Deep Learning

Volker Tresp Winter 2023-2024

Neural Network Winter and Revival

- While Machine Learning was flourishing, there was a Neural Network winter (late 1990's until late 2000's)
- Around 2010 there was a revival which made neural networks again extremely popular; it was restarted by Geoffrey Hinton, Yann LeCun, and Yoshua Bengio (many people now name the 2012 as the year of the breakthrough in deep learning)
- Yann LeCun (New York University and Research) and Yoshua Bengio (Universite de Montreal) are two world-class researchers who never stopped working with neural networks. Geoffrey Hinton (co-inventor of the MLP, Boltzmann machines and others) (Google and University of Toronto) says it all got re-started with the 2006 paper "A fast learning algorithm for deep belief nets" by Hinton, Osindero, and Teh
- In Europe: Juergen Schmidhuber at IDSIA
- Deep networks achieved best results on many tasks/datasets

Turing Award Winners (2018)



Juergen Schmidhuber



Kai Yu



Yu Kai, head of Baidu's Institute of Deep Learning (IDL), demonstrates the smart bike project, DuBike, at the company's headquarters in Beijing. Photo: Simon Song

What Belongs to Deep Learning

- 1. In general: Multi Layer Perceptrons (Neural Networks) with many large hidden layers
- 2. Any Recurrent Neural Network (RNN), in particular LSTMs and GRUs; Transformers (separate slides)
- 3. Convolutional Neural Networks (CNNs)
- 4. Deep Reinforcement Learning (separate slides)
- 5. Representation Learning, including representations for words, entities, predicates, samples
- 6. Deep Generative Models: VAEs, GANs (separate slides)
- 7. Foundation models like BERT, DALLE, and GPT which use self-supervised learning

Artificial Intelligence

 Creating machines that perform functions that require intelligence when performed by people (Kurzweil, 1990)

<u>Games</u>



Q&A



Auton. Driving



Drones, Robots



Translation



Face Recognition



Speech Recognition

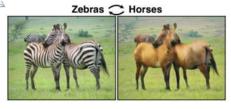


?

Deep Learning

- Deep Learning is the reason for the emerging huge interest in AI
 - Convolutional DL
 - Recurrent DL
 - Reinforcement DL
 - Generative Adversarial Networks (GANs)

CycleGan



Face Recognition



Translation



Speech Recognition



Games



Student Magic: Visual Q&A

"I spy with my little eye ..."

Image	Policy Gradient		Tempered Policy Gradient		
	Is it in left?	No	Is it a person?	No	
	Is it in front?	No	Is it a vehicle?	Yes	
经验 的证据的 "是一个多少	Is it in right?	Yes	Is it a truck?	Yes	
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Is it in middle?	Yes	Is it in front of photo?	No	
	Is it person?	No	In the left half?	No	
	Is it ball?	No	In the middle of photo?	Yes	
	Is it bat?	No	Is it to the right photo?	Yes	
	Is it car?	Yes	Is it in the middle of photo?	Yes	
	Status:	Failure	Status:	Success	
	Is it in left?	No	Is it a giraffe?	Yes	
	Is it in front?	Yes	In front of photo?	Yes	
	Is it in right?	No	In the left half?	Yes	
	Is it in middle?	Yes	Is it in the middle of photo?	Yes	
	Is it person?	No	Is it to the left of photo?	Yes	
	Is it giraffe?	Yes	Is it to the right photo?	No	
	Is in middle?	Yes	In the left in photo?	No	
	Is in middle?	Yes	In the middle of photo?	Yes	
	Status:	Failure	Status:	Success	

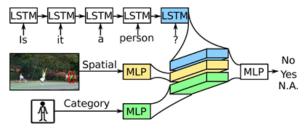
Convolutional DL

- + Recurrent DL
- + Reinforcement DL

Talents, Talents Talents!

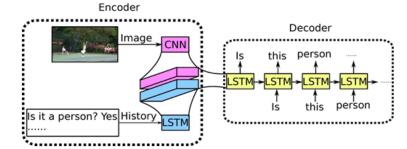
April 02, 2019

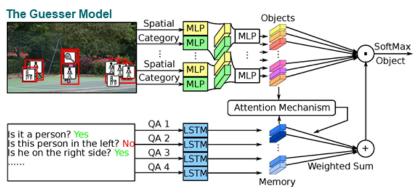
The Oracle Model



Rui Zhao, 2018

The Question-Generator Model



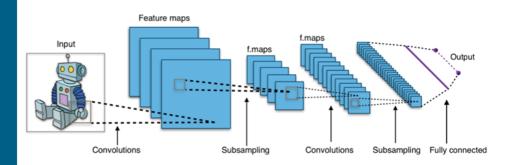


Deep X Technologies behind Artificial Intelligence

- Deep Learning; Machine Learning;
 Data Mining; Statistics
 - More (Labeled) Data
 - Deeper Models
 - New Algorithms
 - End-to-End Training; Differentiable-Computing (no Feature Engineering)
 - Computational Power
 - Community

Deep Knowledge: Facts and Models

- Huge Document Repositories with Rapid IE / QA (IBM Watson)
- Maps with GPS for Autonomous Driving
- Ubiquitous IoT and Big Data in Industry
- Detailed (Patient) Profiles
- Web Content, Wikipedia for Humans
- Knowledge Graphs for Machines





Deep Learning Recipe: What Are the Reasons? (Hinton 2013)

- 1. Take a large data set
- 2. Take a Neuronal Network with many (e.g., 7) large (z.B. 1000 nodes/layer) layers
- 3. Optional: Use GPUs
- 4. Train with Stochastic Gradient Decent (SGD)
- 5. Except for the output layer use rectified linear units: $\max(0,h)$
- 6. Regularize with *drop-out*
- 7. Optional: Initialize weights with unsupervised learning
- 8. If the input is spatial (e.g., a picture), use convolutional networks (weight sharing) with max-pooling

Important Benefits

- A deep network learns complex application-specific features trained on **many data** points (large N)
- ullet Data are given in some feature space (can be raw pixel images); **no additional feature engineering or basis function design is necessary**. Work with the data as they are, also with large M
- A deep architecture can achieve an efficient representation with fewer resources in a hierarchical layered structure
- Composition: In a classifier, an image is analysed by composing low level representations formed in the first processing layers, to generate high level features in the higher layers; a deep generative models composes an image from hierarchical representations

1: Large Data Set

- When decision boundaries are complex, a large data set describes the details of those boundaries
- Details can be captured with a complex (multi-layer) neural network
- "As of 2016, a rough rule of thumb is that a supervised deep learning algorithm will generally achieve acceptable performance with around 5,000 labeled examples per category, and will match or exceed human performance when trained with a dataset containing at least 10 million labeled examples." (Deep Learning, Goodfellow et al.)

2: Large Networks

- It has been possible to train small to medium size problems since the early 1990s
- In deep learning, people work with really large Neural Networks. Example: 10 layers, 1000 neurons/layer
- ResNet from 2015 had 152 layers

3: Graphical Processing Units (GPUs)

- GPUs are highly suited for the kind of number crunching, matrix/vector math involved in deep Neural Networks. GPUs have been shown to speed up training algorithms by orders of magnitude
- Their highly parallel structure makes them more effective than general-purpose CPUs for algorithms where processing of large blocks of data is done in parallel

4: Stochastic Gradient Descent SGD

- Often regular SGD is used where the gradient is calculated on a single training pattern
- "Minibatch SGD" works identically to SGD, except that more than one training example (a "batch" of examples) is used to estimate of the gradient
- Gradient clipping (to avoid huge update steps): if $\|\mathbf{g}\| > v$ then $\mathbf{g} \leftarrow \mathbf{g} v / \|\mathbf{g}\|$. v > 0 is the norm threshold (\mathbf{g} is the gradient vector)
- Local optima do not appear to be a major problem: current thinking is that there are many local optima, but that they are all very good

Adaptive Learning Rates

• (1) AdaGrad (adaptive gradient algorithm) is often used for learning rates to be adaptively altered; let g_j be the gradient for weight w_j accumulated over a minibatch at "time" t

$$w_j := w_j - \frac{\eta}{\sqrt{G_{j,j}}} g_j$$

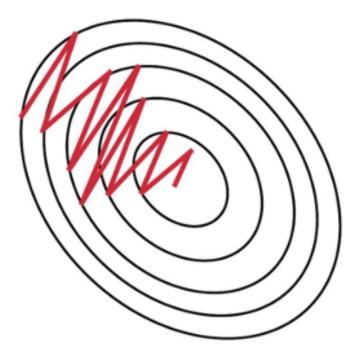
Here, $G_{j,j} = \sum_{\tau=1}^t g_{\tau,j}^2$ is the accumulated squared gradient from the start of the epoch

