DD2437 – Artificial Neural Networks and Deep Architectures (annda)

Lecture 9: **Deep learning fundamentals**

General philosophy and a review of deep architectures

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AI ambition behind Deep Learning

The grand plan is to *”allow computers to model our world well enough to exhibit what we call intelligence”.*

(Bengio, 2006)

- The need for capturing high-level of abstraction
- Hope in learning algorithms that can help to exploit large quantities of available information (big data in the future) and generalise it to new contexts
- The assumption about the need for highly nonlinear (varying) mathematical functions (accounting for variations in the multivariate, often high-dimensional, domain of interest) to model complex behaviours

AI ambition behind Deep Learning

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So, we need

- knowledge
- learning
    - complex functions,
    - from unlabeled data
    - with little human input
- generalisation
- understanding/identifying the underlying explanatory factors

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  - from unlabeled data
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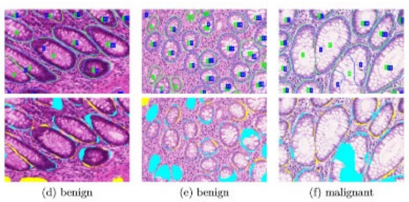
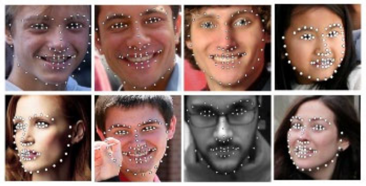
Is there a hope in **DEEP LEARNING in DEEP ARCHITECTURES ?**

Where are we now?

Vision

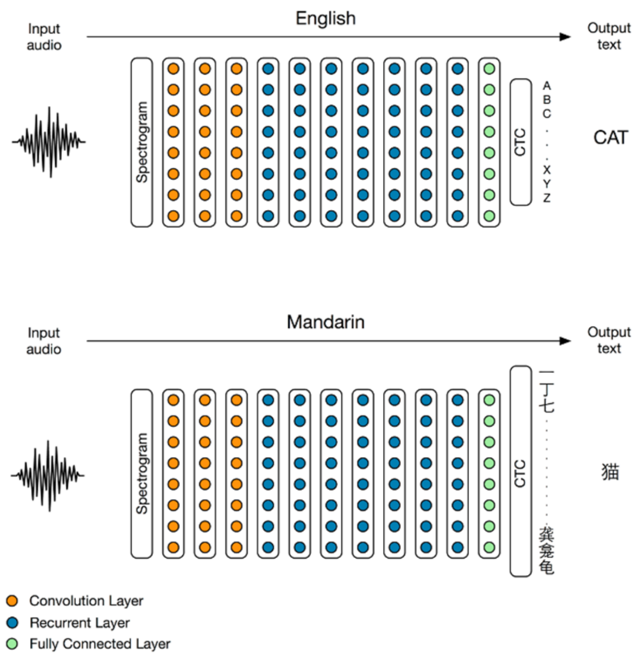


[Nvidia Dev Blog 2017]



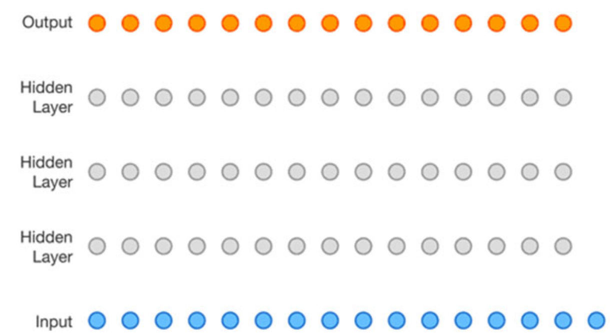
[Facial landmark detection CUHK 2014]

Text-to-speech



[Baidu 2014]

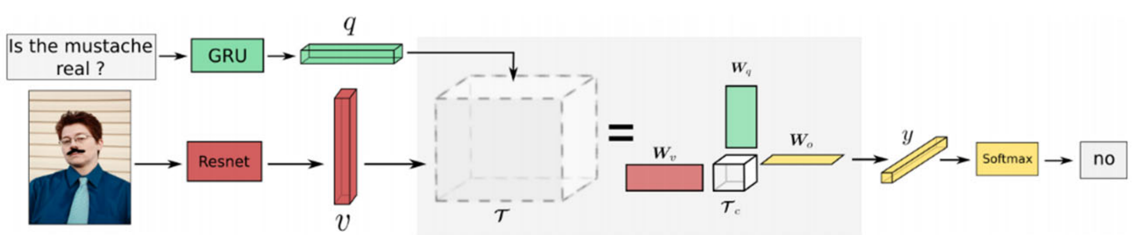
Generative models



[DeepMind 2017]

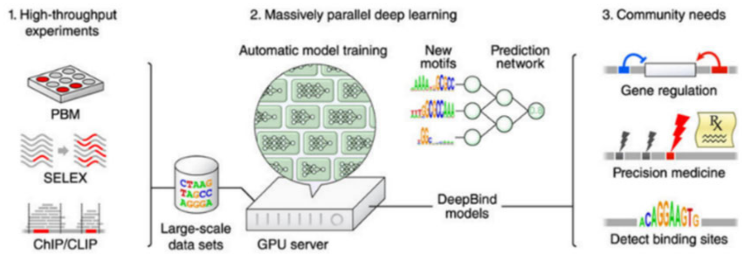
[DeepDream 2015]

Vision + NLP



[VQA - Mutan 2017]

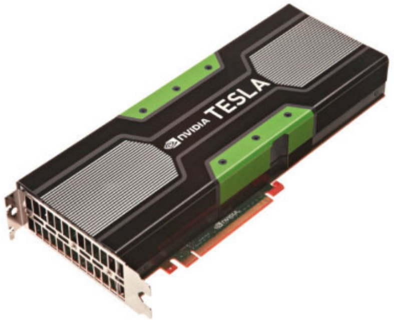
Genomics, computational biology

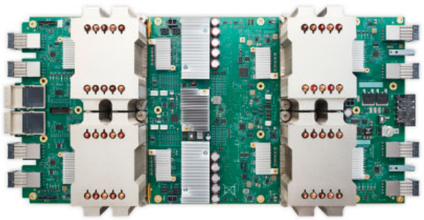


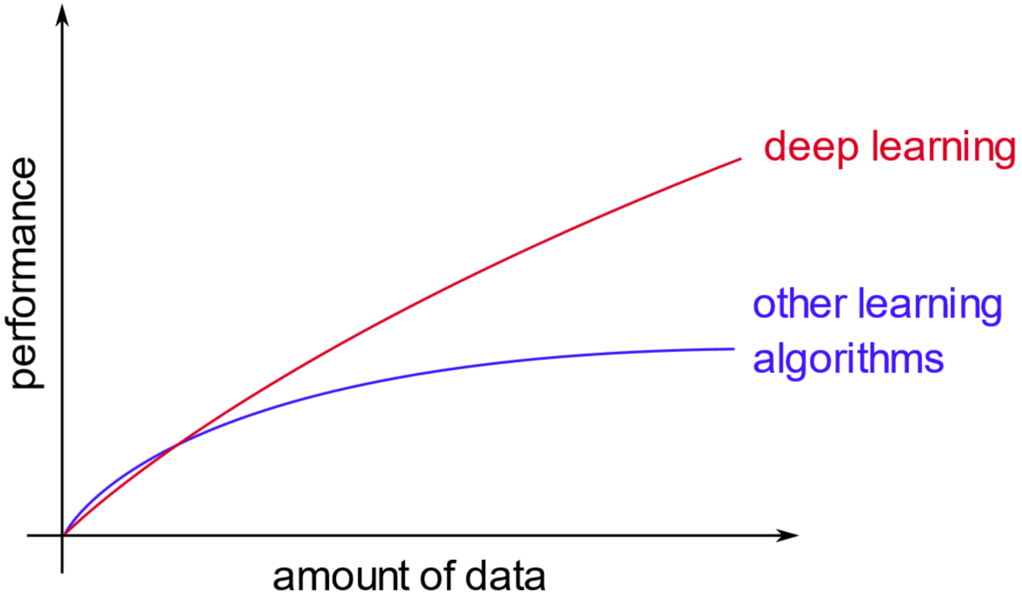
[Deep Genomics 2017]

Where are we now? Why now?

- ➢ computing power, hardware platforms
- ➢ data availability (age of Big Data)
- ➢ more effective algorithms
- ➢ open source tools

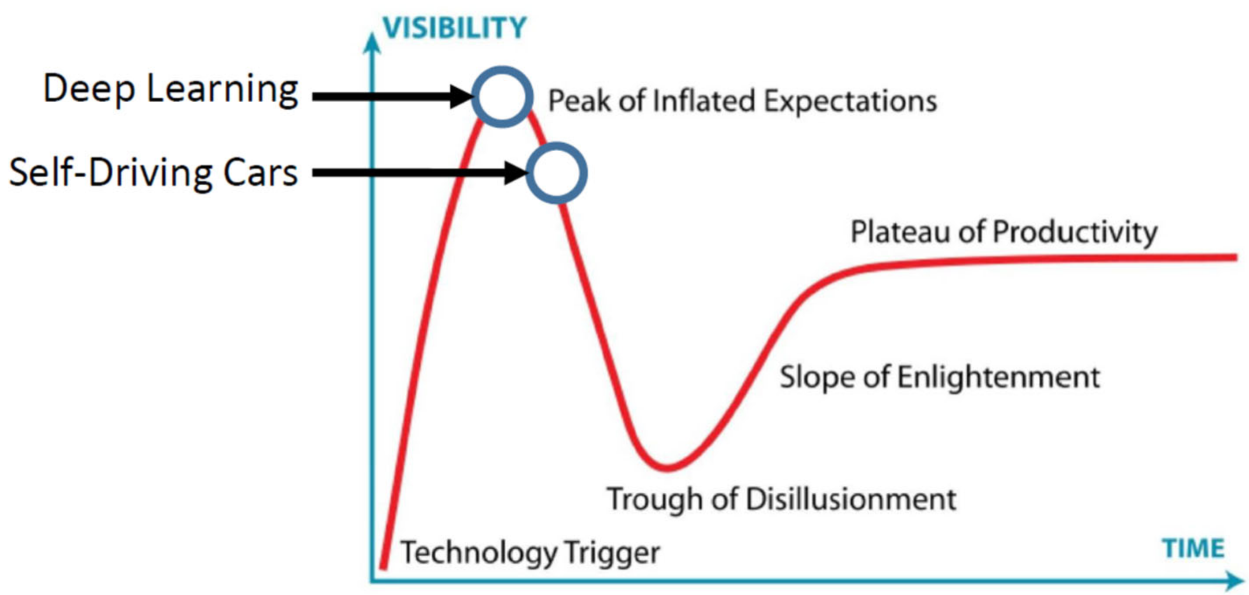






Where are we now? Where are we heading?

