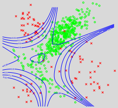

Machine Learning

Lecture *Machine Learning* on March 11-13, 2024

Mario Stanke
Institut für Mathematik und Informatik
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Definition 1 (Artificial Neural Network (NN, Multilayer Perceptron))

A feed-forward artificial neural network with $L \geq 1$ layers of sizes $s_1, \ldots, s_L$ with $n =: s_0$ input variables $\mathbf{x} = (x_1, \ldots, x_n)^T$ and $K := s_L$ output variables $\mathbf{t} = (t_1, \ldots, t_K)^T$ is a function

$$\mathbf{t} = h_{\boldsymbol{\theta}}(\mathbf{x})$$

with parameters

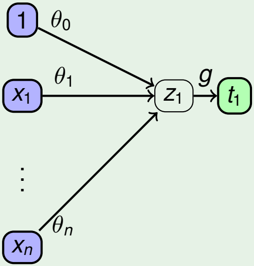
$$\boldsymbol{\theta} = (\Theta^{(0)}, \ldots, \Theta^{(L-1)}) \qquad \text{, where} \quad \Theta^{(\ell)} \in \mathbb{R}^{s_{\ell+1} \times (s_\ell + 1)},$$

defined by the following recursions

$$\begin{aligned}
\mathbf{t} &= \mathbf{g}(\mathbf{z}^{(L)}) \in \mathbb{R}^K \\
\mathbf{z}^{(\ell)} &= \Theta^{(\ell-1)} \mathbf{a}^{(\ell-1)} \in \mathbb{R}^{s_\ell} \qquad (1 \leq \ell \leq L) \\
\mathbf{a}^{(\ell)} &= \begin{pmatrix} a_0^{(\ell)} \\ a_1^{(\ell)} \\ \vdots \\ a_{s_\ell}^{(\ell)} \end{pmatrix} = \begin{pmatrix} 1 \\ \sigma(z_1^{(\ell)}) \\ \vdots \\ \sigma(z_{s_\ell}^{(\ell)}) \end{pmatrix} \qquad (1 \leq \ell < L) \\
\mathbf{a}^{(0)} &= \begin{pmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{pmatrix}.
\end{aligned} \tag{1}$$

Here, σ is called an activation function and we will call $\mathbf{g} : \mathbb{R}^K \to \mathbb{R}^K$ the output activation function.

Linear regression = NN with 1 layer and 1 output variable



$L = 1$ layers

$$\boldsymbol{\theta} = (\theta_0, \theta_1, \ldots, \theta_n) \quad \text{parameters}$$

t_1 one output unit
$x_1, \ldots, x_n$ input units
output activation function $t_1 = g(z_1) = z_1$

$$t_1 = \theta_0 + \sum_{j=1}^{n} \theta_j x_j$$

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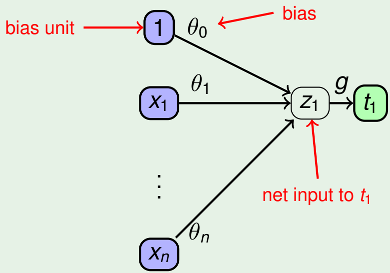

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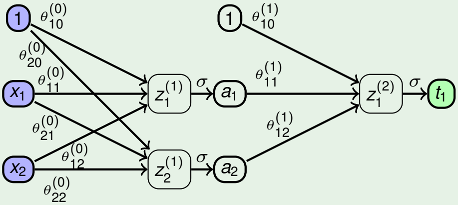
Artificial Neural Networks

NN with 1 hidden layer



$L = 2$ layers, 1 hidden layer, $s_1 = 2$

$$\boldsymbol{\theta} = (\Theta^{(0)}, \Theta^{(1)}) \quad \text{parameters}$$

x_1, x_2 input units, t_1 single output unit with output activation function σ

$$t_1 = \sigma\left(\theta_{10}^{(1)} + \theta_{11}^{(1)} a_1 + \theta_{12}^{(1)} a_2\right) = \sigma\left(\theta_{10}^{(1)} + \theta_{11}^{(1)} \sigma(\theta_{10}^{(0)} + \theta_{11}^{(0)} x_1 + \theta_{12}^{(0)} x_2) + \theta_{12}^{(1)} \sigma(\theta_{20}^{(0)} + \theta_{21}^{(0)} x_1 + \theta_{22}^{(0)} x_2)\right)$$

