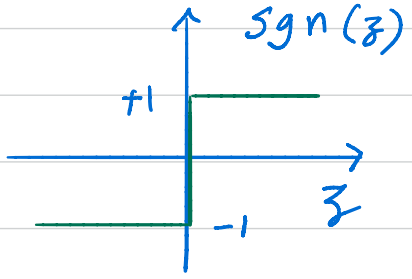
Application: Neural Networks

- Neuron is a non-linear function, which takes $z \in \mathbb{R}$ as input and produces $\sigma(z) \in \mathbb{R}$ as output

$$z \longrightarrow (\sigma) \longrightarrow \sigma(z)$$

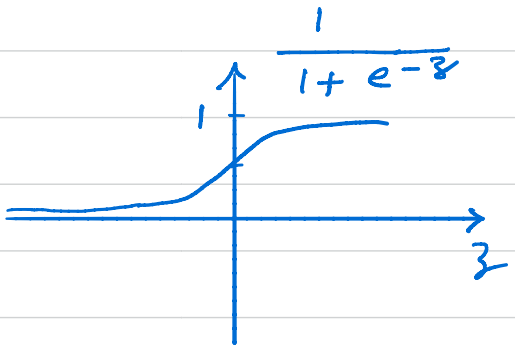
Examples of σ:

(1)



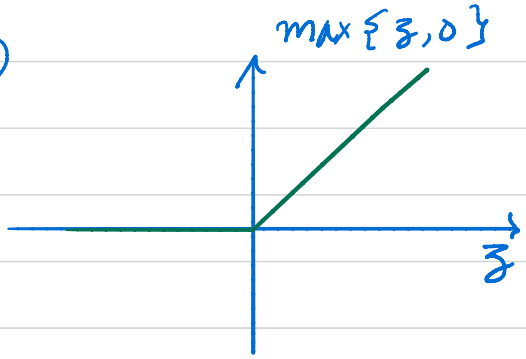
sign

(2)



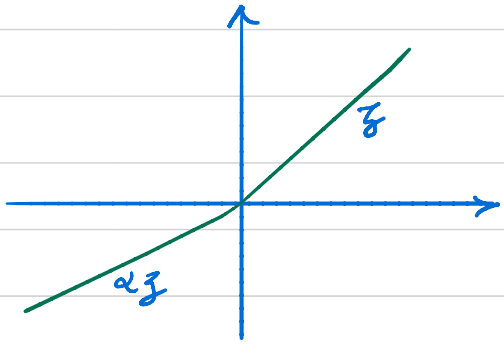
sigmoid

(3)



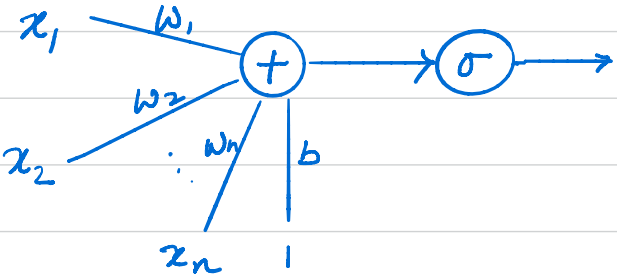
Rectifier Linear Unit (ReLU)

(4)



