INFO 6105
Data Science Engineering Methods and Tools

Lecture 5
Neural Networks

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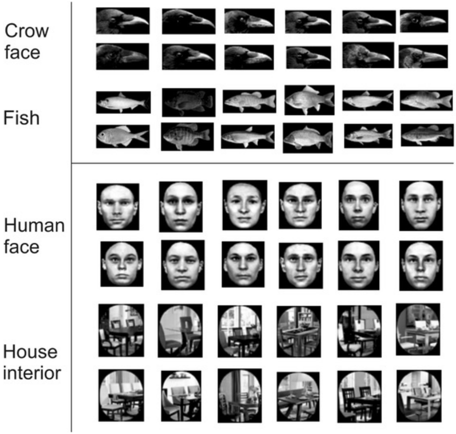
Human Face Detection

Face detection: detect whether a digital image is a human face.



[Source: https://doi.org/10.1007/s00359-017-1211-7]

Human Face Detection

Note that

- images are 567×541 pixels
- each image can be represented as a vector of pixel values

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We can represent the images as

$$(\vec{x}_1, y_1), (\vec{x}_2, y_2), \ldots, (\vec{x}_n, y_n)$$

where $\vec{x}_i \in \mathbb{R}^{306,747}$ and $y_i \in \{0, 1\}$ for i^{th} images with

$$x_{ij} = \text{the value of color in pixel } j \text{ in image } i$$

$$y_i = \begin{cases} 0 & \text{if it is a non-human face} \\ 1 & \text{otherwise} \end{cases}$$

The face detection is a classification problem.

Logistic Regression

Modeling Choice: We choose

$$P(\text{the image is a human fcae given } \vec{x}) = \frac{1}{1+e^{-\vec{\beta}^T\vec{x}}}$$
$$P(y=1|X) = \frac{1}{1+e^{-\beta^T\vec{x}}}$$

where $f(z) = \frac{1}{1+e^{-z}}$ is the *logistic function* and $\vec{\beta}^T = (\beta_0, \beta_1, \ldots, \beta_m)$ are the *model parameters*.

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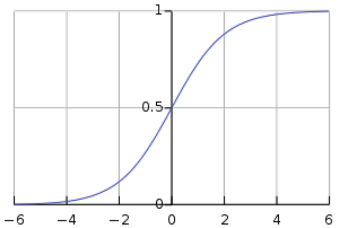
Properties:

- $0 \leq f(z) \leq 1$
- $f(0) = 0.5$
- $f(z) \longrightarrow 1$ as $z \longrightarrow \infty$
- $f(z) \longrightarrow 0$ as $z \longrightarrow -\infty$



How to determine the model parameters?

- Find the model parameters $\vec{\beta}$ such that the predicted probability

$$h_\beta(\vec{x}_i) = P(y_i | \vec{x}_i; \beta)$$

  - is close to one if $y_i = 1$
  - is close to zero if $y_i = 0$

Maximum Likelihood

Note that

$$p(y_i|\vec{x}_i;\beta) = h_\beta(\vec{x}_i)^{y_i} \cdot (1 - h_\beta(\vec{x}_i))^{1-y_i}$$
$$= \begin{cases} h_\beta(\vec{x}_i) & \text{if } y_i = 1 \\ 1 - h_\beta(\vec{x}_i) & \text{if } y_i = 0 \end{cases}$$

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$$

Assuming the data is generated independently, the probability of the observing $y_1, \ldots, y_n$ is given by

$$
\begin{aligned}
L(\beta) = P(Y|\vec{x};\beta) &= \prod_{i=1}^{m} P(y_i|\vec{x}_i;\beta) \\
&= \prod_{i:y_i=1} h_\beta(X_i) \cdot \prod_{i:y_i=0} (1 - h_\beta(\vec{x}_i))
\end{aligned}
$$

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Choose β so as to maximize $L(\beta)$ or equivalently minimize $-\log L(\beta)$.

Maximum Likelihood

Choose β so as to maximize $L(\beta)$ or equivalently minimize $-\frac{1}{n}\log L(\beta)$.

$$\mathcal{L}(\vec{\beta}) := -\frac{1}{n}\log L(\beta) = -\frac{1}{n}\sum_i \left[y_i \log(h_\beta(x_i)) + (1-y_i)\log(1-h_\beta(x_i))\right]$$

where $h_\beta(x_i) = \frac{1}{1+e^{-\beta^T \vec{x}_i}}$.
This does not have an explicit solution, we need to minimize numerically!

