

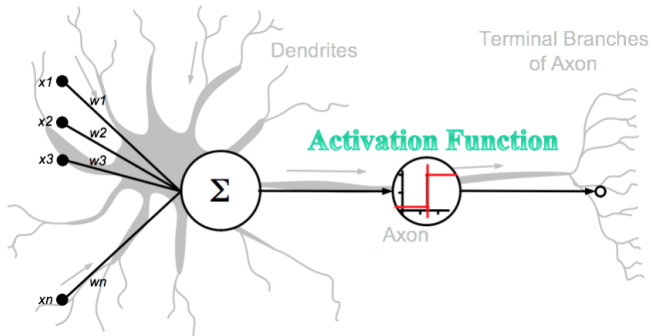
Perceptrons and Neural Networks

F. Noé¹

Deep Learning Classes, FU Berlin 2018

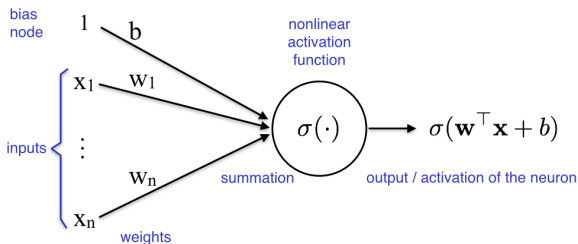
Artificial Neural Networks

Motivation



Artificial Neural Networks

Basic artificial neuron



- Input vector $\mathbf{x} \in \mathbb{R}^n$
- Trainable weights: $\mathbf{w} \in \mathbb{R}^n$ and $b \in \mathbb{R}$
- Fixed nonlinear activation function $f : \mathbb{R} \rightarrow \mathbb{R}$
- Output / activation: $y = \sigma(\mathbf{w}^\top \mathbf{x} + b)$

Perceptron

F. Rosenblatt: The Perceptron: A Probabilistic Model for Information Storage and Organization in the Brain. Phys. Rev. 65, 386-408 (1958)

Single neuron that acts as a binary classifier with

$$\sigma(x) = \begin{cases} 1 & \mathbf{w}^\top \mathbf{x} + b > 0 \\ 0 & \text{otherwise.} \end{cases}$$

Training data $\mathbf{X} \in \mathbb{R}^{N \times n}$, $\mathbf{y} \in \{0, 1\}^N$. Parameters $\mathbf{w} \in \mathbb{R}^n$, $b \in \mathbb{R}$.

Algorithm

- 1 Initialize \mathbf{w}^0 and b^0
- 2 For each training pair (\mathbf{x}_i, y_i) :
 - 1 Predict output: $\hat{y}_i^t = \sigma(\mathbf{w}^\top \mathbf{x} + b)$
 - 2 Update weights:

$$\mathbf{w}^{t+1} = \mathbf{w}^t + (y_i - \hat{y}_i^t) \mathbf{x}_i$$

$$b^{t+1} = b^t + (y_i - \hat{y}_i^t)$$

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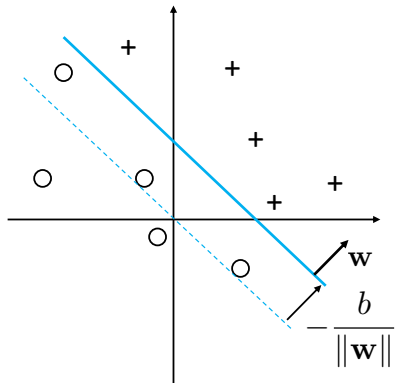
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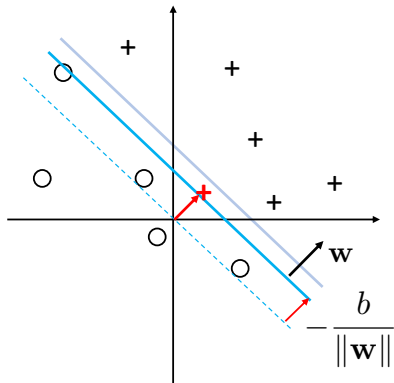
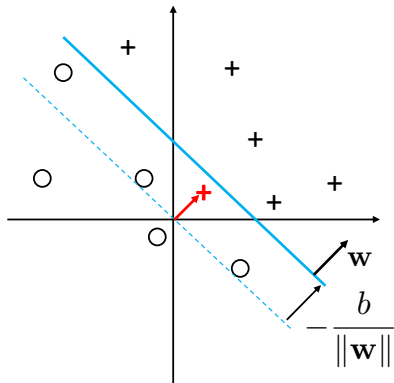
Perceptron

