Sistemas Inteligentes

Logistic Regression and Neural Networks

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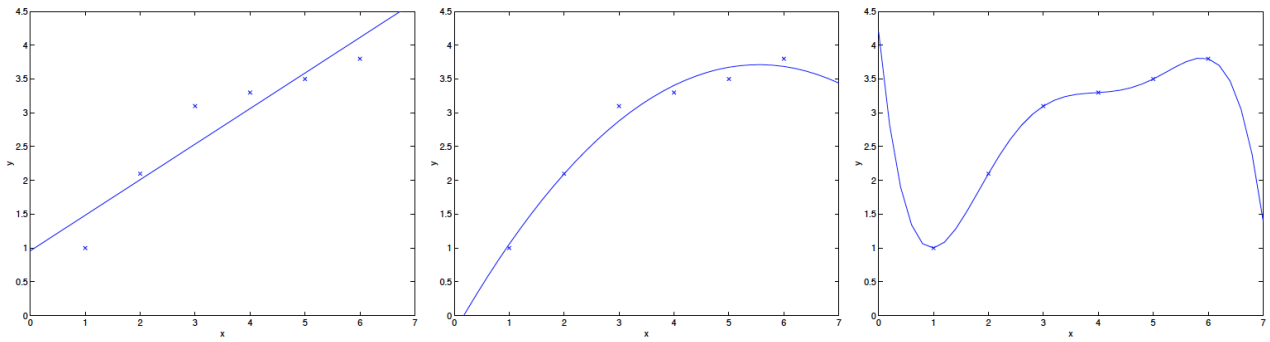
Overfitting

Consider the problem of predicting y from $x \in \mathbb{R}$



- 1) $y = \theta_0 + \theta_1 x$
- 2) $y = \theta_0 + \theta_1 x + \theta_2 x^2$
- 3) $y = \sum_{j=0}^{5} \theta_j x^j$

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- We would not expect this to be a very good predictor of, housing prices (y) for different living areas (x)

Logistic Regression

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- spam classifier: $x^{(i)}$ may be some features of a piece of email, y may be 1 if it is a piece of spam mail, and 0 otherwise
- Given $x^{(i)}$, the corresponding $y^{(i)}$ is also called the label for the training example.

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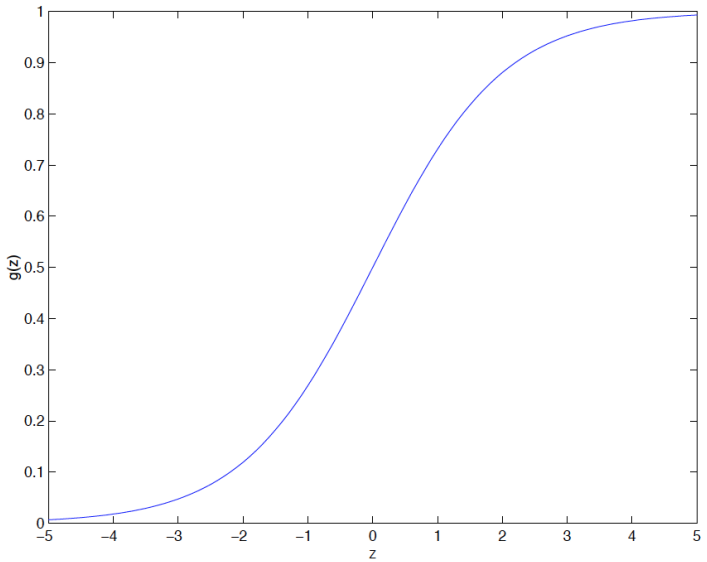
- Thus, the hypotheses $h_\theta(x)$ change:

