Neural Networks

lecturer: Jiří Matas, matas@cmp.felk.cvut.cz

authors: O. Drbohlav , J. Matas

Czech Technical University, Faculty of Electrical Engineering
Department of Cybernetics, Center for Machine Perception
121 35 Praha 2, Karlovo nám. 13, Czech Republic

http://cmp.felk.cvut.cz

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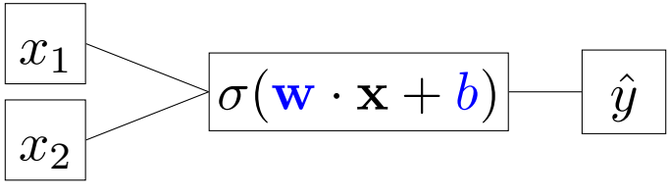
Neural Networks - Motivation (1)

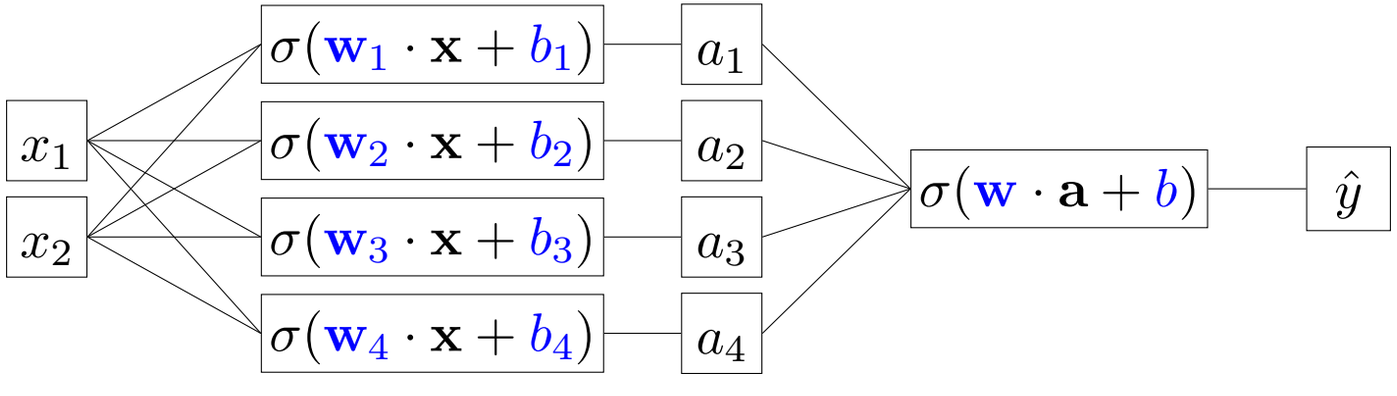
Recall the Perceptron: given the perceptron parameters $\mathbf{w} \in \mathbb{R}^n$ and $b \in \mathbb{R}$, the classification $\hat{y}$ to two classes $\{-1, 1\}$ for a vector $\mathbf{x} \in \mathbb{R}^n$ is performed as

$$\hat{y} = \text{sign}(\mathbf{w} \cdot \mathbf{x} + b)\,, \tag{1}$$

which is an affine (often called linear) function $l(\mathbf{x}) = \mathbf{w} \cdot \mathbf{x} + b$, followed by a non-linear function $\sigma : \mathbb{R} \to \mathbb{R}$, $\sigma(z) = \text{sign}(z)$. The perceptron is also often depicted as follows:

