Neural Networks

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Mathematical Introduction to Machine Learning

Peking University, Fall 2023

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Two-layer neural networks

- A two-layer network defines function define a map from $\mathbb{R}^d$ to $\mathbb{R}^k$

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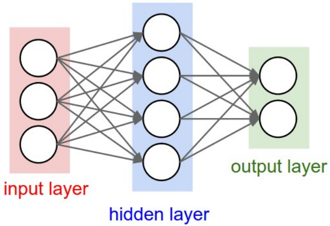
where $A \in \mathbb{R}^{k\times m}, B \in \mathbb{R}^{m\times k}, \boldsymbol{c} \in \mathbb{R}^m$. Here, $\theta = \{A, B, \boldsymbol{c}\}$ are the trainable parameters.



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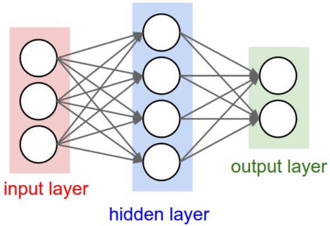

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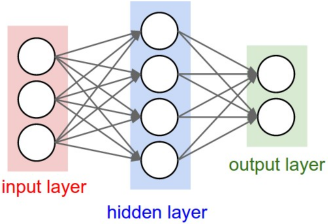

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- m denotes the number of neurons, which is also called the network **width**.

An adaptive feature perspective

- Let $\varphi(\boldsymbol{x}; \boldsymbol{b}, c) = \sigma(\boldsymbol{b} \cdot \boldsymbol{x} + c)$. Two-layer neural networks can be written as

$$f_m(\boldsymbol{x}; \theta) = \sum_{j=1}^{m} \boldsymbol{a}_j \sigma(\boldsymbol{b}_j \cdot \boldsymbol{x} + c_j) = \sum_{j=1}^{m} \boldsymbol{a}_j \varphi(\boldsymbol{x}; \boldsymbol{b}_j, c_j)$$

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  If $\{\boldsymbol{b}_j,c_j\}$ keep fixed after the (random) initialization and only train the outer coefficients $\{\boldsymbol{a}_j\}_j$, we obtain a (random) fixed-feature model.
- However, for neural networks, $\{\boldsymbol{b}_j,c_j\}_j$ are learned from data. Thus, two-layer neural networks can be interpreted as a specific type of adaptive feature methods.

Multilayer fully-connected networks

- A L-layer network is defined as $f(x;\theta) = \boldsymbol{x}^L$, with $\boldsymbol{x}^0 = \boldsymbol{x}$ and

$$\boldsymbol{x}^{\ell+1} = \sigma(W^\ell \boldsymbol{x}^\ell + b^\ell), \quad \ell = 0, 1, \ldots, L-1. \tag{1}$$

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- Layers $1, 2, \ldots, L$ are the hidden layers, and 0 and L are called the input and output layer, respectively. L and $\max\{m_1, \ldots, m_{L-1}\}$ are the depth and width, respectively.

Multilayer fully-connected networks (Cont'd)

- We call $f(\cdot;\theta)$ a **fully-connected** neural networks since $\{W^\ell\}$ are dense matrices.
- Sometimes, it is also called multilayer perceptron (**MLP**) network due to historical reasons.

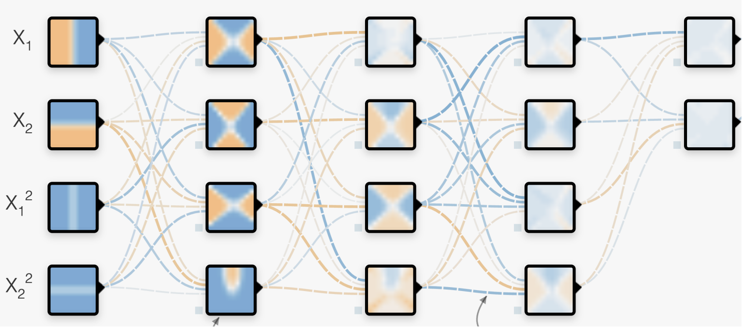


Figure 1: Play with MLP: `https://playground.tensorflow.org`.

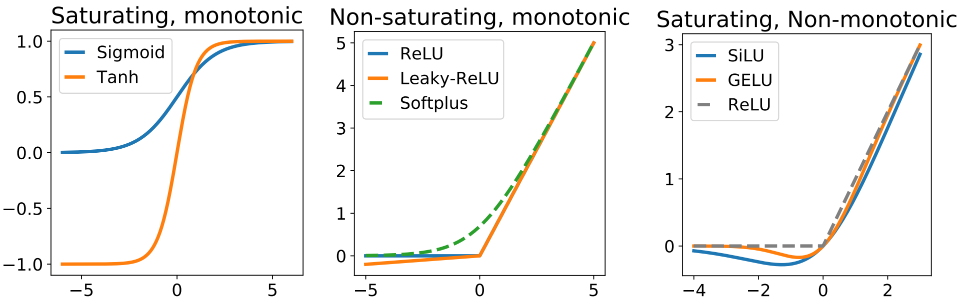
Activation Functions

Saturating	Sigmoid Tanh	$\frac{1}{1+e^{-x}}$ $\frac{e^x-e^{-x}}{e^x+e^{-x}}$
Non-saturating	ReLU Leaky ReLU Parametric ReLU Softplus	$\max(0,x)$ $\max(ax,x)$, where a is a small value, e.g. 0.01 $\max(ax,x)$, with a **learnable** $\ln(1+e^x)$
	GELU SiLU	$x\Phi(x)$ $x\sigma_{\text{sigmoid}}(\beta x)$