Batch Gradient Descent

Start with some initial β and repeatedly take a step in the direction of steepest decrease of $-\log L(\beta)$:

$$\beta_j = \beta_j - \eta \frac{\partial}{\partial \beta_j} \mathcal{L}(\vec{\beta})$$

η is called *learning rate*.

Batch Gradient Descent

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$$\beta_j = \beta_j - \eta \frac{\partial}{\partial \beta_j} \mathcal{L}(\vec{\beta})$$

η is called *learning rate*.

Update Rule: For training examples $(\vec{x}_1, y_1), \ldots, (\vec{x}_n, y_n)$:

$$\beta_j = \beta_j - \frac{\eta}{n} \sum_{i=0}^{n} (h_\beta(\vec{x}_i) - y_i) x_{ij} \qquad\qquad j = 0, 1, \ldots, m$$

Note: The magnitude of the update is proportional to the error term

Stochastic Gradient Descent

In practice, n can be very large and hence the batch gradient descent can be costly.

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An alternative approach is to scan the training data one by one and update the parameters with respect to a single training example. For a single training example (x, y), the update rule is

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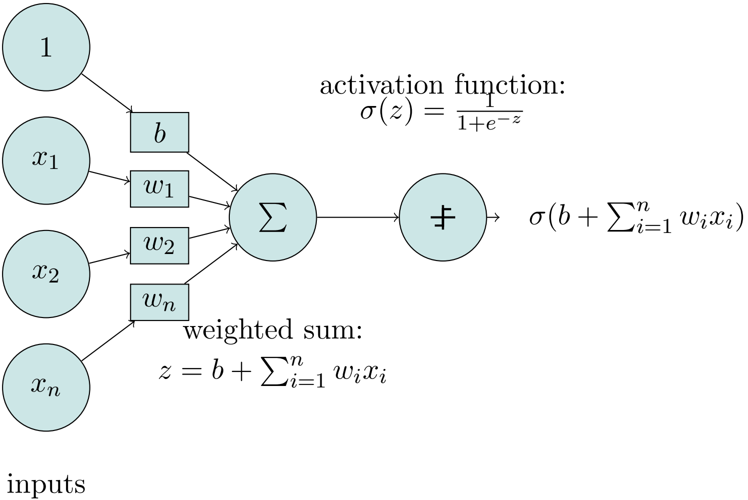
$$\beta_j = \beta_j - \frac{\eta}{n}(h_\beta(\vec{x}) - y_i)x_j \qquad j = 0, 1, \ldots, m$$

For $i = 1, \ldots, m$, update β

$$\beta_j = \beta_j - \frac{\eta}{n}(h_\beta(\vec{x}_i) - y_i)x_{ij} \qquad j = 0, 1, \ldots, m$$

Often, this approach gets β close to the optimal value much faster than batch gradient descent, in particular when the training dataset is large.

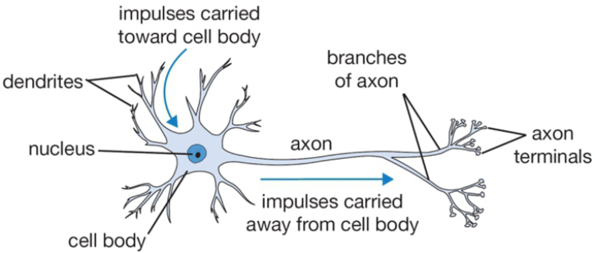
Logistic regression as a Neural Network



The reasoning for this notational difference is conform with standard neural network notation.

Inspiration: The Brain

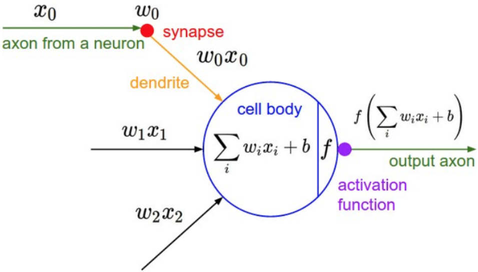
- Neural networks are inspired by biology, e.g., the (human) brain
- Our brain has approximately 86 billion neurons, each of which communicates (is connected) to about $10,000$ other neurons
- The basic computational unit of the brain is called neuron



A cartoon drawing of a biological neuron
[Source: http://cs231n.github.io/neural-networks-1/]

Mathematical Model of a Neuron

- Artificial neurons are called units



A mathematical model of the neuron in a neural network
[Source: http://cs231n.github.io/neural-networks-1/]

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Face Detection

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- A more complex neural network is required:
  - take the single neuron described above and "stack" them together such that one neuron passes its output as input into the next neuron, resulting in a more complex function.
  - take a composition of many different functions

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  - right eye
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- These features can be formulated as functions of the image features.

