An Introduction to Deep Learning

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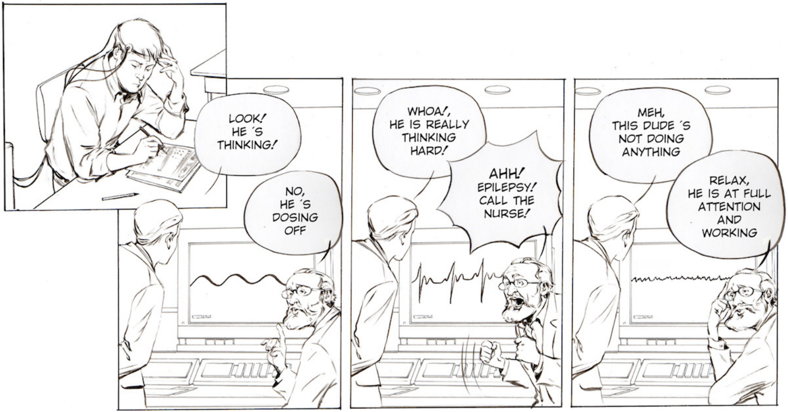
Outline

1. Introduction to feed-forward networks
2. Relation to logistic regression
3. Notes on implementation
4. Illustration using synthetic and real data

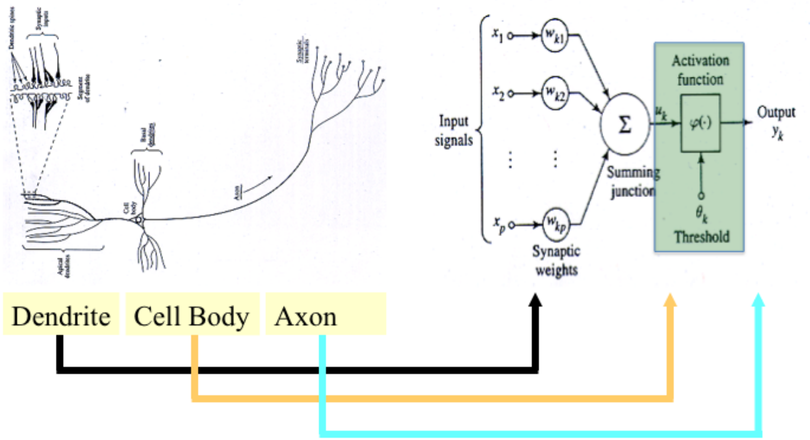
Motivation



The idea: Human intelligence may be due to a learning algorithm. We aim to build algorithms that mimic the brain.[1]

[1] image: https://backyardbrains.com/experiments/EEG

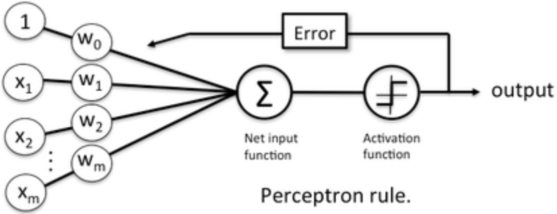
Imitate neurons in the brain: Artificial Neurons



Artificial Neuron (AN): input, weights, and output

Activation functions

The Perceptron (Rosenblatt et al. 1957 & 1962) computes a step function as an activation function.



$$\text{step}(z) = \begin{cases} 1 & z \geq t \\ 0 & z < t \end{cases}, \text{ where } t \text{ is a threshold}$$

As each input is applied to the perceptron its output is compared to the target. To keep the output closer to the target the **learning rule** adjusts the network parameters.

What can a single AN compute?

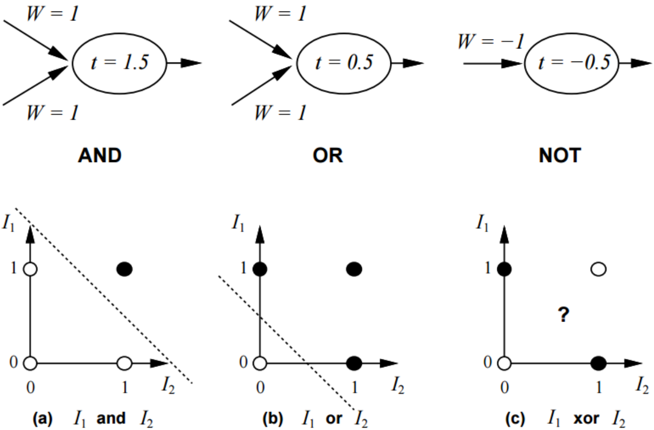
The Perceptron output is given by $y = \mathsf{step}(b + \sum_{j=1}^{p} w_j x_j)$.