Table 1: Commonly used activation functions. $\Phi(\cdot)$ is the CDF of $\mathcal{N}(0,1)$. GELU and SiLU (also called Swish) belongs to the self-gated family: $x\phi(x)$ with ϕ be a CDF.

- ReLU stands for rectified linear unit. The Gaussian error linear unit (GELU) and sigmoid linear unit (SiLU) becomes popular recently.

Comparison of activation functions



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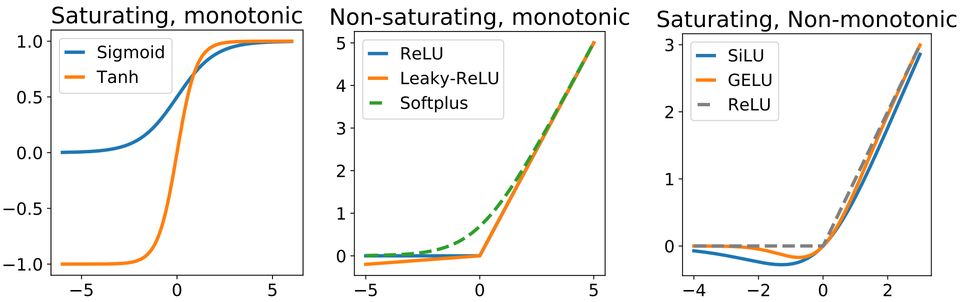

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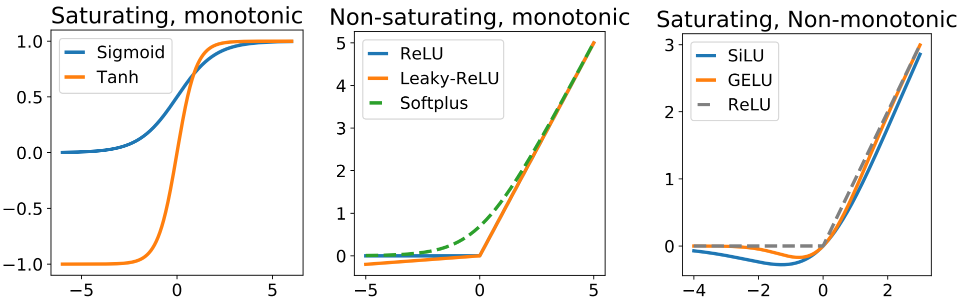

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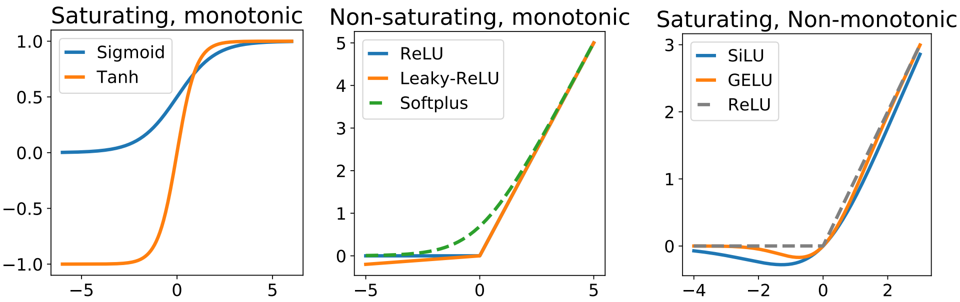

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- For saturating activation functions, $\sigma'(z) \approx 0$ when $|z|$ is relatively large. This is bad for training.
- **Dying ReLU:** For ReLU, if a neuron is dead, it keeps dead for the whole training and cannot be re-activated anymore. Leaky ReLU is proposed to solve the dying ReLU issue.

Universal Approximation Property (UAP)

Theorem 1 (Cybenko 1989)

Let Ω be a compact subset in $\mathbb{R}^d$. Assume that σ is sigmoidal, i.e.

$$\sigma(t) \to \begin{cases} 1 & t \to +\infty \\ 0 & t \to -\infty. \end{cases}$$

For any $f \in C(\Omega)$ and $\varepsilon > 0$, there exist a two-layer neural network $f_m(\boldsymbol{x}; \theta) = \sum_{j=1}^{m} a_j \sigma(\boldsymbol{b}_j^T \boldsymbol{x} + c_j)$ such that

$$\sup_{\boldsymbol{x} \in \Omega} |f(\boldsymbol{x}) - f_m(\boldsymbol{x})| \leq \varepsilon.$$

- The above theorem can be extended to general non-polynomial activation functions, including all the commonly-used activation functions.
- The above theorem says that two-layer neural networks can approximate any continuous function.
- Here, we only state theorem with the proof deferred to the advanced topics.