$$h_\theta(x) = g(\theta^T x) = \frac{1}{1 + e^{-\theta^T x}}$$

- where g is called the logistic or the sigmoid function

$$g(z) = \frac{1}{1 + e^{-z}}$$

Sigmoid Function



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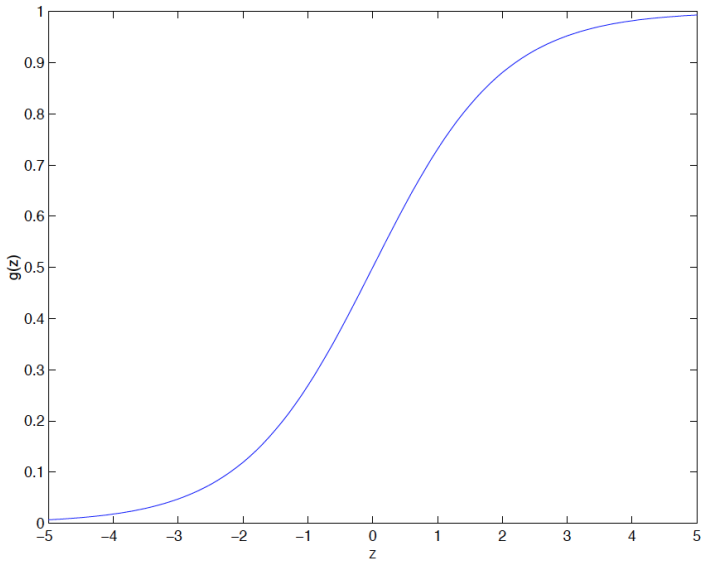

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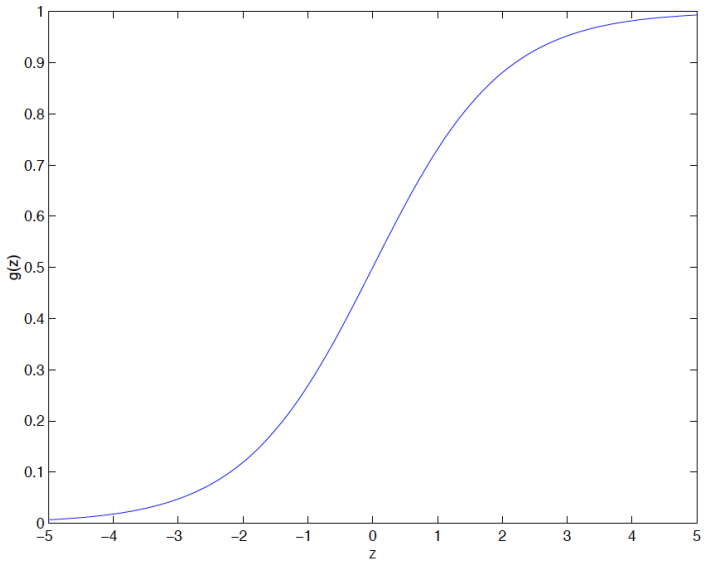

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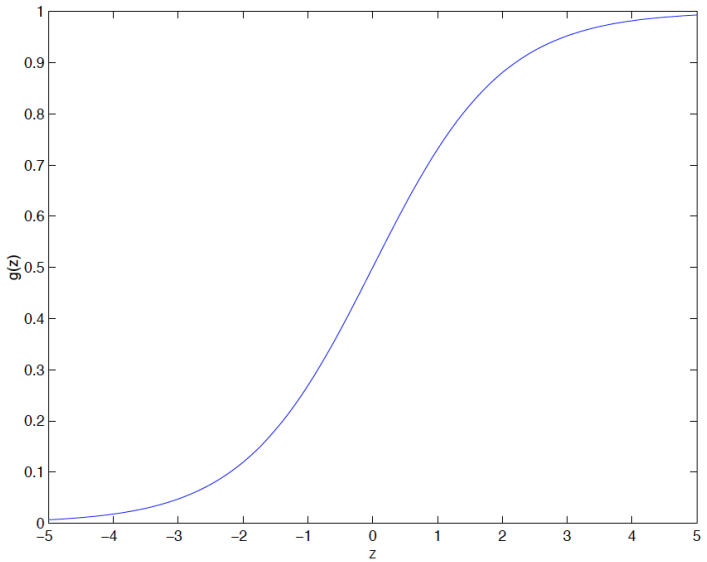