Gartner Hype Cycle



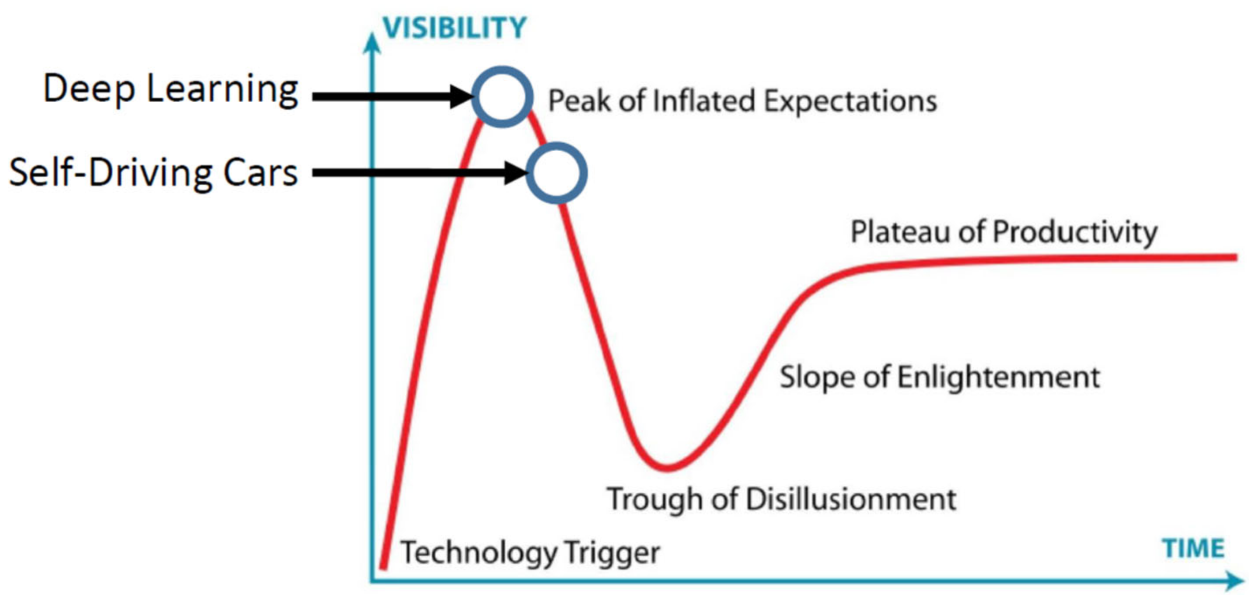
https://deeplearning.mit.edu

Applicability

- no human expertise or expertise hard to formalize
- no underlying physical/math models
- problems with a search space exceeding human capabilities
- tendency to automate and reduce human involvement

Where are we now? Where are we heading?

Gartner Hype Cycle



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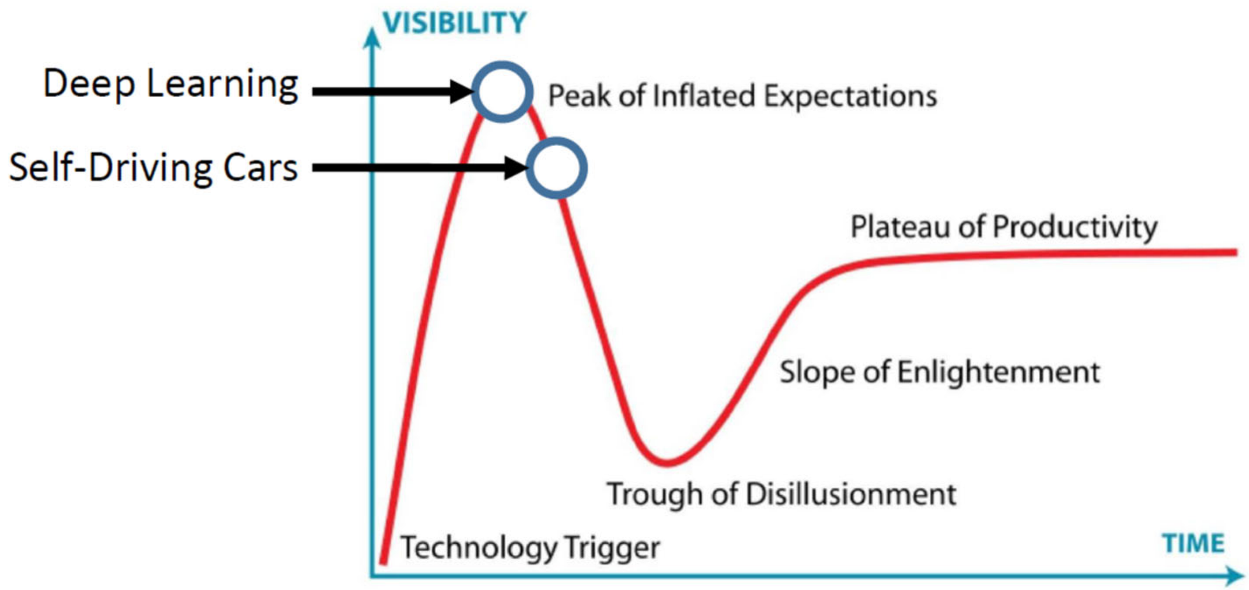

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Is there a hope in

DEEP LEARNING / DEEP ARCHITECTURES ?

Deep Learning: A Critical Appraisal, Gary Marcus 2017

Applicability

- no human expertise or expertise hard to formalize
- no underlying physical/math models
- problems with a search space exceeding human capabilities
- tendency to automate and reduce human involvement

- shallow meaning of "depth"
- lack of transparency
- causality vs correlation
- insufficiently trustworthy
- unintended consequences

Short historical note on deep architectures in ML

- 1943: McCulloch & Pitt's neuron model, Hebbian learning
- 1957: Rosenblatt's perceptron
- 1960: Widrow and Hoff's ADALINE
- 1969: Minsky and Pappert, first "AI winter"
- 1974-1986: Backprop, RBM, neurocognitron (towards CNN)
- 1991: "fundamental DL problem" – unstable gradients
- 1997: LSTM (backprop through time and gates)
- Late 1990's and 2000's: second "AI winter"

Short historical note on deep architectures in ML

- Major breakthrough in 2006
  - the idea to pre-train deep architectures with layer-wise unsupervised learning (groups led by G.E. Hinton, Y. Bengio and Y. LeCun)
  - more efficident parameter estimation methods

[1] Hinton, G. et al. (2006) A fast learning algorithm for deep belief nets. *Neural Computation* 18:1527-1554,

[2] Bengio, Y. et al. (2006) Greedy Layer-Wise Training of Deep Networks, in J. Platt et al. (Eds), Advances in Neural Information Processing Systems 19 (NIPS 2006), pp. 153-160.

[3] Ranzato, M. et al. & Yann LeCun, Y. (2006) Efficient Learning of Sparse Representations with an Energy-Based Model, in J. Platt et al. (Eds), *NIPS*.

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Shared principles in these papers:

- Unsupervised learning of representations is used to (pre-)train each layer.
- Unsupervised training of one layer at a time, on top of the previously trained ones. The representation learned at each level is the input for the next layer.
- Use supervised training to fine-tune all the layers (in addition to one or more additional layers that are dedicated to producing predictions).

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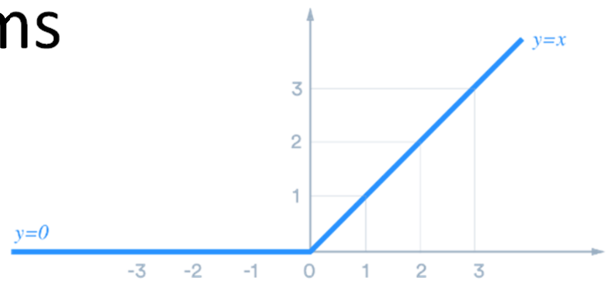
- Major breakthrough in 2006
  - the idea to pre-train deep architectures with layer-wise unsupervised learning (groups led by G.E. Hinton, Y. Bengio and Y. LeCun)
  - more efficident parameter estimation methods
- Enhancements developed to make networks perform more robustly and address new problems
  - 2010: Rectified linear units (ReLU)
  - 2014: Dropout
  - 2014: Generative adversarial networks (GANs)
  - 2015: Batch normalisation



Successful applications as a driver for development

- Convolutional nets (CNNs) in *computer vision*
- Deep learning based *speech recognition* systems developed by Google and Microsoft
- Deep learning is becoming a hot topic in *natural language processing* (NLP)
- Advances in machine translation (RNNs, LSTM)
- Growing importance in reinforcement learning (deep RL)
- Scope of applications massively grows

Trouble with classical multi-layer ANNs

- Hard to train
  - the problem of ***vanishing gradients*** (*diffusion* of gradients) in backpropagation algorithm

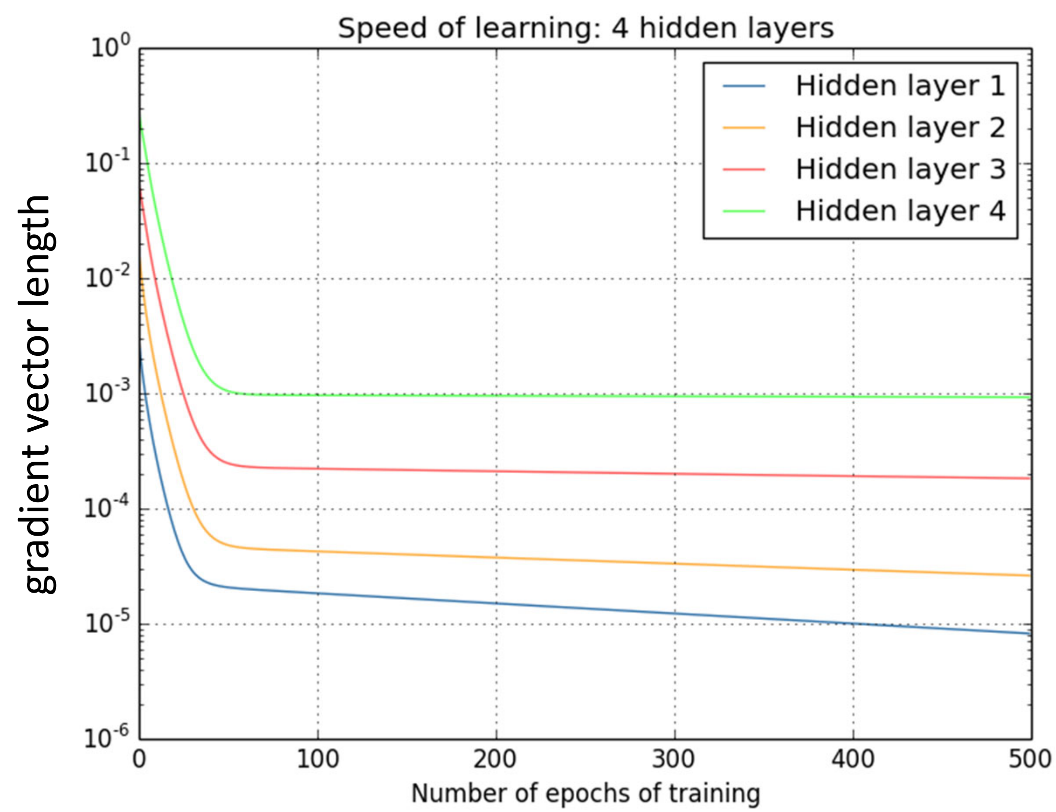
$$\frac{\partial C}{\partial b_1} = \sigma'(z_1) \times w_2 \times \sigma'(z_2) \times w_3 \times \sigma'(z_3) \times w_4 \times \sigma'(z_4) \times \frac{\partial C}{\partial a_4}$$

$$\frac{\partial C}{\partial b_1} = \sigma'(z_1)\overbrace{w_2\sigma'(z_2)}^{<\frac{1}{4}}\overbrace{w_3\sigma'(z_3)}^{<\frac{1}{4}}\underbrace{w_4\sigma'(z_4)\frac{\partial C}{\partial a_4}}_{\text{common terms}}$$

$$w_i \sim \mathbb{N}(0,1); \quad b_i \leq 1$$

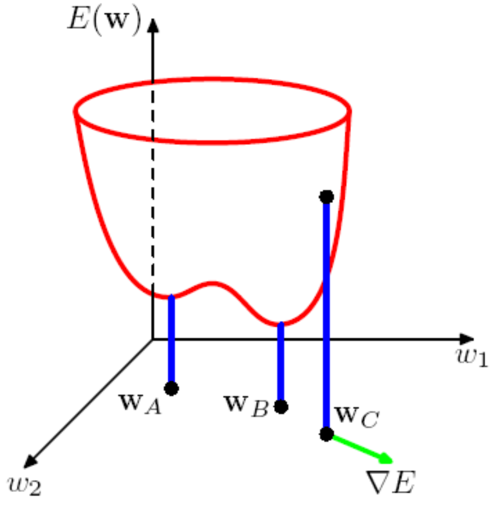
$$\frac{\partial C}{\partial b_3} = \sigma'(z_3)\overbrace{w_4\sigma'(z_4)\frac{\partial C}{\partial a_4}}$$