Perceptron can divide the input space into two regions.

The decision boundary is given by: $b + \sum_{j=1}^{p} w_j x_j = 0$.

Perceptron can learn to classify any linearly separable set of inputs—convergence theorem (Rosenblatt 1962)

Boolean functions



Examples[2] of linearly separable and non separable problems

[2] Veloso, 2001

Learning the XOR function

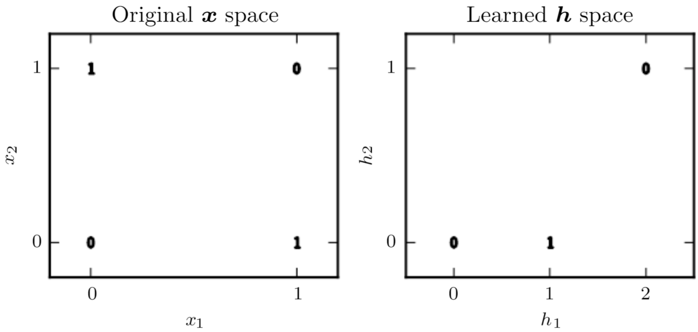
Consider this as a regression problem and use the MSE loss function:

$$\mathsf{MSE}(\theta) = \frac{1}{4} \sum_{\boldsymbol{x} \in \mathcal{X}} (y - f_\theta(\boldsymbol{x}))^2$$

where $\theta = (\boldsymbol{w}, b)$ and $f_\theta(\boldsymbol{x}) = b + \sum_{j=1}^{p} w_j x_j$—a linear model.

Using the normal equations we can minimize $\mathsf{MSE}(\theta)$ w.r.t. $\boldsymbol{w}$ and b in closed form. It gives $\boldsymbol{w} = 0$ and $b = .5$—This gives the model output $.5$ everywhere.

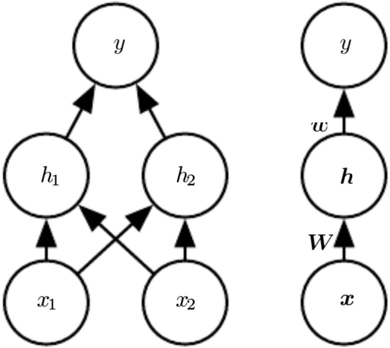
Learning the XOR function



- When $x_1 = 0$, the model's output must increase as x_2 increases
- When $x_1 = 1$, the model's output must decrease as x_2 increases
- A linear model applies a fixed coefficient w_2 to x_2. It cannot use the value of x_1 to change the coefficient w_2 on x_2 and cannot solve this problem.

Intuition behind multilayer neural network

One way to solve the XOR problem is to transform the input by introducing a feed-forward network:



The complete model will then be, in a function form:

$$f(\boldsymbol{x}; \boldsymbol{W}, \boldsymbol{w}, b, \boldsymbol{c}) = f^{(2)}\left(f^{(1)}(\boldsymbol{x}; \boldsymbol{W}, \boldsymbol{c}); \boldsymbol{w}, b\right)$$

What function should $f^{(1)}$ be?

We consider $f^{(2)}$ as a linear function.

We can write the hidden layer output as

$$\boldsymbol{h} = f^{(1)}(\boldsymbol{x}; \boldsymbol{W}, \boldsymbol{c}) = g(\boldsymbol{W}^{\mathsf{T}}\boldsymbol{x} + \boldsymbol{c})$$

What function should $f^{(1)}$ be?

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$$\boldsymbol{h} = f^{(1)}(\boldsymbol{x}; \boldsymbol{W}, \boldsymbol{c}) = g(\boldsymbol{W}^{\mathsf{T}}\boldsymbol{x} + \boldsymbol{c})$$

If $f^{(1)}$ is also linear, then the network as a whole would remain a linear function of its input.