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- $g(z)$ tends towards 0 as $z \to -\infty$
- $g(z)$, and hence $h(x)$, is always bounded between 0 and 1
- $x_0 = 1$, and $\theta^T x = \theta_0 + \sum_{j=1}^{n} \theta_j x_j$

Derivative of the Sigmoid Function

$$
\begin{aligned}
g'(z) &= \frac{d}{dz}\frac{1}{1+e^{-z}} \\
&= \frac{1}{(1+e^{-z})^2}\left(e^{-z}\right) \\
&= \frac{1}{(1+e^{-z})}\cdot\left(1-\frac{1}{(1+e^{-z})}\right) \\
&= g(z)(1-g(z)).
\end{aligned}
$$

Likelihood

Let us assume that

$$p(y = 1|x; \theta) = h_\theta(x)$$

$$p(y = 0|x; \theta) = 1 - h_\theta(x)$$

this can be written more compactly as

$$p(y|x; \theta) = (h_\theta(x))^y (1 - h_\theta(x))^{1-y}$$

Likelihood II

Assuming that the m training examples were generated independently, the likelihood of the parameters is

$$\begin{aligned} L(\theta) &= p(\vec{y}|X;\theta) \\ &= \prod_{i=1}^{m} p(y^{(i)}|x^{(i)};\theta) \\ &= \prod_{i=1}^{m} (h_\theta(x^{(i)}))^{(y(i))}(1-h_\theta(x^{(i)}))^{1-y^{(i)}} \end{aligned}$$

It will be easier to maximize the log likelihood:

$$\begin{aligned} l(\theta) &= \log L(\theta) \\ &= \sum_{i=1}^{m} y^{(i)} \log h(x^{(i)}) + (1-y^{(i)}) \log(1-h(x^{(i)})) \end{aligned}$$

Gradient Ascent

To maximize the likelihood, we can use gradient ascent

$$\theta := \theta + \alpha \nabla_\theta l(\theta)$$

Consider on training example (x, y) and take derivatives to derive stochastic gradient ascent rule:

$$\begin{aligned}
\frac{\partial}{\partial(\theta)} l(\theta) &= \left(y \frac{1}{g(\theta^T x)} - (1-y) \frac{1}{1-g(\theta^T x)} \right) \frac{\partial}{\partial \theta_j} g(\theta^T x) \\
&= \left(y \frac{1}{g(\theta^T x)} - (1-y) \frac{1}{1-g(\theta^T x)} \right) g(\theta^T x)(1 - g(\theta^T x)) \frac{\partial}{\partial \theta_j} \theta^T x \\
&= \left(y(1 - g(\theta^T x)) - (1-y) g(\theta^T x) \right) x_j \\
&= (y - h_\theta(x)) x_j
\end{aligned}$$

Gradient Ascent II

We used the fact that $g'(z) = g(z)(1 - g(z))$, this gives us the stochastic gradient ascent rule

$$\theta_j := \theta_j + \alpha(y^{(i)} - h_\theta(x^{(i)}))x_j^{(i)}$$

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- If we compare to the LMS update rule, it looks identical
- but $h_\theta(x^{(i)})$ is defined as a non-linear function of $\theta^T x^{(i)}$

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- We wish to decide if k should be $0, 1, \ldots$ or 10
- How can we automatically select a model with a good bias and variance tradeoff?
- Assume we have a set of models $M = \{M_1, \ldots, M_d\}$ that we are trying to select among.

First Attempt

Given a training set S

- Train each model M_i on S, to get some hypothesis h_i

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- This algorithm does not work, why?

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- Train each model M_i on S_{train} only, to get some hypothesis h_i
- Select and output the hypothesis h_i that had the smallest error $\hat{E}_{S_{CV}}(h_i)$ on the hold out cross validation set.