Training - Illustration



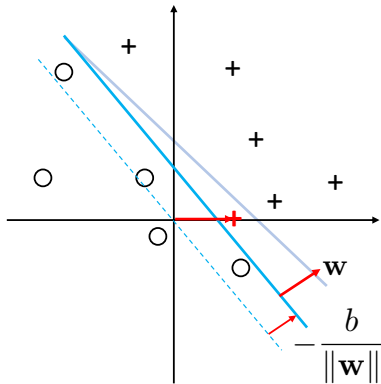
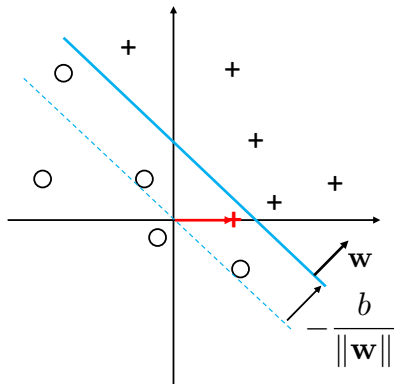
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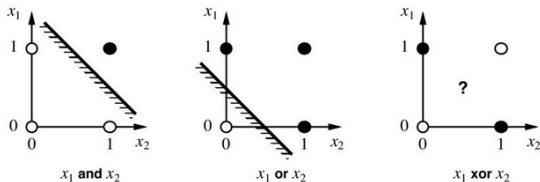
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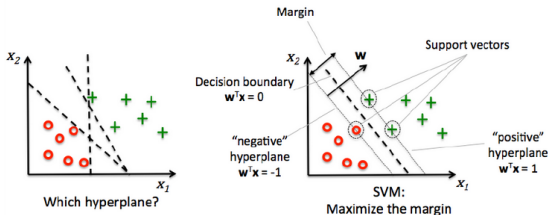
Perceptron

Perceptron can learn linearly separable functions

Perceptron can learn linearly separable functions. Separation plane divides input space in classes $\{0,1\}$ and is defined by normal vector \mathbf{w} and shift b .



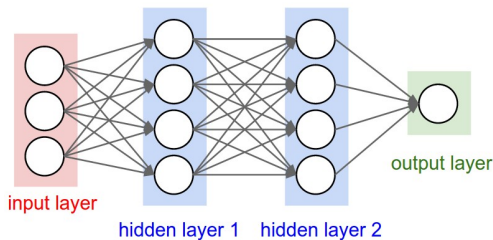
Support vector machine: Perceptron with maximum separation margin.



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Multilayer Feedforward Network / Perceptron

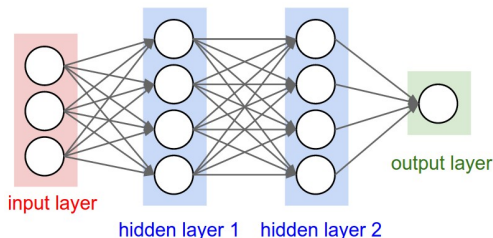


Sequence of linear and nonlinear transforms defined by the recursion:

$$\mathbf{x}^{l+1} = \sigma(\mathbf{W}^l \mathbf{x}^l + \mathbf{b}^l)$$

- L layers indexed by $l = 1, \dots, L$. Input vector $\mathbf{x}^{(0)}$ does not count as a layer.
- $\mathbf{x}^l \in \mathbb{R}^{n_l}$: Activations of n_l neurons at layer l
- Trainable weights $\mathbf{W}^l \in \mathbb{R}^{n_{l-1} \times n_l}$ and biases $\mathbf{b}^l \in \mathbb{R}^{n_l}$ at each layer. W_{ij}^l is connecting neuron j of layer $l-1$ with neuron i of layer l .
- Nonlinear function $\sigma: \mathbb{R} \rightarrow \mathbb{R}$. $\sigma(\mathbf{x}) = [\sigma(x_1), \dots, \sigma(x_n)]^T$ is shorthand for applied element-wise application to vector $\mathbf{x} \in \mathbb{R}^n$.
- Output vector: $\hat{\mathbf{y}} = \mathbf{x}^L$ ($\hat{\mathbf{y}}$: network predictions, \mathbf{y} : training values)