Artificial Neural Networks

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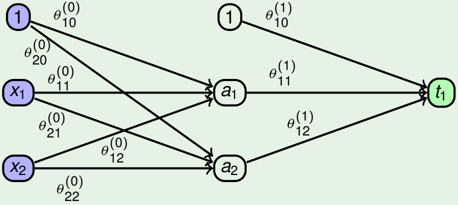

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Artificial Neural Networks

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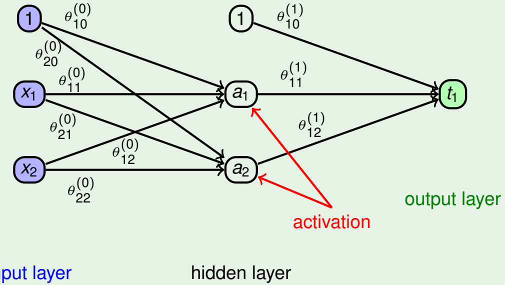

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Training of Artificial Neural Networks

Suppose a *single* training observation

$$\mathbf{y} = (y_1, \ldots, y_K)^T$$

for training input

$$\mathbf{x} = (x_1, \ldots, x_n)^T$$

is given.

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Consider some error function

$$D(\boldsymbol{\theta})$$

that typically depends on training data but that depends on the parameters $\boldsymbol{\theta}$ only through the network output $\mathbf{t}$, e.g. a squared error function.

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$$\frac{\partial D}{\partial \theta_{ji}^{(\ell-1)}}$$

for ℓ, j and i ("gradient" in TensorFlow).

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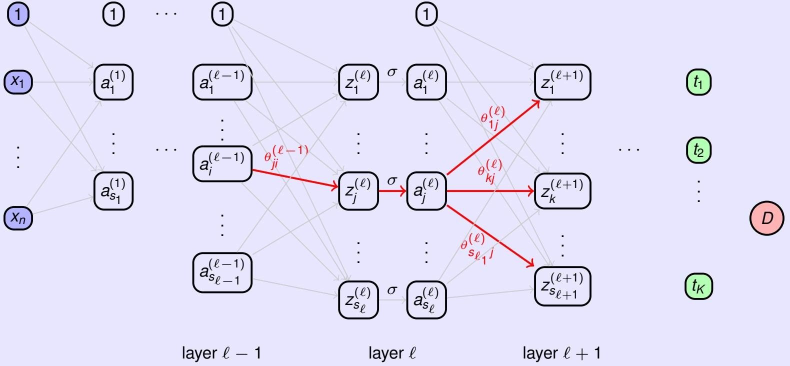
$D(\boldsymbol{\theta})$ may be non-convex and have local, non-global minima.

NN Training: partial derivatives backpropagate through network



From

$$z_j^{(\ell)} = \sum_r \theta_{jr}^{(\ell-1)} a_r^{(\ell-1)}$$

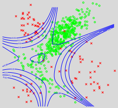
we obain using the univariate chain rule that

$$\frac{\partial D}{\partial \theta_{ji}^{(\ell-1)}} = \frac{\partial D}{\partial z_j^{(\ell)}} a_i^{(\ell-1)}$$

and using the multivariate chain rule that

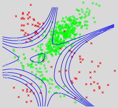
$$\frac{\partial D}{\partial z_j^{(\ell)}} = \left(\frac{\partial D}{\partial z_1^{(\ell+1)}}, \dots, \frac{\partial D}{\partial z_{s_{\ell+1}}^{(\ell+1)}} \right) \begin{pmatrix} \frac{\partial z_1^{(\ell+1)}}{\partial z_j^{(\ell)}} \\ \vdots \\ \frac{\partial z_{s_{\ell+1}}^{(\ell+1)}}{\partial z_j^{(\ell)}} \end{pmatrix}.$$

All derivates can be computed efficiently in one right-to-left pass (“backpropagation algorithm”).
TensorFlow does backprop automatically, for general models.