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  For $j = 1, \ldots, k$
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  - Test the hypothesis h_{ij} on S_j, to get $\hat{E}_{S_{cv}}(h_{ij})$

  The estimated generalization error of the model M_i is then calculated as the average of the $\hat{E}_{S_{cv}}(h_{ij})$'s

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- Pick the model M_i with the lowest estimated generalization error, and retrain that model on the entire training set S. The resulting hypothesis is the output as our final answer.

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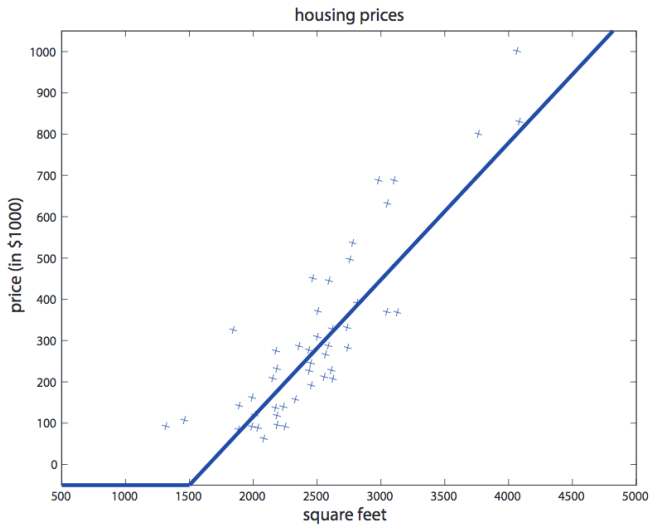
- This method is called leave-one-out cross validation

Neural Networks

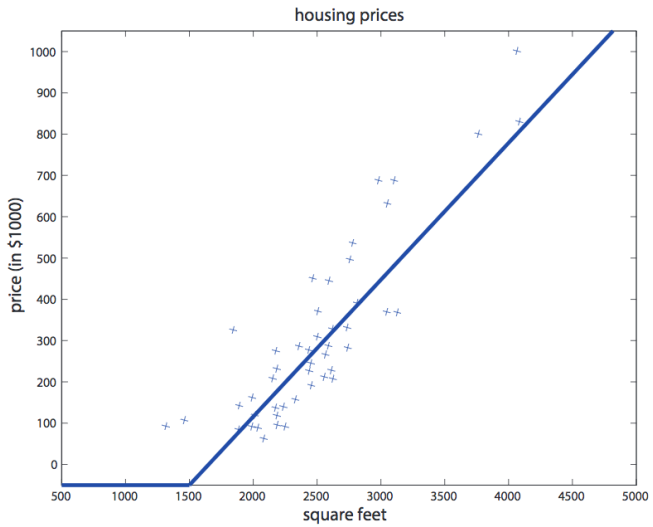
Neural Networks Example

- Recall the housing price prediction problem



Neural Networks Example

- Recall the housing price prediction problem
- We wish to prevent negative housing prices by setting the absolute minimum price as zero:



ReLU Function

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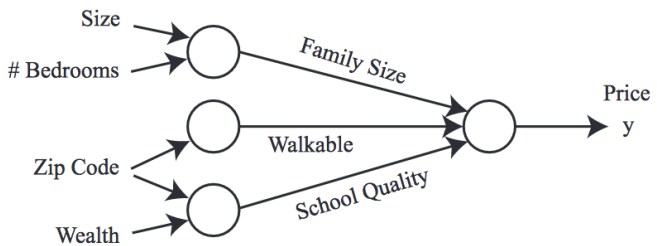
- That results in a more complex function

Housing Prediction Revisited

- features: number of bedrooms, zip code, wealth of the neighborhood



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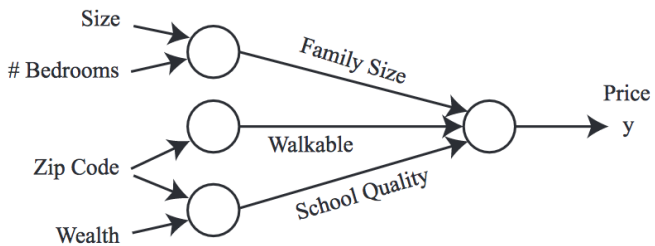