Multilayer Feedforward Network / Perceptron

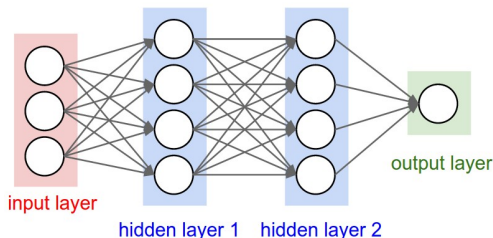


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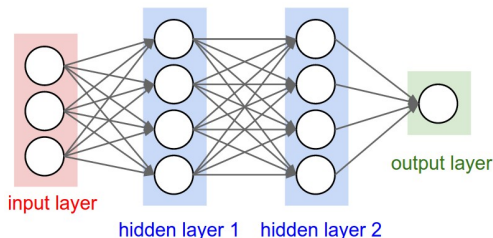


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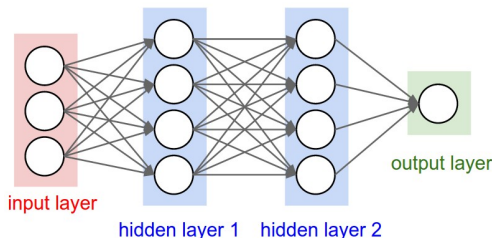


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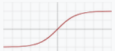

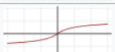



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Common Choices of Nonlinearities





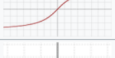

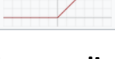
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Binary step		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Logistic (a.k.a. Soft step)		$f(x) = \frac{1}{1 + e^{-x}}$ traditionally used
TanH		$f(x) = \tanh(x) = \frac{2}{1 + e^{-2x}} - 1$
ArcTan		$f(x) = \tan^{-1}(x)$
Softsign ^{[7][8]}		$f(x) = \frac{x}{1 + x }$
Rectified linear unit (ReLU) ^[9]		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$

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Drawback: vanishing gradients. For large input weights, activation function saturates and derivative of output vanishes (especially for deep networks).

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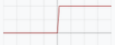



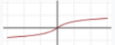

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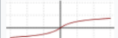
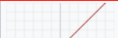
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Non-saturating activation functions – gradients stay finite even for large inputs. Continuously differentiable versions: ELUs and SoftPlus.

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Universal Representation Theorem (URT)

Sloppy formulation: *A neural network with **a single** hidden layer and a monotonically increasing nonlinearity σ can approximate any continuous function $F : \mathbb{R}^{n_0} \mapsto \mathbb{R}^{n_2}$ from inputs \mathbb{R}^{n_0} to outputs \mathbb{R}^{n_2} with arbitrary accuracy given that sufficiently many hidden neurons n_1 are provided.*

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Caveats:

- Existence of network parameters that approximate F does not mean these parameters can be efficiently found.
- Approximation of a function does not mean exact representation, error might be too large for practical purposes.
- For many complex functions, the number of hidden neurons required to achieve acceptable accuracy is unpractical. \rightarrow deep neural networks.