Artificial Neural Networks for Regression

Consider first a single training instance $\mathbf{x} \in R^n$ with a single output $\mathbf{y} \in R^K$.
(We simply average $D(\boldsymbol{\theta})$ over multiple training instances.)



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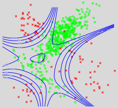

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- Choose the identity function as output activation function $\mathbf{g}$, i.e. $\mathbf{t} = \mathbf{z}^{(L)}$ (unbounded).
- Choose the squared error function

$$D(\boldsymbol{\theta}) := \|\mathbf{t} - \mathbf{y}\|_2^2 = \sum_{k=1}^{K} (t_k - y_k)^2$$

Artificial Neural Networks for Classification

Again, consider first a single training instance. Here, let output $\mathbf{y} \in R^K$ be one-hot encoded such that

$$\mathbf{y} = \mathbf{e}_c = c\text{-th unit vector}$$

if $c \in \{1, 2, \ldots, K\}$ is the true class of the learning instance.

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- Choose the softmax function as output activation function $\mathbf{g}$.

$$\mathbf{t} = \mathbf{g}(z_1, \ldots, z_K) = \frac{1}{\sum_{k=1}^{K} e^{z_k}} \begin{pmatrix} e^{z_1} \\ \vdots \\ e^{z_K} \end{pmatrix}$$

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  Properties:

  - $0 < t_k < 1$, $t_1 + \cdots + t_K = 1$
  - if $z_j \gg z_i$ for $i \neq j$, then $t_j \approx 1$ and $t_i \approx 0$ for $i \neq j$
  - softmax is a generalization of the sigmoid function to more than 2 classes

- If $K = 2$ (binary classification), $t_1 = 1 - t_2$ is often not stored. The same neural network function can then be achieved by setting the output size to 1 and using the logistic sigmoid function as activation.

Artificial Neural Networks for Classification

Cross-entropy error function for multiclass problem

Consider the true class of the training instance to be a random variable $C \in \{1, \ldots, K\}$ with observation c and the output vector $\mathbf{t}$ of the net to be the parameters of a multinomial distribution for C. Then the likelihood is

$$L(\boldsymbol{\theta}) =$$

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and we seek to minimize the negative log-likelihood

$$-\ln L(\boldsymbol{\theta}) = -\ln t_c = -\sum_{k=1}^{K} y_k \ln t_k$$

Artificial Neural Networks for Classification

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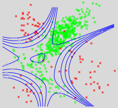
Define the cross-entropy error function

$$D(\boldsymbol{\theta}) = -\sum_{k=1}^{K} y_k \ln t_k.$$



Artificial Neural Networks

Training set

Let

$$\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}$$

be training inputs and

$$\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(m)}$$

be the corresponding training outputs / labels. Let

$$\mathbf{t}^{(i)} = h_\Theta(\mathbf{x}^{(i)}) \qquad (i = 1..m)$$

be the outputs of the NN.

Overfitting

If the model has many parameters, the training may result in a model that fits the training data 'too well', therefore does not generalize well and performs poorly on independent test data. Remedies:

1. Make model less complex, e.g. reduce number of parameters or change model class (e.g. lin. regresion over NN).
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Error function with regularization for neural networks

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An common choice for the regularization term is the (scaled) L2 norm:

$$R(\boldsymbol{\theta}) = \frac{1}{m} \sum_{\ell=0}^{L-1} \sum_{i=1}^{s_\ell} \sum_{j=1}^{s_{\ell+1}} \left(\theta_{ji}^{(\ell)}\right)^2 .$$

Note that the bias terms $\theta_{j0}^{(\ell)}$ are left out (not penalized).