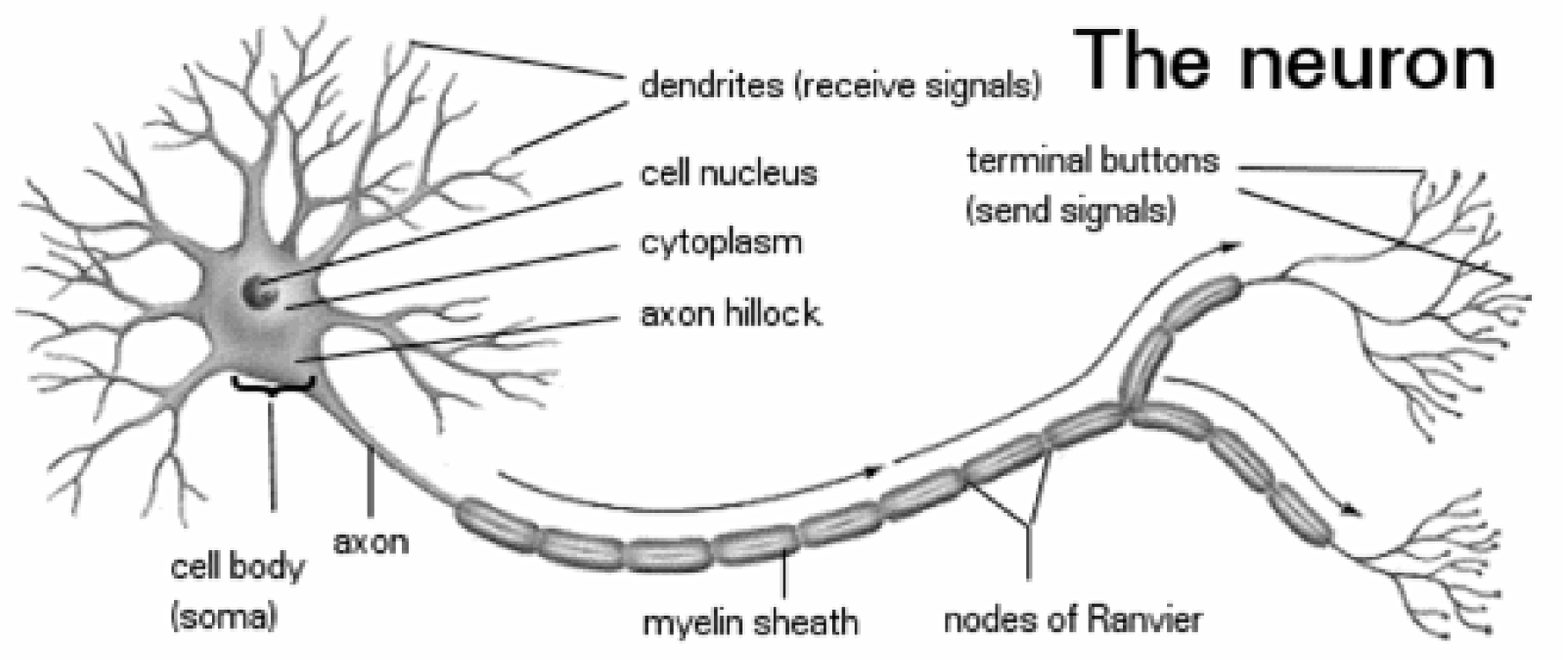


to make the linear combination of elements of the input vector explicit. Perceptron is a linear classifier; these are well understood, have low VC dimension, etc. and thus it is a natural next step to combine them to a more complex classifiers: By letting more of them sharing the input, as well as using their outputs a_i's as inputs to other perceptrons:



Neural Networks - Motivation (2)

'Biological' motivation - a real neuron is known to combine inputs to an output which is then passed to other neurons.



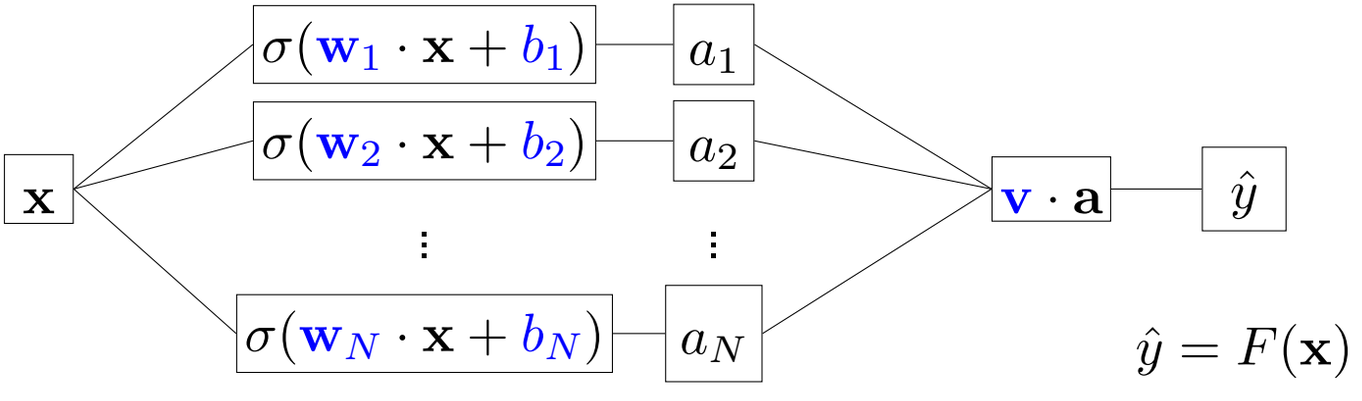
Neural Networks - Motivation (3)