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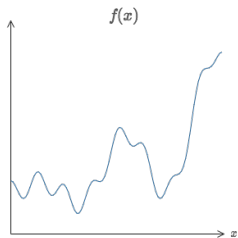
One-dimensional version: Given continuous function $f(x) : \mathbb{R} \mapsto \mathbb{R}$, the URT guarantees that for sufficiently many hidden neurons n_1 , there exist weights $(\mathbf{w}^1, \mathbf{b}^1, \mathbf{w}^2, b^2)$, such that the two-layer neural network function

$$\hat{y}(x) = \sigma \left((\mathbf{w}^2)^\top \sigma(\mathbf{w}^1 x + \mathbf{b}^1) + b^2 \right)$$

approximates the function $f(x)$ with the desired accuracy ε :

$$|\hat{y}(x) - f(x)| < \varepsilon \quad \forall x \in \mathbb{R}.$$

Example: Approximate the following function with $\sigma(z) = (1 + e^{-z})^{-1}$



¹From <http://neuralnetworksanddeeplearning.com/chap4.html>

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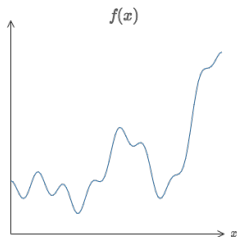
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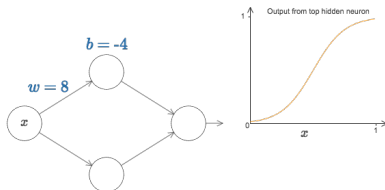
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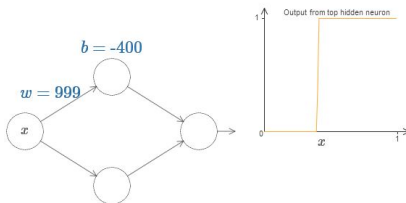
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Universal Representation Theorem (URT)¹

Consider output of one hidden neuron.



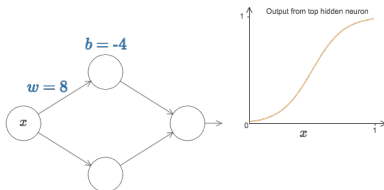
Increasing weight makes the sigmoid more steep, approximating a step function. Use the bias to shift the step where we want it:



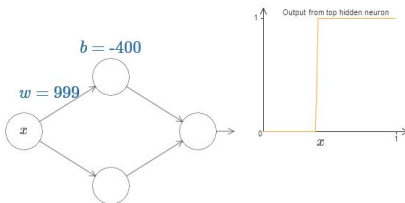
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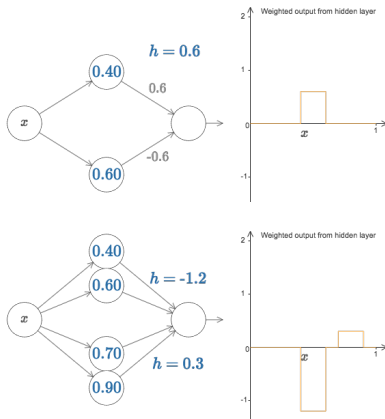
Increasing weight makes the sigmoid more steep, approximating a step function. Use the bias to shift the step where we want it:



¹From <http://neuralnetworksanddeeplearning.com/chap4.html>

Universal Representation Theorem (URT)¹

Characterize each hidden neuron i by the position $s_i = b_i^1/w_i^1$ where it places the step. As the output neuron performs a weighted sum, we can form arbitrary functions as the input to the output nonlinearity:

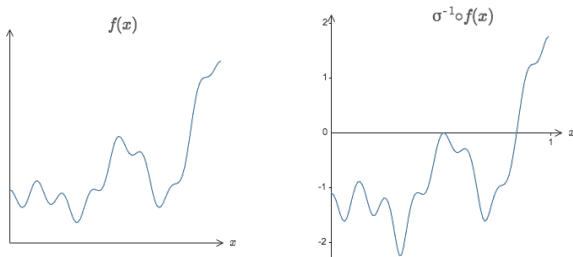


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Universal Representation Theorem (URT)¹

In order to deal with the final nonlinearity, we design the weights such that we approximate $\sigma^{-1}(f(x))$ by the input to the output nonlinearity:

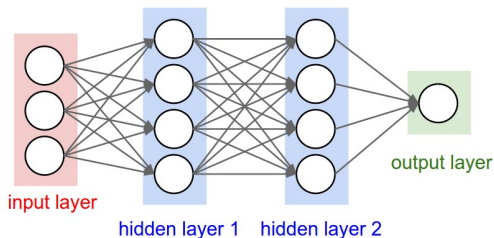
$$f(x) = \sigma(\sigma^{-1}(f(x)))$$



See <http://neuralnetworksanddeeplearning.com/chap4.html> for illustration of multidimensional case.

