Neural Network - Foundations

CORS 2021 Workshop

June 8, 2021

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In this talk

A bit of theory

- decision theory
- empirical risk minimization

Neural networks, with a bit of history

- Perceptron Era (1958-60s)
- Backpropagation Era (1986-90s)
- Deep Learning Era (2006-)

Not covered in this talk: statistical learning (capacity, overfitting, underfitting).

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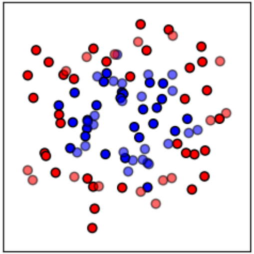
Supervised learning

We have a data set $\mathcal{D} \sim p$ of previously observed (x, y) pairs.

Example

- customer bank records $\rightarrow$ solvency
- patient symptoms $\rightarrow$ disease
- apartment address, surface, year $\rightarrow$ price
- mushroom picture $\rightarrow$ variety



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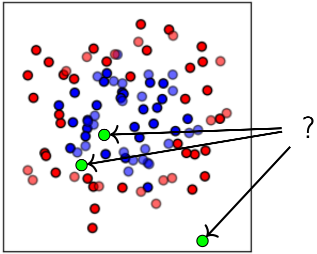

Objective: for any new observation x, make a prediction $\hat{y}$.

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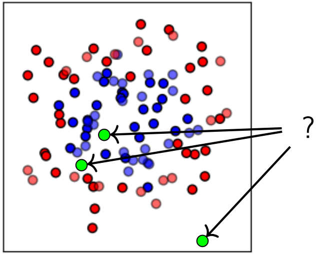

Objective: for any new observation x, make a prediction $\hat{\mathrm{y}}$.

Find a mapping h from an input space $\mathcal{X}$ to an output space $\mathcal{Y}$,

$$\mathrm{h} : \mathcal{X} \rightarrow \mathcal{Y}.$$

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Decision theory

Cost of $\hat{y}$ instead of y ? Loss function

$$L : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}_{\geq 0}.$$

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Decision theory

Cost of $\hat{y}$ instead of y ? Loss function

$$L : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}_{\geq 0}.$$

Risk of $\hat{y}$? Expected cost

$$\mathbb{E}_{y|x}[L(\hat{y}, y)] = \sum_{y} p(y \mid x) \times L(\hat{y}, y) \quad \text{(classification)}.$$

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Decision theory

Cost of ŷ instead of y ? Loss function

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Risk of ŷ ? Expected cost

$$\mathbb{E}_{y|x}[L(\hat{y}, y)] = \sum_{y} p(y \mid x) \times L(\hat{y}, y) \quad \text{(classification)}.$$

Optimal mapping ? Risk-minimizing prediction

$$h^{\star}_{L}(x) = \arg\min_{\hat{y}} \mathbb{E}_{y|x} L(\hat{y}, y).$$

Plug-in risk minimization

$\mathcal{D}$ a set of i.i.d. data samples $\{(\mathrm{x}, \mathrm{y})^{(i)}\}_{i=1}^{N}$ drawn from $p(\mathrm{x}, \mathrm{y})$,
$\mathcal{Q}$ a restricted probabilistic model (e.g. parametric distribution).

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Learning: empirical likelihood maximization given $\mathcal{D}$

$$q^\star = \arg\max_{q \in \mathcal{Q}} \sum_{(\mathrm{x},\mathrm{y}) \in \mathcal{D}} \log q(\mathrm{y}|\mathrm{x}).$$

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Inference: risk minimization given $q^{\star}$

$$\mathrm{h}^{\star}(\mathrm{x}) = \arg\min_{\hat{\mathrm{y}}} \sum_{\mathrm{y}} q^{\star}(\mathrm{y}|\mathrm{x}) L(\hat{\mathrm{y}}, \mathrm{y})$$

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Example: binary classification

Loss function:

$$
\begin{array}{cc|cc}
\multicolumn{2}{c|}{L} & \multicolumn{2}{c}{\hat{y}} \\
 & & 0 & 1 \\
\hline
\multirow{2}{*}{y} & 0 & 0 & 2 \\
 & 1 & 5 & 0
\end{array}
$$

Expected loss:

$$\mathbb{E}_{y|x}[L(1, y)] = p(y = 0|x) \times 2$$
$$\mathbb{E}_{y|x}[L(0, y)] = p(y = 1|x) \times 5$$

Prediction rule:

$$h^{\star}(x) = [p(y = 1|x) > 28.6\%] \, .$$

All we need is to estimate $p(y|x)$.

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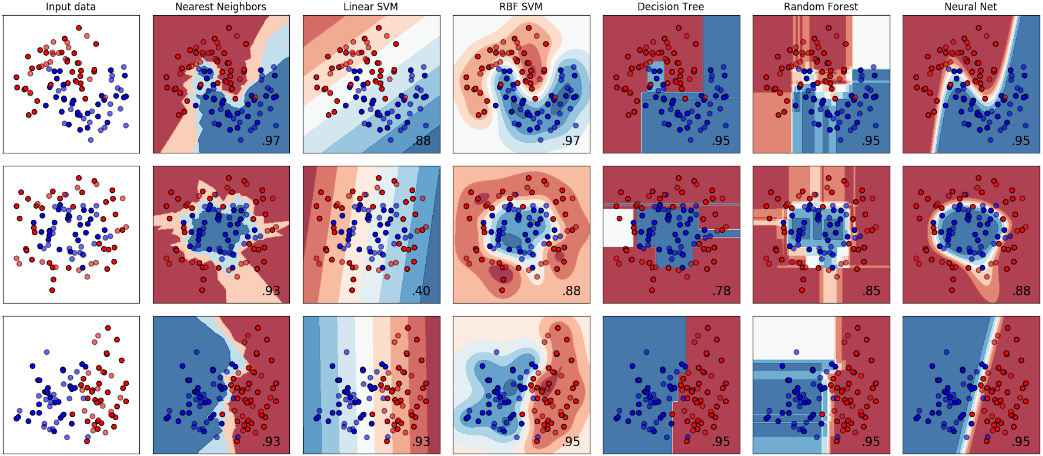
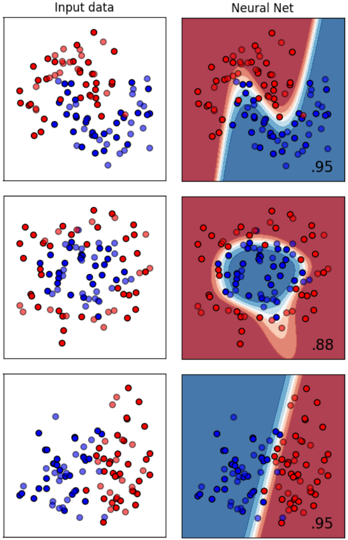
Decision boundaries