• (2) Momentum term

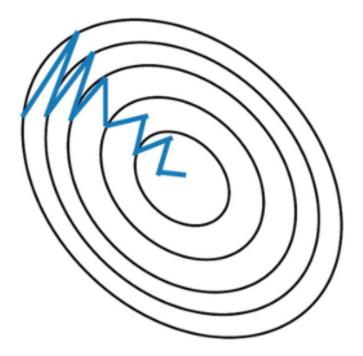
$$\tilde{g}_j := \beta \tilde{g}_j + (1 - \beta)g_j$$

$$w_j := w_j - \eta \tilde{g}_j$$

• (3) Adam (Adaptive Moment Estimation) (very popular)



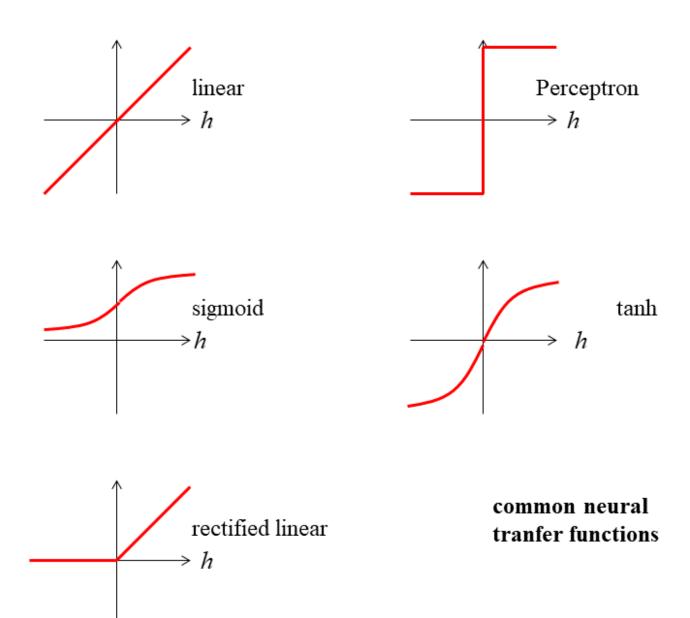
Stochastic Gradient Descent withhout Momentum

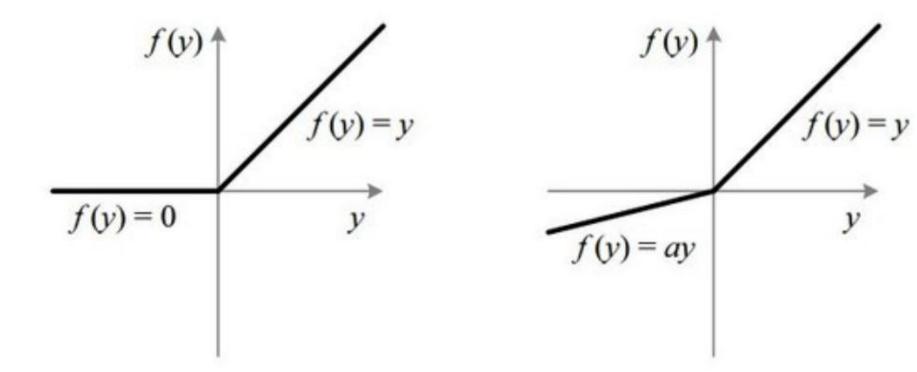


Stochastic Gradient
Descent with
Momentum

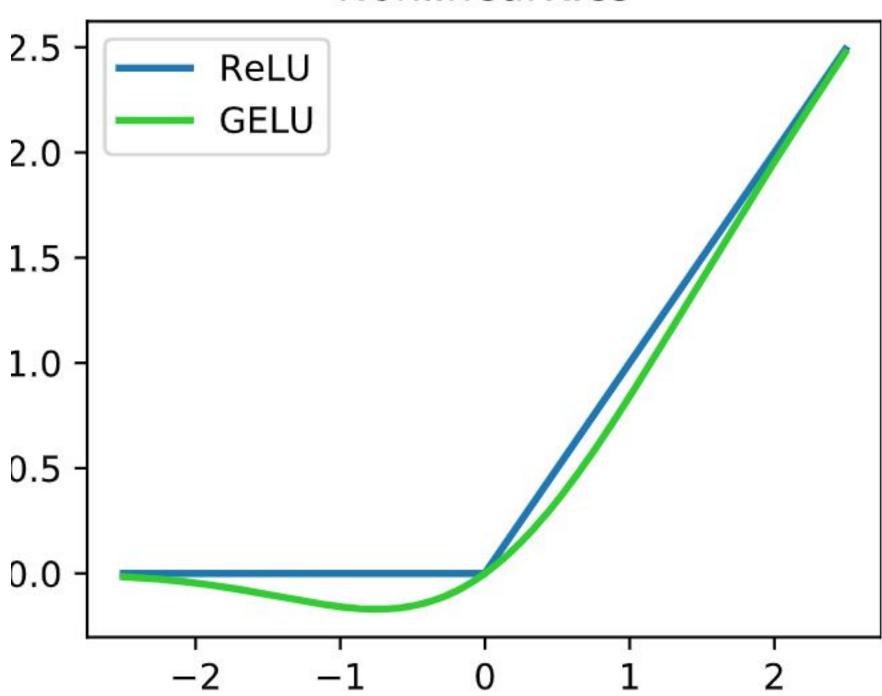
5: Rectified Linear Function

- The transfer function of a Rectified Linear Unit (ReLU) is max(0,h)
- Reduces the effects of the vanishing gradient problem which can occur with sigmoid neurons! They learn much faster!
- Seems odd since some neurons become insensitive to the error, but a sufficient number stays active
- Leads to sparse gradients and to a sparse solution
- Leaky ReLU "fixes" problems with "dead" neurons; GELU (Gaussian Error Linear Unit) "fixes" problems with the discontinuity at the origin
- For training classification tasks, the output layer has sigmoidal activation functions and the cross-entropy cost function is used





Nonlinearities



6A: Drop-Out Regularization

- For each training instance: first remove 50% of all hidden units, randomly chosen. Only calculate error and do adaptation on the remaining network
- \bullet For testing (prediction): use all hidden units but multiply all outgoing weights by 1/2
- This is like a committee machine, where each architecture is a committee member, but committee member share weights
- Works better than stopped training! No stopping rule required!
- Can even do drop-out in the input layer, thus different committee members see different inputs!
- Hinton: use a large enough neural network so that it overfits on your data and then regularize using drop out
- Goodfellow (DL): Dropout provides an inexpensive approximation to training and evaluating a bagged ensemble of exponentially many neural networks
- Variant: DropConnect (dropout of single connections)

6B: Weight Regularization

- Weight decay works
- ullet But even better: for each neuron, normalize the incoming weight vector to have the same maximum length. Thus if $\|\mathbf{w}\| > \alpha$