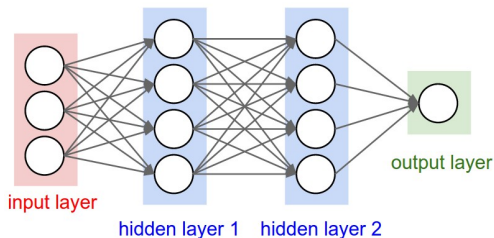
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Multilayer Feedforward Network



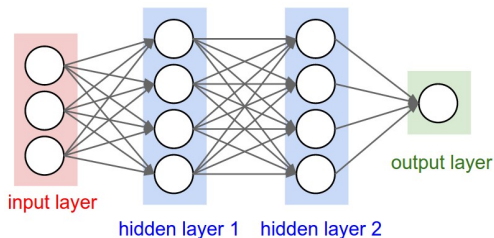
- **Network architecture** is typically the most complex model decision:
 - Number of hidden layers $L - 1$ and number of neurons (n_1, \dots, n_{L-1}) .
 - Type of activation functions σ .
 - Layer types (dense, convolutional, etc. – more details later)
 - Additional regularization terms, e.g. promoting sparsity.
- **Choosing the network architecture:**
 - In principle: Hyperparameter selection problem.
 - In practice: Engineering problem, problem specific architecture.
 - Depends on amount and type of data and available computational resources.
- Intuition: number of parameters should be large enough to prevent underfitting (Advani and Saxe, 2017).

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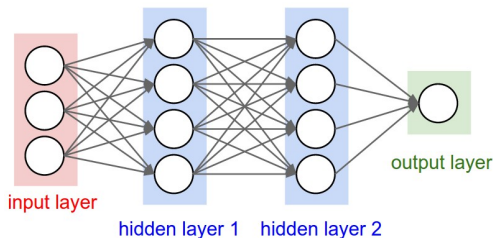
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Training Multilayer Neural Networks

Cost or **loss function** C quantifies performance of network with parameters θ to predict observations \mathbf{X} .

Learning network weights

$$\hat{\theta} = \arg \min_{\theta} C(\mathbf{X}, \mathbf{Y}, \theta)$$

Minimizing *cost* $C \equiv$ maximizing *score* $-C$. Often we just write $C(\theta)$.

Example: for supervised learning with features $\mathbf{X} = (\mathbf{x}_i)_{i=1\dots N}$ and labels $\mathbf{Y} = (\mathbf{y}_i)_{i=1\dots N}$. Neural network prediction $\hat{\mathbf{y}}_i(\mathbf{x}_i, \theta)$. Error vector $\Delta_i = \mathbf{y}_i - \hat{\mathbf{y}}_i(\mathbf{x}_i, \theta)$.

- **Regression:** L2 error. Becomes mean square error for 1d-outputs.

$$C_{L2}(\mathbf{X}, \theta) = \frac{1}{N} \sum_{i=1}^N \|\Delta_i\|_2^2 = \frac{1}{N} \sum_{i=1}^N \Delta_i^T \Delta_i$$

- **Classification** to K categories $(s_i)_{i=1,\dots,N}$. Define **one-hot encoding**:

$$y_{im} = \begin{cases} 1 & \text{if } s_i = m \\ 0 & \text{otherwise,} \end{cases}$$

and use L2 error. More common choice: categorical cross-entropy

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Neural networks are usually trained with some form of gradient descent:

Simple gradient descent algorithm

- ➊ Initialize θ_0
- ➋ For $t = 0, \dots, T - 1$ or until converged:
 - ➊ Compute gradient $\mathbf{g}(\theta_t) = \nabla_{\theta} C(\theta_t)$
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- How do we compute the gradient $\nabla_{\theta} C(\theta_t)$?
- Networks are functions of functions, so we will need to use the chain rule of differentiation.
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- **Notation** (reminder): L Layers indexed by $l = 1, \dots, L$. $\mathbf{x}^l \in \mathbb{R}^{n_l}$: Activations of n_l neurons at layer l . Network output: $\hat{\mathbf{y}} = \mathbf{x}^L$.