Error function with regularization for regression

$$E(\boldsymbol{\theta}) = \frac{1}{m}\left\{\sum_{i=1}^{m}\sum_{k=1}^{K}\left(t_k^{(i)} - y_k^{(i)}\right)^2 + \lambda\sum_{\ell=0}^{L-1}\sum_{i=1}^{s_\ell}\sum_{j=1}^{s_{\ell+1}}\left(\theta_{ji}^{(\ell)}\right)^2\right\} \tag{2}$$

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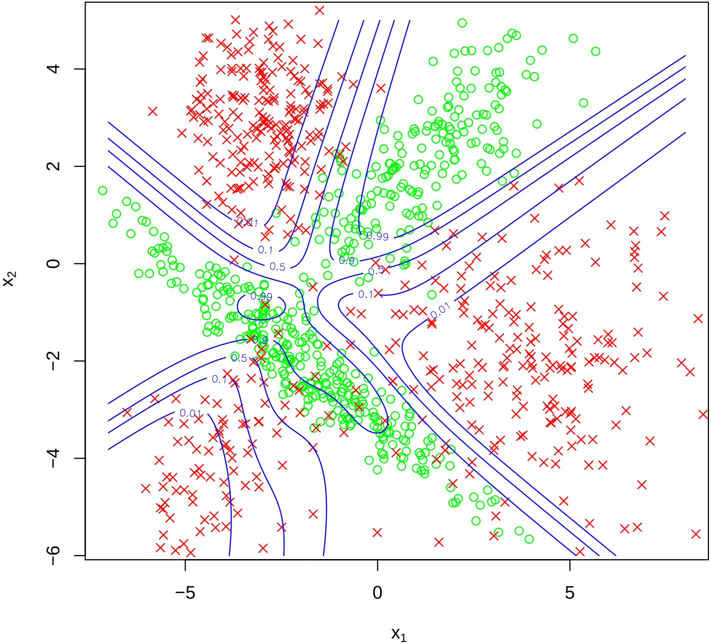
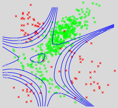
Error function with regularization for classification

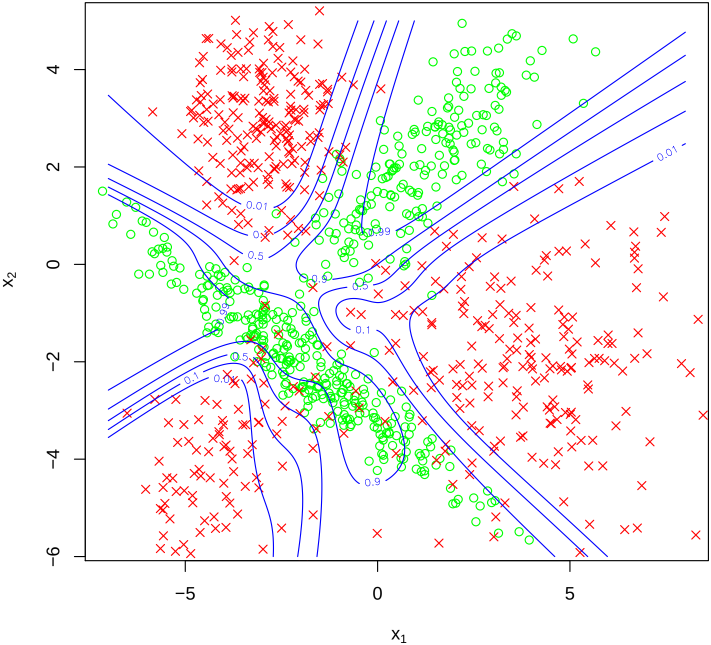
$$E(\boldsymbol{\theta}) = \frac{1}{m}\left\{-\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)} \ln t_k^{(i)} + \lambda\sum_{\ell=0}^{L-1}\sum_{i=1}^{s_\ell}\sum_{j=1}^{s_{\ell+1}}\left(\theta_{ji}^{(\ell)}\right)^2\right\} \tag{3}$$

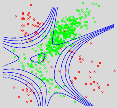
1 hidden layer of size 5, $\lambda = 0$ (no regularization)