$$\mathbf{w} \to \alpha \frac{1}{\|\mathbf{w}\|} \mathbf{w}$$

Backpropagation is performed through the normalization

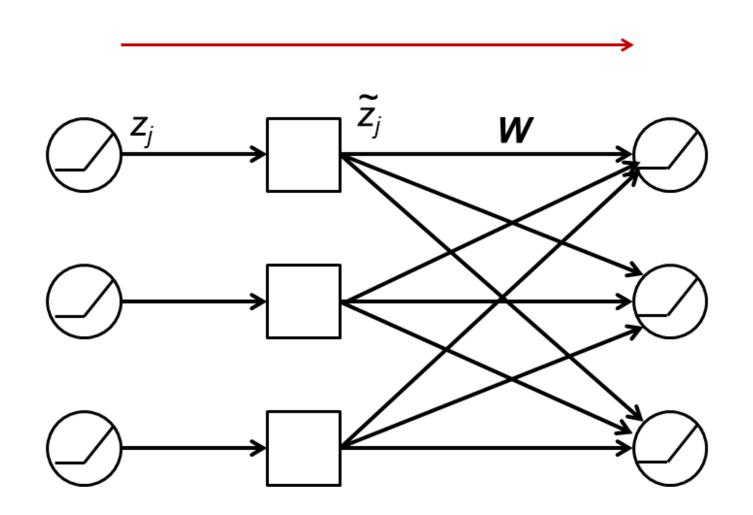
6C: Batch Normalization

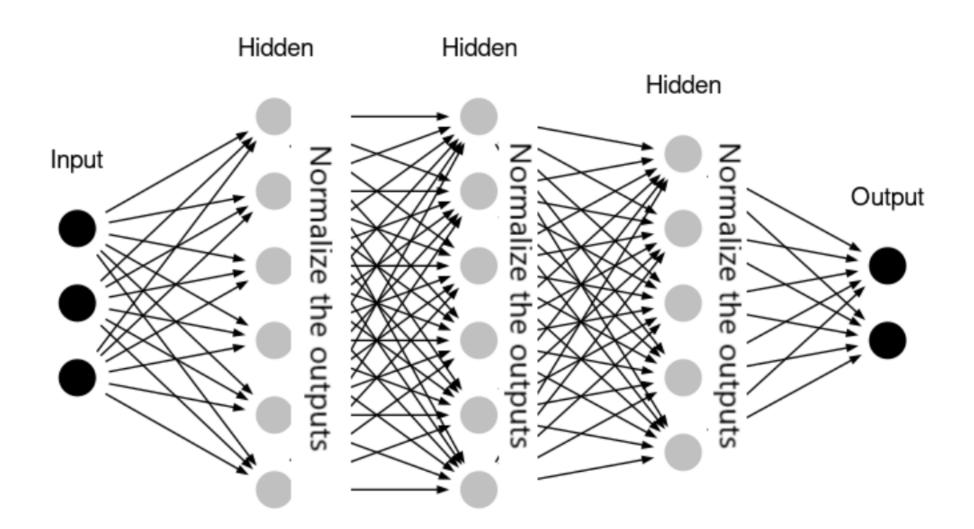
- Batch-Normalization is an algorithmic method which makes the training of Deep Neural Networks (DNN) faster and more stable
- ullet Batch normalization: Let z_j be the output (activation) of a neuron after applying the nonlinear transfer function. Then each neuron z_j is normalized as

$$\tilde{z}_j = \frac{z_j - \mu_j}{\sqrt{\sigma_j^2 + \epsilon}}$$

- Mean μ_j and variance σ_j^2 of that neuron are calculated **over a small batch**. Back-propagation is performed through these operations. $\epsilon>0$ is a small number, to ensure stability
- Batch normalization can be applied after the ReLU (as discussed here) or before the ReLU
- It is provided by all major frameworks; the details of the implementation are involved

Batch Normalization



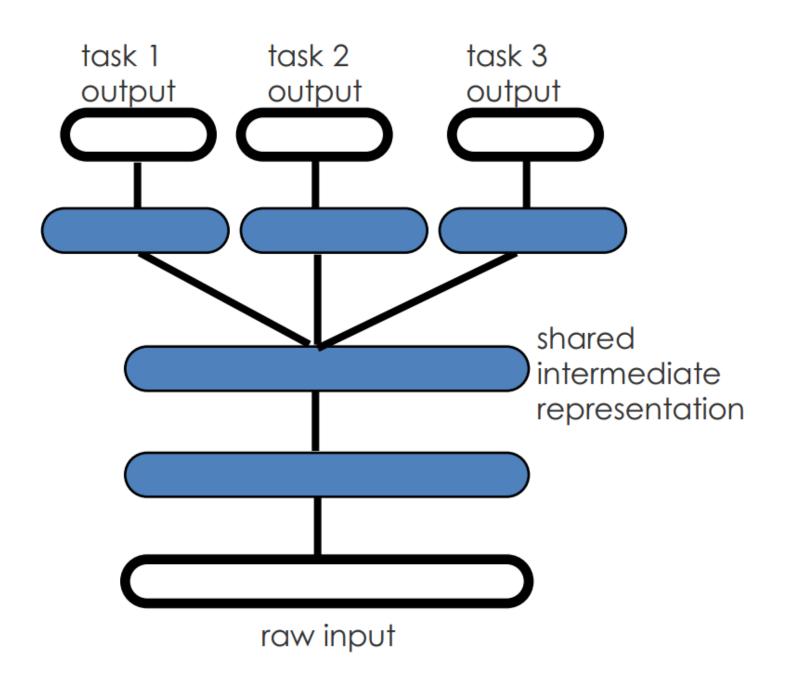


7: Initialize Weights with Unsupervised Learning

- The first layer is initialized with the encoder part of an autoencoder (see lecture on manifolds)
- Alternatively: Several layers are initialized by a stacked autoencoder
- Not as popular anymore: Restricted Boltzmann Machine (RBM) for Deep Boltzmann Machines (DBMs) and Deep Belief Networks (DBNs)
- New in 2021: Pretraining is coming back with strong force in the form of "contrastive learning"!

Multitask Learning and Pretrained Models

- The idea is to learn several tasks by sharing common representations (same learned "basis functions" with different output weights)
- One task might be trained on a huge data set: this is then called the "pretrained model"
- For a new task (data set), only the last layer is adapted and the remaining network is inherited from the pretrained network (there are many variants on this basic idea)
- Current research: few-shot learning, one-shot learning, zero-shot learning



Facebook's Deep Face: Face Recognition as Multi-Task Learning

- Build a deep learning NN to classify many face images from 4000 persons. Thus there
 are 4000 outputs, one for each person
- The next to last layer is used as a representation for any face image (also for faces and persons not in the training set)
- Note that here, the representation is close to the output layer
- Much effort is spent in the input layers to normalize the facial images
- C: convolutional layer. M: max-pooling layer. The subsequent layers (L4, L5 and L6) are locally connected, like a convolutional layer they apply a filter bank, but every location in the feature map learns a different set of filters.

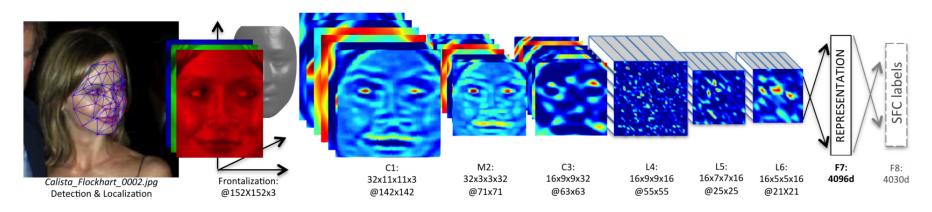


Figure 2. **Outline of the** *DeepFace* **architecture**. A front-end of a single convolution-pooling-convolution filtering on the rectified input, followed by three locally-connected layers and two fully-connected layers. Colors illustrate feature maps produced at each layer. The net includes more than 120 million parameters, where more than 95% come from the local and fully connected layers.

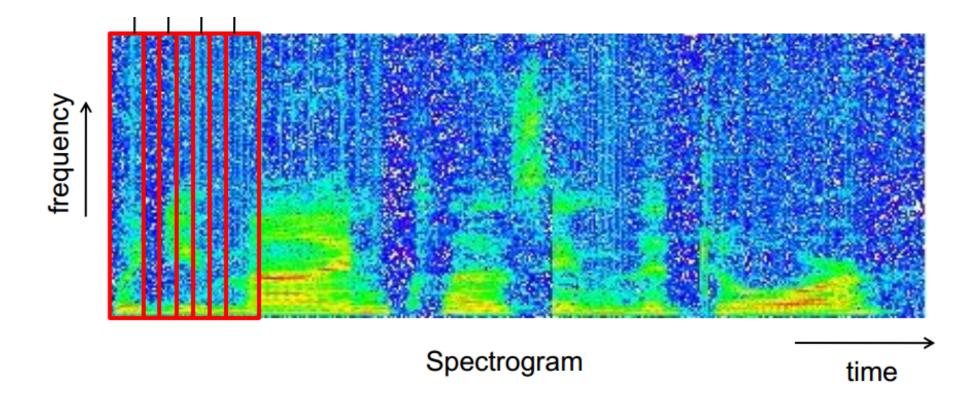
Android Server Architecture for Speech Recognition (2013)

- Part of speech recognition with Hidden Markov Models (HMMs): predict a state in the HMM (State) using a frequency representation of the acoustic signal in a time window (Frame)
- The Neural Network is trained to learn P(State|Frame)
- 4-10 layers, 1000-3000 nodes / layer, no pre-training
- Rectified linear activations: y=max(0,x)
- Full connectivity between layers,
- Softmax output (cross-entropy cost function) (see lecture on linear classifiers)

cont'd

• Features:

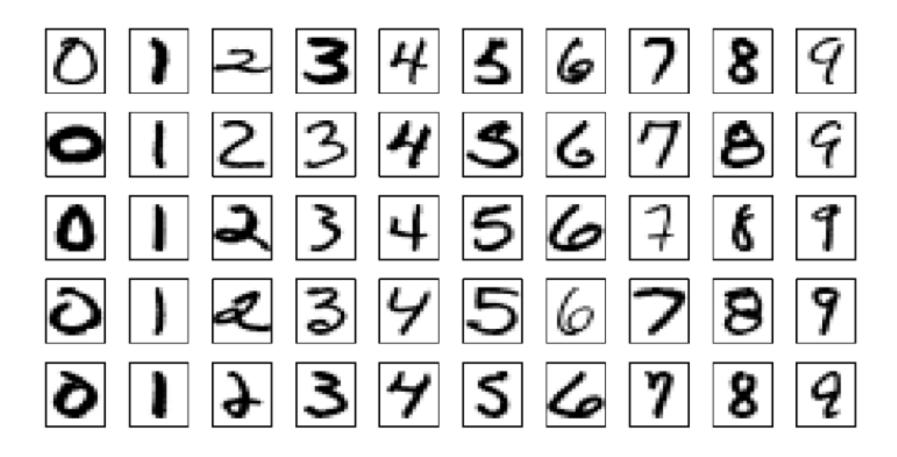
- 25ms window of audio, extracted every 10ms.
- log-energy of 40 Mel-scale filterbanks, stacked for 10-30 frames.
- Training time: 2-3 weeks using GPUs!
- Online: Android uses the server solution. Offline: Small Neural Network on the Smart Phone
- Advantage: Speaker independent! Now used by Google, Microsoft, IBM, replacing Gaussian mixture models (30% reduction in error)
- Even more improvement on the task of object recognition in images (from 26% error to 16% error)) using 1.2 million training images. With convolutional neural networks.



task	Hours of training data	Deep net+HMM	GMM+HMM same data	GMM+HMM more data
Switchboard	309	16.1	23.6	17.1 (2k hours)
English Broadcast news	50	17.5	18.8	
Bing voice search	24	30.4	36.2	
Google voice input	5870	12.3		16.0 (lots more)
Youtube	1400	47.6	52.3	

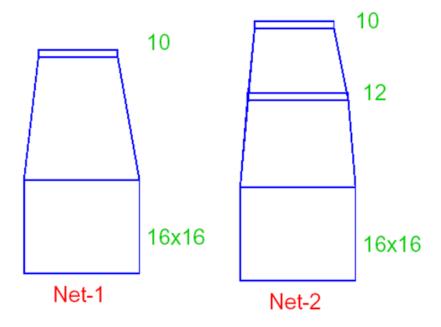
8: Convolutional Neural Networks (CNNs)

Recognition of Handwritten Digits



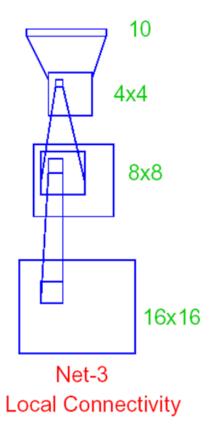
Recognition of Handwritten Digits using Neuronal Networks

- \bullet Example: 16×16 grey-valued pictures; 320 training images, 160 test images
- Net-1: No hidden layer: corresponds to 10 Perceptrons, one for each digit
- Net-2: One hidden layer with 12 nodes; fully connected ("normal MLP")



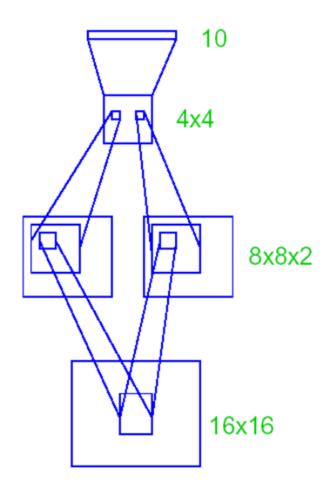
Neuronal Network with Local Connectivity: Net-3

- In the following variants, the complexity was reduced
- Net-3: Two hidden layers with local connectivity (but no weight sharing yet): motivated by the local receptive fields in the brain
 - Each of the 8×8 neurons in the first hidden layer is only connected to 3×3 input neurons from a receptive field
 - In the second hidden layer, each of the 4 \times 4 neurons is connected to 5 \times 5 neurons in the first hidden layer
 - Net-3 has less than 50% of the weights of Net-2, but more neurons



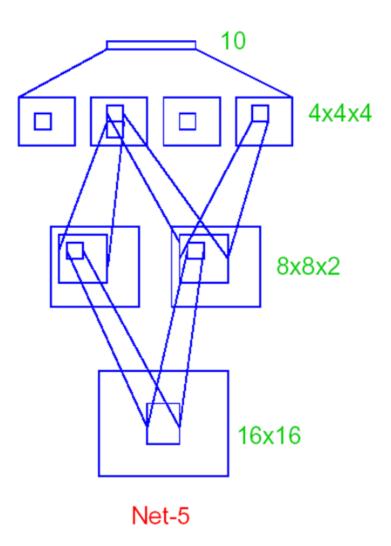
Neuronal Networks with Weight-Sharing (Net-4)

- Net-4: Two hidden layers with local connectivity and weight-sharing
- ullet All receptive fields in the left 8 imes 8 block have the same weights; the same is true for all neurons in the right 8 imes 8 block
- ullet The 4 imes 4 block in the second hidden layer, as before



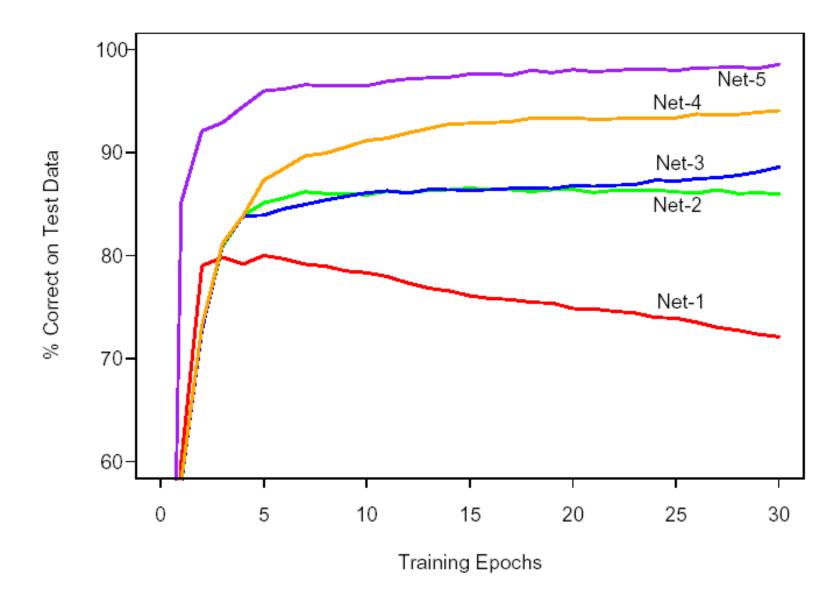
Neural Networks with Weight Sharing (Net-5)

• Net-5: Two hidden layers with local connectivity and two layers of weight-sharing



Learning Curves

- One training epoch is one pass through all data
- The following figure shows the performance on the test set
- Net-1: One sees overfitting with increasing epochs
- Net-5: Shows best results without overfitting



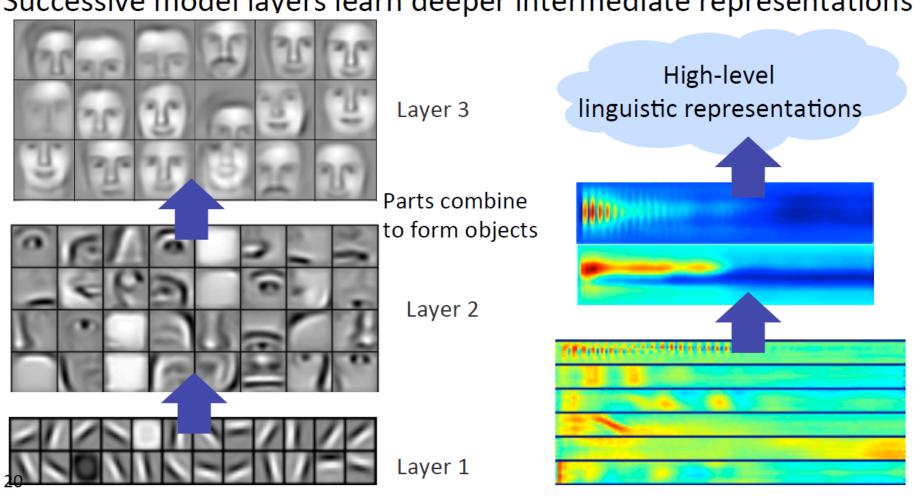
Statistics

• Net-5 has best performance. The number of free parameters (1060) is much smaller than the total number of parameters (5194)

TABLE 11.1. Test set performance of five different neural networks on a hand-written digit classification example (Le Cun, 1989).