http://scikit-learn.org/

Artificial Neural Network (ANN)



Pros:

- + state-of-the-art on many hard problems
- + scale well to large data sets

Cons:

- – requires large data sets
- – no theoretical guarantee
- – more an art than a science

Covered in this lecture !

Perceptron Era (1958-60s)

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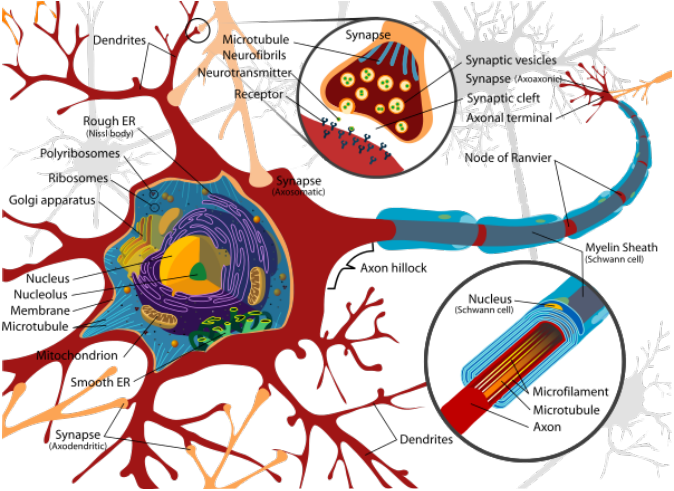
Biological neurons

Extremely complicated cells.

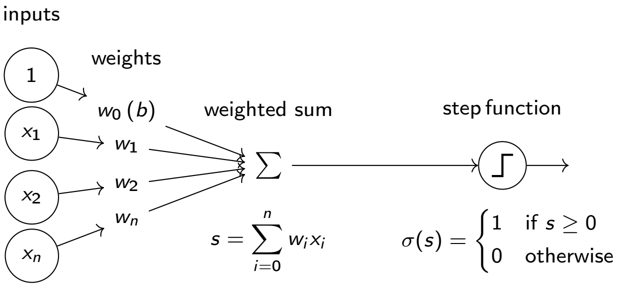
In a nutshell:

- Receives electrical pulses from dendrites (input).
- Accumulates electrical potential.
- Above a certain threshold, fires off along its axon (output).



McCuloch-Pitts artificial neuron

A simplified mathematical model of how neurons operate.



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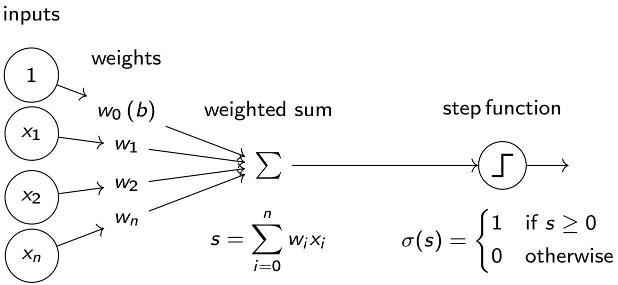

$$s = \sum_{i=0}^{n} w_i x_i$$

$$\sigma(s) = \begin{cases} 1 & \text{if } s \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

Can model logical gates: AND, OR, NOT.

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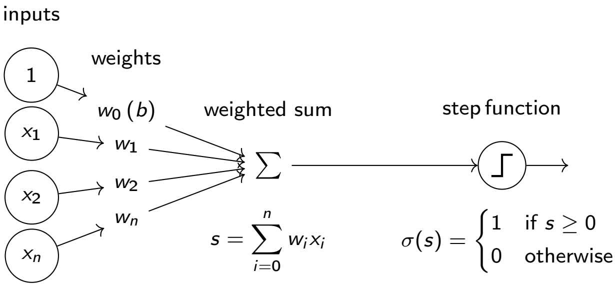

Can model logical gates: AND, OR, NOT.

In NN jargon, that's a linear model: $h(\mathrm{x}) = \sigma(\mathrm{w}^\intercal \mathrm{x} + b)$.

W. S. McCulloch and W. Pitts (1943). A logical calculus of the ideas immanent in nervous activity.

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Rosenblatt's perceptron

$\mathcal{D}$ a training set of input-output pairs (x, y), with $x \in \mathbb{R}^n$ and $y \in \{0, 1\}$.

F. Rosenblatt (1957). The perceptron, a perceiving and recognizing automaton. Tech. rep. Project Para., Cornell Aeronautical Laboratory

Rosenblatt's perceptron

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$\mathcal{D}$ a training set of input-output pairs (x, y), with $x \in \mathbb{R}^n$ and $y \in \{0, 1\}$.

Start with random weights, and iterate over the training examples

- if target is 1 and output is 0:
  - increase weights w_i where x_i is positive
  - decrease weights w_i where x_i is negative
- if target is 0 and output is 1:
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Formally: $\mathrm{w} \leftarrow \mathrm{w} + \alpha(y - \sigma(\mathrm{w}^\intercal \mathrm{x}))\mathrm{x}$, with α the learning rate. Gradient descent ?