Universal Approximation Theorem. Another strong motivation for forming such combinations of simple classifiers is the theorem which states that if $\sigma : \mathbb{R} \to \mathbb{R}$ is a nonconstant, bounded and continuous function and f is a continuous function on unit hypercube $[0,1]^n$ then for any $\epsilon > 0$ there exists $N \in \mathbb{N}$, $v_i, b_i \in \mathbb{R}$ and $\mathbf{w}_i \in \mathbb{R}^n$ such that

$$F(\mathbf{x}) = \sum_{i=1}^{N} v_i \sigma(\mathbf{w}_i \cdot \mathbf{x} + b_i)\,, \text{ and} \tag{2}$$

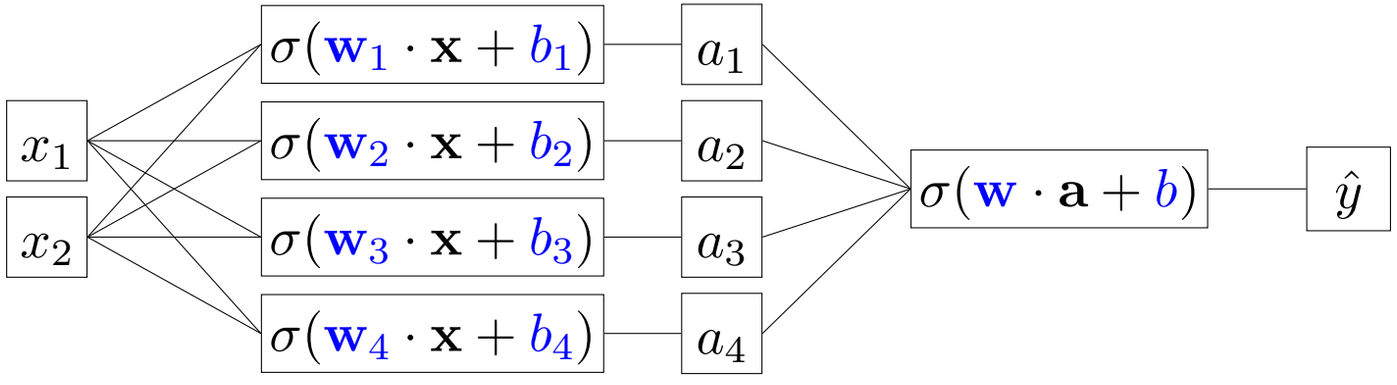
$$|F(\mathbf{x}) - f(\mathbf{x})| < \epsilon\,, \quad \forall \mathbf{x} \in [0,1]^m \tag{3}$$

By comparison, we see that the approximation is exactly captured by the following network with single hidden layer and linear output:



Layers, Concise Equivalent Representation

The network



input layer hidden layer output layer

can be rewritten in a more concise form as follows:

$$\text{(in)} \xrightarrow{\mathbf{x}\in\mathbb{R}^2} \boxed{\sigma(\overset{\mathbf{W}\in\mathbb{R}^{4\times 2},\mathbf{b}\in\mathbb{R}^4}{\mathbf{W}\mathbf{x}+\mathbf{b}})} \xrightarrow{\mathbf{a}\in\mathbb{R}^4} \boxed{\sigma(\overset{\mathbf{w}\in\mathbb{R}^4,b\in\mathbb{R}}{\mathbf{w}\cdot\mathbf{a}+b})} \xrightarrow{\hat{y}\in\mathbb{R}} \text{(out)} \tag{4}$$

where we introduced a convention that for $\sigma\colon \mathbb{R} \to \mathbb{R}$ and $\mathbf{z} \in \mathbb{R}^k$,
$\sigma(\mathbf{z}) = [\sigma(z_1), \sigma(z_2), ..., \sigma(z_k)]^\top$, i.e. the function is applied per component of the vector $\mathbf{z}$.

A network with M hidden layers can be written as (here shown with affine output layer)

$$\text{(in)} \xrightarrow{\mathbf{a}_1=\mathbf{x}\in\mathbb{R}^n} \Bigg[\overset{\textbf{hidden layers}}{\boxed{\sigma(\mathbf{W}_i\mathbf{a}_i+\mathbf{b}_i)}} \xrightarrow{\mathbf{a}_{i+1}}\Bigg]_{i=1}^{M} \rightarrow \overset{\textbf{output layer}}{\boxed{\mathbf{W}_{M+1}\mathbf{a}_{M+1}+\mathbf{b}_{M+1}}} \xrightarrow{\hat{\mathbf{y}}\in\mathbb{R}^K} \text{(out)} \tag{5}$$