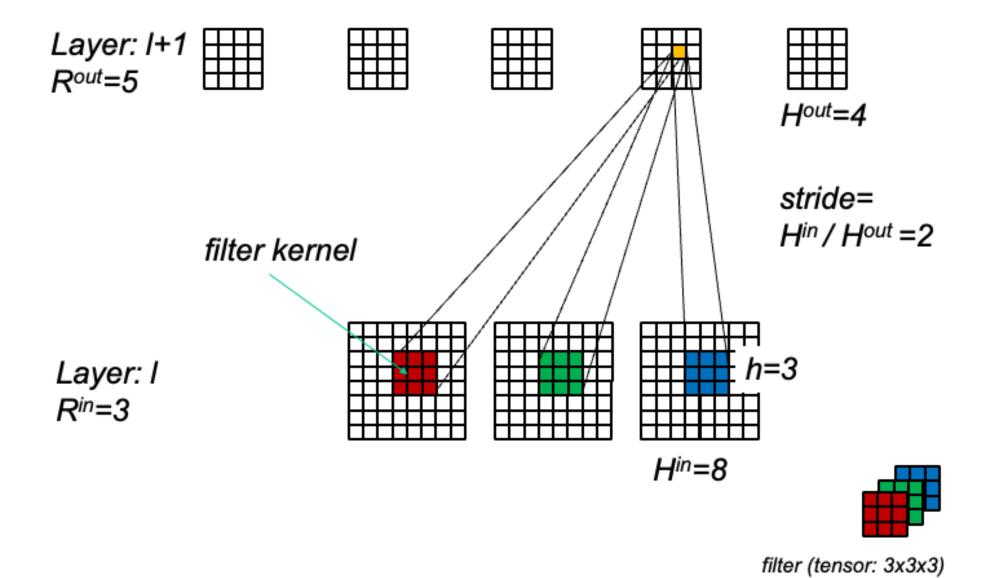
	Network Architecture	Links	Weights	% Correct
Net-1:	Single layer network	2570	2570	80.0%
Net-2:	Two layer network	3214	3214	87.0%
Net-3:	Locally connected	1226	1226	88.5%
Net-4:	Constrained network 1	2266	1132	94.0%
Net-5:	Constrained network 2	5194	1060	98.4%

Successive model layers learn deeper intermediate representations



Details of Convolutional Layers

- ullet The current layer l might consist of R^{in} sub-layers of size $H^{in} imes H^{in}$
- ullet The next layer l+1 might consist of R^{out} sub-layers of size $H^{out} imes H^{out}$
- This implies that one has R^{out} filter kernels (one for each output sub-layer)
- ullet Each filter consists of R^{in} filter kernels, each of size $h \times h$, where typically the kernel support h is $h << H^{in}$
- ullet The each filter is then a tensor of dimension (size) $h imes h imes R^{in}$
- ullet The *stride* is H^{in}/H^{out} ; often the stride is 1; by using a larger stride, $H^{out} < H^{in}$ I can down-sample the image
- Note that I might need to pad the image with zeros



•	1	0	0	0	0	0	0	0	0	0	0
36		0	0	0	0	0	0	0	0	0	0
		0	0							0	0
		0	0								
		0	0								0
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		•				36					•
	30										

The input volume is $32 \times 32 \times 3$. If we imagine two borders of zeros around the volume, this gives us a $36 \times 36 \times 3$ volume. Then, when we apply our conv layer with our three $5 \times 5 \times 3$ filters and a stride of 1, then we will also get a $32 \times 32 \times 3$ output volume.

Inductive Bias

- One says that the different nets, i.e., Net-1, ..., Net-5 have different "inductive bias"
- They make different implicit assumptions about the function class

Representation Learning and Convolutional Neural Networks in Sentence Classification

• Representation Learning and Convolutional Neural Networks in Sentence Classification

Nonlinear Mappings: Tensor Modelling as Representation Learning in NLP

Mapping indices to value!

Sentence class, e.g., sentiment

Deep CNN, ..., often pretrained

My friend Max likes Mary very much

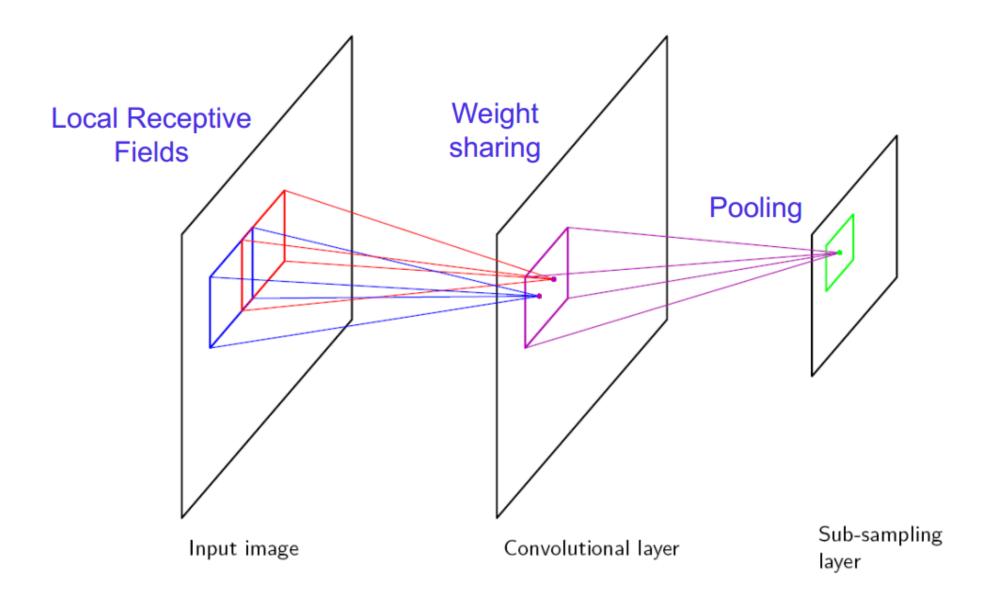
- Pretrained embeddings from dictionaries and then adapted for task
- No feature engineering: NLP for everyone!

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Pooling

- For example, one could compute the mean (or max) value of a **particular feature** over a **region of the image**. These summary statistics are much lower in dimension (compared to using all of the extracted features) and can also improve results (less over-fitting). We aggregation operation is called this operation pooling, or sometimes **mean pooling** or **max pooling** (depending on the pooling operation applied).
- Max-pooling is useful in vision for two reasons: (1) it reduces the computational complexity for upper layers and (2) it provides a form of translation invariance
- Since it provides additional robustness to position, max-pooling is thus a "smart" way of reducing the dimensionality of intermediate representations.
- Mean pooling is related to a convolutional layer with a rectangular (uniform) kernel and a large stride

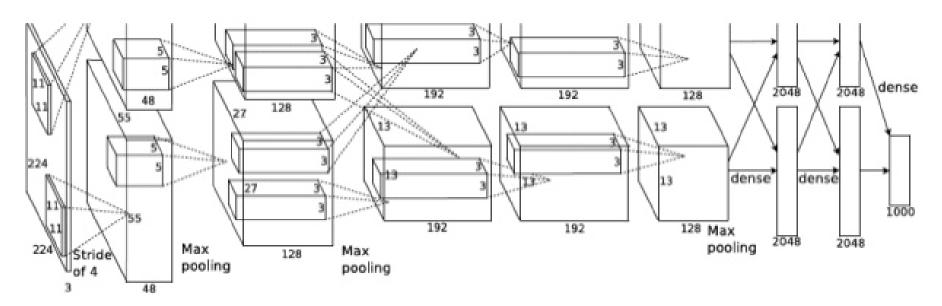


Architectures

- The next slide shows AlexNet
- Alternatives: Inception (Google), Visual Geometry Group (VGG) (Oxford)