Nielsen, 2015



Trouble with classical multi-layer ANNs

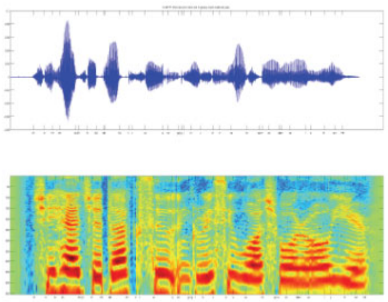
- Hard to train
  - the problem of *vanishing gradients* (*diffusion* of gradients) in backpropagation algorithm
  - it is really about unstable gradients
  - non-convex optimisation
    - local minima
    - susceptibility to overfitting

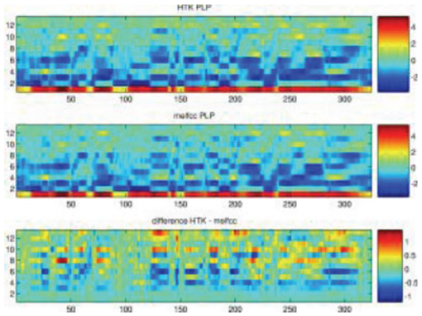


Learning high-level features – data representations

Traditional pattern recognition

- Human-designed representations (hand-engineered features)





- Focus on optimisation to make best predictions
- Importance of data labels in supervised learning

$$(\boldsymbol{x}, y)$$

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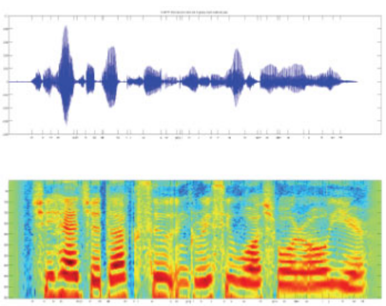
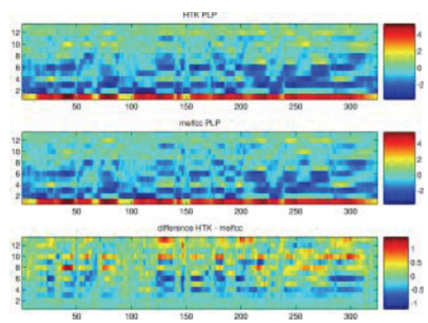




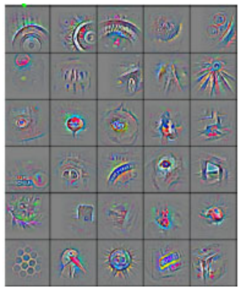
- Focus on optimisation to make best predictions
- Importance of data labels in supervised learning

$$(x, y)$$

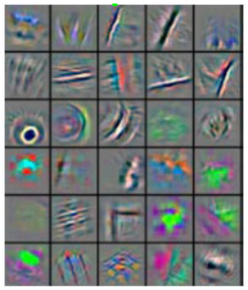
Deep learning approach

- Representation learning where good features are automat. learnt
- Potential to learn multiple levels of representation in DL algorithms

high level



middle level

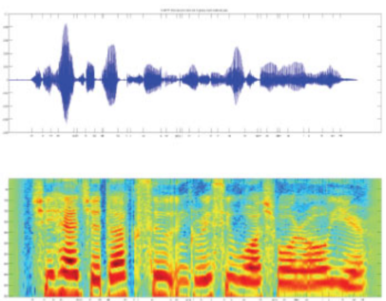


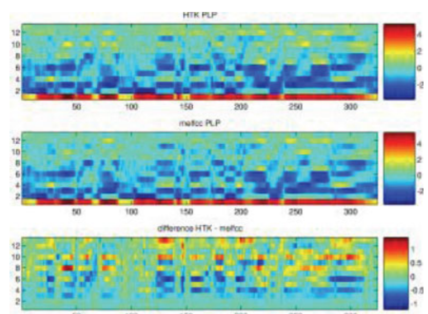
low level

Learning high-level features – data representations

Traditional pattern recognition

- Human-designed representations (hand-engineered features)





- Focus on optimisation to make best predictions
- Importance of data labels in supervised learning

$$(\boldsymbol{x}, \color{red}{y})$$

Deep learning approach

- Representation learning where good features are automat. learnt
- Potential to learn multiple levels of representation in DL algorithms

high level

BUT: ***Extracting low-level features specific to the problem domain helps a lot!***

Learning high-level features – data representations

Traditional pattern recognition

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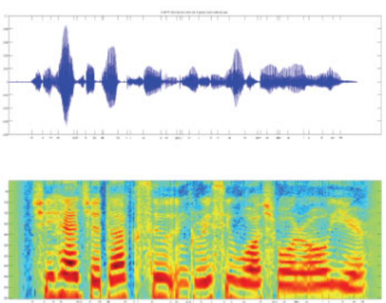

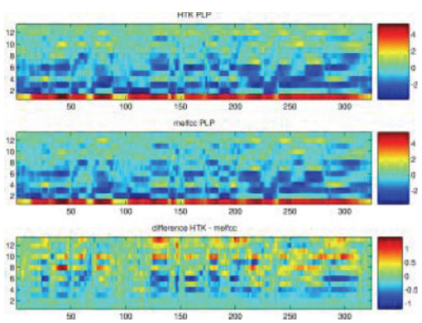

- Focus on optimisation to make best predictions
- Importance of data labels in supervised learning

$$(x, y)$$

Deep learning approach

- Representation learning where good features are automat. learnt
- Potential to learn multiple levels of representation in DL algorithms
- For example,

character –> word –> word group, phrase –> clause –> sentence –> story

pixel –> edge –> motif –> object

sample –> spectral feature –> sound –> phoneme –> word

Learning high-level features – data representations

Traditional pattern recognition

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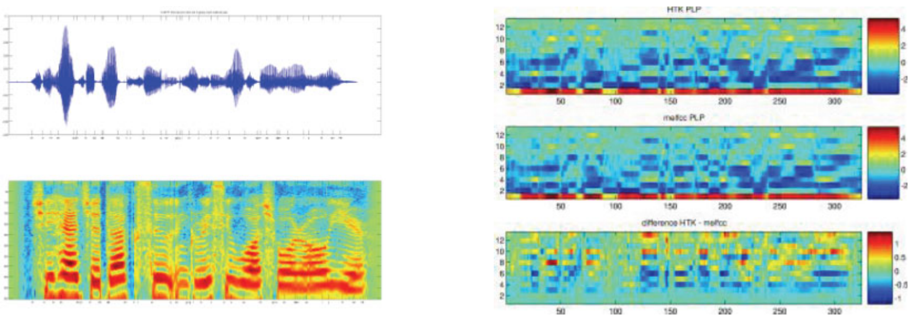


- Focus on optimisation to make best predictions
- Importance of data labels in supervised learning

$$(x, y)$$

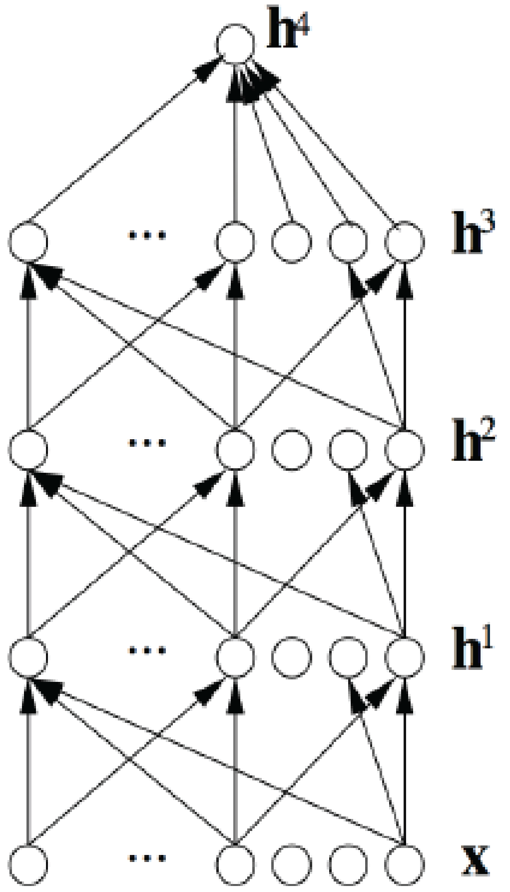
Deep learning approach

- Representation learning where good features are automat. learnt
- Potential to learn multiple levels of representation in DL algorithms
- Good predictions are v. important but so is <u>data representation</u>
- Both unsupervised and supervised mode is heavily exploited – <u>unlabeled data are also useful</u>

What is depth in ML?

- Depth of architecture
  - the number of levels of composition of nonlinear op function learnt
  - the length of the longest path from input to output in th

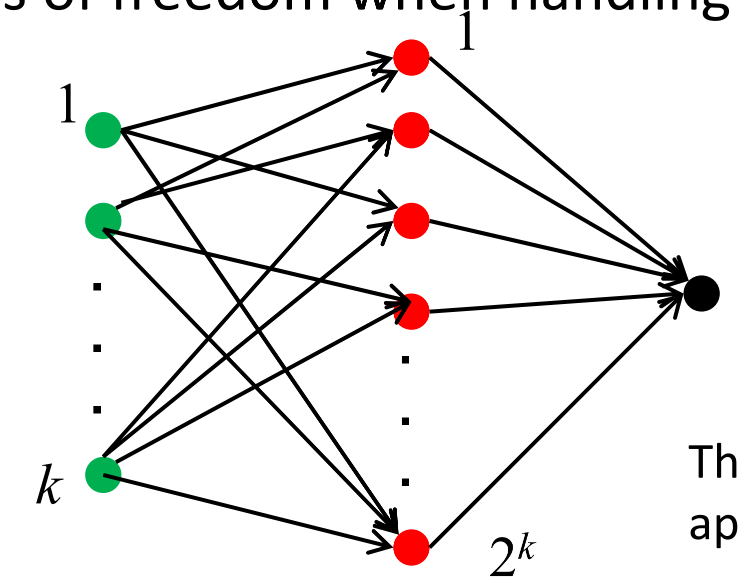
- Deep learning
  - using multiple layers of inf. processing stages architectures for pattern recognition and representation
  - originally, focus on (*incremental*) learning of feature hier



Motivation for deep structures

Why go deep? Do we need deep structures?

- Expressive power and compactness of models (*expressibility* and *efficiency*)
  - enhances generalisation, especially with limited training examples
  - less degrees of freedom when handling complexity and nonlinearity – exponential gain



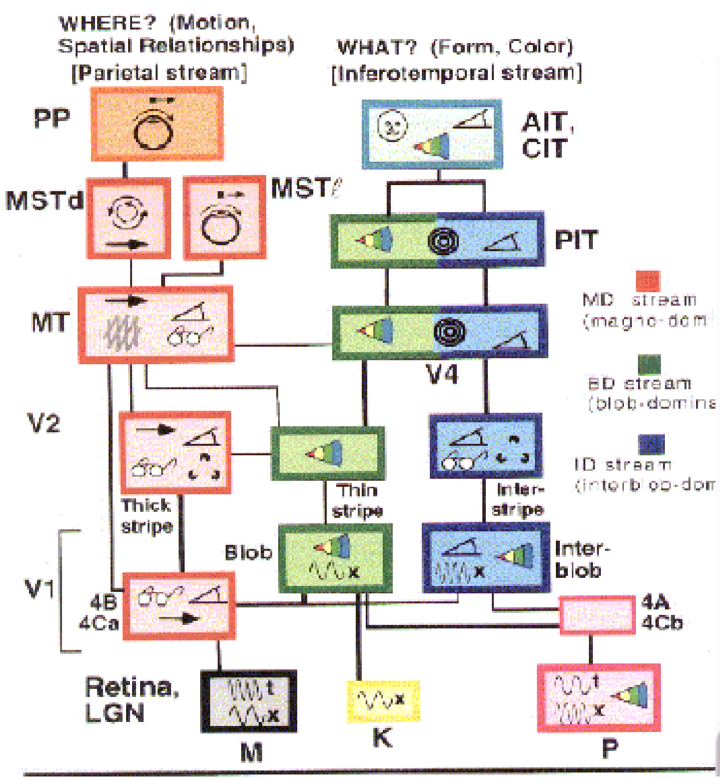
Shallow structure may need exponential size of hidden layer(s)