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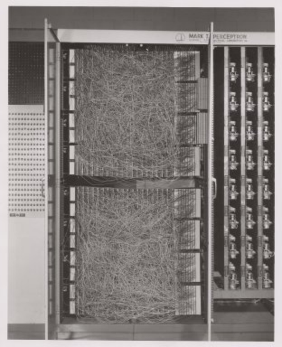
Rosenblatt's perceptron

Custom hardware implementation: Mark I Perceptron

- input: 20×20 photocells
- weights: potentiometers
- learning: electric motors



Classifies simple shapes correctly.

Machine learning is born!

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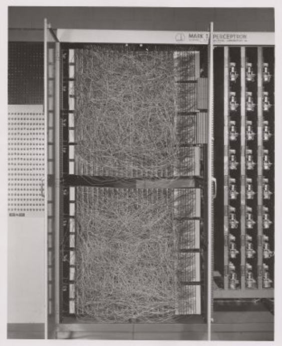

Classifies simple shapes correctly.

Machine learning is born!

« The Navy revealed the embryo of an electronic computer today that it expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence [. . .] Dr. Frank Rosenblatt, a research psychologist at the Cornell Aeronautical Laboratory, Buffalo, said Perceptrons might be fired to the planets as mechanical space explorers. »
New-York Times, 1958

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1969: First NN winter

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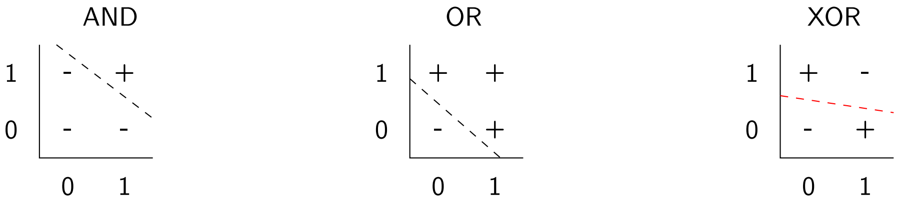
1969: First NN winter

Critical analysis by Minsky and Papert (MIT lab).

Linearity limits, can not learn the simple XOR function.



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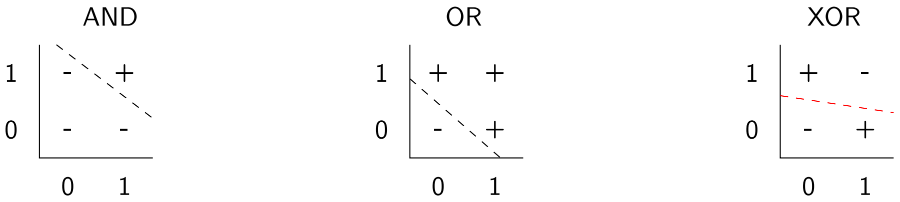

Non-linearity requires a multilayer perceptron (MLP).

Rosenblatt's algorithm does not work for multiple layers.

$\Longrightarrow$ Massive disillusionment, freeze to funding and publications.

M. Minsky and S. Papert (1969). Perceptrons An Introduction to Computational Geometry.

Backpropagation Era (1986-90s)

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Gradient descent

Gradient descent (GD): $\theta \leftarrow \theta - \alpha \Delta \theta$, with α the learning rate.

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Gradient descent

Gradient descent (GD): $\theta \leftarrow \theta - \alpha\Delta\theta$, with α the learning rate.

Batch GD: compute gradients over the whole training set $\mathcal{D}$

$$\Delta\theta = \frac{\partial \sum_{(\mathsf{x},\mathsf{y})\in\mathcal{D}} L(\mathsf{h}(\mathsf{x}),\mathsf{y})}{\partial\theta} = \sum_{(\mathsf{x},\mathsf{y})\in\mathcal{D}} \frac{\partial L(\mathsf{h}(\mathsf{x}),\mathsf{y})}{\partial\theta}$$

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Mini-batch GD: compute gradients over a small subset $\mathcal{D}_{mb} \subset \mathcal{D}$

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Stochastic GD: compute gradients over a single example $(x, y) \in \mathcal{D}$

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$\Longrightarrow$ all of these will reach a local minima ($\alpha \to 0$).

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$$\Delta\theta = \frac{\partial L(\mathrm{h}(\mathrm{x}), \mathrm{y})}{\partial\theta}$$

$\implies$ all of these will reach a local minima ($\alpha \to 0$).

Noisy but fast updates often more efficient. Also, can escape local minima !

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Back-propagation

Proposed in the 70s, rediscovered in the 80s by several groups.

P. Werbos (1974). Beyond Regression: New Tools for Prediction and Analysis in the Behavioral Sciences.

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Back-propagation

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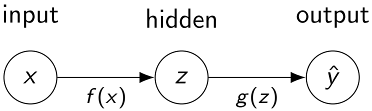
Multi-layer network: composition of functions $h = g \circ f$



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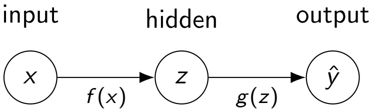

Gradient: chain rule of calculus

$$\frac{\partial \hat{y}}{\partial x} = \frac{\partial z}{\partial x} \frac{\partial \hat{y}}{\partial z}.$$

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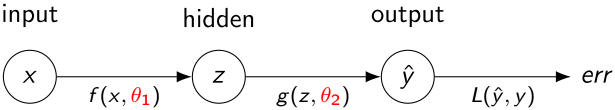
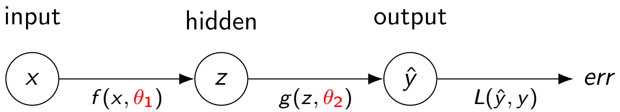
Back-Propagation