Housing Prediction Revisited

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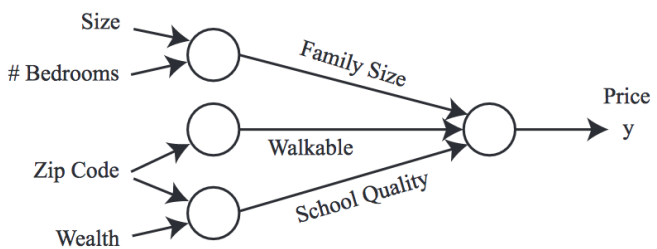
- Given three derived features (Family size, walkable school quality), the price of the home depends on these features



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- Goal NN: automatically determine three relevant features so as to predict the price of a house

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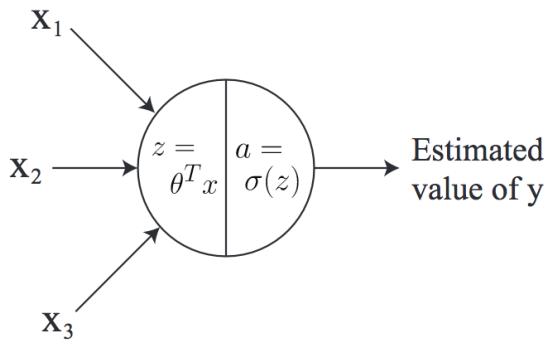
- $a_1^{[1]}$ denote the output value of the first hidden unit in the first hidden layer
- The input layer is layer 0, the first hidden layer is 1 and the output is layer 2.

Notation

$$
\begin{aligned}
x_1 &= a_1^{[0]} \\
x_2 &= a_2^{[0]} \\
x_3 &= a_3^{[0]}
\end{aligned}
$$

Logistic Regression as Neuron



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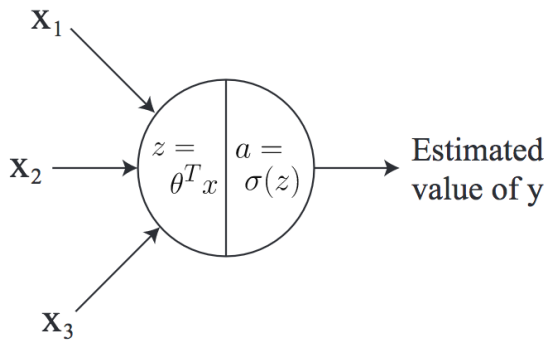

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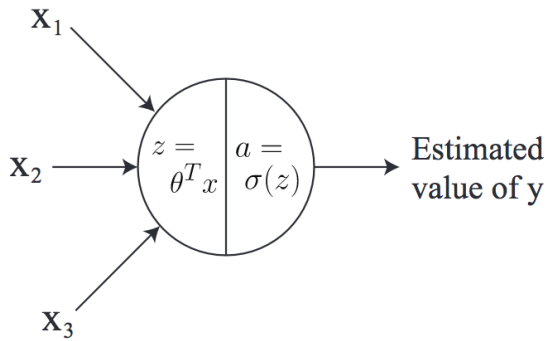

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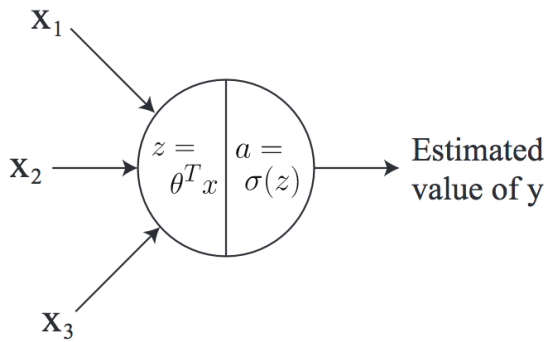