$$\mathbf{x}^{l+1} = \sigma(\mathbf{W}^l \mathbf{x}^l + \mathbf{b}^l)$$

- Trainable weights $\mathbf{W}^l \in \mathbb{R}^{n_l \times n_{l-1}}$ and biases $\mathbf{b}^l \in \mathbb{R}^{n_l}$ at each layer. W_{ij}^l is connecting neuron j of layer $l-1$ with neuron i of layer l .
- Nonlinear activation functions $\sigma: \mathbb{R} \rightarrow \mathbb{R}$, applied element-wise.
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Backpropagation

- Loss gradient with respect to the activations of the output neurons:

$$\frac{\partial C}{\partial \hat{y}_i} = \frac{\partial C}{\partial \mathbf{x}_i^L}$$

- Depends on the definition of the loss function. For mean square error:

$$C(\mathbf{X}, \theta) = \frac{1}{N} \sum_{k=1}^N c(\mathbf{x}_k, y_k, \theta) \quad \frac{\partial C(\mathbf{X}, \theta)}{\partial \hat{y}_i} = \frac{1}{N} \sum_{k=1}^N \frac{\partial c(\mathbf{x}_k, y_k, \theta)}{\partial \hat{y}_i}$$

with

$$c(\mathbf{x}, y, \theta) = \frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i(\mathbf{x}, \theta))^2 \quad \frac{\partial c(\mathbf{x}, y, \theta)}{\partial \hat{y}_i} = 2(\hat{y}_i(\mathbf{x}, \theta) - y_i)$$

Loss function needs to be differentiable.

- Loss-specific derivatives can be implemented with the loss functions in a neural network package.

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Backpropagation

- **Error:** Loss gradient with respect to the i th weighted input

$$\mathbf{e}_i^l = \frac{\partial C}{\partial z_i^l} = \underbrace{\frac{\partial c(\mathbf{x}, y, \theta)}{\partial \hat{y}_i}}_{\text{loss derivative}} \frac{\partial \hat{y}_i}{\partial z_i^l} = \frac{\partial c(\mathbf{x}, y, \theta)}{\partial \sigma(z_i^l)} \frac{\partial \sigma(z_i^l)}{\partial z_i^l} = \frac{\partial c(\mathbf{x}, y, \theta)}{\partial \sigma(z_i^l)} \underbrace{\sigma'(z_i^l)}_{\text{activation derivative}}$$

The derivative of the fixed activation function can be implemented along with that function, e.g.:

$$\sigma(z) = \frac{1}{1 + e^{-z}} \quad \sigma'(z) = \sigma(z)(1 - \sigma(z)) = \frac{e^{-z}}{(1 + e^{-z})^2}$$

- **Backpropagate error** to earlier layers using

$$z_j^{l+1} = \sum_k w_{jk}^{l+1} x_k^l + b_j^{l+1};$$

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- **Compute gradients** at each layer using $z_i^l = \sum_k w_{ik}^l x_k^{l-1} + b_i^l$:

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- **Weight update:**

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Forward- and Backpropagation