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We can write the hidden layer output as

$$\boldsymbol{h} = f^{(1)}(\boldsymbol{x}; \boldsymbol{W}, \boldsymbol{c}) = g(\boldsymbol{W}^{\mathsf{T}}\boldsymbol{x} + \boldsymbol{c})$$

So we must use a nonlinear activation function for g. A popular nonlinear activation function g is rectified linear unit (ReLU)

$$g(z) = \mathsf{max}\{0, z\}$$

A feed-forward network solution to XOR

We wish the network to perform well on the four cases

$$\boldsymbol{X} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix}, \boldsymbol{y} = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}$$

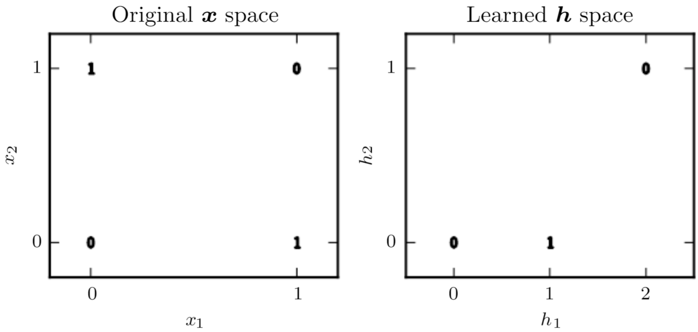
We can specify a two-layer network solution to XOR as

$$\boldsymbol{W} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \boldsymbol{c} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}, \boldsymbol{w} = \begin{bmatrix} 1 \\ -2 \end{bmatrix}, b = 0$$

The complete network is given by

$$f(\boldsymbol{x}; \boldsymbol{W}, \boldsymbol{w}, b, \boldsymbol{c}) = \boldsymbol{w}^{\mathsf{T}} \max\{0, \boldsymbol{W}^{\mathsf{T}} \boldsymbol{x} + \boldsymbol{c}\} + b$$

A feed-forward network solution to XOR



In the proposed network, the nonlinear hidden layer has mapped both $\boldsymbol{x} = [1, 0]$ and $\boldsymbol{x} = [0, 1]$ to a single point in feature space, $\boldsymbol{h} = [1, 0]$.

A linear model can now describe the function as increasing in h_1 and decreasing in h_2.

Activation functions

Modern ANs use a variety of activation functions that are smoother than the step function.

Linear - no input squashing

$$y = x$$

Logistic sigmoid - squash input into $[0, 1]$

$$y = \mathsf{sigmoid}(x) = \frac{1}{1 + \exp(-x)}$$

Hyperbolic tangent - squash input into $[-1, 1]$

$$y = \mathsf{tan}(x) = \frac{\exp(x) - \exp(-x)}{\exp(x) + \exp(-x)}$$

Rectified linear unit

$$y = \mathsf{max}\{0, x\}$$

Relation to logistic regression

Let $p(y = 1 \mid X = \boldsymbol{x}) = p(\boldsymbol{x}; \boldsymbol{w})$ be the conditional probability that a particular sample belongs to class 1 given its predictors $\boldsymbol{x}$. We write the logistic regression model as

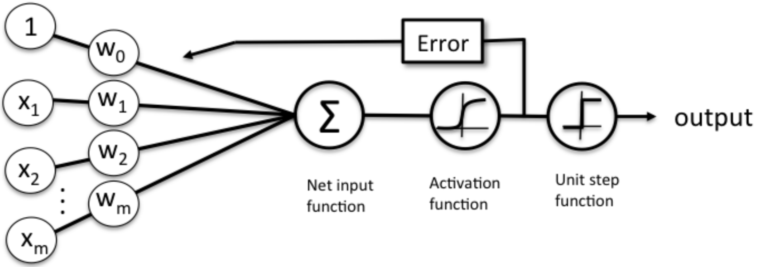
$$\text{logit}\left(p(\boldsymbol{x}; \boldsymbol{w})\right) = w_0 + \boldsymbol{w}^{\mathsf{T}}\boldsymbol{x}$$

Solving for $p(\boldsymbol{x}; \boldsymbol{w})$ gives

$$p(\boldsymbol{x}; \boldsymbol{w}) = \text{sigmoid}\left(w_0 + \boldsymbol{w}^{\mathsf{T}}\boldsymbol{x}\right)$$

To minimize misclassification rate, one should predict $y = 1$ when $p \geq .5$, and vice versa.—i.e. guess 1 whenever $w_0 + \boldsymbol{w}^{\mathsf{T}}\boldsymbol{x} \geq 0$ and 0 otherwise. So logistic regression gives a linear classifier.

Relation to logistic regression



Schematic of a logistic regression classifier. [3]

Learning parameters $\boldsymbol{w}$ and b: maximum likelihood estimation

- Perceptron algorithm: online and error-driven.
- Logistic regression: batch algorithms—e.g. gradient descent, limited-memory BFGS, or online algorithms—stochastic gradient descent.