Remarks

The universal approximation theorem is an analog of Weierstrass Theorem in mathematical analysis which asserts that on compact domains, continuous functions can be approximated by polynomials.

By itself, it does not explain the success of neural network approximations over polynomial approximations (in high dimensions).

Convolutional Networks

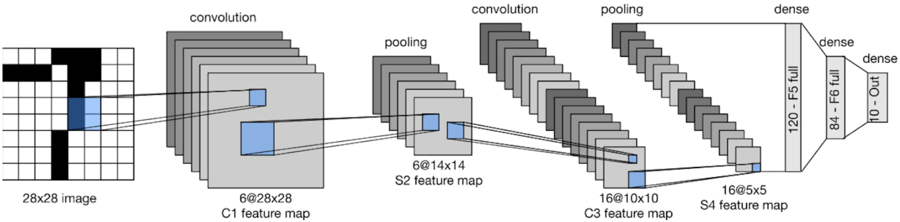

Figure 2: LeNet-5 for MNIST dataset

- Convolutional networks are similar to fully connected networks,

$$f(x) = \mathcal{A}^{(L)} \circ \sigma \circ \mathcal{A}^{(L-1)} \circ \cdots \circ \sigma \circ \mathcal{A}^{(1)} x.$$

The only difference is that $\mathcal{A}^{(\ell)} \boldsymbol{z} = \boldsymbol{z} * \boldsymbol{w}^{\ell} + \boldsymbol{b}^{\ell}$ is a convolutional transformation.

1D Convolutional transform

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$$y_s = \sum_{i=1}^{k} x_{s+i} w_i, \quad \forall s = 1, \cdots, n-k+1.$$

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- **Matrix Form:** The convolutional transform can be written in a matrix form. For example, if $\boldsymbol{w} = (w_1, w_2, w_3)^T \in \mathbb{R}^3$, we have

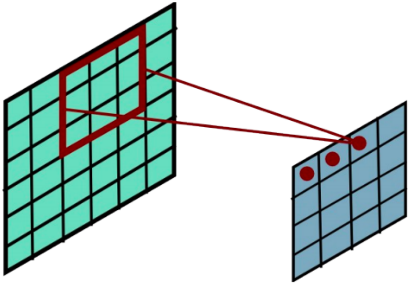
$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{n-3+1} \end{pmatrix} = \begin{pmatrix} w_1 & w_2 & w_3 & \cdots & 0 & 0 & 0 \\ 0 & w_1 & w_2 & w_3 & \cdots & 0 & 0 \\ 0 & 0 & w_1 & w_2 & w_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & w_1 & w_2 & w_3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix}.$$

The matrix corresponds to general $\boldsymbol{w} \in \mathbb{R}^k$ is given similarly.

2D convolutional transform

We can similarly define the "valid" convolutional transform for $x \in \mathbb{R}^{d \times d}$. Then, the filter $w \in \mathbb{R}^{k \times k}$ is a small matrix. Let $y = x * w \in \mathbb{R}^{(n-k+1)\times(n-k+1)}$, then

$$y_{s,t} = \sum_{i,j=1}^{k} x_{s+i,t+j} w_{i,j}.$$



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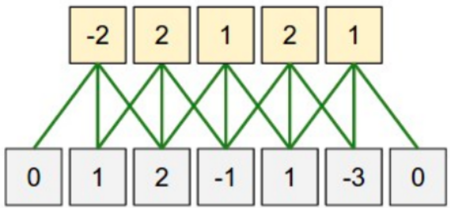
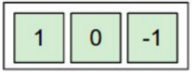
- **Visualization**: $x = (1, 2, -1, 1, -3) \in \mathbb{R}^5, w = (1, 0, -1)^T \in \mathbb{R}^3$. Then $y = x * w = (-2, 2, 1, 2, 1) \in \mathbb{R}^5$.





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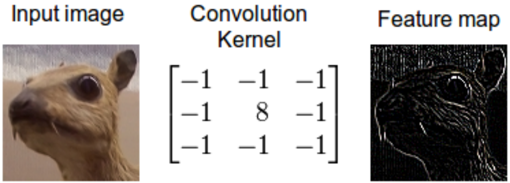

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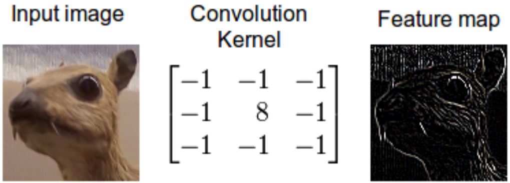

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- The fully-connected linear transform: $W\boldsymbol{x} + b$, is not easy to capture the local structures.

Motivation to use convolutional transforms (Cont'd)

- Translation invariance.
- The number of parameters to be learned for convolutional transforms are much smaller than that of fully-connected linear transforms. It is also much efficient to compute former than the latter.