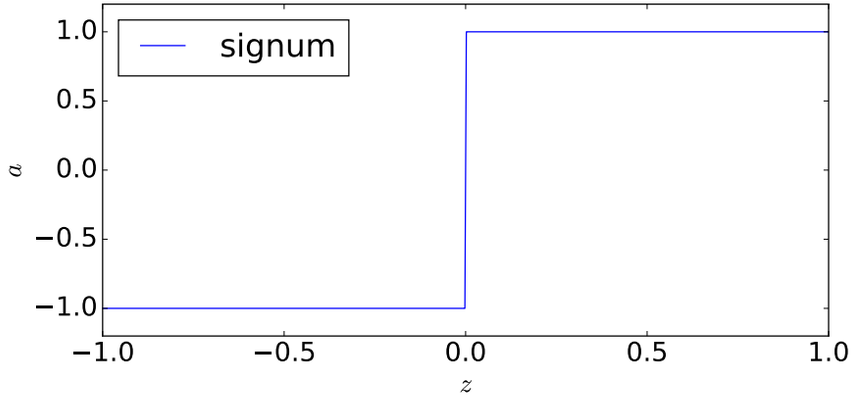
Layer Anatomy

$$\text{(in)} \xrightarrow{\mathbf{a}_1=\mathbf{x}\in\mathbb{R}^n} \Big[\underbrace{\boxed{\sigma(\mathbf{W}_i\mathbf{a}_i+\mathbf{b}_i)}}_{\text{hidden layers}} \xrightarrow{\mathbf{a}_{i+1}}\Big]_{i=1}^{M} \rightarrow \underbrace{\boxed{\mathbf{W}_{M+1}\mathbf{a}_{M+1}+\mathbf{b}_{M+1}}}_{\text{output layer}} \xrightarrow{\hat{\mathbf{y}}\in\mathbb{R}^K} \text{(out)} \quad (6)$$

Each hidden layer of an NN is composed of an affine function, followed by a non-linearity.

Non-linear functions

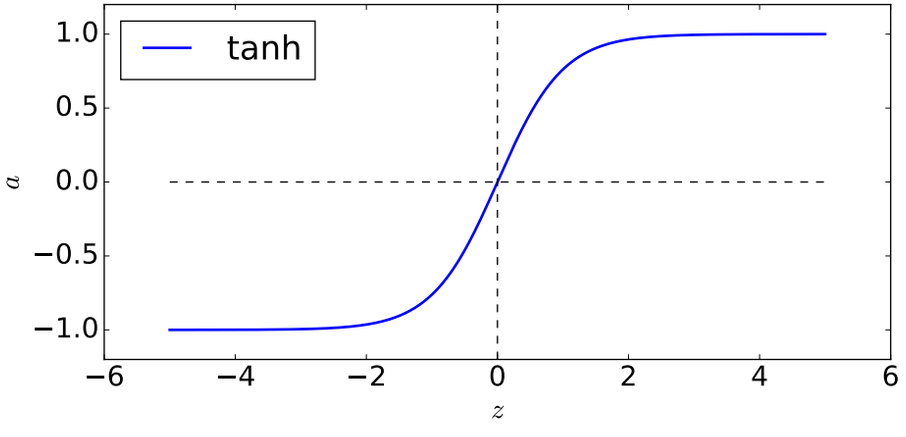
- $\sigma(z) = \text{sign}(z)$: used for the original perceptron. Unusable for an NN because this non-linear function is discontinuous and not differentiable at 0, and everywhere else has zero gradient. So, once we would like to optimize the parameters of the combination of perceptrons, gradient descent and other methods based on first and second order approximations could not proceed. This is why the original sign function has been replaced by functions with 'nicer' properties.