AlexNet

- Similar framework to LeCun'98 but:
 - Bigger model (7 hidden layers, 650,000 units, 60,000,000 params)
 - More data (10⁶ vs. 10³ images)
 - GPU implementation (50x speedup over CPU)
 - Trained on two GPUs for a week



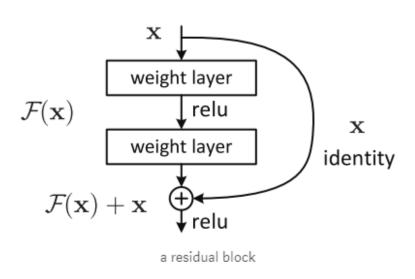
A. Krizhevsky, I. Sutskever, and G. Hinton, ImageNet Classification with Deep Convolutional Neural Networks, NIPS 2012

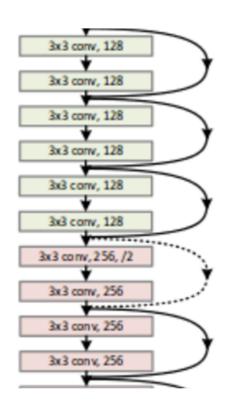
Deep Residual Network

- The next figure shows a Deep Residual Network (ResNet) (2015)
- A ResNet of 152 layers became world champion in the ImageNet data base
- Other special architectures used in image classification: AlexNet (5 convolutional layers) (2012), VGG network (19 convolutional layers) (2014), GoogleNet (Inception) (22 convolutional layers) (2015), and many variants

Input Image

.



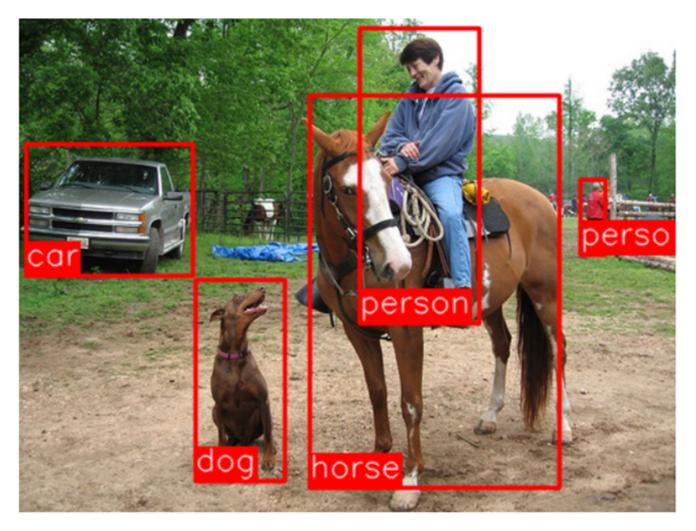


152 layers in total

Output Classes

Regional CNN

- Task: Finding bounding boxes in images (object detection, object segmentation)
- R-CNN, Fast R-CNN, Faster R-CNN, Mask R-CNN



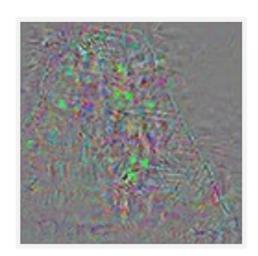
Object detection algorithms such as R-CNN take in an image and identify the locations and classifications of the main objects in the image. Source: https://arxiv.org/abs/1311.2524.

Adversarial Examples

- Deep high-performing DNNs can be fooled by examples intentionally constructed by using an optimization procedure to search for an input that is very close to a real data point and produces a very different label
- A good explanation might be that training data lies on a manifold and for new data on the same manifold, performance is very good: the adversarial examples are away from the manifold and, there, the model behaves rather unpredictable (see lecture on manifolds)
- Adversarial training are attempts to make DNNs less prone to adversarial examples (active research area)



Original image Temple (97%)



Perturbations



Adversarial example
Ostrich (98%)

Where from here?

- There will never be enough labelled data to learn it all
- The Google cat recognizer sees more cat images than any child and is not as good
- If one assumes that cat features are not encoded genetically, then **unsupervised learning**, i.e., understanding the world's statistics might do the job! First attempts: RBM, all sorts of Clustering, autoencoders, ...
- Foundation models like BERT and DALLE might be the next big thing: they are trained in a self-supervised manner without any labelled data!

Explainability using Heat Maps

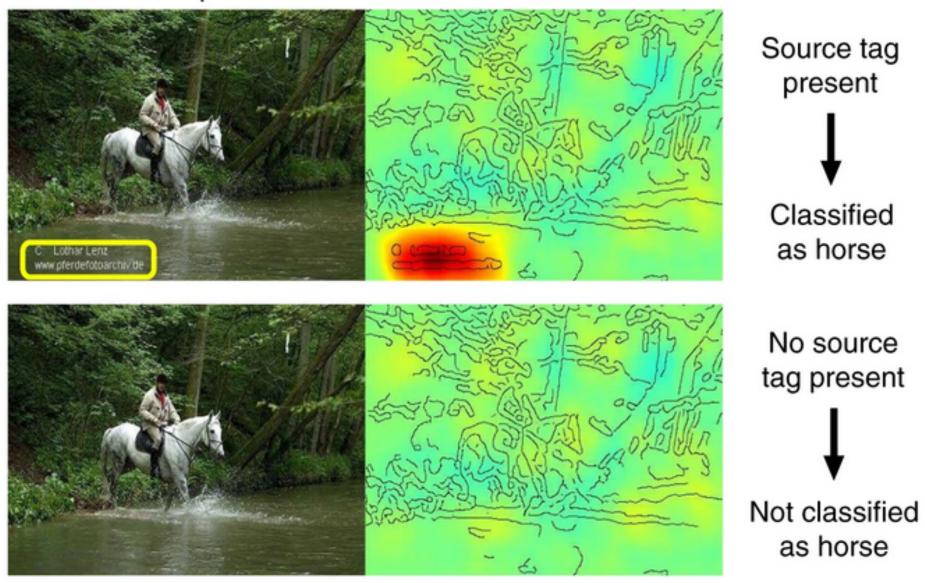
- Getting insights in the working of a DNN is important for many reasons, e.g., for debugging
- "Clever Hans" effect: the classifier pays attention to features in the image, irrelevant for the task
- Many approaches have been proposed
- ullet A simple approach would evaluate for a particular image i

$$\frac{\partial \hat{y}_i(\mathbf{x}_i)}{\partial x_{i,j}}$$

and interpret this quantity (or the square of it) as the relevance of input j for predicting y in the context of image i; if displayed as an image, this is called a heatmap

- ullet Note that in a linear model, $\widehat{y} = \sum w_j x_j$, this is simply w_j
- Popular approaches: Layer-wise Relevance Propagation (LRP), Deep Taylor, Grad-CAM

Horse-picture from Pascal VOC data set



Brahimi, Mohammed, Saïd Mahmoudi, Kamel Boukhalfa, and Abdelouhab Moussaoui. "Deep interpretable architecture for plant diseases classification." In 2019 Signal Processing: Algorithms, Architectures, Arrangements, and Applications (SPA), IEEE, 2019.

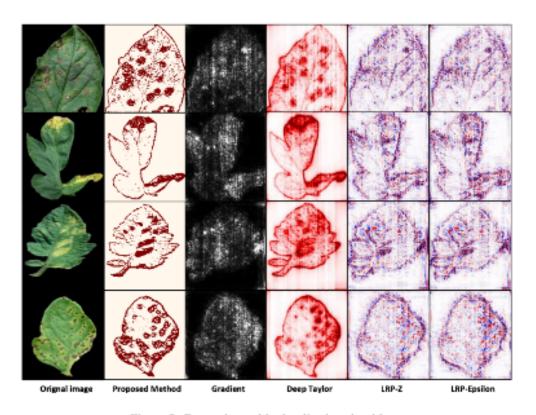
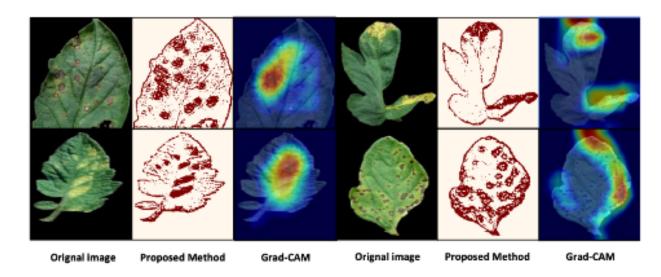


Figure 5: Comparison with visualization algorithms.