Forward pass: composition of functions

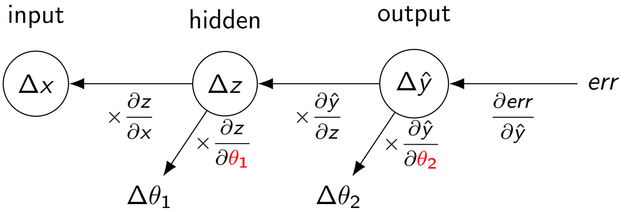


Back-Propagation

Forward pass: composition of functions



Backward pass: chain rule of calculus



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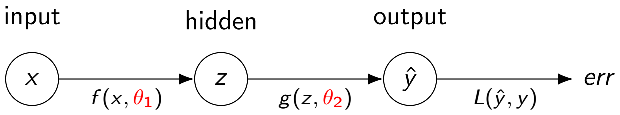
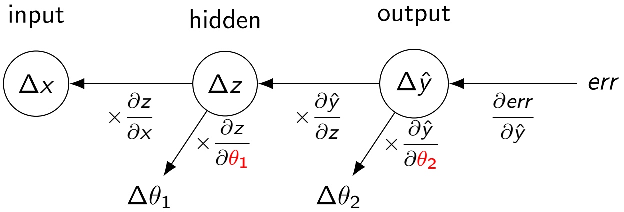
Back-Propagation

Forward pass: composition of functions



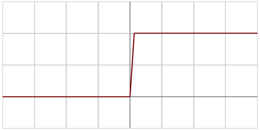
Backward pass: chain rule of calculus



$\Longrightarrow$ all we need is f, g and L differentiable.

Activation functions

Step function: non-differentiable...



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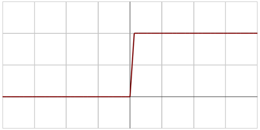
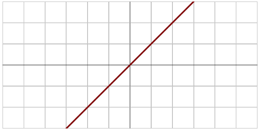


Identity: linear model



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Activation functions

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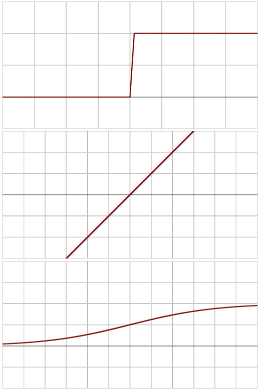
Identity: linear model

Logistic (sigmoid)

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



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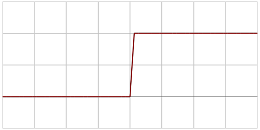

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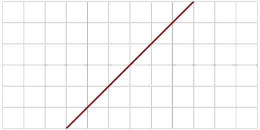

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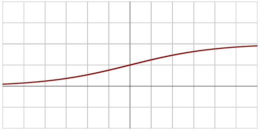
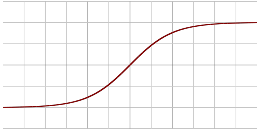
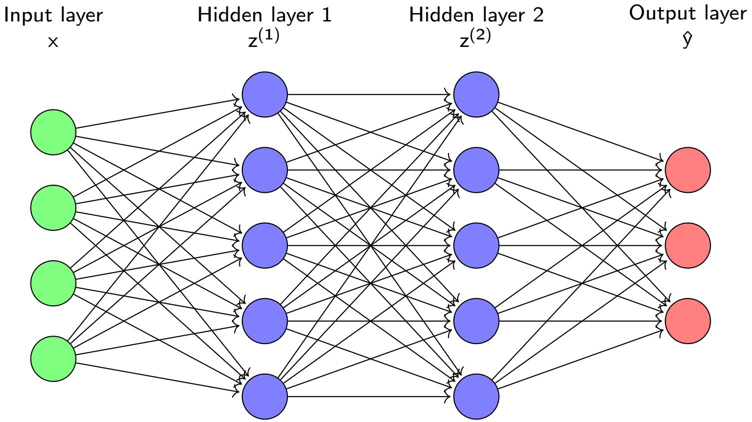


Hyperbolic tangent (tanh)

$$\sigma(x) = \frac{2}{1 + \exp^{-2x}} - 1$$

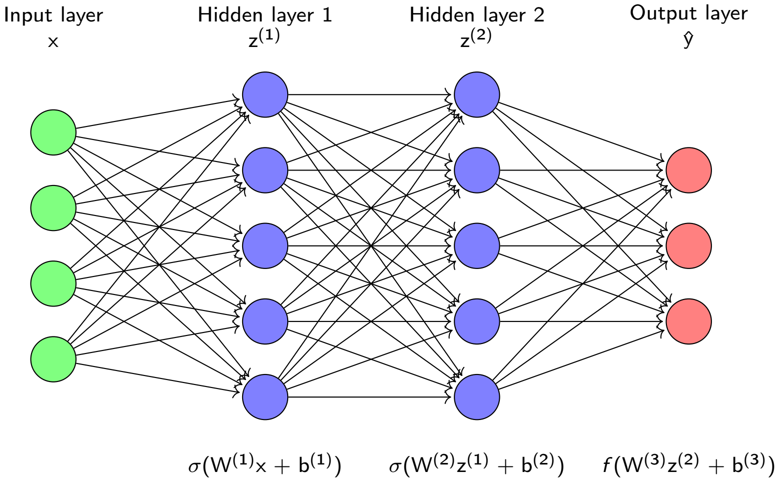


Multilayer feed-forward neural network



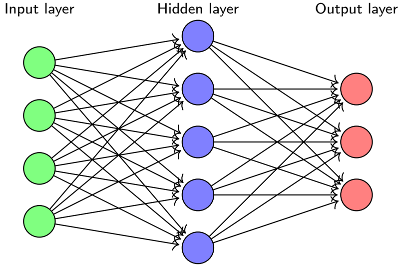
$\sigma(W^{(1)}x + b^{(1)})$ $\sigma(W^{(2)}z^{(1)} + b^{(2)})$ $f(W^{(3)}z^{(2)} + b^{(3)})$

Multilayer feed-forward neural network



Demo time `http://playground.tensorflow.org`

MLPs are universal approximators



A single hidden layer with sufficiently many hidden units can approximate any $\mathcal{X} \mapsto \mathcal{Y}$ mapping to any desired degree of accuracy.

In other words: infinite capacity.

