfellow, I., Bengio, Y. & Courville, A. 2016. Deep Learning, Cambridge (MA), MIT Press.

<https://mitpress.mit.edu/books/deep-learning>

Geometric deep learning: going beyond Euclidean data

Michael M. Bronstein, Joan Bruna, Yann LeCun, Arthur Szlam, Pierre Vandergheynst

Many signal processing problems involve data whose underlying structure is non-Euclidean, but may be modeled as a manifold or (combinatorial) graph. For instance, in social networks, the characteristics of users can be modeled as signals on the vertices of the social graph [1]. Sensor networks are graph models of distributed interconnected sensors, whose readings are modeled as time-dependent signals on the vertices. In genomics, gene expression data are modeled as signals defined on the regulatory network [2]. In neuroscience, graph models are used to represent anatomical and functional structures of the brain. In computer graphics and vision, 3D objects are modeled as Riemannian manifolds (surfaces) endowed with properties such as color texture. Even more complex examples include networks of operators, e.g., functional correspondences [3] or difference operators [4] in a collection of 3D shapes, or orientations of overlapping cameras in multi-view vision ("structure from motion") problems [5].

The complexity of geometric data and the availability of very large datasets (in the case of social networks, on the scale of billions) suggest the use of machine learning techniques. In particular, deep learning has recently proven to be a powerful tool for problems with large datasets with underlying Euclidean structure.

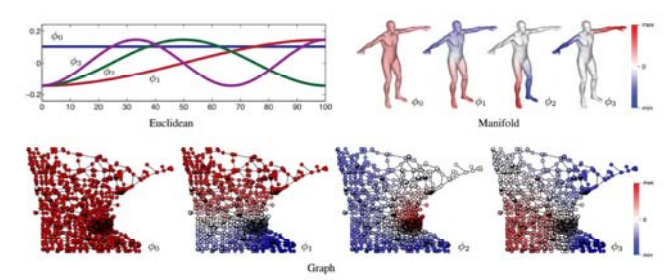
The purpose of this paper is to overview the problems arising in relation to geometric deep learning and present

Constructions that leverage the statistical properties of the data, in particular stationarity and compositionality through local statistics, which are present in natural images, video, and speech [18, 19] are one of the key reasons for the success of deep neural networks in these domains. These statistical properties have been related to physics [20] and formalized in specific classes of convolutional neural networks (CNNs) [21, 22, 23]. For example, one can think of images as functions on the Euclidean space (plane), sampled on a grid. In this setting, stationarity is owed to shift-invariance, locality is due to the local connectivity, and compositionality stems from the multi-resolution structure of the grid. These properties are exploited by convolutional architectures [24], which are built of alternating convolutional and downsampling (pooling) layers. The use of convolutions has a two-fold effect. First, it allows extracting local features that are shared across the image domain and greatly reduces the number of parameters in the network with respect to generic deep architectures (and thus also the risk of overfitting), without sacrificing the expressive capacity of the network. Second, as we will show in the following, the convolutional architecture itself imposes some priors about the data, which appear very suitable especially for natural images [25], [22].

While deep learning models have been particularly successful when dealing with signals such as speech, images, or video,



Thank you!



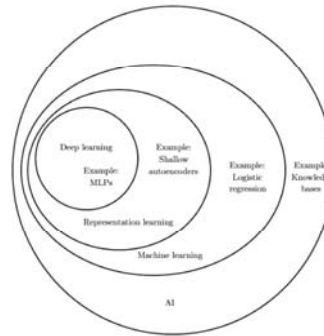
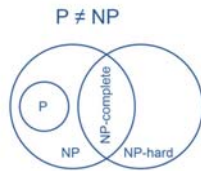
Bronstein, M. M., Bruna, J., Lecun, Y., Szlam, A. & Vandergheynst, P. 2016. Geometric deep learning: going beyond Euclidean data. arXiv preprint arXiv:1611.08097.

Appendix



<http://playground.tensorflow.org>

- **P**: algorithm can solve the problem in polynomial time (worst-case running-time for problem size n is less than $F(n)$)
- **NP**: problem can be solved and any solution can be verified within polynomial time ($P \subseteq NP$)
- **NP-complete**: problem belongs to class NP and any other problem in NP can be reduced to this problem
- **NP-hard**: problem is at least as hard as any other problem in NP-complete but solution cannot necessarily be verified within polynomial time



Goodfellow, I., Bengio, Y. & Courville, A. 2016. Deep Learning, Cambridge (MA), MIT Press, Chapter 1, p.9

Open Problem: How to avoid negative transfer?