Channels

Assume the input is an image.

- Let h^ℓ denote output of the ℓ-th layer. $h^\ell \in \mathbb{R}^{W_\ell \times H_\ell \times C_l}$ is a 3-order tensor. h^ℓ is called a **feature map** with shape (width W_ℓ) $\times$ (height H_ℓ) $\times$ (channels C_ℓ).

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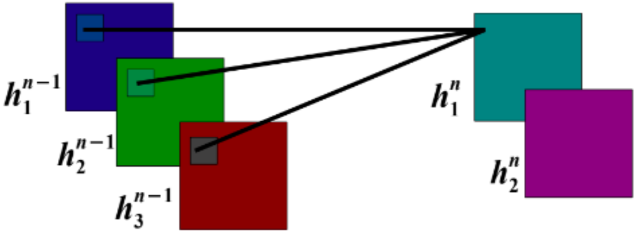
- Consider the input h^0. $C_0 = 1$ for a grayscale image; $C_0 = 3$ for a color image. The different channels store different information.
- It is expected that as we go deeper, the information stored at different channels becomes eventually "disentangled ". For example, when extracting features from an image of human, we would like that channel 1 represents "eye"; channel 2 represents "leg"; channel 3 represents "hand", etc.

A convolutional layer

A convolutional layer performs the convolution transform along the width and height dimensions and the **fully-connected** transform along the channel dimension.



Convolutional layer (Cont'd)

- Let $h^i \in \mathbb{R}^{W_i \times H_i \times C_i}$ and $h^o \in \mathbb{R}^{W_o \times H_o \times C_o}$ denote the input and output feature map, respectively. The filter $w \in \mathbb{R}^{k \times k \times C_i \times C_o}$ is 4-**order tensor** and bias $b \in \mathbb{R}^{C_o}$.

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  - "$*$" denotes the convolution transform with an appropriate padding.

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- "$*$" denotes the convolution transform with an appropriate padding.
- b^t is the bias corresponding to t-th channel of output feature map.

Convolutional layer (Cont'd)

- Let $h^i \in \mathbb{R}^{W_i \times H_i \times C_i}$ and $h^o \in \mathbb{R}^{W_o \times H_o \times C_o}$ denote the input and output feature map, respectively. The filter $w \in \mathbb{R}^{k \times k \times C_i \times C_o}$ is 4-**order tensor** and bias $b \in \mathbb{R}^{C_o}$.
- Mathematically, a convolutional layer makes the following transform:

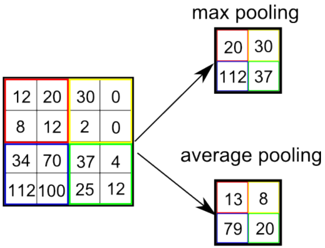
$$h^o_t = \sum_{s=1}^{C_i} h^i_s * w^{s,t} + b^t,$$

  where

  - $w^{s,t} \in \mathbb{R}^{k \times k}$ denotes the filter from the s-th channel of input to the t-th channel of output.
  - h^o_t is the t-th channel of output feature map.
  - h^i_s is the s-th channel of input feature map.
  - "$*$" denotes the convolution transform with an appropriate padding.
  - b^t is the bias corresponding to t-th channel of output feature map.
- Note that (w, b) will be learned from the data.

Pooling Layer

- **Pooling (Down-sampling):** There are two types of pooling: max pooling and average pooling.



- **Pooling Layer:** $\mathbb{R}^{W \times H \times C} \mapsto \mathbb{R}^{\frac{W}{k} \times \frac{H}{k} \times C}$.
  - Pooling is performed for each channel. No across channel transformation.
  - No learnable parameters.
- **Motivation:**
  - Decreasing the spatial dimension can reduce the memory usage. Hence, we can increase the number of channels without running out of the GPU memory.
  - For image classification problems, coarse graining does not lose too much category information.

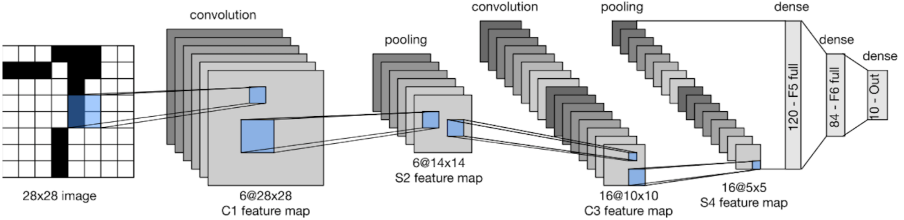
A Closer Look at LeNet-5

- **MNIST:** Handwritten Digits, $60,000$ training examples, $10,000$ test examples. Each sample is a 28×28 grayscale image.

- **Task:** build a classifier: $f(x) : \mathbb{R}^{28 \times 28 \times 1} \mapsto \mathbb{R}^{10}$, with $f_i(x) \in [0, 1]$ and $\sum_{i=1}^{10} f_i(x) = 1$.