K. Hornik, M. B. Stinchcombe, and H. White (1989). Multilayer feedforward networks are universal approximators.

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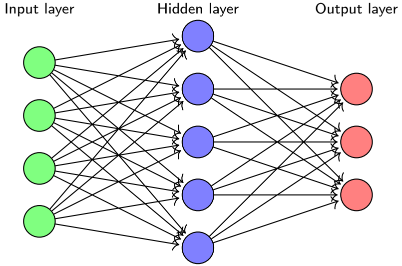
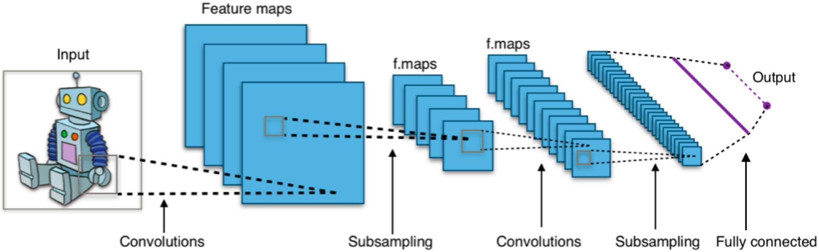


Strong theoretical argument at the time. Still, are NNs useful ?

- k-NN has infinite capacity;
- decision trees have infinite capacity;
- requires an exponential number of hidden neurons.

K. Hornik, M. B. Stinchcombe, and H. White (1989). Multilayer feedforward networks are universal approximators.

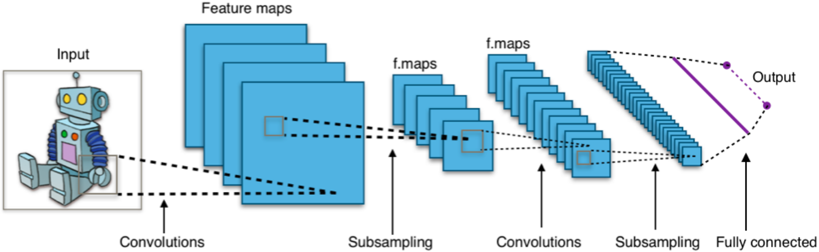
Convolutional neural networks



Typical CNN layer: convolution + max pooling

- convolutions $\rightarrow$ weight sharing, less free parameters
- max pooling $\rightarrow$ translation invariance, dimensionality reduction

Convolutional neural networks



Typical CNN layer: convolution + max pooling

- convolutions $\rightarrow$ weight sharing, less free parameters
- max pooling $\rightarrow$ translation invariance, dimensionality reduction

Leverages spatial / temporal structures

- image processing (2D spatial convolutions)
- signal processing (1D temporal convolution)

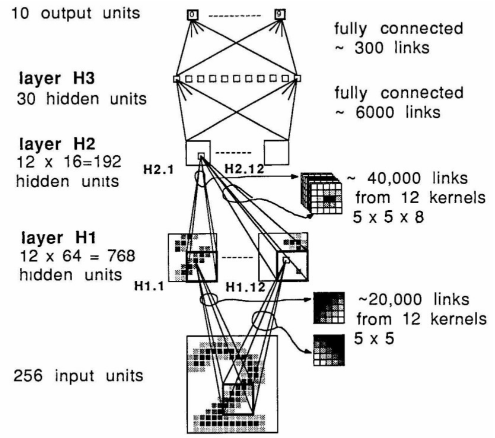
Handwritten digit recognition: LeNet-5

SUN 4/260 16.67 MHz, 128 MB

- *tanh* activations
- L_2 loss
- Stochastic GD

https://youtu.be/FwFduRA_L6Q

At some point in the 90s, read about 10-20% of all the checks in the US.



Y. LeCun et al. (1989). Backpropagation Applied to Handwritten Zip Code Recognition.

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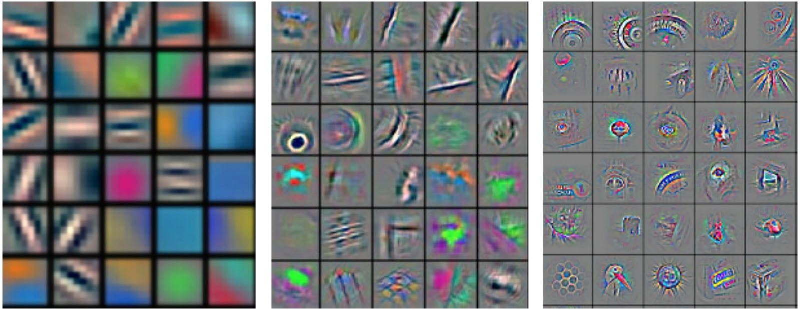
CNN feature maps



https://distill.pub/2017/feature-visualization/

Intuition:

- lower layers = low-level features (edges, blobs)
- higher layers = high-level features

M. D. Zeiler and R. Fergus (2014). Visualizing and Understanding Convolutional Networks.

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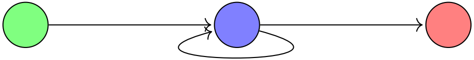
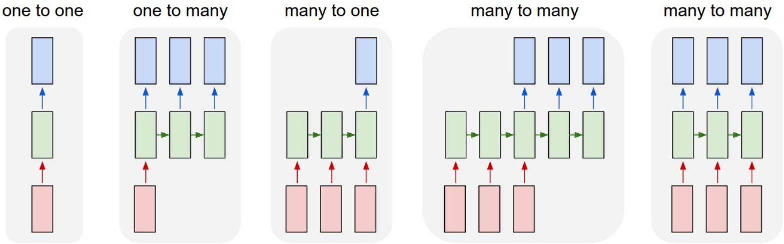
Recurrent neural networks

Time-delayed connections $\implies$ memory.