- 1 **Activation at input layer:** Input activations x_i^0 .
- 2 **Feedforward:** For each layer, compute weighted sum and nonlinear transformation, and thus activations of neurons x_j^l .
- 3 **Error at output layer:** Calculate the error of output layer using the derivatives of the cost function.
- 4 **Backpropagate the error:** Propagate the error backwards and compute Δ_j^l for all layers.
- 5 **Calculate gradients:** $\frac{dC}{db_i^l}$ and $\frac{dC}{dw_{ij}^l}$ of cost function with respect to all trainable weights.
Neural network packages (Theano, TensorFlow, PyTorch, Autograd, ...) have gradients defined for all elementary functions. This permits automatic differentiation using the product rule for composite functions.
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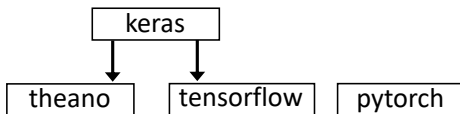
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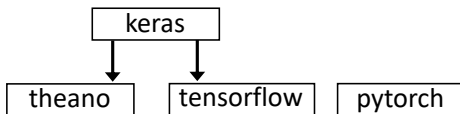
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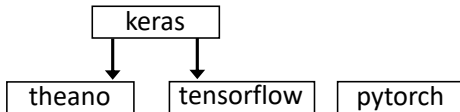
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- 2 **Feedforward:** For each layer, compute weighted sum and nonlinear transformation, and thus activations of neurons x_j^l .
- 3 **Error at output layer:** Calculate the error of output layer using the derivatives of the cost function.
- 4 **Backpropagate the error:** Propagate the error backwards and compute Δ_j^l for all layers.
- 5 **Calculate gradients:** $\frac{dC}{db_i^l}$ and $\frac{dC}{dw_{ij}^l}$ of cost function with respect to all trainable weights.
Neural network packages (Theano, TensorFlow, PyTorch, Autograd, ...) have gradients defined for all elementary functions. This permits automatic differentiation using the product rule for composite functions.
- 6 **Train:** Change weights b_j^l and w_{ij}^l in the direction opposite gradient.



- **keras**: high-level python package.
 - Easy to learn, but limited flexibility
 - Runs on CPUs (slow) and NVidia GPUs (via theano, tensorflow)
 - Recommended installation: direct pip install of the newest compatible keras and tensorflow packages.
- **theano, tensorflow**: low-level python packages for GPU-accelerated tensor operations.
 - Harder to learn, maximum flexibility and speed.
 - Mathematical code defines a graph with operations as nodes and tensors passed along the edges.
 - Before executing, GPU code for graph is generated and compiled.
 - Derivatives are defined for basic operators, enabling automatic backprop for most code.
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- **pytorch**: simplified low-level python package for GPU-accelerated tensor operations.
 - Learning curve between keras and tensorflow.
 - Allows dynamic changes in network structures.
 - More intuitive than tensorflow because operations are executed on demand (dynamic linking of precompiled modules instead of code generation)
 - Recommended installation: conda

Steps in neural network training

❶ **Data preparation:** collect data, featurize and preprocess it:

- ❶ Benchmark datasets can be downloaded via NN packages (e.g. MNIST, CIFAR)
- ❷ Featurization means to define a vector or tensor representation of the data which can be processed by NN packages.
- ❸ Splitting into training and test data (size of test set should be related to complexity of learning task - e.g. 80/20 for MNIST with 10 classes, 50/50 for ImageNet with 1000 classes)
- ❹ Shuffle data sets.
- ❺ Center data: subtract mean over all samples from each sample.
- ❻ Rescale data: when approximately normal, divide the standard deviation. Otherwise, rescaled by the maximum absolute value to move data to interval $[-1, 1]$. Rescaling ensures that the weights of the DNN are of a similar order of magnitude.
- ❼ Data augmentation, i.e. distorting data samples from the existing dataset in some way to enhance size the dataset, e.g. to exploit invariances.

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- 1 **Data preparation:** collect data, featurize and preprocess it:
- 2 **Network model:** Define layers and connectivity, i.e. architecture of the network
- 3 **Loss function:** Define or implement the cost / loss function that should be minimized.
- 4 **Optimizer:** Choose the Optimizer (e.g. ADAM, RMSprop)
- 5 **Train model:** Feed data into (model / loss / optimizer) structure in order to train it, often in minibatches.
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Key advances in deep network training

Until 2009, deep networks were rarely used as training them seemed too difficult. Key advances that enabled the training of deep networks include:

- **Rectifiers:** Changing from activation functions such as logistic, tanh or arctan to rectifiers (ReLU, ELU, SoftPlus) avoids the vanishing gradient problem, makes the loss surface less “frustrated” and thus improves convergence.
- **Stochastic Gradient Descent:** Changing from full gradient descent to stochastic gradient descent resulted in significant reduction of the computational cost to convergence (cheaper iterations and ability to escape flat local minima and saddle points)
- **GPU implementations** of neural networks (Theano, TensorFlow), the resulting computational speedup, and the flexibility of automatic differentiation.

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Data versus learning performance