Tools

- **Torch7** is used at facebook, Deep Mind and several groups at Google (based on LuaJIT which is similar to Python)
- **PyTorch** is an open-source machine learning library for **Python**, based on Torch (initial release 2016) [Comment: Currently the most important/popular framework]
- **GP-GPU-CUDA:** Facebook, NYU, and Google/Deep Mind all have custom CUDA back-ends for fast/parallel convolutional network training (CUDA (Compute Unified Device Architecture) is a parallel computing platform and programming model implemented by the graphics processing units (GPUs) that they produce. CUDA gives program developers direct access to the virtual instruction set and memory of the parallel computational elements in CUDA GPUs)
- **Theano:** Python library. Popular in the deep learning community. Theano family:
 - Blocks + Fuel: Blocks and Fuel are machine learning frameworks for Python developed by the Montreal Institute of Learning Algorithms (MILA) at the University of Montreal. Blocks is built upon Theano (also by MILA) and allows for rapid

- prototyping of neural network models. Fuel serves as a data processing pipeline and data interface for Blocks.
- **Keras:** Keras is a minimalist, highly modular neural networks library, written in Python and capable of running on top of either TensorFlow or Theano.
- Lasagne: Lasagne is a lightweight library to build and train neural networks in Theano.
- PyLearn2: Pylearn2 is a machine learning library.
- **TensorFlow:** TensorFlow is an open source software library for machine learning in various kinds of perceptual and language understanding tasks. Under development: **Tensor Processing Unit (TPU) custom chip**
- **Deeplearning4j** is an open source deep learning library for Java and the Java Virtual Machine
- Caffe is a deep learning framework made with expression, speed, and modularity in mind. It is developed by the Berkeley Vision and Learning Center (BVLC) and by community contributors. Yangqing Jia created the project during his PhD at UC Berkeley.

Time-line of some Breakthroughs

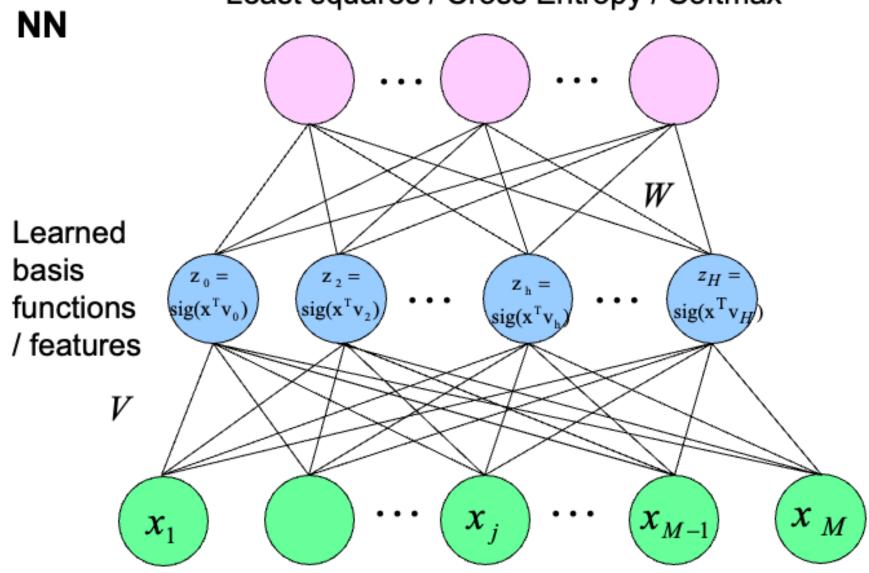
- Object recognition (2012): AlexNet is the name of a convolutional neural network, originally written with CUDA to run with GPU support, which competed in the ImageNet Large Scale Visual Recognition Challenge in 2012. The network achieved a top-5 error of 15.3%, more than 10.8 percentage points ahead of the runner up. AlexNet was designed by the SuperVision group, consisting of Alex Krizhevsky, Geoffrey Hinton, and Ilya Sutskever
- Speech Recognition (2012): Microsoft Chief Research Officer Rick Rashid demonstrates a speech recognition breakthrough via machine translation that converts his spoken English words into computer-generated Chinese language.
- Face recognition (2014): Facebooks Deep Face. Asked whether two unfamiliar photos of faces show the same person, a human being will get it right 97.53 percent of the time. New software developed by researchers at Facebook can score 97.25 percent on the same challenge, regardless of variations in lighting or whether the person in the picture is directly facing the camera.

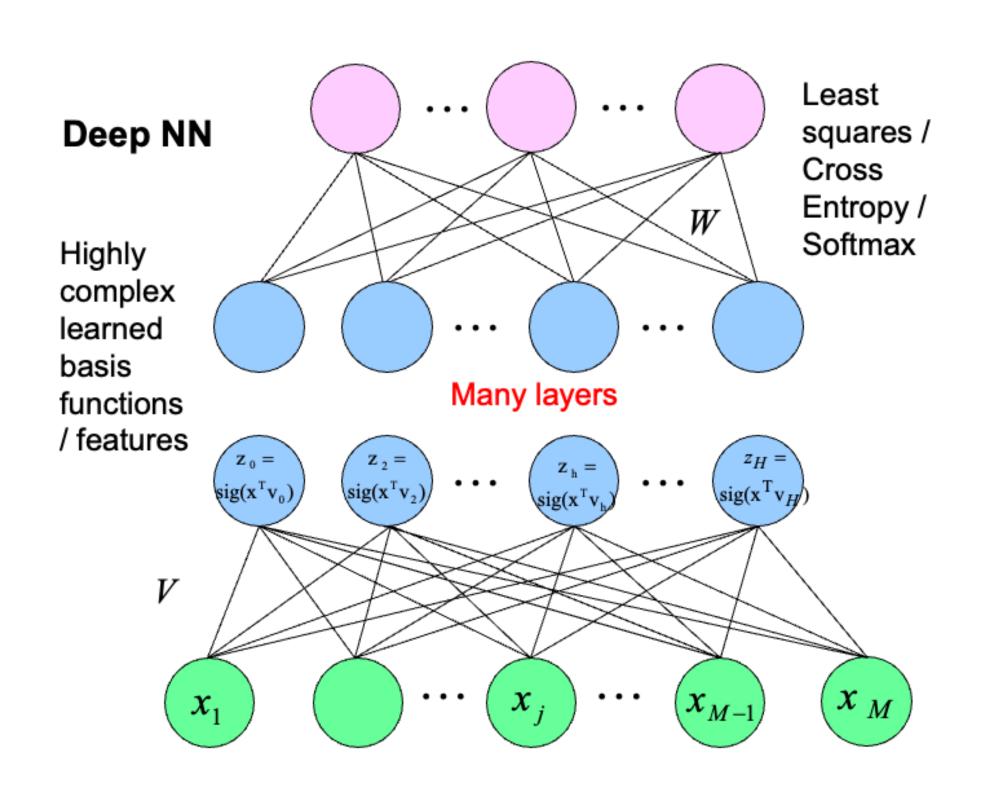
- Generative AI (Images) (2014): GANs have been used to produce samples of photo-realistic images for the purposes of visualising new interior/industrial design, shoes, bags and clothing items or items for computer games' scenes
- ResNet (2015)
- Machine translation (2016): Google Translate began using neural machine translation (NMT)
- Computer and Board Games (2014++): Playing Atari with Deep Reinforcement Learning (2014); spectacular successes of AlphaGo (2015) and AlphaZero (2017) in Go, Chess, and other board games using reinforcement learning
- Protein structure prediction (2020): AlphaFold is an artificial intelligence (AI) program developed by DeepMind, which performs predictions of protein structure
- Chatbots (2022): ChatGPT (Chat Generative Pre-trained Transformer) is a large language model-based chatbot developed by OpenAI; see also ing Bard (Google, based on LaMDA and PaLM), LLaMA (Meta)
- Autonomous driving / Advanced driver-assistance system (e.g., Horizon Robotics)

Deep Learning also Learns Fancy Basis Functions / Features

- Following our analysis of a neural network, also a deep neural network learns basis functions
- The difference is that, due to the many hidden layers, these basis functions now can be highly complex

Least squares / Cross Entropy / Softmax





Why does Deep Learning Work so Well?