Can process non i.i.d. data (sequences):



Back-propagation through time (BPTT) $\implies$ vanishing / exploding gradients...

http://karpathy.github.io/2015/05/21/rnn-effectiveness/

The vanishing gradient problem

Chain rule $\approx$ geometric sequence

- derivatives $\frac{\partial \sigma(x)}{x} < 1 \implies$ vanishing gradient
- derivatives $\frac{\partial \sigma(x)}{x} > 1 \implies$ exploding gradient

Related to:

- activation function σ
- initial weight initialization

Affects MLPs with many layers, and recurrent neural nets.

- hard to train deep networks;
- hard to learn long-term dependencies.

Limitations

Gradient descent: no theoretical guarantee

- non-convex optimization problem (hidden layers)
- quality of the local minimum ?

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Outperformed by other models in the 2000s (random forest, SVM).

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Backpropagation: vanishing / exploding gradients

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Computer resources: limited at the time

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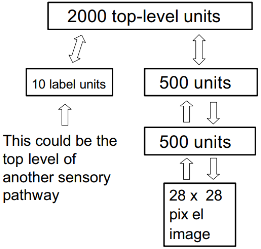
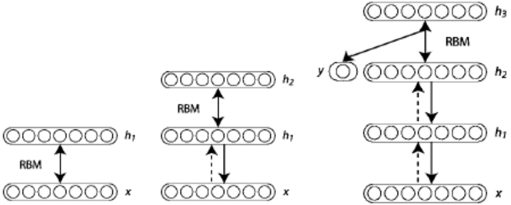
Outperformed by other models in the 2000s (random forest, SVM).

Despite some irrefutable successes, neural networks lose popularity.
$\implies$ Second NN winter.

Deep Learning Era (2006-)

2006 Deep belief network (DBN)





(a) Train RBM for $\mathbf{x}$ (b) Train RBM for $\mathbf{h}^1$ (c) Train RBM for $\mathbf{h}^2$ and y

Unsupervised layer-by-layer pre-training (weight initialization).
$\Longrightarrow$ successful training of deep neural nets is possible.

1.25% error on MNIST without convolutions ! (0.95% with CNNs)

Generative model of digit images (MNIST).

G. E. Hinton, S. Osindero, and Y. W. Teh (2006). A Fast Learning Algorithm for Deep Belief Nets.

2006 Resurgence: Deep belief network (DBN)

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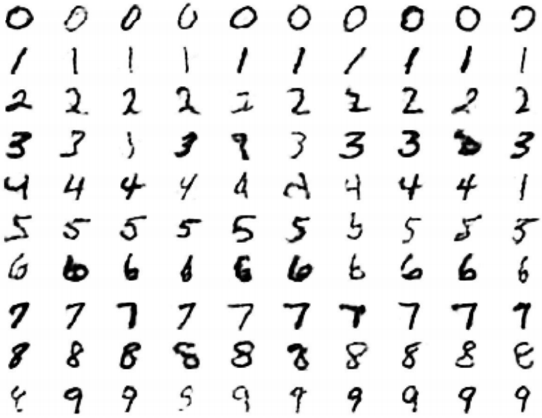
Generative model: "Looking into the mind of a neural network".



G. E. Hinton, S. Osindero, and Y. W. Teh (2006). A Fast Learning Algorithm for Deep Belief Nets.

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Computational power

Forward / backward passes highly parallel by nature.

Use GPUs instead of CPUs for training ? $\implies$ 70x speed-up.

R. Raina, A. Madhavan, and A. Y. Ng (2009). Large-scale deep unsupervised learning using graphics processors.

Q. V. Le et al. (2012). Building high-level features using large scale unsupervised learning.

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DBN training on Youtube images by Google

- 16 000 parallel CPUs
- $\sim$ 1 billion weights (Hinton's 2006 DBN $\sim$ 1M)

«We never told it during the training, 'This is a cat'. It basically invented the concept of a cat.» *Jeff Dean*

One of the neurons.

R. Raina, A. Madhavan, and A. Y. Ng (2009). Large-scale deep unsupervised learning using graphics processors.

Q. V. Le et al. (2012). Building high-level features using large scale unsupervised learning.

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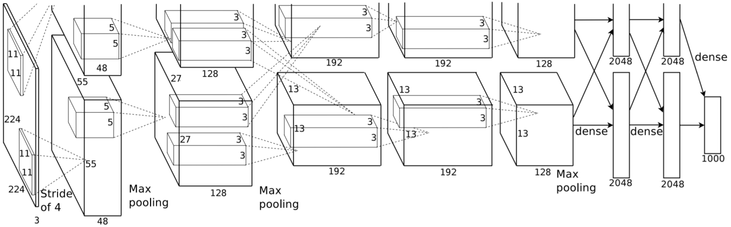
2012 Tsunami: AlexNet

Successful supervised training of a deep convolutional network on GPUs.



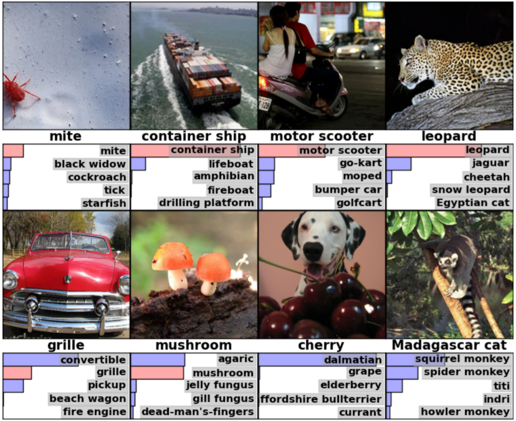
- one week training on two gaming GPUs (Nvidia GTX 580, 3GB)
- 5 convolutional layers + 3 fully-connected layers
- relu activation functions (non-saturating neurons)
- dropout (regularization)
- data augmentation (cropping + translations)