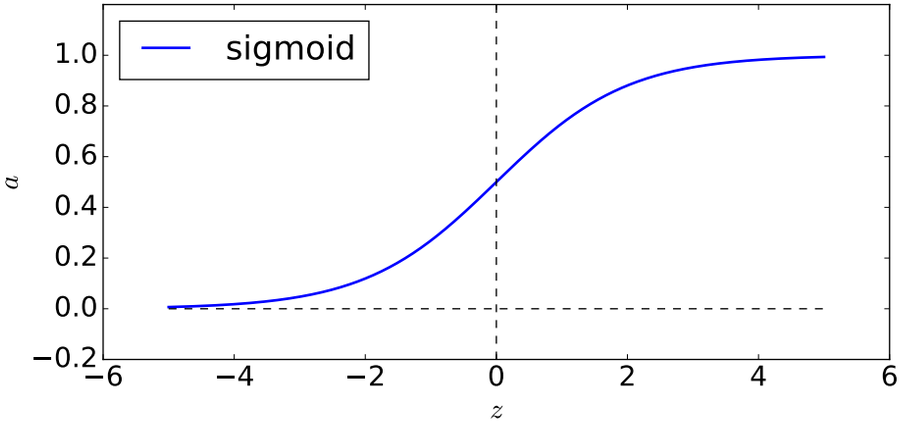


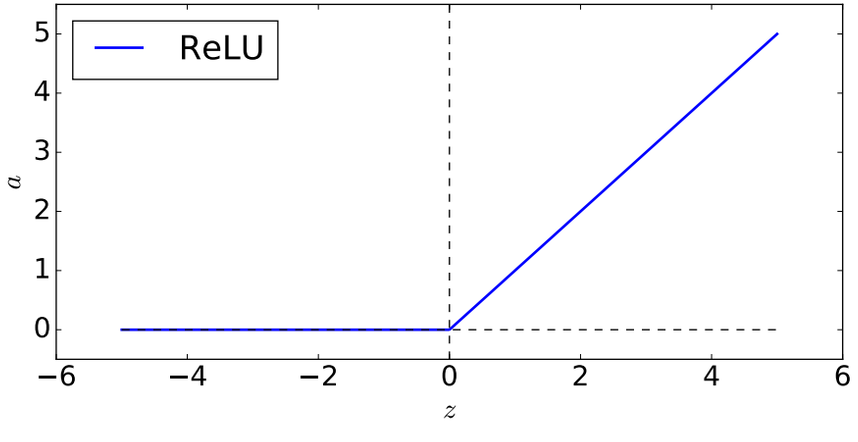
Layer Anatomy, Non-Linear Functions

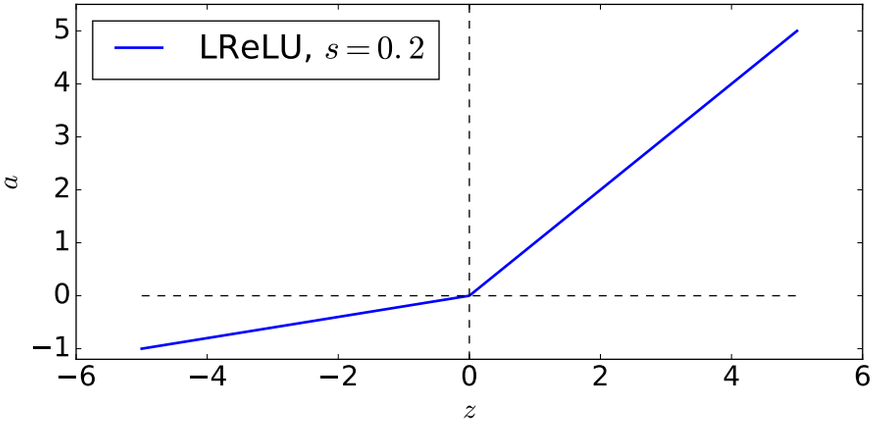
Non-linear functions

- $\sigma(z) = 1/(1+e^{-z})$: logistic sigmoid, $\sigma : \mathbb{R} \to [0, 1]$
- $\sigma(z) = \tanh(z) = (e^{z} - e^{-z})/(e^{z} + e^{-z})$: tanh sigmoid, $\sigma : \mathbb{R} \to [-1, 1]$
- $\sigma(z) = \max(0, z)$: ReLU (rectified linear unit)
- $\sigma(z) = \max(0, z) + \min(0, sz)$ $(0 < s < 1)$: Leaky ReLU
- Many other









Output Layer and Loss Functions. K-class Classification (1)

So far, we have made a general assumption that the output of NN is a K-element vector $\hat{\mathbf{y}} \in \mathbb{R}^K$. Now we will discuss what form the output should take and how we will measure how good the output is.

K-class Classification. We may formally number the classes as $1, 2, ..., K$. But if classes are not ordinal, these numbers are really just labels; it doesn't mean that objects from classes 2 and 3 are in some sense closer than objects from classes 1 and K, say. Therefore, it would make no sense to have a one-dimensional output $\hat{y}$ trying to predict the class label. Instead, the output layer will consist of an affine function producing a K-dimensional vector, followed by the **softmax** which will convert it to class probabilities:

output layer

$$\xrightarrow{\mathbf{a}_{M+1}} \boxed{\mathbf{W}_{M+1}\mathbf{a}_{M+1} + \mathbf{b}_{M+1}} \xrightarrow{\mathbf{z}\in\mathbb{R}^K} \boxed{\text{softmax}} \xrightarrow{\hat{\mathbf{y}}\in\mathbb{R}^K} (\text{out}) \tag{7}$$

with

$$[\text{softmax}(\mathbf{z})]_k = \frac{\exp z_k}{\sum_{l=1}^{K} \exp z_l}\,. \tag{8}$$

For representing the class y of the training data point $(\mathbf{x}, y)$, **one-hot** representation is used which simply makes a K-dimensional vector which is everywhere zero except for the y-th component which is 1:

$$\text{onehot}(y) = [\delta_{1y}, \delta_{2y}, ...\delta_{Ky}]^\top = [0, 0, ..., \underset{\substack{\uparrow\\ \text{y-th place}}}{1}, ..., 0]^\top \in \mathbb{R}^K \tag{9}$$

Output Layer and Loss Functions. K-class Classification (2)

For a training data point $(\mathbf{x}, y)$, how to measure how far the prediction $\hat{\mathbf{y}} \in [0,1]^K$ for $\mathbf{x}$ is from the target vector $\mathbf{y} = \text{onehot}(y) \in \{0,1\}^K$?