[3] http://rasbt.github.io/mlxtend/user_guide/classifier/LogisticRegression/

Gradient-based learning

The nonlinearity of a neural network causes most interesting loss functions to become non-convex

- Optimization procedure – using iterative, gradient-based optimizers that drive the cost function to a very low value
- Cost function, $C(\theta)$ – they are more or less the same as those for other parametric models, such as linear models

Cost function

We define the loss functional $\mathcal{L}(f_\theta, z)$ based on the network, e.g., squared error, the negative conditional log-likelihood. Here, $z = (x, y)$ and $f_\theta(x)$ is the predictive function for y given θ.

We define the cost function as

$$C(\theta) = \int \mathcal{L}(f_\theta, z) P(z) dz$$

We typically write this as an average—*training loss*

$$C(\theta) = \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}(f_\theta, z)$$

Gradient descent (GD) algorithm[4]

We find a θ that minimizes the cost

- By solving $\frac{\partial C(\theta)}{\partial \theta} = 0$ we can find the minima, maxima, and saddle points.
- In general, we cannot find the solutions of this equation. So we seek numerical optimization methods
- *local descent*: iteratively modify θ so as to decrease $C(\theta)$, until we reach a local minima

$$\theta^{(t+1)} = \theta^{(t)} - \epsilon \frac{\partial C(\theta^{(t)})}{\partial \theta^{(t)}},$$

ϵ is the learning rate

[4] http://www.iro.umontreal.ca/~pift6266/H10/notes/gradient.html

Stochastic gradient descent (SGD) algorithm

- We use the fact that $C(\theta)$ is an average over i.i.d. samples
- Make updates much often

$$\theta^{(t+1)} = \theta^{(t)} - \epsilon \frac{\partial \mathcal{L}(\theta^{(t)}, z)}{\partial \theta^{(t)}},$$

  z is an the next sample from the training set.—It can be implemented online
- The update direction is a random variable whose expectation is the true gradient of interest.

Output units

The output layer provides additional transformation from the hidden features $\boldsymbol{h}$ to complete the network's indented task.

Linear units for Gaussian output distributions: the output units based on an affine transformation with no nonlinearity

- Given hidden features $\boldsymbol{h}$, we define outputs $f_\theta(\boldsymbol{x}) = \boldsymbol{w}^\mathsf{T}\boldsymbol{h} + b$
- It's typically used to produce the mean of a conditional Gaussian distribution $p(y|\boldsymbol{x}, \theta) = \mathcal{N}(f_\theta(\boldsymbol{x}), \mathsf{I})$

Cost function: the negative log-likelihood

The neural network defines a conditional distribution $p(y \mid \boldsymbol{x}, \theta)$.

Suppose we use MLE for parameter estimation. Then, it's natural to use the cost function as the negative log-likelihood:

$$C(\theta) = -\mathsf{E}_{\boldsymbol{x},y} \log p_{\mathsf{model}}(y|\boldsymbol{x}, \theta)$$

Example

if $p_{\mathsf{model}}(y|\boldsymbol{x}, \theta) = \mathcal{N}(f_\theta(\boldsymbol{x}), \mathsf{I})$, then we have

$$C(\theta) = \frac{1}{2} \mathsf{E}_{\boldsymbol{x},y} \|y - f_\theta(\boldsymbol{x})\|^2 + \text{const.}$$

Output units

Sigmoid units for Bernoulli output distributions: e.g. a binary classification problem

Given hidden features $\boldsymbol{h}$, we define the output as

$$\mu = \text{sigmoid}(\eta) = \text{sigmoid}\left(\boldsymbol{w}^{\mathsf{T}}\boldsymbol{h} + b\right)$$

Bernoulli distribution and logistic sigmoid

For a Bernoulli distribution with $y \in \{0, 1\}$ that represents either success of failure, and $0 \leq \mu \leq 1$ representing the probability of success, we have

$$
\begin{aligned}
p(y \mid \mu) &= \mu^y (1-\mu)^{(1-y)} && (1) \\
&= \exp\{y \log \mu + (1-y) \log(1-\mu)\} && (2) \\
&= \exp\left\{y \log \frac{\mu}{1-\mu} + \log(1-\mu)\right\} && (3)
\end{aligned}
$$

Comparing this expression with the density of an exponential family distribution $p(y \mid \eta) = h(x) \exp\{\eta \, \mathsf{T}(y) - \mathsf{A}(\eta)\}$,