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

2012 Tsunami: AlexNet

ImageNet Large Scale Visual Recognition Challenge (ILSVRC) 2012

- crowd-sourced image annotation
- 1000 classes
- 1.3 million training examples



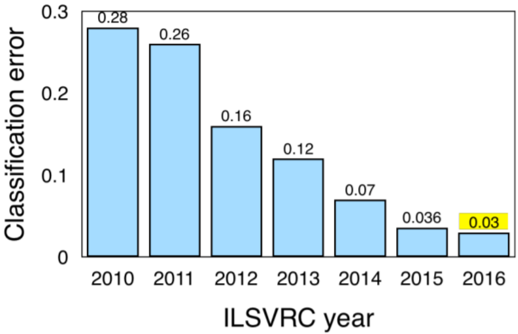
The only NN competitor, AlexNet, wins by a large margin

- 15.3% top-5 error rate, compared to 26.2% for second entry

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

2012 Tsunami: AlexNet

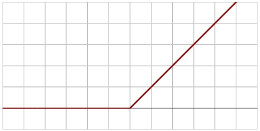
Since 2012: overflow of CNN competitors, test error continually decreases



Modern activation functions

Rectified linear unit (relu)

$$\sigma(x) = \begin{cases} x & \text{if } x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$



P. Ramachandran, B. Zoph, and Q. Le (2017). Swish: a Self-Gated Activation Function.

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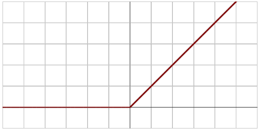
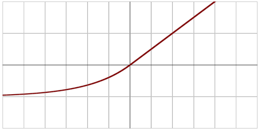


Exponential linear unit (elu)

$$\sigma(x) = \begin{cases} x & \text{if } x \geq 0 \\ \exp(x) - 1 & \text{otherwise} \end{cases}$$



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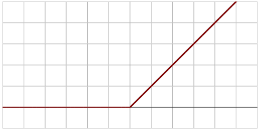

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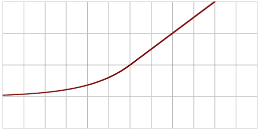
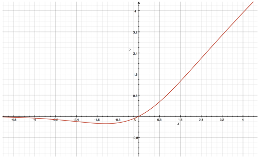


Google's activation (swish)

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



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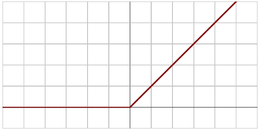

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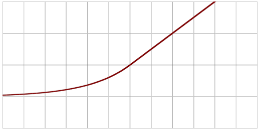

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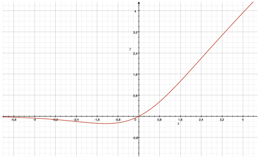


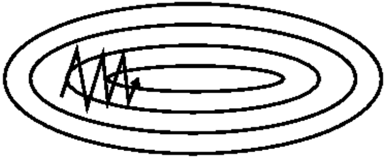
$\Longrightarrow$ non-saturating neurons.

P. Ramachandran, B. Zoph, and Q. Le (2017). Swish: a Self-Gated Activation Function.

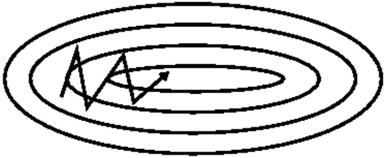
Modern gradient descent algorithms

Momentum:

$$\Delta\theta \leftarrow \beta\Delta\theta + (1-\beta)\frac{\partial L}{\partial \theta} \quad \text{with } \beta \in]0,1[,$$
$$\theta \leftarrow \theta - \alpha\Delta\theta.$$



No momentum



Momentum

$\implies$ faster convergence, especially with SGD.

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Modern gradient descent algorithms

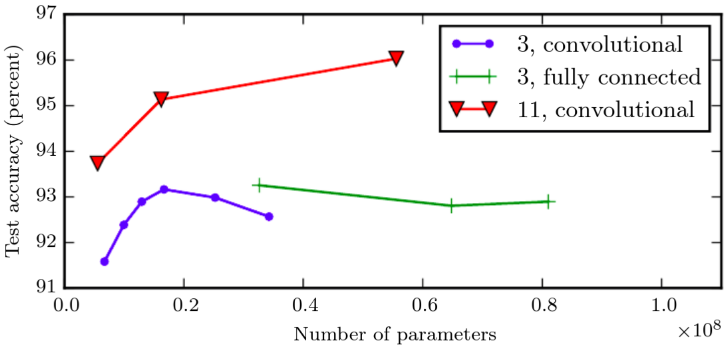
Adaptive moment estimation (adam): first and second order statistics

$$
\begin{aligned}
m &\leftarrow \beta_1 m + (1-\beta_1)\frac{\partial L}{\partial \theta} && \text{(mean)},\\
v &\leftarrow \beta_2 v + (1-\beta_2)\left(\frac{\partial L}{\partial \theta}\right)^2 && \text{(uncentered variance)},\\
\hat{m} &= \frac{m}{1-\beta_1} && \text{(bias correction)},\\
\hat{v} &= \frac{v}{1-\beta_2} && \text{(bias correction)},\\
\theta &\leftarrow \theta - \alpha\frac{\hat{m}}{\sqrt{\hat{v}}+\epsilon}.
\end{aligned}
$$

$\Longrightarrow$ really fast, often used by default.

D. P. Kingma and J. L. Ba (2015). Adam: a Method for Stochastic Optimization.

Deeper is better than wider

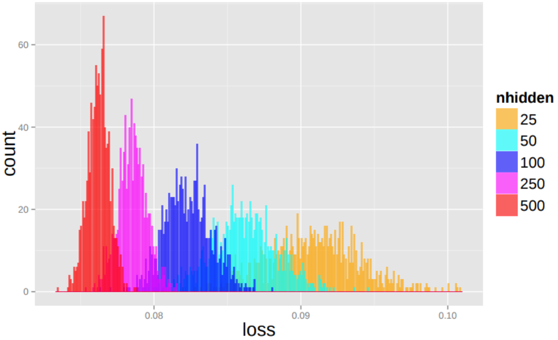


I. Goodfellow, Y. Bengio, and A. Courville (2016). Deep Learning.

Local minima is not an issue with large networks

Analogy to spin glasses

«For large-size decoupled networks the lowest critical values [. . .] are located in a well-defined band lower-bounded by the global minimum. The number of local minima outside that band diminishes exponentially with the size of the network.»