A Closer Look at LeNet-5

- **LeNet-5:** Convolutional layers + Fully-connected layers + Softmax.



feature extractor (5×5 filter)

classifier

A Closer Look at LeNet-5

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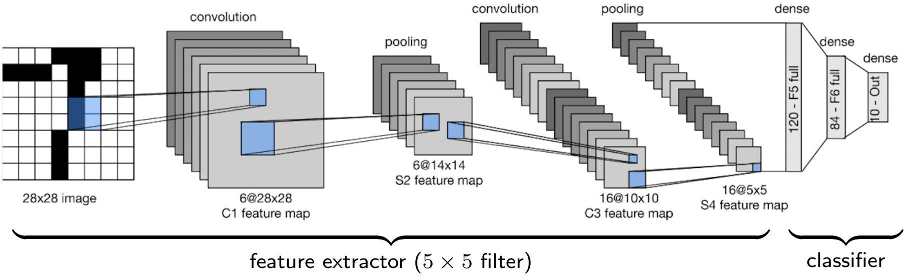

- The outputs before the softmax layer are usually called logits. Then, **softmax layer** converts logits to a probability: $\mathbb{R}^k \mapsto \mathbb{R}^k$ $p_i(x) = \frac{e^{x_i}}{\sum_{i=1}^{k} e^{x_i}}$, which gives the predicted probability over the classes.

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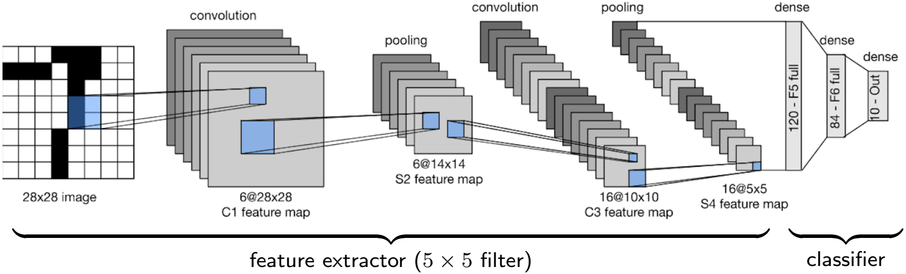

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- **One useful principle:** While decreasing the spatial dimension, increase the number of channels.

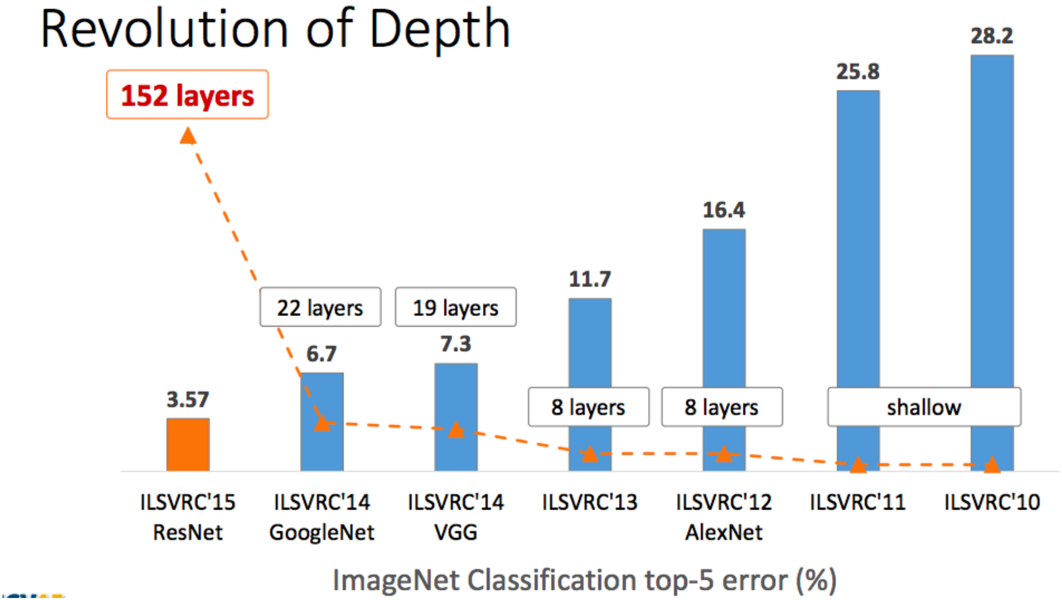
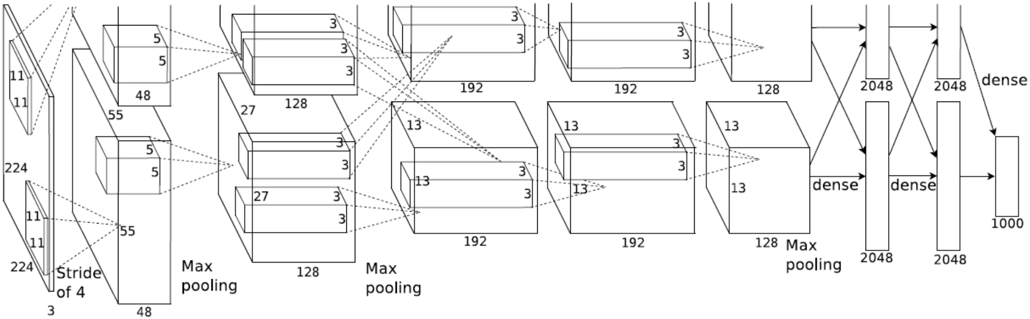


Figure 4: Taken from Kaiming He's slide.