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Comparing this expression with the density of an exponential family distribution $p(y \mid \eta) = h(x) \exp\{\eta \, \mathsf{T}(y) - \mathsf{A}(\eta)\}$, where η is the natural parameter, $\mathsf{T}(y)$ is the sufficient statistic, $\mathsf{A}(\eta)$ is the log partition function, and $h(x)$ is a normalizing constant,

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\end{aligned}
$$

Comparing this expression with the density of an exponential family distribution $p(y \,|\, \eta) = h(x) \exp\{\eta \, \mathsf{T}(y) - \mathsf{A}(\eta)\}$, we have

$$
\begin{aligned}
\eta &= \log \frac{\mu}{1-\mu} - \text{log odds} & (4)\\
\to \mu &= \text{sigmoid}(\eta) & (5)
\end{aligned}
$$

Parameter estimation via MLE

We assume we have a training set $\mathcal{X} = (\boldsymbol{x}_i, y_i), i = 1, 2, \ldots, n$. Our goal is to maximize the log likelihood:

$$\log p(\mathcal{X} \mid \theta) = \sum_{i=1}^{n} \log p(\boldsymbol{x}_i, y_i \mid \theta).$$

We factor the log likelihood into an unconditional term $p(\boldsymbol{x})$ that we ignore and a conditional term $p(y \mid \boldsymbol{x})$ that we focus.

Let $z_i = \mathsf{I}(y_i == 1)$ and $\mu_i = p(y_i = 1 \mid \boldsymbol{x}_i)$—a logistic linear function of $\boldsymbol{x}_i$ for a single layer network. We can write the conditional density of the dataset as

$$\mathcal{L} = \prod_{i=1}^{n} \mu_i^{z_i} (1 - \mu_i)^{1 - z_i}$$

Parameter estimation via MLE

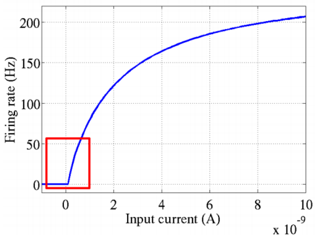
We wish to maximize the log likelihood:

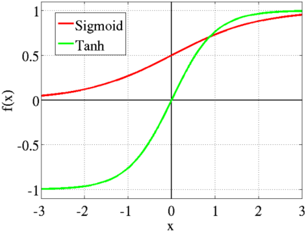
$$\log \mathcal{L} = \sum_{i=1}^{n} z_i \log \mu_i + (1 - z_i) \log (1 - \mu_i)$$

The negative of this log likelihood is a *cross entropy* between the indicator variables z and the posterior probabilities μ.

This also shows that the cross entropy is a natural cost function for binary classification problem (Jordan 1995)

Hidden units: sigmoid and hyperbolic tangent[5]

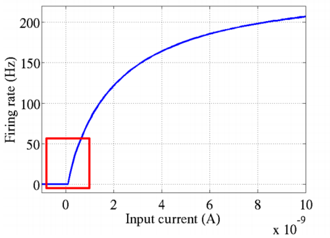


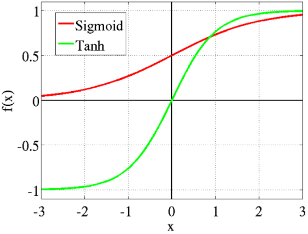


Common neural activation function motivated by biological data (left) and sigmoid and hyperbolic tangent (right).

[5] Glorot (2011)

Hidden units: sigmoid and hyperbolic tangent[5]

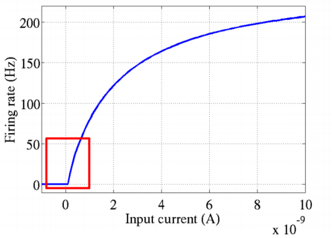


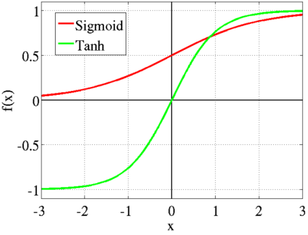


During training sigmoidal units saturate across most of their domain—they saturate to a high value when z is very positive and vice versa. It can make gradient-based learning very difficult.