- A number of different theories are being developed
- We follow Tomaso Poggio, who addresses approximation theory, optimization, and learning theory
- Youtube: DALI 2018 Tomaso Poggio: Deep Networks: Three Theory Questions
- Mhaskar, Hrushikesh, Qianli Liao, and Tomaso Poggio. "When and why are deep networks better than shallow ones?" Thirty-First AAAI Conference on Artificial Intelligence. 2017.
- Heuristic scaling laws: errors decrease proportionately to (1) computational power and
 (2) data set size and (3) number of parameters

Approximation theory and Case Ic (compositional functions). (When and why are deep networks better than shallow networks?)

- Given any function out of a target function class: what is the best fit a DNN (with some architectural constraints) can obtain
- Both shallow and deep networks can approximate a function equally well/badly, in case we cannot make any particular assumptions on the target function class, except for smoothness. This is our Case I (curse)
- Both suffer from the curse of dimensionality; the **number of required parameters** grows as $\mathcal{O}\left(accuracy^{M \times roughness}\right)$ (see previous lecture on approximation theory)

Compositional Functions

• If we go from generic functions $f(\cdot)$ to a compositional function (functions of functions of functions of functions, ...) and each of those functions only depends on a small number of arguments, then the number of required parameters for a DNN is

$$\mathcal{O}\left(M \times accuracy^2 \times roughness^2\right)$$

(roughness = K is the Lipschitz constant for the target function class; the smaller K, the smoother the function)

• This result can, e.g., be found in: "Why and When Can Deep-but Not Shallow-networks Avoid the Curse of Dimensionality: A Review" Tomaso Poggio et al., International Journal of Automation and Computing, 2017. Theorem 4.

Compositional Functions (cont'd)

• Example of a compositional formula

$$f(x_1, \dots, x_8) =$$

$$h3(h21(h_{11}(x_1, x_2), h_{12}(x_3, x_4)), h_{22}(h_{13}(x_5, x_6), h_{14}(x_7, x_8)))$$

 So we can consider compositional function as a new Case Ic (compositional) of target functions

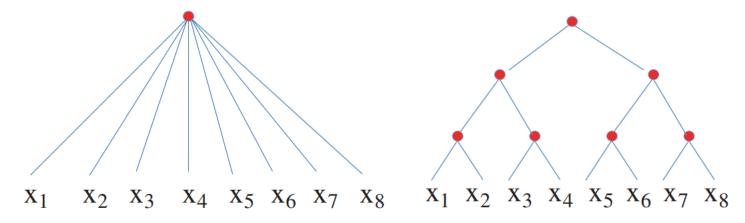


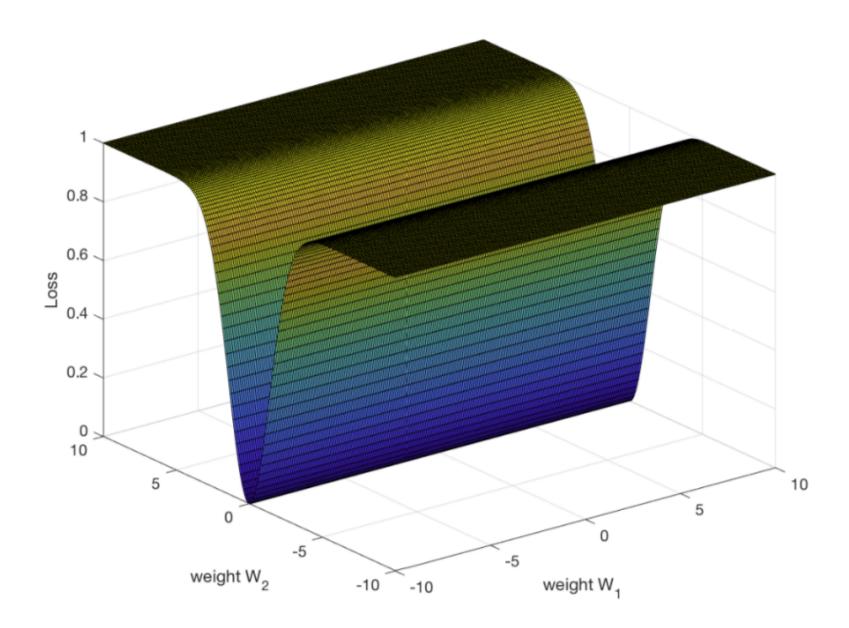
Figure 1: On the left a shallow universal network in 8 variables and N units which can approximate a generic function $f(x_1, \dots, x_8)$. On the right, a binary tree hierarchical network in n=8 variables, which approximates well functions of the form $f(x_1, \dots, x_8) = h_3(h_{21}(h_{11}(x_1, x_2), h_{12}(x_3, x_4)), h_{22}(h_{13}(x_5, x_6), h_{14}(x_7, x_8)))$. Each of the n-1 nodes consists of Q smoothed ReLU units with Q(n-1) = N and computes the ridge function (Pinkus 1999) $\sum_{i=1}^{Q} a_i (\langle \mathbf{v}_i, \mathbf{x} \rangle + t_i)_+$, with $\mathbf{v}_i, \mathbf{x} \in \mathbb{R}^2$, $a_i, t_i \in \mathbb{R}$. Each term, that is each unit in the node, corresponds to a "channel". In a binary tree with n inputs, there are $log_2 n$ levels and a total of n-1 nodes. Similar to the shallow network, a hierarchical network can approximate any continuous function; the text proves how it approximates a compositional functions better than a shallow network. No invariance is assumed here.

Comparison

Target F.	Model F.	Parameters		$\epsilon = 0.1$		Reference
Smooth	Fixed BFs	0 ($\left(extit{accuracy}^{M imes extit{roughness}} ight)$	O(1	$0^{M \times roughness}$	e.g., Poggio
C_f	NN	0	$\left(M imes$ accuracy $ imes C_f^2 ight)$	0 ($\left(10M \times C_f^2\right)$	Barron
Composit.	DNN	$\mathcal{O}(M)$	\times accuracy ² \times roughness ²)	\mathcal{O} (100	$M \times roughness^2$	Poggio

Optimization: What is the landscape of the empirical risk?

- With over-parametrization $(M_p >> N)$, the global optima of the cost functions are degenerate and thus take on more volume in parameter space and are easier to find by SGD
- So, as confirmed empirically, over-parameterized DNNs do not have major problems with local optima
- Another "blessing of dimensionality"
- Poggio: "Over-parametrized deep networks have many global minimizers that are generically degenerate; other critical points of the gradient are generically isolated."
- Poggio: "SGDL (a variant of SGD) finds with very high probability large volume, zero minimizers; empirically SGD behaves in a similar way."



Learning Theory and Overfitting (Learning Theory: How can deep learning generalize so well and not overfit?)

- ullet How many training data points N are required to obtain a good model?
- When the optimum is degenerate, the number of parameters well defined by the data, i.e., the effective number of parameters $M_{\it eff}$, is much smaller than the number of parameters in the DNN, M_p
- Terms estimating the difference between generalization error and training error (i.e., the overfitting) contain expressions like M_p/N : we get overfitting with many parameters M_p and few data points N
- ullet Thus, if we can substitute $M_p \to M_{\it eff}$, overfitting is largely reduced!
- ullet Thus, also for a good generalization performance, over-parameterizations ($M_p>>N$) does not hurt, as long as $M_{\it eff}$ is small

How Many Data Points?

• One estimates for the required number of data points (sample size),

$$\frac{N_{shallow}}{N_{deep}} \approx \epsilon^{-M}$$

With $\epsilon = 0.1$,

$$N_{shallow} \approx 10^{M} \times N_{deep}$$

ullet Thus a shallow network with one hidden layer requires 10^M more data points for training than a deep neural network, to achieve comparable performance

Summary

- Poggio: "Theorem: Much used variants of SGD Batch Normalization and Weight Normalization - perform minimization with unit norm constraint, which is equivalent to maximize margin under norm constraint" (thus the DNN is regularized)
- Poggio: "Theorem: Standard gradient descent implicitly performs minimization with unit norm constraint"
- Poggio: "Together the theorems explain why the training of over-parametrized deep networks satisfy the classification bounds leading to generalization despite over-parametrization"

Conclusions

- Why is this a lecture on Machine Learning and not Deep Learning?
- "If you only know deep learning, you're pretty shallow" (VT)