AlexNet: 2012



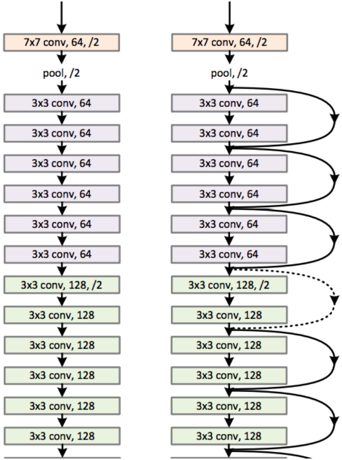
Contribution:

- BIG LeNet!
- deep CNN, GPU Acceleration. (Jürgen Schmidhuber team did the same thing in 2011.)
- ReLU and ImageNet.

VGG: 2014

- Small (3×3) convolutional layer.
- Better architecture-design principles.

Residual Networks (ResNets): 2015



Vanilla net

$$x^{\ell+1} = h(x^\ell; \theta^\ell)$$

Residual net

$$x^{\ell+1} = h(x^\ell; \theta^\ell) + x^\ell$$

$h(\cdot; \theta^l)$ can be a fully-connected or convolutional neural network.

- In ResNets, we learn the residual $h(\cdot; \theta^\ell)$ instead of the full map $\mathrm{Id} + h(\cdot; \theta^\ell)$.

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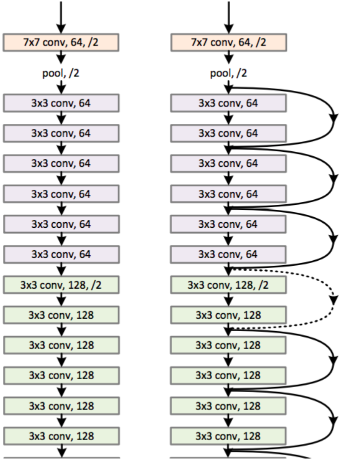

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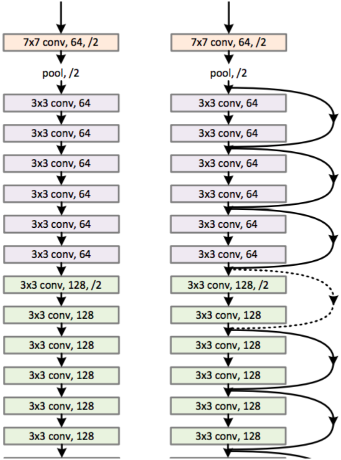

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- Residual and vanilla nets have the same expressivity: $\boldsymbol{x} = \mathtt{ReLU}(\boldsymbol{x}) - \mathtt{ReLU}(-\boldsymbol{x})$.
- Skip connections can be more general, e.g. connecting the input to the output directly.

Recurrent neural networks

Motivation

Sequence predictions:

- Speech-to-text and text-to-speech.
- Machine translation.
- Sentiment analysis.
- Caption generalization.

When both input and output are sequence, this task is called **sequence-to-sequence** prediction.

Abstraction:

- **Input:** $\boldsymbol{x} = (x_1, x_2, \ldots, x_T)$ with $x_t \in \mathbb{R}^{d_x}$.
- **Output:** $\boldsymbol{y} = (y_1, y_2, \ldots, y_T)$ with $y_t \in \mathbb{R}^{d_y}$.
- **Target:**

$$y_t = H_t(x_1, \ldots, x_t).$$

  Non Markovian process!

Recurrent neural networks

- **Code/Feature:** $\boldsymbol{h} = (h_1, h_2, \ldots, h_T)$, with $h_t \in \mathbb{R}^{d_h}$ encodes the information of $(x_1, x_2, \ldots, x_t)$ through
$$h_t = f(x_t, h_{t-1}).$$

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- **Model output**:
$$y_t = g(y_{t-1}, h_t)$$
- **Parameterization:** Use fully or convolutional networks to parameterize f and g.
- Note that f and g are shared among all time t's.