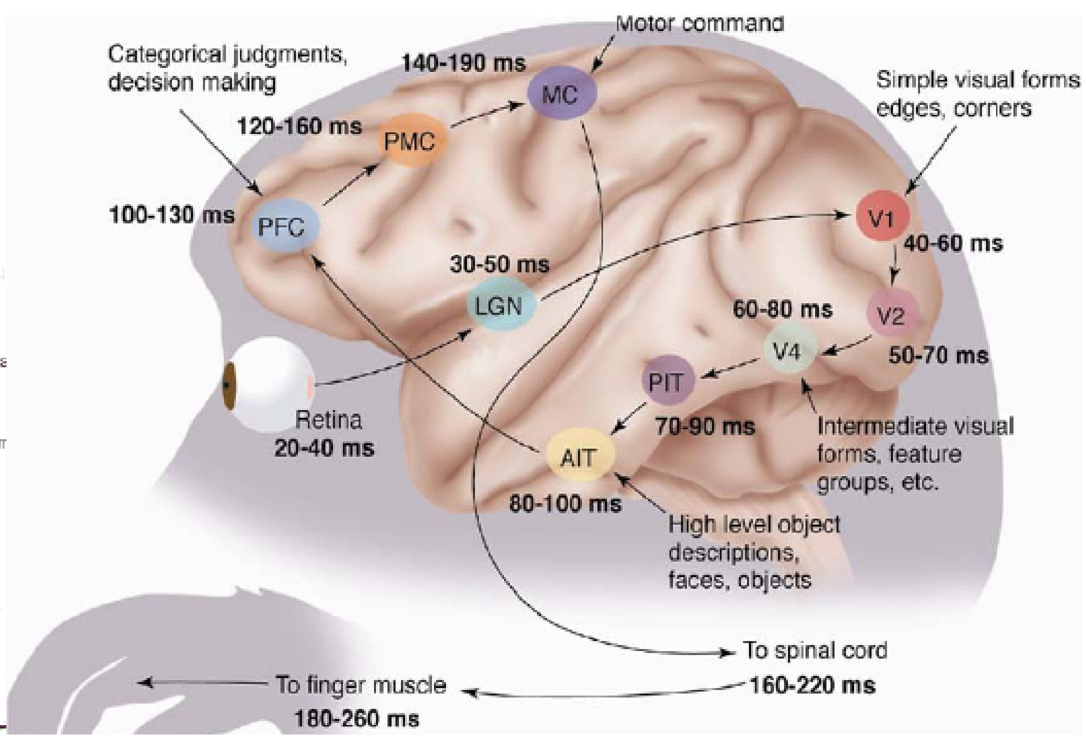
The universal approximation theorem and approximation costs.

Motivation for deep structures

Why go deep? Do we need deep structures?

- Inspirations from hierarchical brain organisation





LeCun & Ranzato, 2013

Motivation for deep structures

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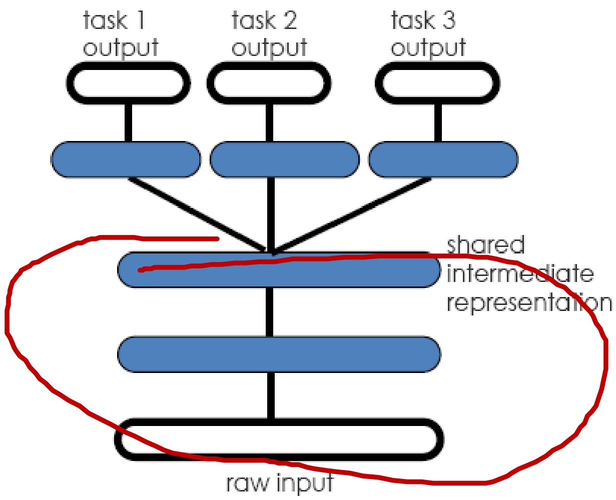
- Inspirations from hierarchical brain organisation
- Cognitive inspiration – multiple levels of abstraction

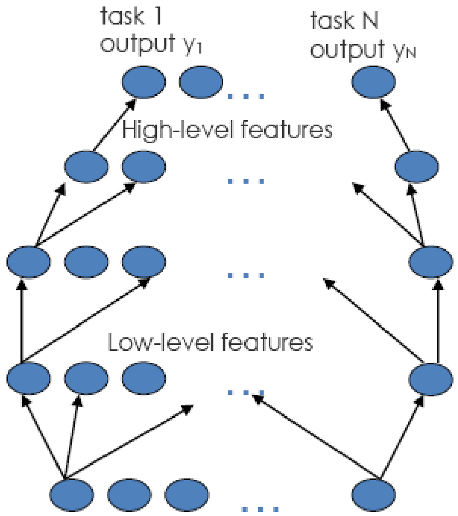
Motivation for deep structures

Why go deep? Do we need deep structures?

- Finally, ...

  multiple levels of representations facilitate transfer and multi-task learning (hierarchy of representations, non-local generalisation)

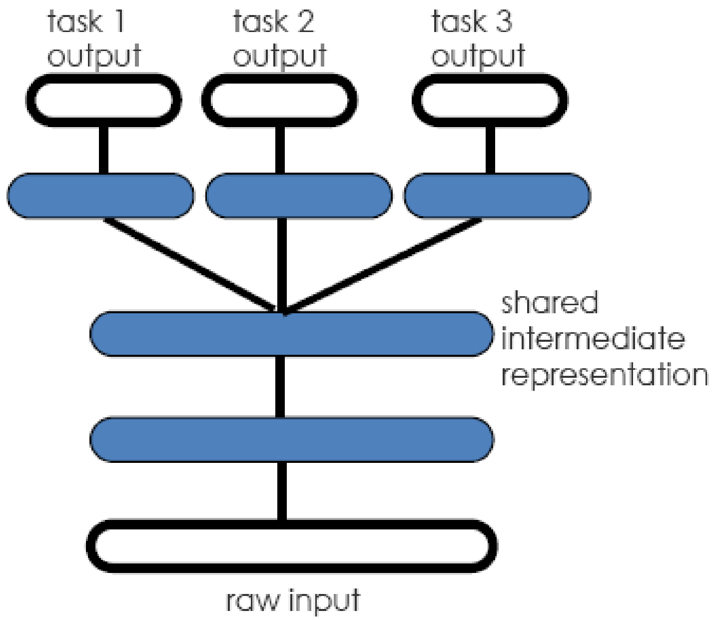




Lee, 2011

Representation learning – the essence

- Learning (distributed) representations
  - learning features as part of DL algorithms
  - multiple levels of abstraction and complexity (hierarchy)
  - **multi-task** or transfer learning



Bengio and Delalleau, 2013

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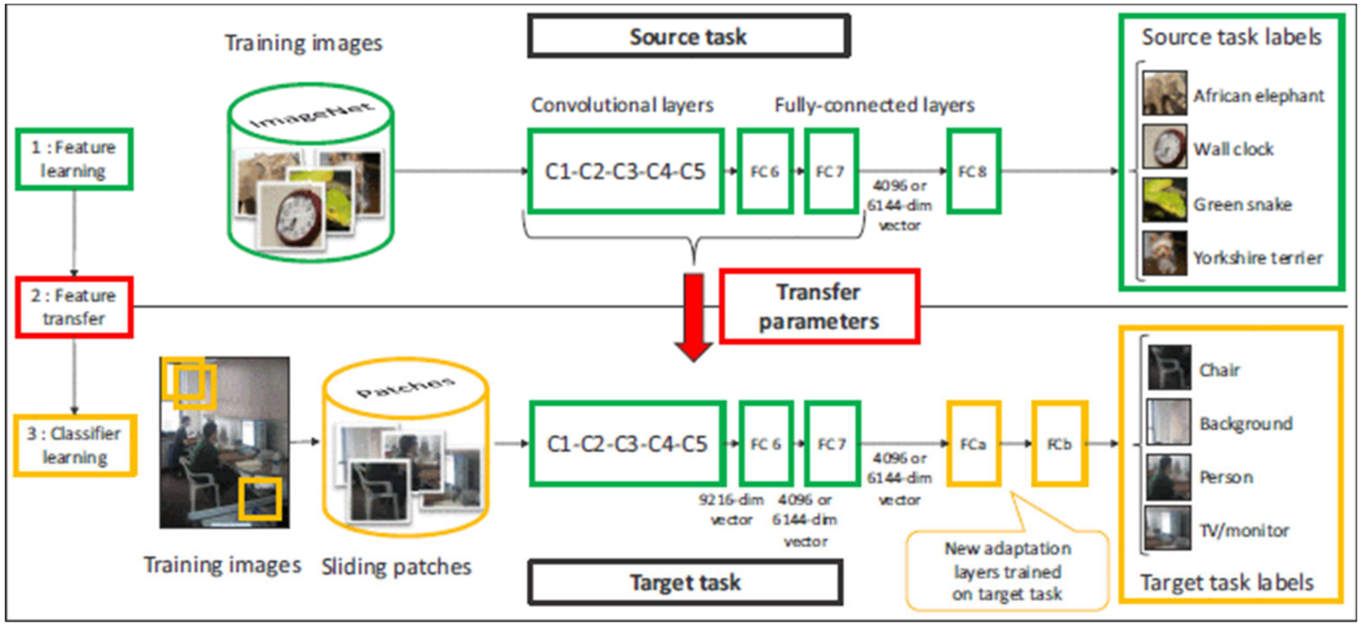

Oquab et al., 2014

Representation learning – the essence

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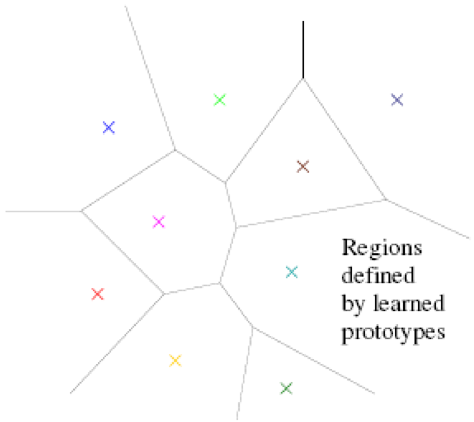
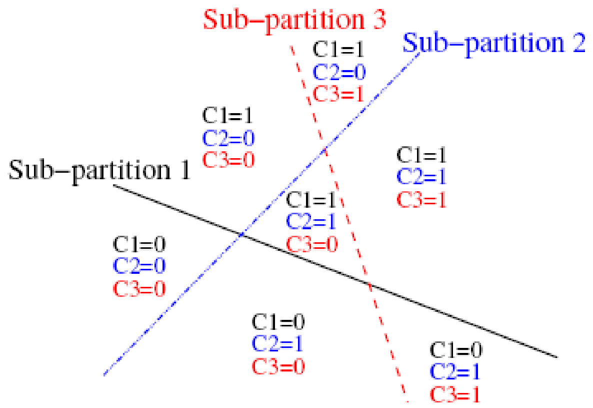
  - multiple levels of abstraction and complexity (hierarchy)
  - multi-task or transfer learning
  - facilitates non-local generalisation (multi-clustering)