A. Choromanska et al. (2015). The Loss Surfaces of Multilayer Networks.

Recent developments

Architectures

- Residual networks, 1000+ layers
- Transformer networks (text)
- Graph neural networks (proteins, networks)

Normalization techniques (stabilizes gradients)

- Batch norm
- Layer norm, instance norm, group norm
- Weight norm

Core ingredients: compositional architectures + differentiable operations + backpropagation.

See also `https://bmk.sh/2019/12/31/The-Decade-of-Deep-Learning/`

Neural Network - Foundations

CORS 2021 Workshop

Thank you!

Maxime Gasse, Polytechnique Montréal

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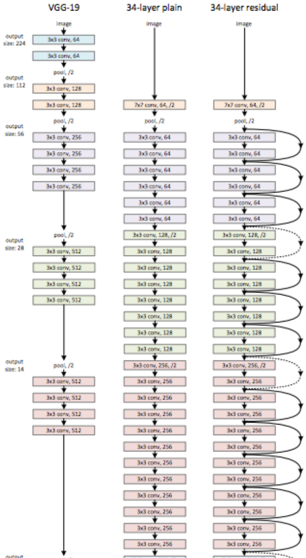
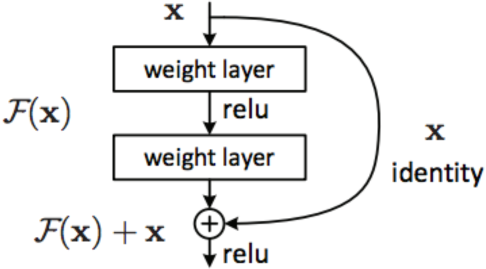
Residual networks





A residual block

State-of-the-art on many tasks (AlphaGo Zero)

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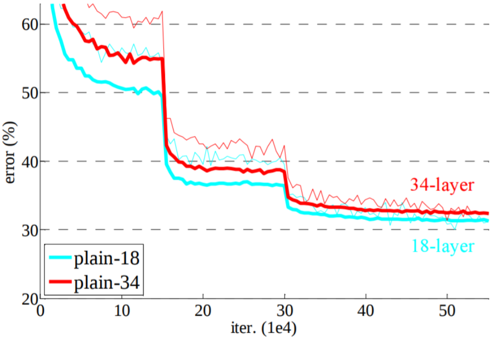
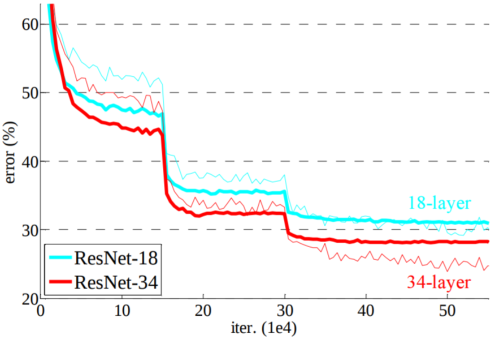
Residual networks





Scales up to a thousand layers
(but actually exploits paths of $<$ 30 layers).

K. He et al. (2015). Deep Residual Learning for Image Recognition.

A. Veit, M. J. Wilber, and S. J. Belongie (2016). Residual Networks Behave Like Ensembles of Relatively Shallow Networks.

Generative Adversarial Networks (GANs)

« *Adversarial training is the coolest thing since sliced bread* » *Yann LeCun*

T. Karras et al. (2017). Progressive Growing of GANs for Improved Quality, Stability, and Variation.

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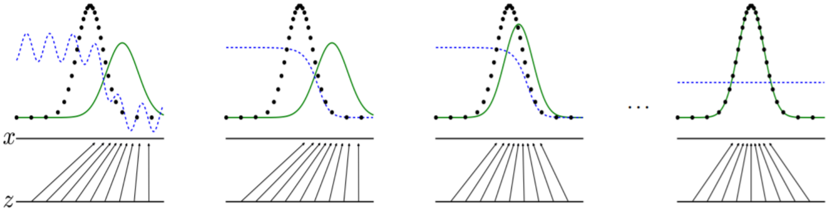
Generative Adversarial Networks (GANs)

Real samples $x \sim p(x)$, fake samples $G(z) \sim q(x)$ where $z \sim U(0,1)^M$.

Generator network $G : \mathcal{Z} \to \mathcal{X}$.
Discriminator network $D : \mathcal{X} \to \mathbb{R}$ (bounded).

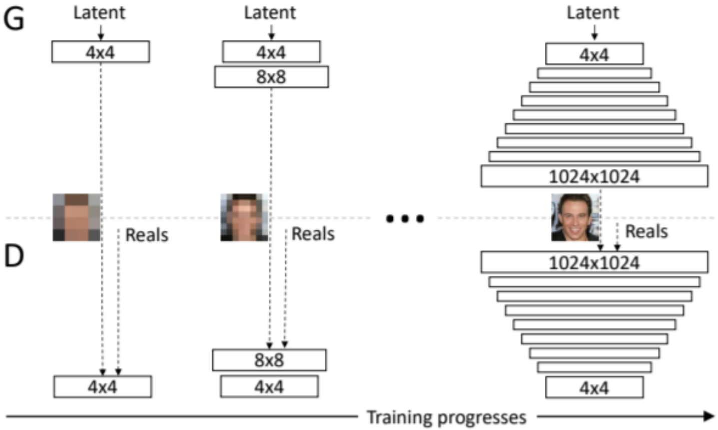
Two-player min-max game:
$G^\star, D^\star = \arg\min_G \max_D \mathbb{E}_{x,z}[D(x) - D(G(z))]$



Optimal point: Nash equilibrium.

I. J. Goodfellow et al. (2014). Generative Adversarial Nets.

Realistic face image generation



https://youtu.be/XOxxPcy5Gr4

T. Karras et al. (2017). Progressive Growing of GANs for Improved Quality, Stability, and Variation.