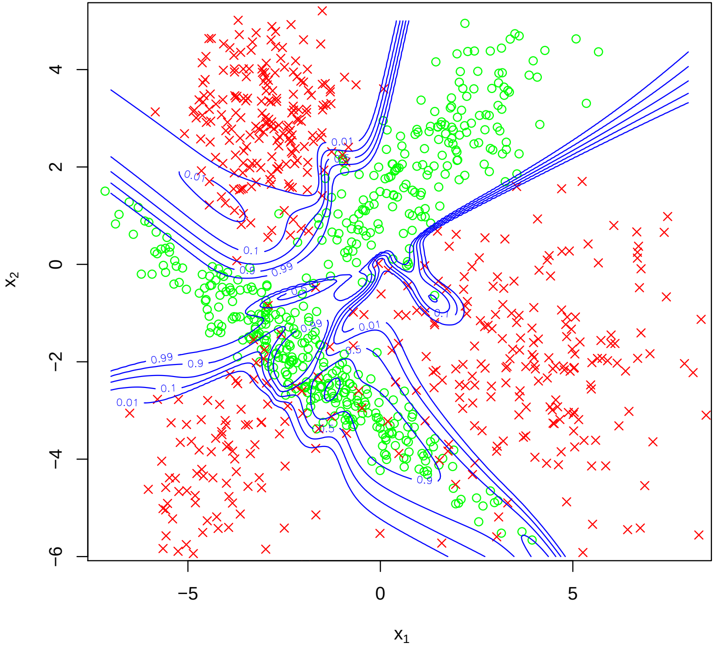


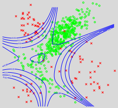
2 hidden layers of size 8 each, $\lambda = 0$ (no regularization)



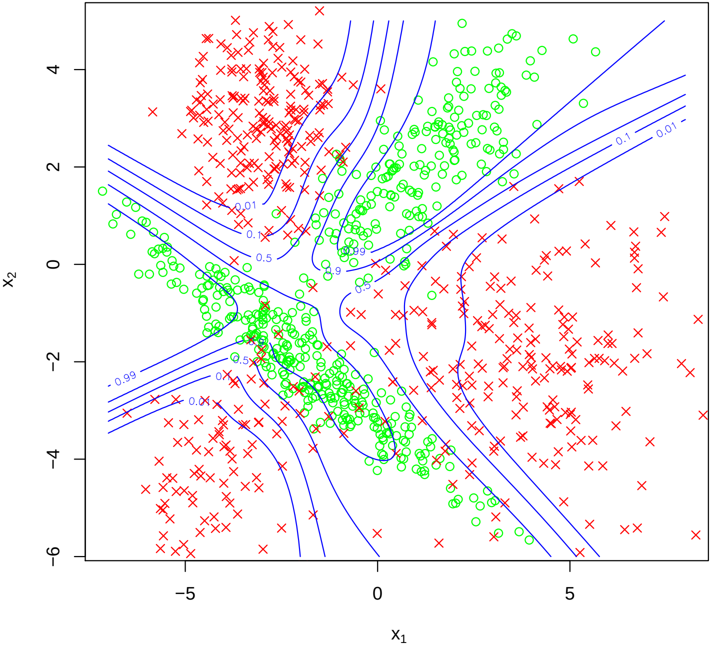


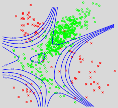
2 hidden layers of size 20 each, $\lambda = 0$ (no regularization)