LOCAL CLUSTERING



MULTI-CLUSTERING



Bengio and Delalleau, 2013

Representation learning – the essence

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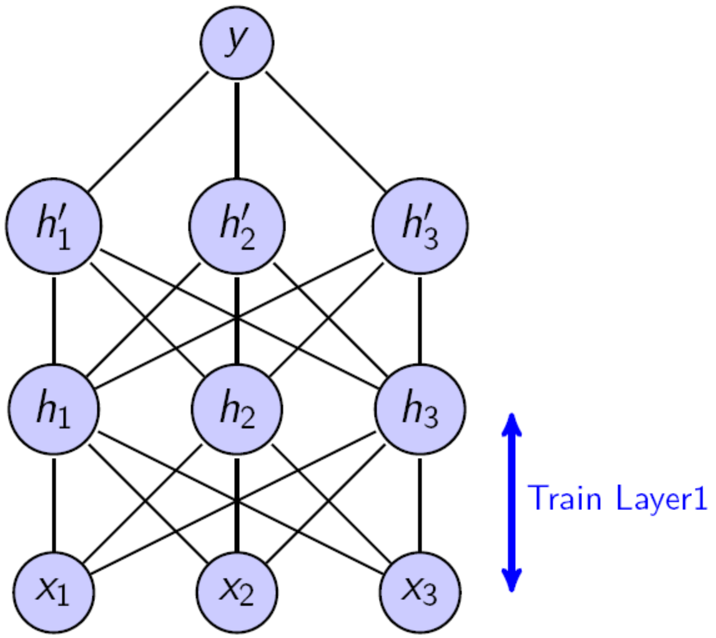
  - multiple levels of abstraction and complexity (hierarchy)
  - multi-task or transfer learning
  - facilitates non-local generalisation (multi-clustering)
  - sparse coding

General theme of the early deep learning protocol – deep belief networks, stacked autoencoders

- Greedy layer-wise unsupervised pre-training
  + supervised tuning (the legacy of Hinton, Bengio and LeCun)



Single layer at a time

Hinton et al., 2006
Duh, 2013

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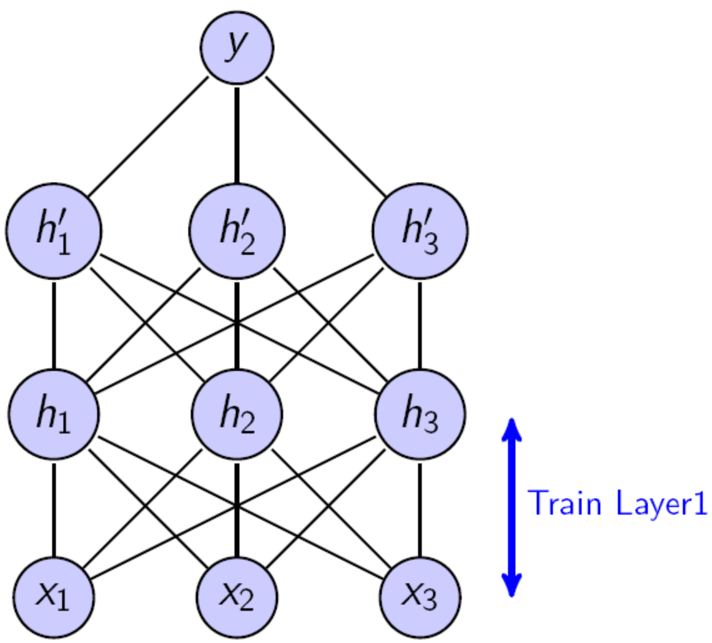
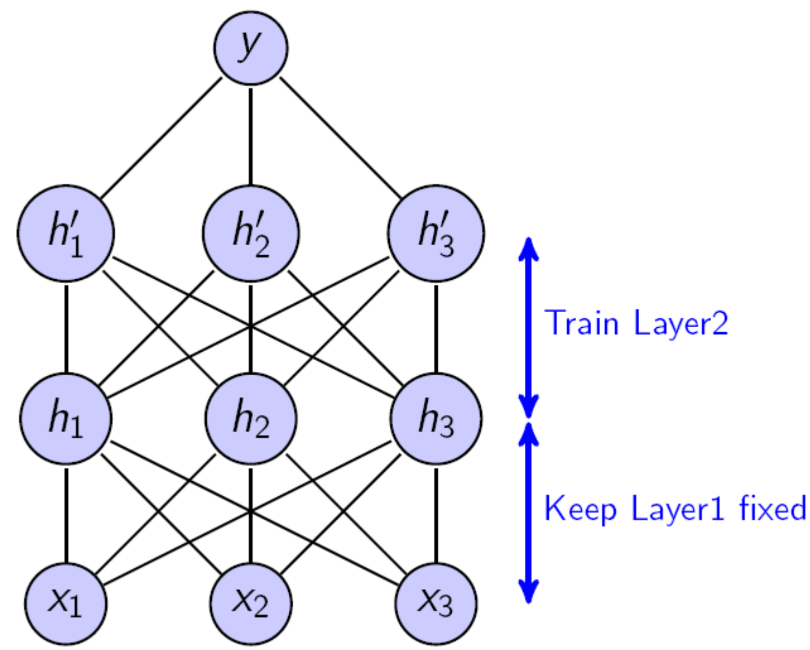


Single layer at a time



Train another layer while keeping the lower layer fixed

Hinton et al., 2006
Duh, 2013

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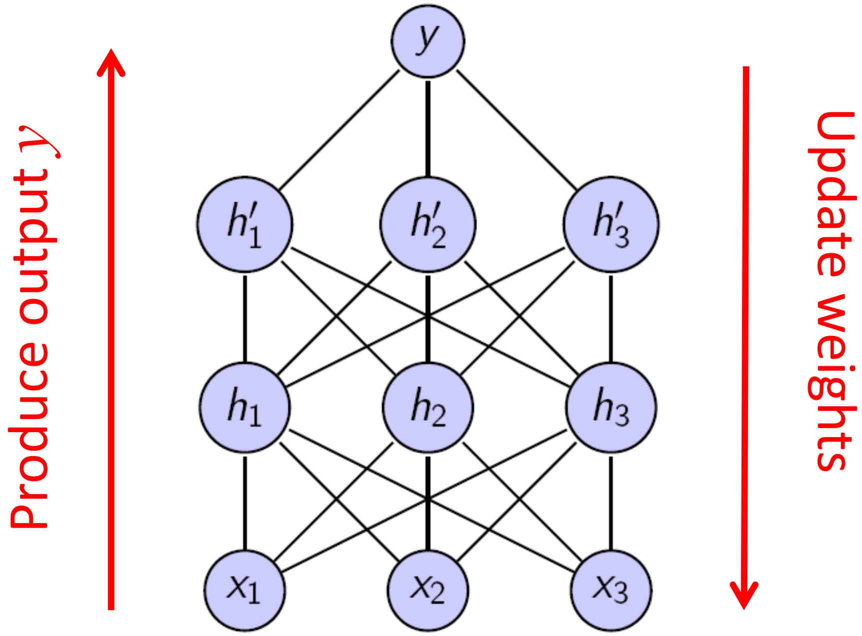

Gradient-based fine tuning

1. Add a classifier layer and retrain globally the entire structure.
2. Train only a supervised classifier on top and keep other layers fixed.

Hinton et al., 2006
Duh, 2013
LeCun & Ranzato, 2013

Hypothetical role of unsupervised pre-training

- Regularisation hypothesis (Erhan et al., 2010)
  - Pre-training minimises variance
  - It also helps to control complexity for architectures with large sizes of hidden layers
  - Acts like an implicit penalisation term – regularisation

Hypothetical role of unsupervised pre-training

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- Optimisation hypothesis (Bengio et al., 2007)

Hypothetical role of unsupervised pre-training

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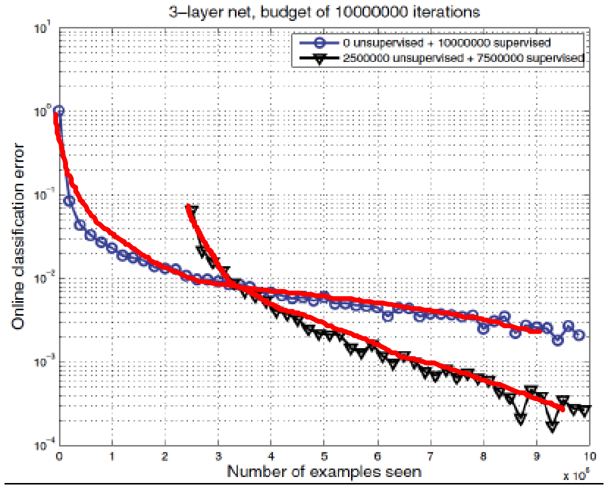
  - Pre-training minimises variance
  - It also helps to control complexity for architectures with large sizes of hidden layers
  - Acts like an implicit penalisation term – regularisation

- Optimisation hypothesis (Bengio et al., 2007)
  - pre-training finds a better initial condition for further gradient-based optimisation
  - good initial conditions are very important
  - it facilitates training of the entire architecture (lower and higher layers benefit from tuning)



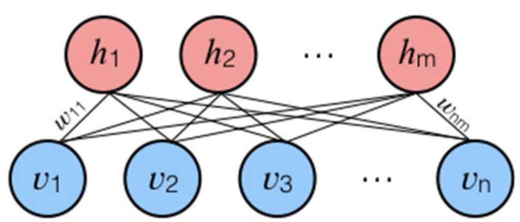
The fate of “pretraining” concept

- Pretraining actually sparked off developments in deep learning *(“revived DNNs from obscurity”, McKay*)
- The original ideas: *learning input distribution is useful and initialization is important*
- Now, unsupervised pretraining has mostly been abandoned due to more advanced regularization techniques and ReLU units
- However, pretraining concept has inspired much of the modern research in transfer learning

Fundamental network architecture and learning types

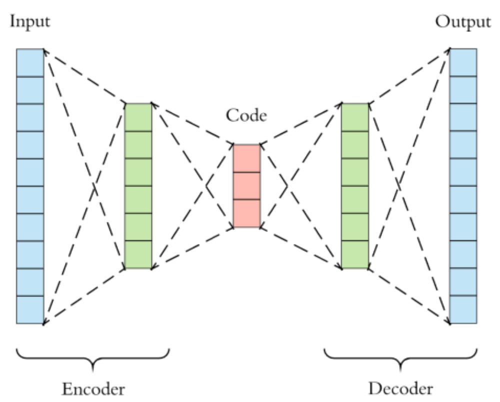
Restricted Boltzmann machine (RBM) layer

(contrastive divergence for pre-training)

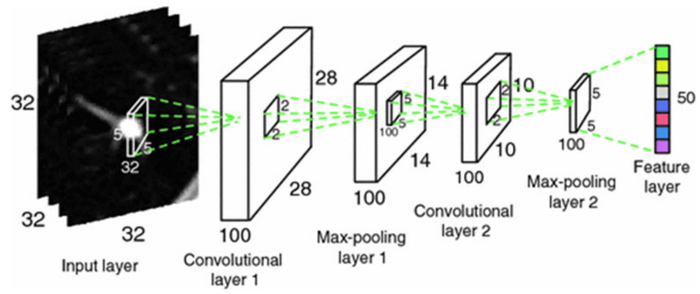


Autoencoder (AE) layer

(gradient descent based algorithms for pre-training)



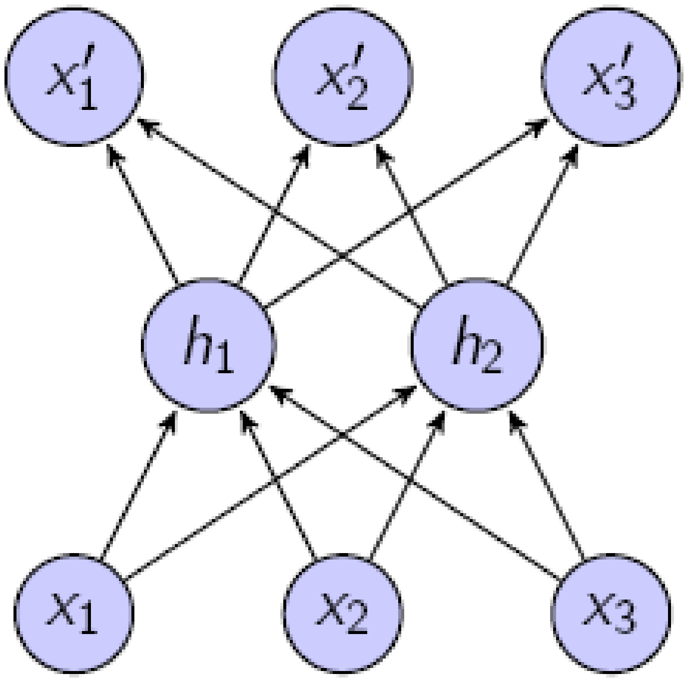
Convolutional neural networks (CNNs)