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- notational difference, before $z = \theta^T x$, now $z = w^T x + b$ (W will denote a matrix)

Activation functions

$a = g(z)$, where $g(z)$ is some activation function:

$$g(z) = \frac{1}{1+e^{-z}} \qquad \text{(sigmoid)}$$
$$g(z) = \max(z, 0) \qquad \text{(ReLU)}$$
$$g(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}} \qquad \text{(tanh)}$$

In general, $g(z)$ is a non-linear function

NN computation

- The first hidden unit in the fist hidden layer will perform: $z_1^{[1]} = {W_1^{[1]}}^T x + b_1^{[1]}$ and $a_1^{[1]} = g(z_1^{[1]})$

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- W_1 is the first row of W, a matrix of parameters
- $W_1^{[1]} \in \mathbb{R}^3$ and $b_1^{[1]} \in \mathbb{R}$
- second and third hidden units (first hidden layer):

$$\begin{aligned} z_2^{[1]} &= {W_2^{[1]}}^T x + b_2^{[1]} \text{ and } a_2^{[1]} = g(z_2^{[1]}) \\ z_3^{[1]} &= {W_3^{[1]}}^T x + b_3^{[1]} \text{ and } a_3^{[1]} = g(z_3^{[1]}) \end{aligned}$$

NN computation II

The output layer performs:

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

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

$$a^{[1]} = \begin{bmatrix} a_1^{[1]} \\ a_2^{[1]} \\ a_3^{[1]} \\ a_4^{[1]} \end{bmatrix}$$

For regression tasks one typically does not apply a non-linear function to $a_1^{[2]}$

Vectorization

One must be careful when using for loops. In order to compute hidden unit activations in the first layer, we must compute:

$$\begin{array}{ccc} z_1^{[1]} = {W_1^{[1]}}^T x + b_1^{[1]} & \text{and} & a_1^{[1]} = g(z_1^{[1]}) \\ \vdots & & \vdots \\ z_4^{[1]} = {W_4^{[1]}}^T x + b_4^{[1]} & \text{and} & a_4^{[1]} = g(z_4^{[1]}) \end{array}$$

Deep Learning algorithms have high computational requirements. As a result, code will run very slowly if you use for loops

Vectorizing the Output Computation

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

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- $a^{[1]} = g(z^{[1]})$, use vectorized libraries (element-wise operations, e.g. ./ element-wise division Octave)

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- To compute the output layer's activations:

$$\underbrace{z^{[2]}}_{1\times1} = \underbrace{W^{[2]}}_{1\times4}\underbrace{a^{[1]}}_{4\times1} + \underbrace{b^{[2]}}_{1\times1} \quad \text{and} \quad \underbrace{a^{[2]}}_{1\times1} = g(\underbrace{z^{[2]}}_{1\times1})$$

Vectorization Over Training Examples

Training set with three examples:

$$\begin{aligned} z^{[1](1)} &= W^{[1]}x^{(1)} + b^{[1]} \\ z^{[1](2)} &= W^{[1]}x^{(2)} + b^{[1]} \\ z^{[1](3)} &= W^{[1]}x^{(3)} + b^{[1]} \end{aligned}$$

Vectorization

$$X = \begin{bmatrix} | & | & | \\ x^{(1)} & x^{(2)} & x^{(3)} \\ | & | & | \end{bmatrix}$$

$$Z^{[1]} = \begin{bmatrix} | & | & | \\ z^{[1](1)} & z^{[1](2)} & z^{[1](3)} \\ | & | & | \end{bmatrix} = W^{[1]}X + b^{[1]}$$

Putting it together

Suppose we have a training set $(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})$, where $x^{(i)}$ is a picture and $y^{(i)}$ is a binary label for whether the picture contains a cat or not

- Initialize the parameters $W^{[1]}, b^{[1]}, W^{[2]}, b^{[2]}$ to small random numbers

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- This maximization procedure corresponds to training the neural network