[5] Glorot (2011)

Hidden units: sigmoid and hyperbolic tangent[5]





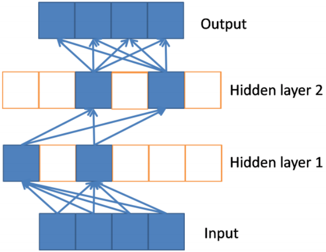
The hyperbolic tangent has a steady state at 0, hence is preferred from the optimization standpoint. It forces an antisymmetry around 0 which is absent in biological neurons.

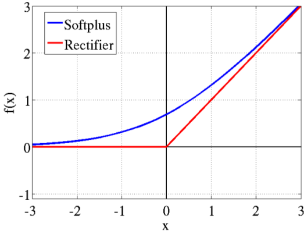
[5] Glorot (2011)

Hidden units: ReLU

A popular choice of activation function for hidden units[6]

$$g(z) = \max\{0, z\}$$





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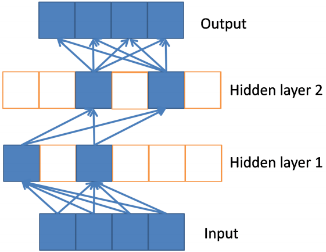

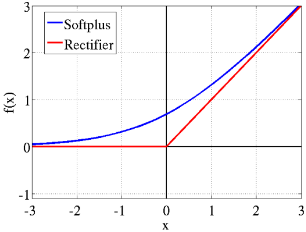

One can safely disregard nonlinearity (Goodfellow et al. 2016): "... neural network training algorithms do not usually arrive at a local minimum of the cost function, but instead merely reduce its value significantly"

[6] Glorot (2011)

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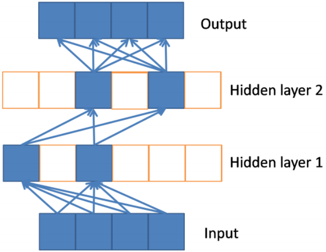

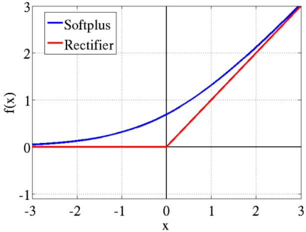

Non-linearity in the network comes from the path selection associated with individual neurons being active or not. Once the subset of neurons is selected, the output is a linear function of the input.

[6] Glorot (2011)

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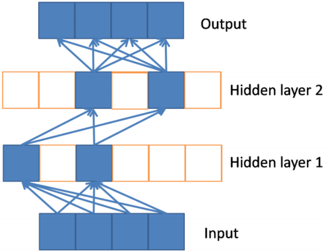

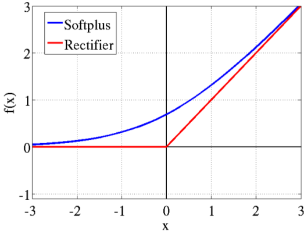

ReLU allows a network to easily obtain sparse representations.

[6] Glorot (2011)

An overview of back-propagation algorithm

Computing an analytical expression for the gradient is straightforward, but numerical evaluation of such an expression can be expensive over the network.—**backprop** gives an inexpensive procedure to evaluate this gradient.

backprop uses the chain rule of calculus: Suppose $\boldsymbol{x} \in \mathbb{R}^m, \boldsymbol{y} \in \mathbb{R}^n$, $g : \mathbb{R}^m \to \mathbb{R}^n, f : \mathbb{R}^n \to \mathbb{R}$. If $\boldsymbol{y} = g(\boldsymbol{x}), z = g(\boldsymbol{y})$, then

$$\frac{\partial z}{\partial x_i} = \sum_j \frac{\partial z}{\partial y_j} . \frac{\partial y_j}{\partial x_i}$$

We can generalize this procedure to vectors and tensors in a multilayer neural network.

Notes on architectural considerations

In practice, the overall structure of the network is important: how many units it should have and how these units should be connected to each other.

Alternatives to feed-forward networks

- Convolutional Neural Networks — imitates human memory
- Auto Encoders — unsupervised learning and dimensionality reduction

Hands on experiments

Datasets

- A synthetic spiral dataset with multiple classes
- The MNIST data set with 0-9 handwritten characters

Algorithm: A basic back-propagation algorithm implementation with one hidden layer

Link to R scripts: `http://bit.ly/deep-learning-stats`

Links to serious implementations

Deep learning frameworks, which uses CPU and GPU

- TensorFlow with R
  `https://rstudio.github.io/tensorflow/index.html`
- Theano with python
  `http://deeplearning.net/software/theano`

Available R packages

- neuralnet
- deepnet
- h2o

Questions?