Vanilla Recurrent Network

- **Update Formulation:**

$$
\begin{aligned}
h_t &= \mathtt{tanh}(W_{hh}h_{t-1} + W_{hx}x_t) \\
y_t &= W_{yh}h_t
\end{aligned}
$$

Vanilla Recurrent Network

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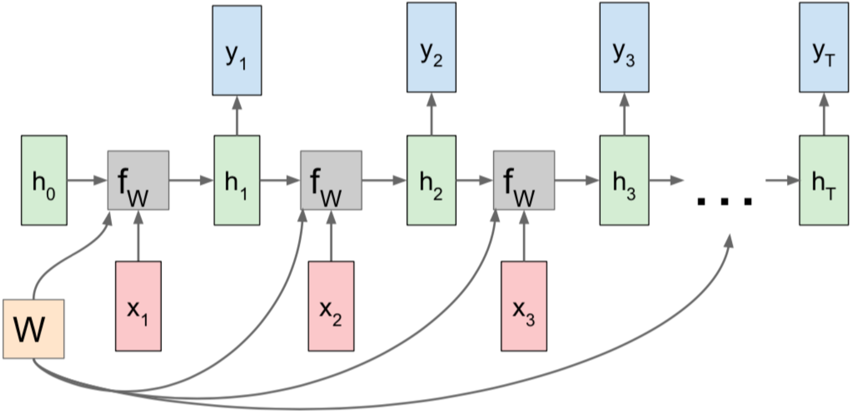
- **Visualization:**



Long Short Term Memory (LSTM)

- **Gate update:**

$$\begin{pmatrix} f_t \\ i_t \\ o_t \end{pmatrix} = \texttt{sigmoid}\begin{pmatrix} W_f x_t + U_f h_{t-1} + b_f \\ W_i x_t + U_i h_{t-1} + b_i \\ W_o x_t + U_o h_{t-1} + b_o \end{pmatrix}$$

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- **Memory update:**

$$c_t = (1 - f_t) \odot c_{t-1} + i_t \odot \texttt{tanh}\left(W_c x_t + U_c h_{t-1} + b_c\right)$$
$$h_t = o_t \odot c_t$$

where $o_t, f_t, i_t \in [0, 1]$ represent the output gate, forget gate and input gate, respectively. $\odot$ denotes the hadamard product.

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- **Key Factors:**
  - The extra state c_t is used to store long time memory.

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- **Key Factors:**
  - The extra state c_t is used to store long time memory.
  - Gate mechanism.

What if the output and input have different lengths?

Geometric Deep Learning: Symmetry-Preserving Neural Networks

Consider an invariance group G, e.g., the permutation, translation, and rotation groups. For any $x \in \mathcal{X}$, suppose $\sigma \cdot x \in \Omega$ for any $\sigma \in G$.

- **Invariance:** $f : \mathcal{X}^d \mapsto \mathbb{R}$ is said to be G-invariant if $f(\sigma \cdot x) = f(x)$ for any $\sigma \in G$.

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We will focus on constructing networks satisfying certain invariances.

Permutation symmetry

- A function $f : \mathbb{R}^{n \times d} \mapsto \mathbb{R}$ is said to be permutation invariant if

$$f(\boldsymbol{x}_{\sigma(1)}, \ldots, \boldsymbol{x}_{\sigma(n)}) = f(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n), \tag{2}$$

  for any permutation $\sigma \in S_n$ and $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \mathbb{R}^d$.
- We can also understand f as a function over the **set** $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$.

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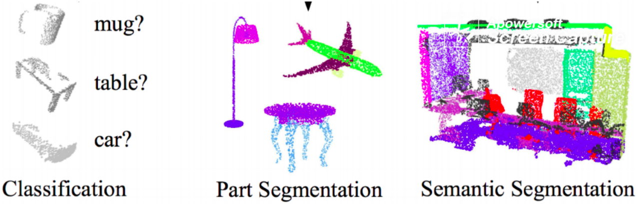
Example:

- $f(x_1, \dots, x_n) = \max\{x_1, \dots, x_n\}$.
- $f(x_1, \dots, x_n) = \sum_{i=1}^n x_i$.

Applications

- Point cloud.



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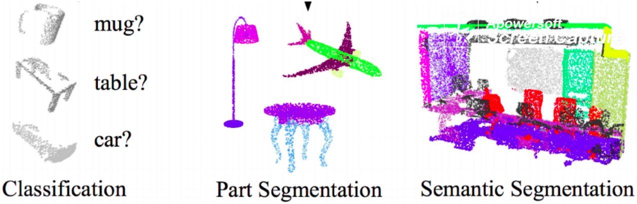

- Wave functions of bosons in quantum physics.

Applications

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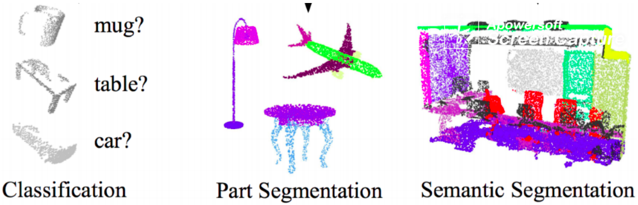


- Wave functions of bosons in quantum physics.
- Energy function of a molecule. The energy should keep unchanged if we swap two identical atoms.

Deep set models

Given the one-particular feature extractor $g : \mathbb{R}^d \mapsto \mathbb{R}^m$ and $\phi : \mathbb{R}^m \mapsto \mathbb{R}^1$, the deep set model is given by

$$(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n) \mapsto \phi\Big(\sum_{j=1}^{n} g(\boldsymbol{x}_j)\Big)$$

In practice, we can replace g and ϕ with neural nets. The corresponding models are called **deep sets**).