Greedy layer-wise unsupervised pre-training, which is increasingly omitted once **ReLU** units are employed

Network can be initialised without any pre-training, though transfer learning is often exploited

Autoencoders



Decoder: $x' = \sigma(W'h + d)$

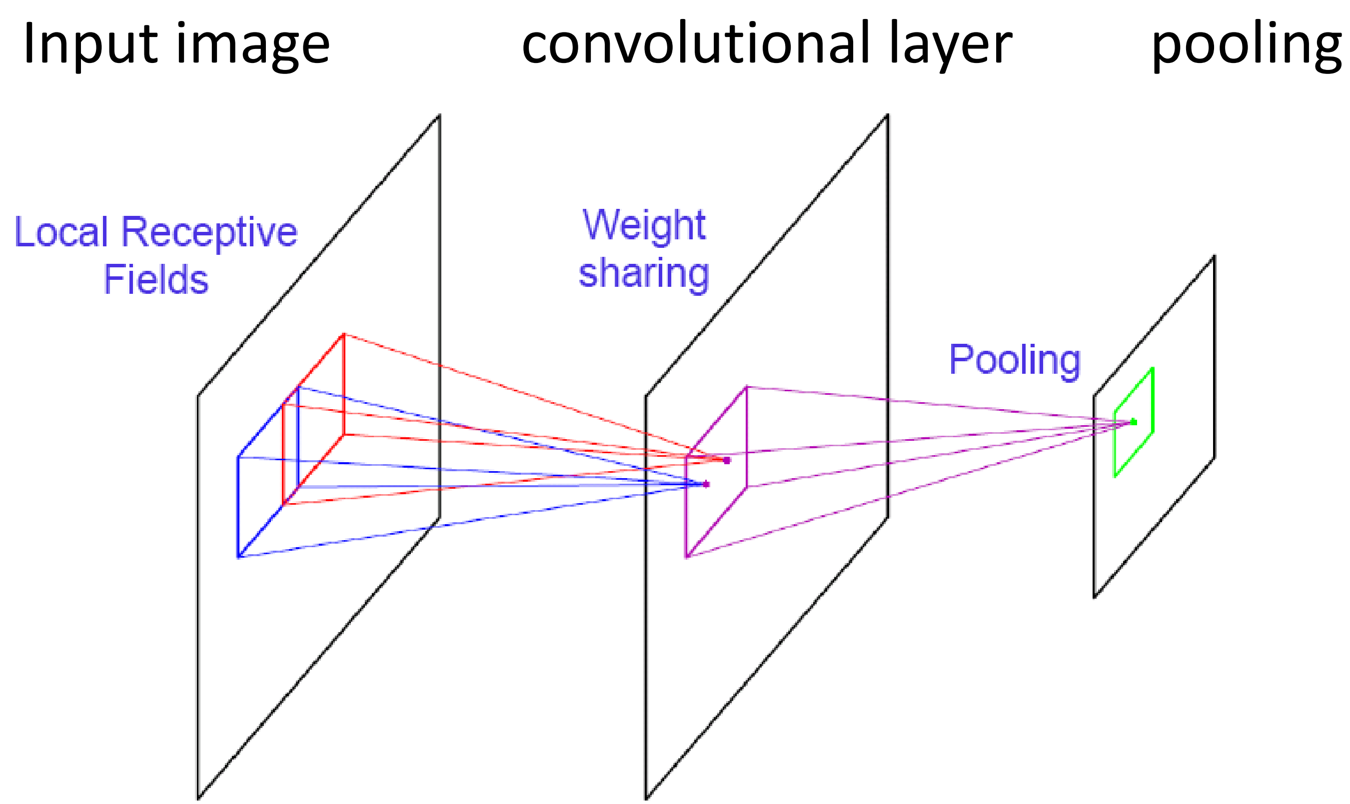
Encoder: $h = \sigma(Wx + b)$

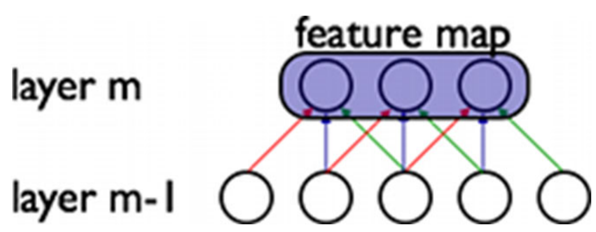
Encourage h to give small reconstruction error:

- e.g. $Loss = \sum_m ||x^{(m)} - DECODER(ENCODER(x^{(m)}))||^2$
- Reconstruction: $x' = \sigma(W'\sigma(Wx + b) + d)$

(REF)

Convolutional neural networks (CNNs)

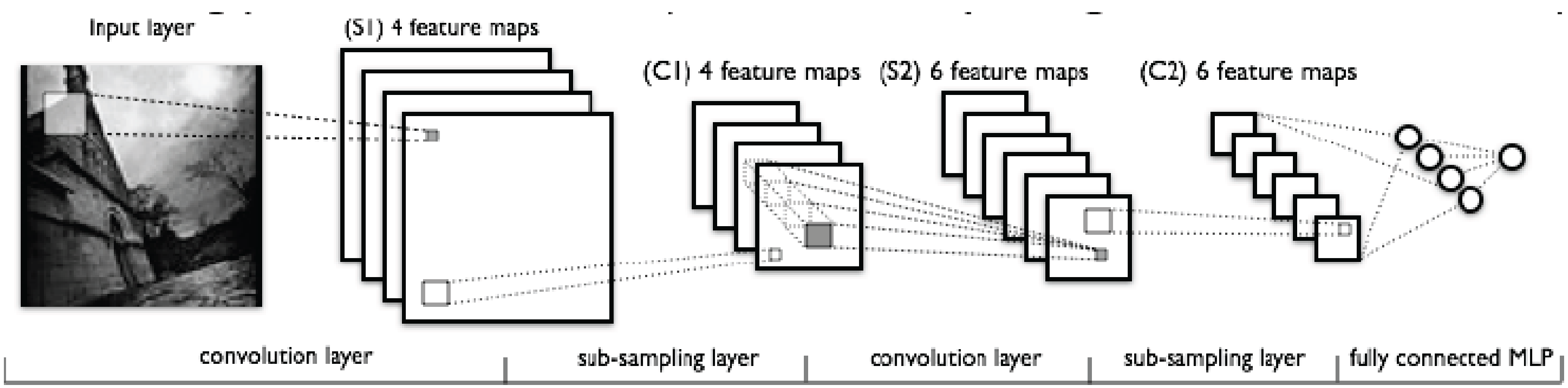


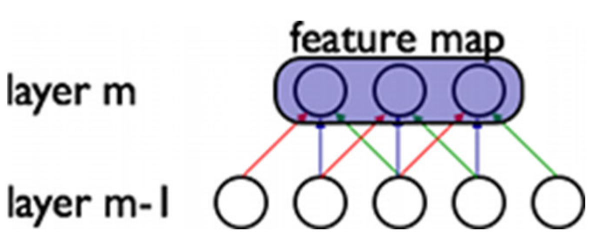


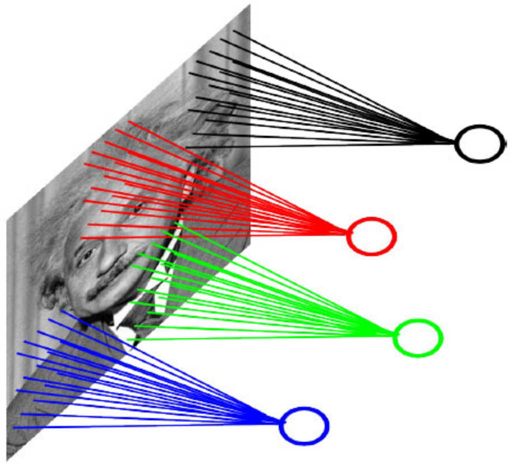
LeCun et al., 1989

Convolutional neural networks (CNNs)

Input image convolution pooling



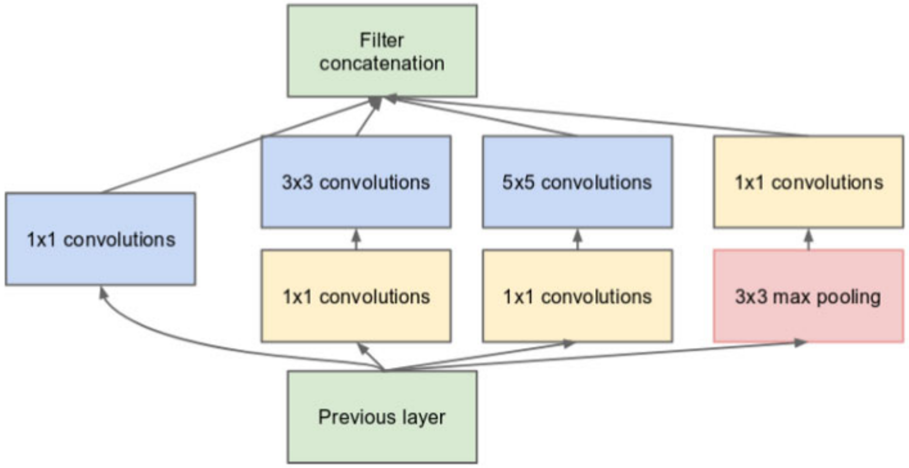




LeCun et al., 1989

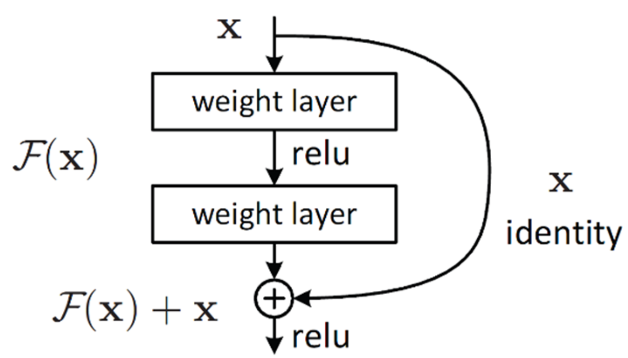
Key variants of CNNs

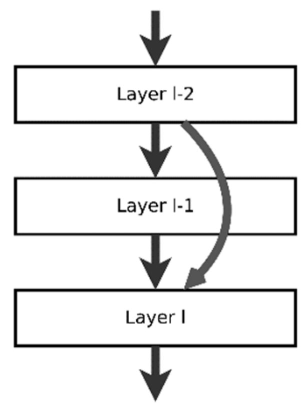
1. VGGNet (Simonyan and Zisserman, 2014)
   - extending up to 19 layers (previously 8 was used)
2. GoogLeNet with Inception (Szegedy et al., 2015)

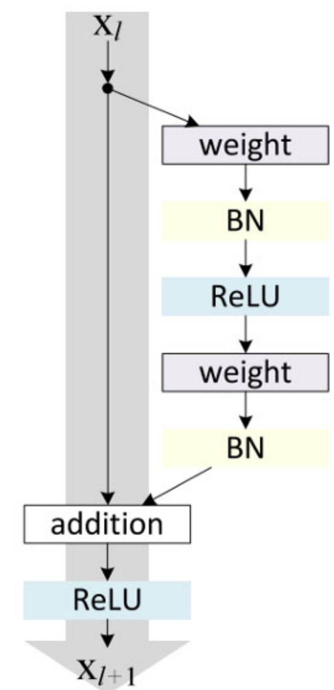


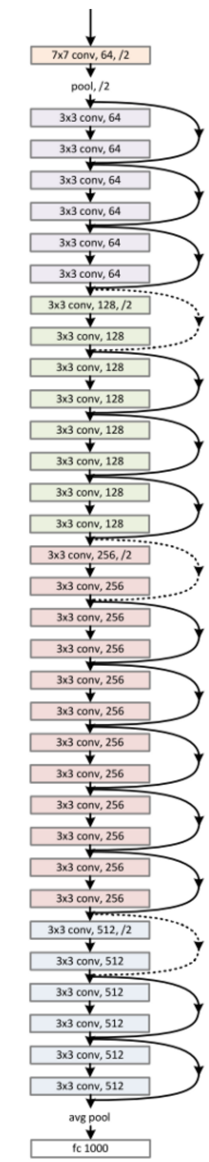
Key variants of CNNs

1. VGGNet (Simonyan and Zisserman, 2014)
   - extending up to 19 layers (previously 8 was used)
2. GoogLeNet with Inception (Szegedy et al., 2015)
3. ResNet (He at al., 2016)