- Squared difference:

$$J(\hat{\mathbf{y}}, \mathbf{y}) = \|\hat{\mathbf{y}} - \mathbf{y}\|^2 . \tag{10}$$

  This loss $= 0$ when the prediction matches the target and > 0 otherwise.

- Negative log-likelihood. To avoid confusion, let us denote the index of the target class l, $l = y$ for training data point $(\mathbf{x}, y)$.

$$J(\hat{\mathbf{y}}, \mathbf{y}) = -\mathbf{y}^\top \log \hat{\mathbf{y}} = -\sum_{i=1}^{K} y_i \log \hat{y}_i = -\log \hat{y}_l . \tag{11}$$

Example: K-class logistic regression. The class conditionals $\hat{\mathbf{y}}(\mathbf{x}) = [p(1|\mathbf{x}), p(2|\mathbf{x}), ..., p(K|\mathbf{x})] \in \mathbb{R}^K$ can be written as ($\mathbf{W} \in \mathbb{R}^{n \times K}$, $\mathbf{b} \in \mathbb{R}^K$):

$$\text{(in)} \xrightarrow{\mathbf{x} \in \mathbb{R}^n} \boxed{\mathbf{W}\mathbf{x} + \mathbf{b}} \xrightarrow{\mathbf{z} \in \mathbb{R}^K} \boxed{\text{softmax}} \xrightarrow{\hat{\mathbf{y}} \in \mathbb{R}^K} \text{(out)} \tag{12}$$

Output Layer and Loss Functions. 2-class Classification

For two classes, the output $\hat{y}$ of the NN can be 1-dimensional, modeling the class posterior $p(1|\mathbf{x}) \in [0, 1]$. The posterior $p(2|\mathbf{x})$ is computed simply as $1 - \hat{y}$.

Example: 2-class logistic regression. The posteriors $p(1|\mathbf{x})$, $p(2|\mathbf{x})$ are modeled as $(\mathbf{x}, \mathbf{w} \in \mathbb{R}^n, b \in \mathbb{R})$:

$$p(1|\mathbf{x}) = \frac{1}{1 + e^{-(\mathbf{w}\cdot\mathbf{x}+b)}}, \qquad p(2|\mathbf{x}) = 1 - p(1|\mathbf{x}) \tag{13}$$

This can be written as a single-neuron NN with output $\hat{y} = p(1|\mathbf{x})$:

$$\text{(in)} \xrightarrow{\mathbf{x}} \boxed{\sigma(\mathbf{w} \cdot \mathbf{x} + b)} \xrightarrow{\hat{y}} \text{(out)} \tag{14}$$

where $\sigma(z) = 1/(1 + e^{-z})$ is the logistic sigmoid non-linearity.

Recall that negative log-likelihood loss has been used for the 2-class logistic regression:

$$J(\hat{y}, y) = -[y \log \hat{y} + (1 - y) \log(1 - \hat{y})] \tag{15}$$

where class labels y have conveniently been changed as $(1, 2) \mapsto (1, 0)$. The procedure for finding the optimal parameters $\boldsymbol{\theta} = \{\mathbf{w}, b\}$ was the gradient descent.

Output Layer and Loss Functions. Regression

The NN can of course also be used for regression, that is, finding a function which predicts a target $\mathbf{y} \in \mathbb{R}^K$ which is not constrained to represent probability distribution.

Squared difference is an obvious choice for such a problem.

Training the NN

Let the training data be $\mathcal{T} = \{(\mathbf{x}_1, \mathbf{y}_1), (\mathbf{x}_2, \mathbf{y}_2), ..., (\mathbf{x}_N, \mathbf{y}_N)\}$, where without loss of generality we assume that class labels y_i's have been converted to their one-hot representations $\mathbf{y}_i$'s if needed. Let $\boldsymbol{\theta}$ denote all parameters of the NN. We want to minimize

$$J(\mathcal{T}; \boldsymbol{\theta}) = \sum_{(\mathbf{x},\mathbf{y}) \in \mathcal{T}} J(\hat{\mathbf{y}}(\mathbf{x}), \mathbf{y}) \,. \tag{16}$$