Face Detection

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- Given the image features, we might decide that the problem of face detection depends on whether the image has
  - left eye
  - right eye
  - nose
  - mouth
- These features can be formulated as functions of the image features.
- Given these four derived features, we may conclude that the face detection depends on these four features.

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Neural Networks

- We have described this neural network as if we already have the insight to determine these four factors (left eye, right eye, nose, mouth) ultimately affect the decision.
- Part of the magic of a neural network is that all we need are the input features x and the output y while the neural network will figure out everything in the middle by itself.

Neural Network Formulation

Suppose we have

- four input features x_1, x_2, x_3, x_4 which are collectively called the input layer,
- five hidden units which are collectively called the hidden layer
- one output unit called the output layer

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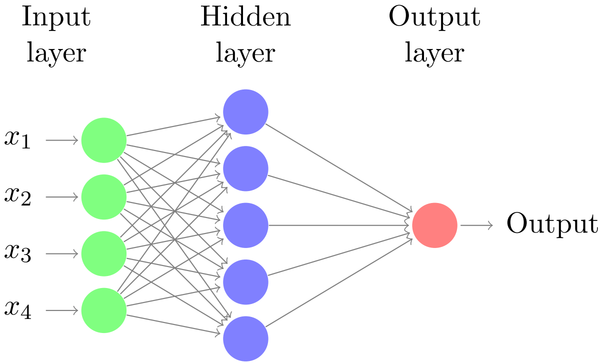
Notes:

- The term hidden layer is called "hidden" because we do not have the ground truth/training value for the hidden units.
- This is in contrast to the input and output layers, both of which we know the ground truth values from $(\vec{x}_i, y_i)$.

Neural Network Architecture

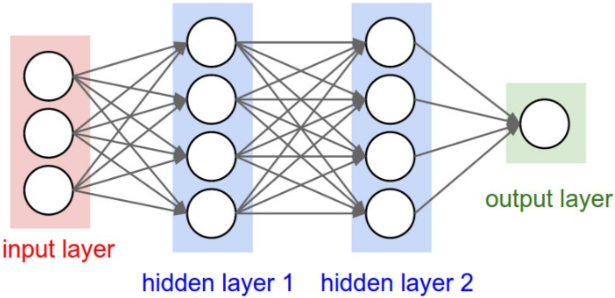
A neural network with one layer of five hidden units:



- Each unit computes its value based on linear combination of values of units that point into it, and an activation function
- a 2-layer neural network (One layer of hidden units, One output layer)

Multi-Layer Neural Network

A 3-layer neural net with 3 input units, 4 hidden units in the first and second hidden layer and 1 output unit



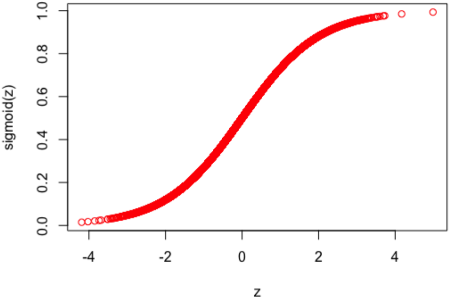
source: http://cs231n.github.io/neural-networks-1/

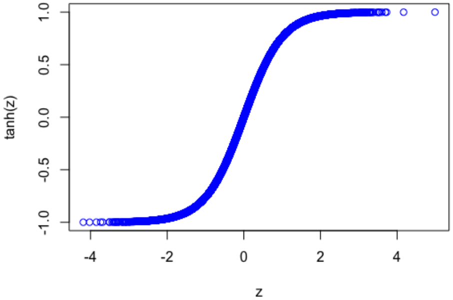
- A N-layer neural network has
  - N -1 layers of hidden units and
  - One output layer

Activation Functions

Most commonly used activation functions:

- Sigmoid: $\sigma(z) = \frac{1}{1+\exp(-z)}$
- Tanh: $\tanh(z) = \frac{\exp(z)-\exp(-z)}{\exp(-z)+\exp(-z)}$
- ReLU (Rectified Linear Unit): $\mathrm{ReLU}(z) = \max(0, z)$



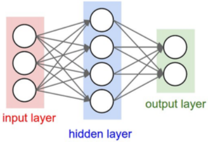


Neural Network Training

We only need to know two algorithms

- Forward pass: calculate the model output
- Backward pass: update the model parameters

Forward pass



Output of the network can be written as:

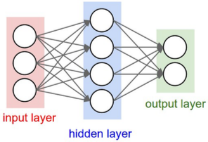
- Hidden layer:

$$h_j(x) = f(b_j^{[1]} + \sum_{i=1}^{D} x_i w_{ji}^{[1]})$$

- Output layer:

$$o_k(x) = g(b_k^{[2]} + \sum_{j=1}^{J} h_j(x) w_{kj}^{[2]})$$

Forward pass



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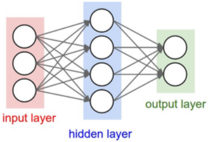
where

- j indexing hidden units, k indexing the output units, D number of inputs
- Activation functions f , g are sigmoid/logistic, tanh, or rectified linear (ReLU)

Forward pass

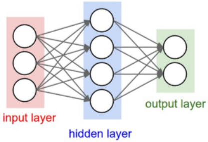


- Computation for the first hidden unit in the first hidden layer:

$$z_1^{[1]} = W_1^{[1]} x + b_1^{[1]} \text{ and } a_1^{[1]} = f(z_1^{[1]})$$

  - $W \in \mathbb{R}^{3\times 4}$ is a matrix of parameters and W_1 refers to the first row of this matrix.
  - The parameters associated with the first hidden unit is the vector $W^{[1]} \in \mathbb{R}^3$ and the scalar $b^{[1]} \in \mathbb{R}$.

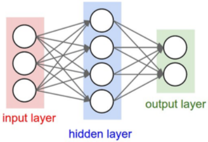
Forward pass



- Computation for the second, third, forth hidden units in the first hidden layer:

$$z_2^{[1]} = W_2^{[1]} x + b_2^{[1]} \text{ and } a_2^{[1]} = f(z_2^{[1]})$$
$$z_3^{[1]} = W_3^{[1]} x + b_3^{[1]} \text{ and } a_3^{[1]} = f(z_3^{[1]})$$
$$z_4^{[1]} = W_4^{[1]} x + b_4^{[1]} \text{ and } a_4^{[1]} = f(z_4^{[1]})$$

Forward pass



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$$z_4^{[1]} = W_4^{[1]}x + b_4^{[1]} \text{ and } a_4^{[1]} = f(z_4^{[1]})$$

- Computation for the output layer:

$$z_1^{[2]} = W_1^{[2]}a^{[1]} + b_1^{[2]} \text{ and } a_1^{[2]} = g(z_1^{[2]})$$
$$z_2^{[2]} = W_2^{[2]}a^{[1]} + b_2^{[2]} \text{ and } a_2^{[2]} = g(z_2^{[2]})$$

where $a^{[1]}$ is defined as the concatenation of all first layer

Forward pass

Forward pass can be implemented efficiently using matrix operations in Python:

$$\underbrace{\begin{bmatrix} z_1^{[1]} \\ \vdots \\ \vdots \\ z_4^{[1]} \end{bmatrix}}_{z^{[1]} \in \mathbb{R}^{4\times 1}} = \underbrace{\begin{bmatrix} - & W_1^{[1]^T} & - \\ - & W_2^{[1]^T} & - \\ & \vdots & \\ - & W_4^{[1]^T} & - \end{bmatrix}}_{W^{[1]} \in \mathbb{R}^{4\times 3}} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}}_{x \in \mathbb{R}^{3\times 1}} + \underbrace{\begin{bmatrix} b_1^{[1]} \\ b_2^{[1]} \\ \vdots \\ b_4^{[1]} \end{bmatrix}}_{b^{[1]} \in \mathbb{R}^{4\times 1}}$$

[source: cs229.stanford.edu/notes/cs229-notes-deep_learning.pdf]

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  where o_i is the output given $\vec{x}_i$.
- Gradient descent:

$$W^{t+1} = W^t - \eta \frac{\partial J}{\partial W^t}$$

  where η is the learning rate and J is the loss function

Useful Derivatives

name	function	derivative
Sigmoid	$\sigma(z) = \frac{1}{1+\exp(-z)}$	$\sigma(z) \cdot (1 - \sigma(z))$
Tanh	$\tanh(z) = \frac{\exp(z)-\exp(-z)}{\exp(z)+\exp(-z)}$	$1/\cosh^2(z)$
ReLU	$\mathrm{ReLU}(z) = \max(0, z)$	$\begin{cases} 1, & \text{if } z > 0 \\ 0, & \text{if } z \leq 0 \end{cases}$

Training Neural Networks

- Back-propagation: an efficient method for computing gradients needed to perform gradient-based optimization of the weights in a multi-layer network

Loop until convergence:

- For each example $(\vec{x}_i, y_i)$
  1. Forward pass: Given input $\vec{x}_i$, propagate activity forward $(x_i \rightarrow \mathrm{a}_i^{[1]} \rightarrow o_i)$
  2. Backward pass: Propagate gradients backward
  3. Update each weight via gradient descent