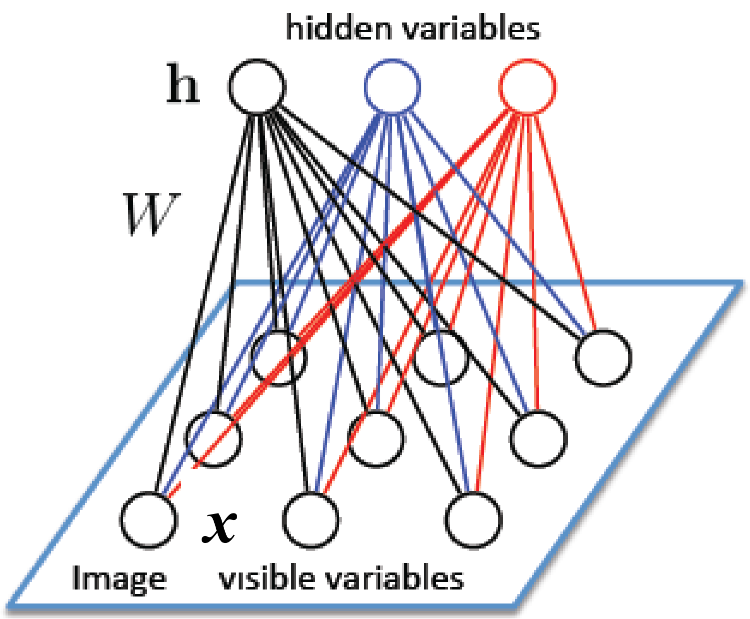






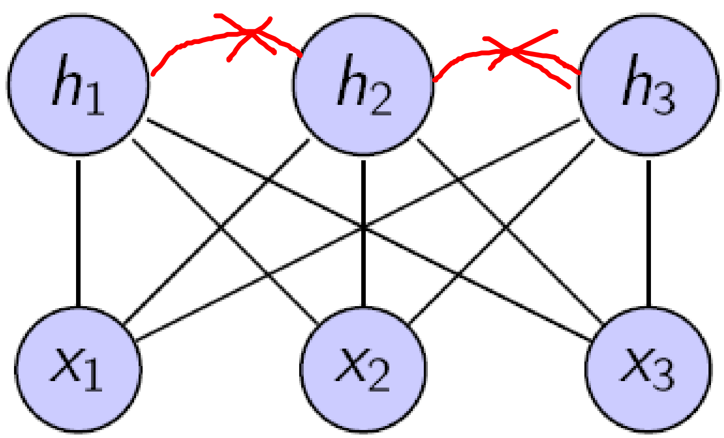


Restricted Boltzmann machine (RBM)



In traditional RBM, x_i and h_j are binary random variables

Simple energy-based model

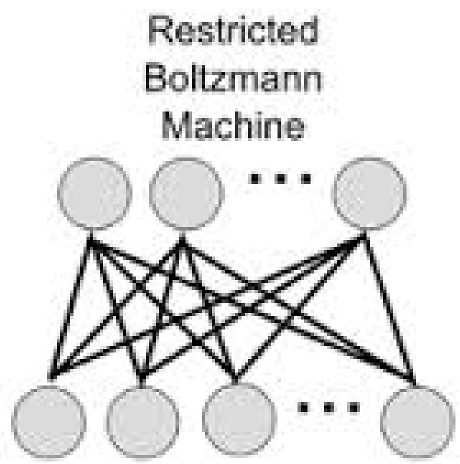


$$p(x,h) \sim e^{-E_\theta(x,h)}$$

$$E_\theta(x,h) = -x'Wh - b'x - d'h$$

The idea is to optimise log-likelihood with the use of approximative Gibbs sampling – Constrastive Divergence algorithm

Restricted Boltzmann machine (RBM)



Visible and hidden units are conditionally independent given one another

$$p(\boldsymbol{h} \mid \boldsymbol{v}) = \prod_i p(h_i \mid \boldsymbol{v})$$

$$p(\boldsymbol{v} \mid \boldsymbol{h}) = \prod_j p(v_j \mid \boldsymbol{h})$$

Following the principle of maximising log likelihood by means of gradient ascent, one obtains:

$$\Delta w_{ji} = \varepsilon \frac{\partial L(\mathbf{W})}{\partial w_{ji}} = \varepsilon \left(\langle v_j h_i \rangle_{\text{data}} - \langle v_j h_i \rangle_{\text{model}} \right)$$

Restricted Boltzmann machine (RBM)

$$P(h_i = 1 \mid \boldsymbol{v}) = \frac{1}{1 + \exp\left(-bias_{h_i} - \boldsymbol{v}^{\mathrm{T}} \mathbf{W}_{:,i}\right)}$$

$$P(v_j = 1 \mid \boldsymbol{h}) = \frac{1}{1 + \exp\left(-bias_{v_j} - \mathbf{W}_{j,:}\, \boldsymbol{h}\right)}$$

$\Rightarrow$

Visible and hidden units are conditionally independent given one another

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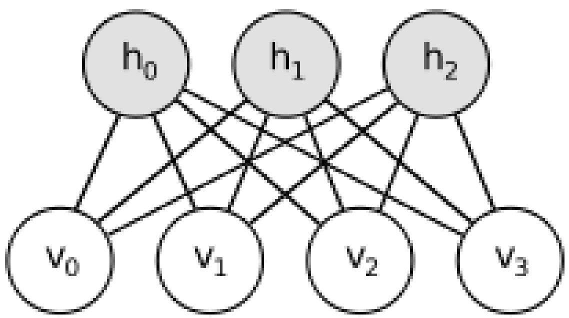
RBM learning with Contrastive Divergence (CD)



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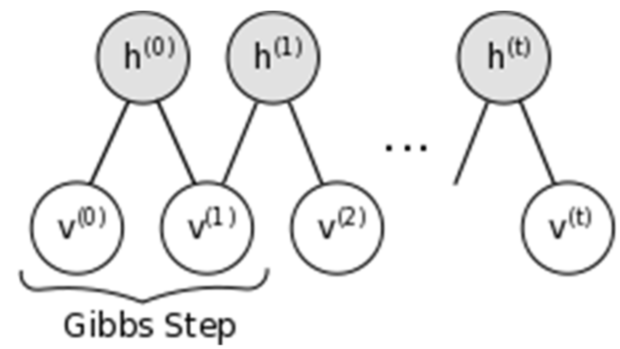
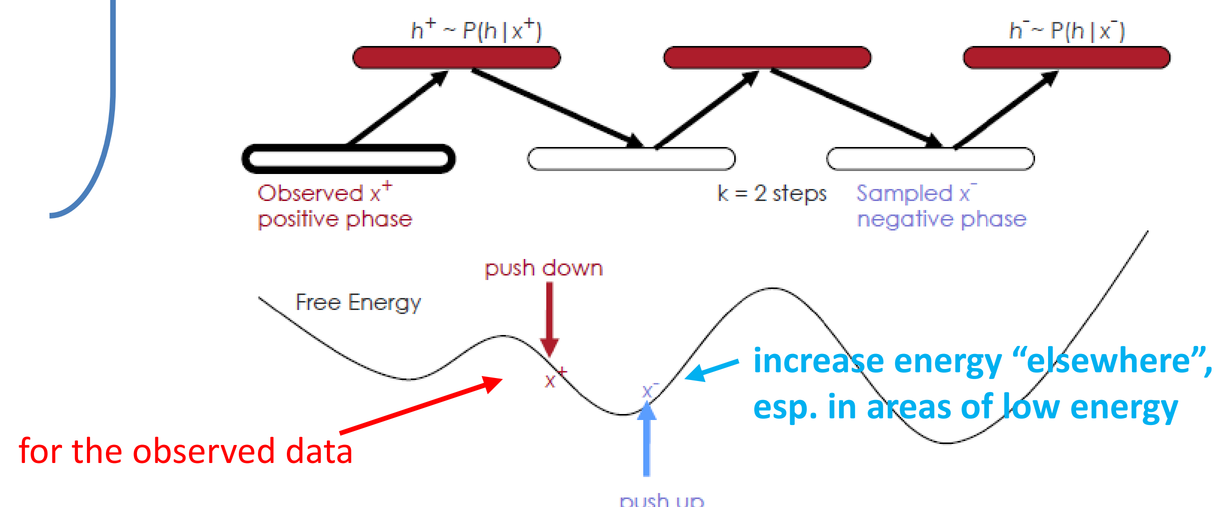
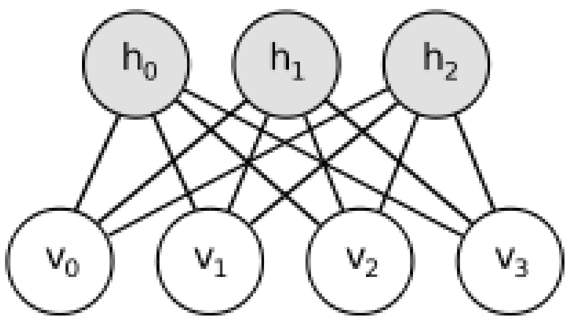
Gibbs sampling





Hinton, 2003

RBM learning with Contrastive Divergence (CD)



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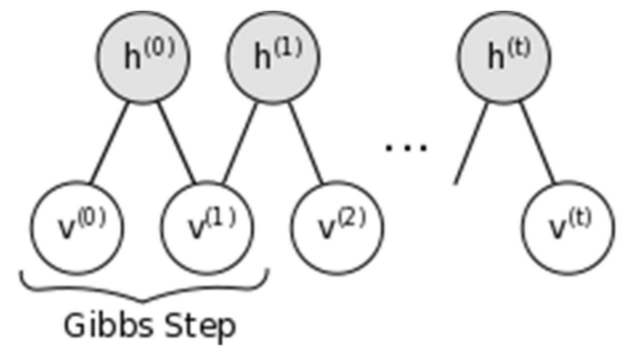
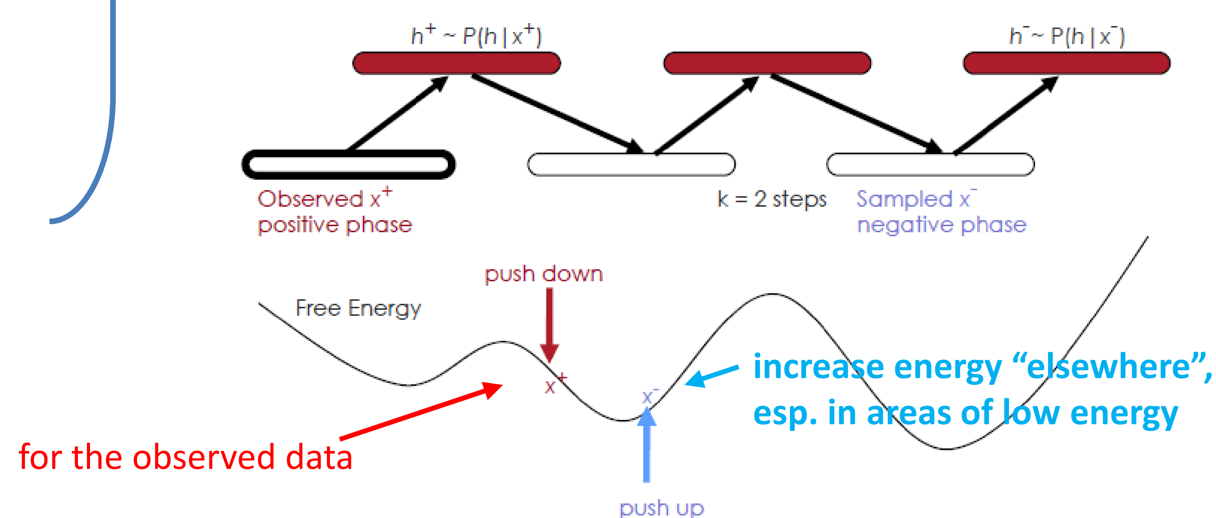