Gradient-based methods are used most of the time for minimizing the loss function $J(\mathcal{T}; \boldsymbol{\theta})$ w.r.t. $\boldsymbol{\theta}$. We need to evaluate the gradient of loss w.r.t. the NN parameters, $\frac{\partial J(\hat{\mathbf{y}}(\mathbf{x}), \mathbf{y})}{\partial \boldsymbol{\theta}}$, in order to use it for updates of the gradient-descent type:

$$\boldsymbol{\theta}_{t+1} \leftarrow \boldsymbol{\theta}_t - \mu \sum_{(\mathbf{x},\mathbf{y}) \in \mathcal{T}' \subseteq \mathcal{T}} \frac{\partial J(\hat{\mathbf{y}}(\mathbf{x}), \mathbf{y})}{\partial \boldsymbol{\theta}} \tag{17}$$

where μ is the learning rate and the summation is not necessarily over the entire dataset.

Computing gradient (1)

When computing the gradient, we will make use of the chain rule. Let $f\colon \mathbb{R}^n \to \mathbb{R}$ and $g\colon \mathbb{R}^m \to \mathbb{R}^n$. For $\mathbf{x} \in \mathbb{R}^m$, let $\mathbf{y} = g(\mathbf{x})$. Let us consider the composition of these functions, $f(g(\mathbf{x})) = f(\mathbf{y})$ ($f \circ g\colon \mathbb{R}^m \to \mathbb{R}$). There holds

$$\frac{\partial f(g(\mathbf{x}))}{\partial x_k} = \sum_{i=1}^{n} \frac{\partial f}{\partial y_i} \frac{\partial y_i}{\partial x_k}. \tag{18}$$

This can be written in a matrix form,

$$\frac{\partial f(g(\mathbf{x}))}{\partial \mathbf{x}} = \frac{\partial f}{\partial \mathbf{y}} \frac{\partial \mathbf{y}}{\partial \mathbf{x}} = f'\mathbf{y}', \tag{19}$$

where $f' = \partial f/\partial \mathbf{y}$ and $\mathbf{y}' = \partial \mathbf{y}/\partial \mathbf{x}$ are Jacobian matrices:

$$f' = \left[\frac{\partial f}{\partial y_1}, \frac{\partial f}{\partial y_2}, ..., \frac{\partial f}{\partial y_n}\right], \tag{20}$$

$$\mathbf{y}' = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \dots & \frac{\partial y_1}{\partial x_m} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \dots & \frac{\partial y_2}{\partial x_m} \\ \vdots & & \ddots & \vdots \\ \frac{\partial y_n}{\partial x_1} & \frac{\partial y_n}{\partial x_2} & \dots & \frac{\partial y_n}{\partial x_m} \end{bmatrix} \tag{21}$$

Example: Gradient by Back Propagation (1)

Let us have the following network:

$$\xrightarrow[\mathbf{a}_1=\mathbf{x}]{\mathbf{a}_1\in\mathbb{R}^n} \boxed{\mathbf{W}_1\mathbf{a}_1+\mathbf{b}_1} \xrightarrow{\mathbf{z}_2\in\mathbb{R}^{m_2}} \boxed{\sigma} \xrightarrow{\mathbf{a}_2\in\mathbb{R}^{m_2}} \boxed{\mathbf{W}_2\mathbf{a}_2+\mathbf{b}_2} \xrightarrow{\mathbf{z}_3\in\mathbb{R}^{m_3}} \dots \tag{22}$$

$$\boxed{\sigma} \xrightarrow{\mathbf{a}_3\in\mathbb{R}^{m_3}} \boxed{\mathbf{W}_3\mathbf{a}_3+\mathbf{b}_3} \xrightarrow{\hat{\mathbf{y}}\in\mathbb{R}^K} \boxed{J(\hat{\mathbf{y}},\mathbf{y})}$$

where the non-linearities have been explicitly put to the chain. The set of NN parameters is $\boldsymbol{\theta}=\{\mathbf{W}_1,\mathbf{W}_2,\mathbf{W}_3,\mathbf{b}_1,\mathbf{b}_2,\mathbf{b}_3\}$. For the loss, let us consider $J(\hat{\mathbf{y}},\mathbf{y})=\|\hat{\mathbf{y}}-\mathbf{y}\|^2$.