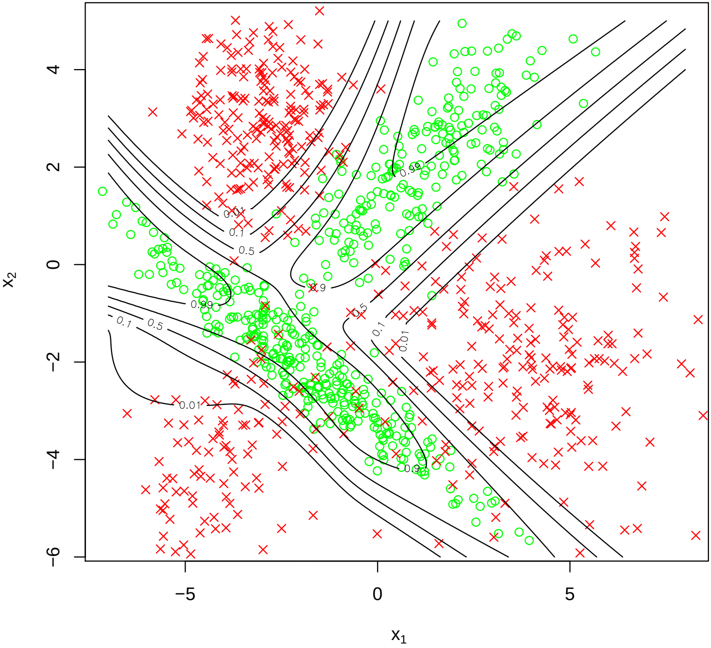


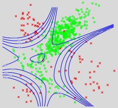
2 hidden layers of size 20 each, $\lambda = 0.1$ (with regularization)





Posterior probability of class (theoretical optimum if distr. was known)



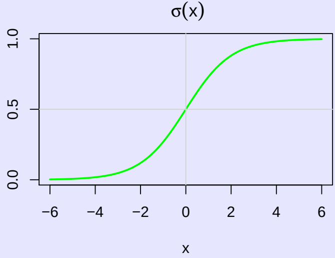


Activation Functions

Logistic sigmoid, `tf.nn.sigmoid`

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

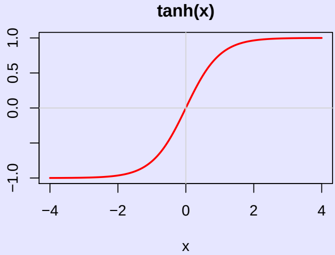
$$\sigma' = \sigma(1 - \sigma)$$



Tangens hyperbolicus

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

$$\tanh'(x) = 1 - (\tanh(x))^2$$

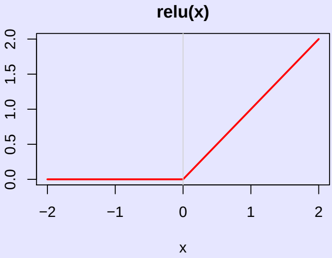


Rectified linear unit (ReLU), `tf.nn.relu`

$$\text{relu}(x) = x^+ = \max\{0, x\}$$

$$\text{relu}'(x) = \begin{cases} 1 & \text{, if } x > 0 \\ 0 & \text{, if } x < 0 \end{cases}$$

$\text{relu}'(0) := 1$ (arbitrary)



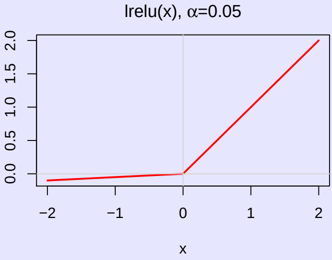
Leaky rectified linear unit (Leaky ReLU), `tf.nn.leaky_relu`

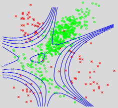
$$\text{lrelu}(x) = \max\{\alpha x, x\}$$

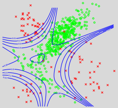
$$\text{lrelu}'(x) = \begin{cases} 1 & \text{, if } x > 0 \\ \alpha & \text{, if } x < 0 \end{cases}$$

$\text{lrelu}'(0) := 1$ (arbitrary)

$\alpha = 0.01$







Activation Functions

Vanishing gradients

- vanishing gradient problem:
  - during backprop in each layer, a derivative of the activation function is multiplied
  - for NNs with many layers (deep networks) this can result in gradients that are practically zero (“vanishing”), in particular for the sigmoid function
- ReLU
  - most frequently chosen
  - introduced in 2010

    (Nair and Hinton, “Rectified linear units improve restricted Boltzmann machines”, *Proc. ICML*, 2010)
  - The derivative is either 0 or 1. Can lead to sparse gradients.