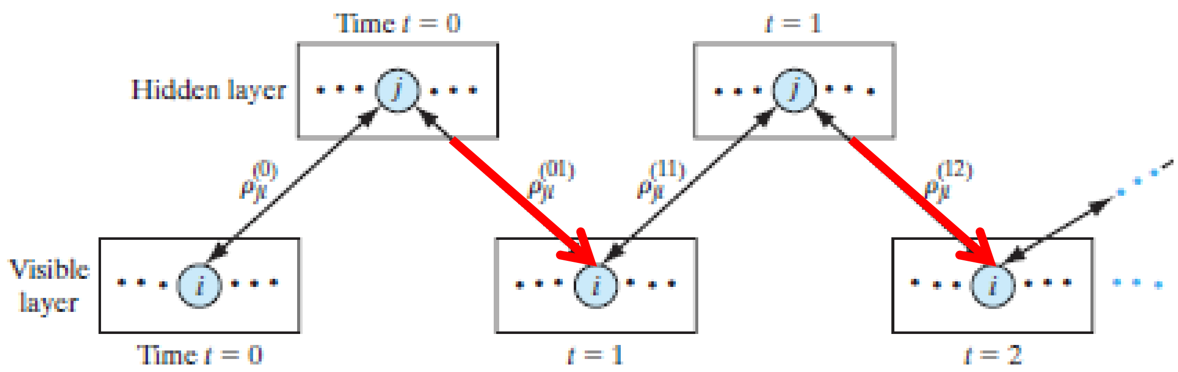
Hinton, 2003

GOOD TO KNOW:

Contrastive Divergence does not optimise the likelihood but it works effectively!

CD$_k$ recipe for training RBM

Gibbs sampling



1) Clamp the visible units with an input vector and update hidden units.

$$P(h_i = 1 \mid \boldsymbol{v}) = \left(1 + \exp\left(-bias_{h_i} - \boldsymbol{v}^{\mathrm{T}} \mathbf{W}_{:,i}\right)\right)^{-1}$$

2) Update all the visible units in parallel to get a **reconstruction**.

$$P(v_j = 1 \mid \boldsymbol{h}) = \left(1 + \exp\left(-bias_{v_j} - \mathbf{W}_{j,:} \boldsymbol{h}\right)\right)^{-1}$$

3) Collect the statistics for correlations after *k* steps using mini-batches and update weights:

$$\Delta w_{j,i} = \frac{1}{N} \sum_{n=1}^{N} \left(v_j^{(n)} h_i^{(n)} - \hat{v}_j^{(n)} \hat{h}_i^{(n)} \right)$$

From RBM to Gaussian-Bernoulli RBM

Bernoulli-Bernoulli (binary-binary)

$$p(v_i = 1|\mathbf{h}) = g\left(\sum_j W_{ij} h_j + b_i\right)$$

$$p(h_j = 1|\mathbf{v}) = g\left(\sum_i W_{ij} v_i + a_j\right)$$

Gaussian-Bernoulli (real/cont.-binary)

$$p(v_i = x|\mathbf{h}) = \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left(-\frac{\left(x - b_i - \sigma_i \sum_j h_j W_{ij}\right)^2}{2\sigma_i^2}\right),$$

$$p(h_j = 1|\mathbf{v}) = g\left(b_j + \sum_i W_{ij} \frac{v_i}{\sigma_i}\right),$$

Visible units are real-valued whereas hidden units remain binary.

Salakhutdinov, 2015

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<u>Visible units are real-valued</u> whereas hidden units remain binary.

The derivative of the log-likelihood:

$$\frac{\partial \log P(\mathbf{v};\theta)}{\partial W_{ij}} = \mathbb{E}_{P_{\text{data}}}\left[\frac{1}{\sigma_i} v_i h_j\right] - \mathbb{E}_{P_{\text{model}}}\left[\frac{1}{\sigma_i} v_i h_j\right]$$

Salakhutdinov, 2015

Generative vs discriminative approach

1. Generative deep architectures
    - describe statistical distributions of data and associated classes, P(X,Y)
    - characterise higher-order correlational structure of data for pattern analysis (suitable for holistic training of complex systems)
    - energy-based models including auto-encoders

Generative vs discriminative approach

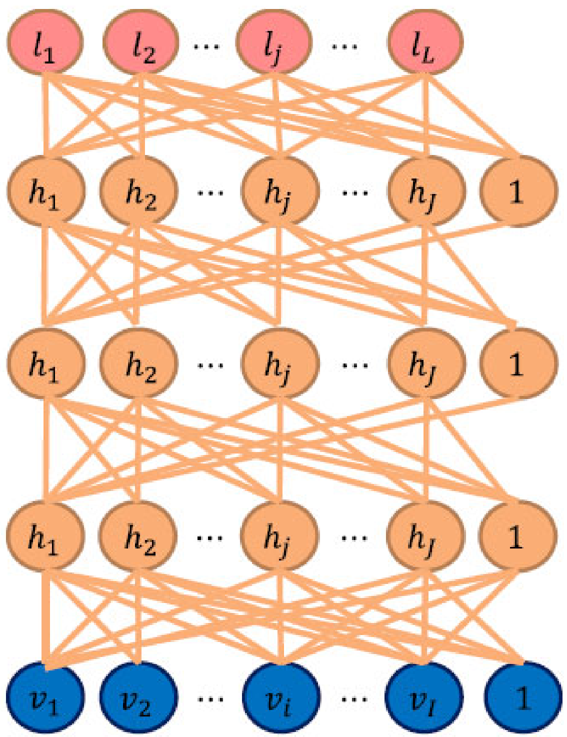
1. Generative deep architectures
   - describe statistical distributions of data and associated classes, P(X,Y)
   - characterise higher-order correlational structure of data for pattern analysis (suitable for holistic training of complex systems)
   - energy-based models including auto-encoders

2. Discriminative deep architectures
   - provide discriminative power for pattern classification by characterising the posterior distribution P(Y|X)
   - HMM, CNN, DBN-DNN

Generative vs discriminative approach

3. Hybrid deep architectures

- the goal is discrimination but is helped by the outcc modelling in deep architectures
- at the heart of early ideas for deep learning proposed and LeCun – unsupervised learning + supervised tuning
- deep belief networks (DBNs) are considered as a precu hybrid deep architectures.



Deng, 2013

Why does deep learning seem to work?

- the notion of *”cheap learning”*
  - exponentially fewer parameters than ”generic” degrees of freedom (”swindle”)
  - we take advantage of the special nature of problems at hand:

    the laws of physics select a particular class of functions that are sufficiently “mathematically simple” to allow “cheap learning” to work

    benefitting from *smoothness*, *symmetry*, *invariance*, *locality* (local interactions boosting sparseness)

Henry W. Lin and Max Tegmark, Why does deep and cheap learning work so well?, arXiv:1608.08225

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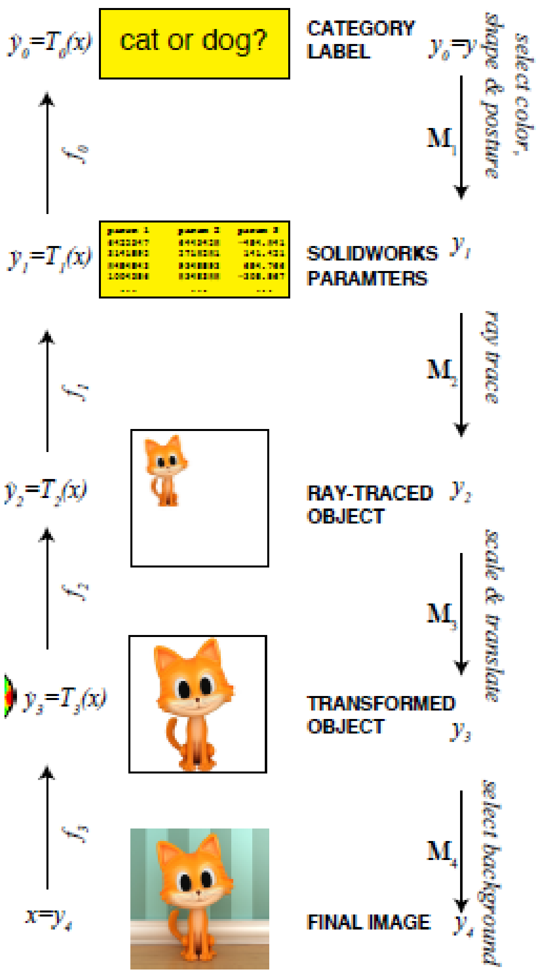
- *”no-flattening” theorems*
  - “flattening polynomials is exponentially expensive, with 2^n neurons required to multiply n numbers using a single hidden layer, a task that a deep network can perform using only $\sim 4n$ neurons”

Henry W. Lin and Max Tegmark, Why does deep and cheap learning work so well?, arXiv:1608.08225

Why does deep learning seem to work?

- ***hierarchical*** structure of the physical world
  - hierarchy of the objects and hierarchy of generative processes to untangle
  - decomposition of the generative process into a hierarchy of simpler steps helps reduce the number of parameters ("swindle" paradox)



Henry W. Lin and Max Tegmark, Why does deep and cheap learning work so well?, arXiv:1608.08225

Key challenges ahead

I. Theoretical challenges

- insufficiently tight generalisation bounds (VC dimension)
- difficulty in theoretical handling of complexity of learning in deep architectures (”hard to prove anything”)
- is it just another (very efficient) parameterisation of solutions?

II. Visualisation, interpretation, *explanation*

- **explainable** deep networks (factors underlying inference outcomes)
- strong initiatives towards visualising and interpreting data representations (particularly in the realm of CNNs)
- how can the process of learning be monitored and controlled?

Key challenges ahead

III. Functionality

- multi-task learning, transfer learning
- multi-modal information processing
- local, incremental learning, self-organisation
- not addressing yet challenges brain-like computing has ambition for

BUT: Is it really the direction for machine intelligence in the spirit of general AI?

Key challenges ahead

III. Functionality

- multi-task learning, transfer learning
- multi-modal information processing
- local, incremental learning, self-organisation
- not addressing yet challenges brain-like computing has ambition for

IV. Computational challenges

- need for lowering computational costs (”equivalent” networks, performance cost etc.)
- need for better use of data and existing networks (pre-trained)
- dedicated hardware platforms

Summary

- The era of deep learning
- What is the motivation for deep network architectures?
  - expressive power (*expressibility*) and compactness (*efficiency*)
  - hierarchical brain (cortex) organisation
  - multiple levels of abstraction
  - multiple **levels of representations** suitable for multi-task learning
- ***Learning data representations*** in deep learning approach vs *hand-engineering features* in traditional pattern recognition
- Problem with unstable gradients
- Learning protocol for DBNs, stacked autoencoders:
  - PHASE I: greedy layer-wise unsupervised pre-training (autoencoders or RBMs)
  - PHASE II: supervised tuning with gradient descent-like optimisation (the last layers or the entire network)

Summary

- Hypotheses about the role of unsupervised pre-training: *regularisation* vs *optimisation* hypotheses
- However, currently there is a trend to avoid pre-training and employ **ReLU units** (less risk for overfitting and local minima), batch normalisation, dropout
- What does DL have to offer?
  - learning data representations at multiple levels
  - hierarchy of distributed features (multi-task and transfer learning, non-local generalisation, mitigating the effect and consequences of curse of dimensionality)
  - good performance (large-scale problems) with relatively compact models --> the driving force behind R&D
  - semi-supervised learning opportunities
- Still plenty of challenges ahead!