1. Compute $\mathbf{v}_3=\frac{\partial J}{\partial\hat{\mathbf{y}}}\big|_{\hat{\mathbf{y}}}$. This is a row vector, $\mathbf{v}_3\in\mathbb{R}^K$, $\mathbf{v}_3=2(\hat{\mathbf{y}}-\mathbf{y})^\top$.
2. $\frac{\partial J}{\partial\mathbf{b}_3}=\mathbf{v}_3\frac{\partial\hat{\mathbf{y}}}{\partial\mathbf{b}_3}\big|_{\mathbf{a}_3}=\mathbf{v}_3\mathbb{1}=\mathbf{v}_3$
3. $\frac{\partial J}{\partial(\mathbf{W}_3)_{kl}}=\mathbf{v}_3\frac{\partial\hat{\mathbf{y}}}{\partial(\mathbf{W}_3)_{kl}}=\mathbf{v}_3[0,0,...,(\mathbf{a}_3)_l,...,0,0]^\top=(\mathbf{v}_3)_k(\mathbf{a}_3)_l$

   $\uparrow$

   at k-th element

   So, arranging partial derivatives of J w.r.t. elements of $\mathbf{W}_3\in\mathbb{R}^{K\times m_3}$ to a matrix of the same dimensions then we can write

$$\frac{\partial J}{\partial\mathbf{W}_3}=\begin{bmatrix}\frac{\partial J}{\partial(\mathbf{W}_3)_{11}} & \frac{\partial J}{\partial(\mathbf{W}_3)_{12}} & \dots & \frac{\partial J}{\partial(\mathbf{W}_3)_{1m_1}}\\ \frac{\partial J}{\partial(\mathbf{W}_3)_{21}} & \frac{\partial J}{\partial(\mathbf{W}_3)_{22}} & \dots & \frac{\partial J}{\partial(\mathbf{W}_3)_{2m_1}}\\ \vdots & \ddots & & \\ \frac{\partial J}{\partial(\mathbf{W}_3)_{K1}} & \frac{\partial J}{\partial(\mathbf{W}_3)_{K2}} & \dots & \frac{\partial J}{\partial(\mathbf{W}_3)_{Km_1}}\end{bmatrix}=\mathbf{v}_3{}^\top\mathbf{a}_3{}^\top \tag{23}$$

Example: Gradient by Back Propagation (2)

Let us have the following network:

$$\xrightarrow[\mathbf{a}_1=\mathbf{x}]{\mathbf{a}_1\in\mathbb{R}^n} \boxed{\mathbf{W}_1\mathbf{a}_1+\mathbf{b}_1} \xrightarrow{\mathbf{z}_2\in\mathbb{R}^{m_2}} \boxed{\sigma} \xrightarrow{\mathbf{a}_2\in\mathbb{R}^{m_2}} \boxed{\mathbf{W}_2\mathbf{a}_2+\mathbf{b}_2} \xrightarrow{\mathbf{z}_3\in\mathbb{R}^{m_3}} \dots \tag{24}$$

$$\boxed{\sigma} \xrightarrow{\mathbf{a}_3\in\mathbb{R}^{m_3}} \boxed{\mathbf{W}_3\mathbf{a}_3+\mathbf{b}_3} \xrightarrow{\hat{\mathbf{y}}\in\mathbb{R}^K} \boxed{J(\hat{\mathbf{y}},\mathbf{y})}$$

4. Compute $\mathbf{v}_2 = \mathbf{v}_3\frac{\partial\hat{\mathbf{y}}}{\partial\mathbf{a}_3}\Big|_{\mathbf{a}_3}\frac{\partial\mathbf{a}_3}{\partial\mathbf{z}_3}\Big|_{\mathbf{z}_3} = \mathbf{v}_3\mathbf{W}_3\text{diag}[\sigma'(\mathbf{z}_3)] = (\mathbf{v}_3\mathbf{W}_3)\odot\sigma'(\mathbf{z}_3)$;
   Here $\sigma'(\mathbf{x}) = [\sigma'(x_1),\sigma'(x_2),...,\sigma'(x_n)]$ with $\mathbf{x}\in\mathbb{R}^n$ and σ' the derivative of σ, $\text{diag}(\mathbf{x})$ for $\mathbf{x}\in\mathbb{R}^n$ forms an n-by-n diagonal matrix with elements of $\mathbf{x}$ on the diagonal, and $\odot$ is the Hadamard (element-wise) product.
5. $\frac{\partial J}{\partial\mathbf{b}_2} = \mathbf{v}_2$
6. $\frac{\partial J}{\partial\mathbf{W}_2} = \mathbf{v}_2{}^\top\mathbf{a}_2{}^\top$
7. Compute $\mathbf{v}_1 = \mathbf{v}_2\mathbf{W}_2\text{diag}[\sigma'(\mathbf{z}_2)] = (\mathbf{v}_2\mathbf{W}_2)\odot\sigma'(\mathbf{z}_2)$
8. $\frac{\partial J}{\partial\mathbf{b}_1} = \mathbf{v}_1$
9. $\frac{\partial J}{\partial\mathbf{W}_1} = \mathbf{v}_1{}^\top\mathbf{a}_1{}^\top$