Approximation of permutation-invariant functions

- UAP guarantees that any continuous permutation-invariant function can be approximated by neural networks. But the networks are not permutation invariant.
- Can we construct models that has UAP while preserving the symmetry?

The following theorem shows deep sets are universal [2].

Theorem 2 (Han et al. 2019)

Let $f : \mathbb{R}^{n\times d} \mapsto \mathbb{R}$ be a permutation invariant and continuous differentiable function. Let Ω be a compact subset of $\mathbb{R}^d$. For any $\varepsilon \in (0, \sqrt{nd}n^{-1/d})$, there exits $g : \mathbb{R}^d \mapsto \mathbb{R}^m$, $\phi : \mathbb{R}^m \mapsto \mathbb{R}$ such that

$$\sup_{\boldsymbol{x}\in\Omega} \left| f(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n) - \phi\Big(\sum_{j=1}^{n} g(\boldsymbol{x}_j)\Big) \right| \leq \varepsilon,$$

where m, the number of feature variables, satisfies that $m \geq O\left(\frac{2^n (nd)^{\frac{nd}{2}}}{\varepsilon^{nd} n!}\right)$

[2] Universal approximation of symmetric and anti-symmetric functions

Translation and rotation invariance

- Let $X = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)^T \in \mathbb{R}^{n\times d}$. A function $f : \mathbb{R}^{n\times d} \mapsto \mathbb{R}$ is said to be translation invariant if

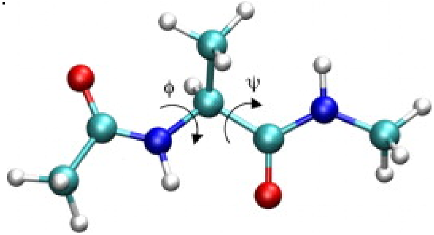
$$f(\boldsymbol{x}_1 + \boldsymbol{b}, \ldots, \boldsymbol{x}_n + \boldsymbol{b}) = f(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n), \qquad \forall \boldsymbol{b} \in \mathbb{R}^d,$$

and to be rotational invariant if

$$f(U\boldsymbol{x}_1, \ldots, U\boldsymbol{x}_n) = f(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n),$$

for any orthogonal rotational matrix U. Note that the the translation and rotation are applied to each "particle".

Application: Molecular modeling.



Network designing

- Let r_c be a pre-specified cut-off radius. Define the neighbor of atom i by

$$\mathcal{N}_i = \{j \in [n] : \|\boldsymbol{x}_j - \boldsymbol{x}_i\| \leq r_c\},$$

  and $n_i = |\mathcal{N}_i|$.

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- For each $\mathcal{N}_i$, define

$$R_i := (\boldsymbol{x}_{j_1} - \boldsymbol{x}_i, \ldots, \boldsymbol{x}_{j_{n_i}} - \boldsymbol{x}_i)^T \in \mathbb{R}^{n_i \times d}$$

  for $j_k \in \mathcal{N}_i$. Then, the matrix

$$\Omega_i = R_i^T R_i$$

  is invariant with respect to both translation and rotation.

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- Consider the function of the following form

$$f(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n) = \sum_{i=1}^{n} h_i(\Omega_i).$$

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  It is obvious that f is invariant to translation and rotation.
- Parameterize $\{h_i\}$ with neural network models.

The effect of symmetry preservation

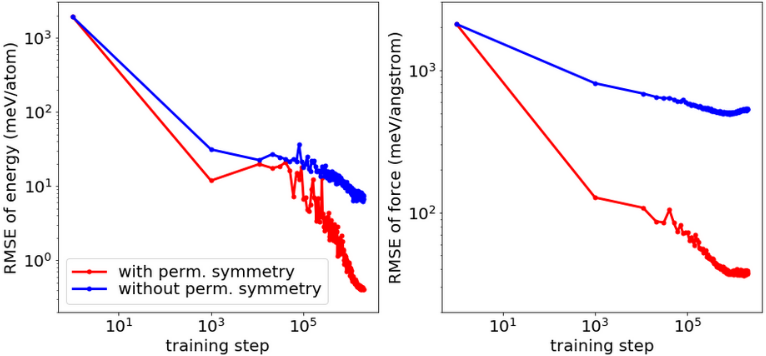

Figure 5: The effect of symmetry preservation on testing accuracy.

We refer to `https://geometricdeeplearning.com/` for more resources on this topic.

Summary

- Fully-connected networks
- Convolutional networks
- Recurrent neural networks.
- Residual neural networks.
- Symmetry-preserving networks: permutation, translation, and rotation invariance.

Other important but uncovered architectures: **Transformer, Graph neural network**.

Reading:

- MLP: https://www.deeplearningbook.org/contents/mlp.html
- CNN:
  - https://indoml.com/2018/03/07/student-notes-convolutional-neural-networks-cnn-introduction/
  - https://www.deeplearningbook.org/contents/convnets.html
- RNN: https://www.deeplearningbook.org/contents/rnn.html
- Geometric Deep Learning: https://geometricdeeplearning.com/.