Leaky ReLU

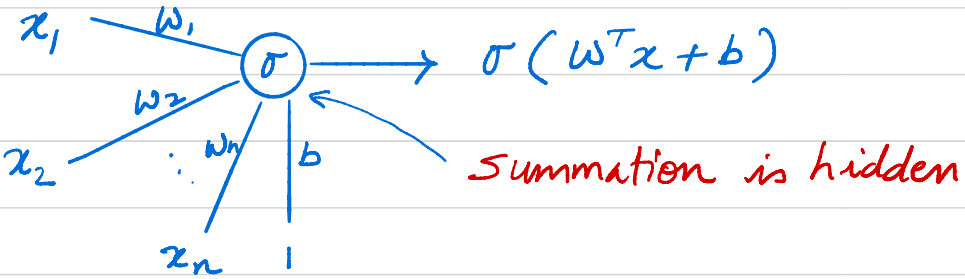
Vector Input



$$\sigma(w^T x + b)$$

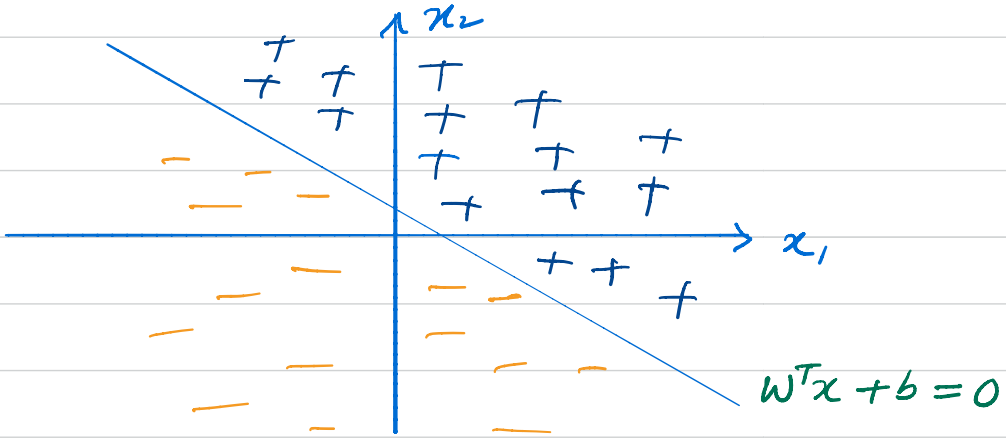
b: bias

Simplified Representation



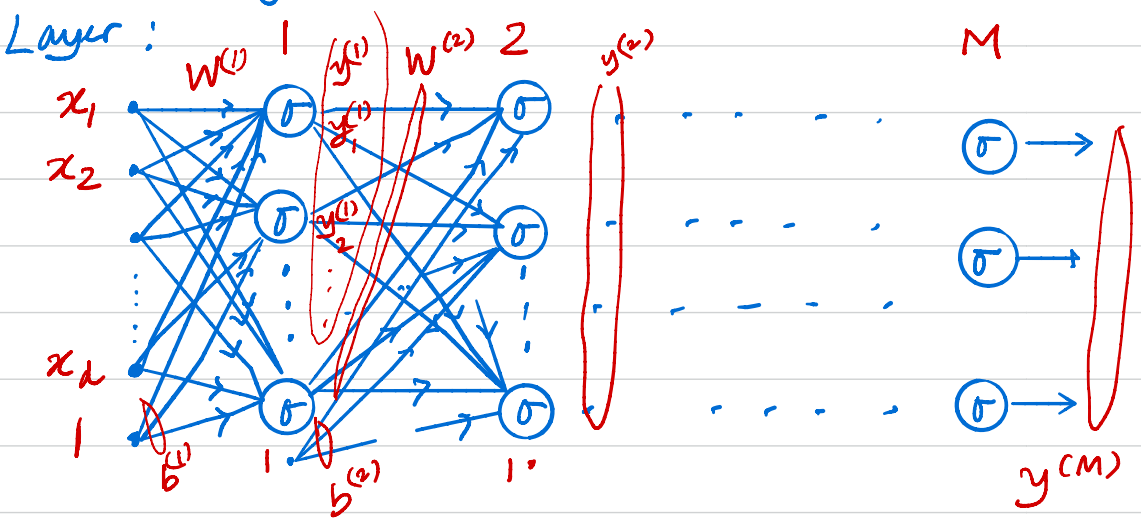
- bias b is important, e.g., if σ is the sgn function, we can output $+1$ if $w^T x \geq -b$
  -1 if $w^T x < -b$
  instead of $w^T x \gtrless 0$.

$w^T x + b = 0$ is a hyperplane in $\mathbb{R}^n$.
and neuron simply divides the input space into two parts corresponding to $+1$ and -1



Multilayer NN's allow us to divide high dimensional space in more complicated ways and approximate functions mapping inputs and outputs of NN

Multilayer Neural Network (Feed Forward)



Note: Last layer may require special processing to make $\hat{y}$ belong to desired output space

- number of neurons in each layer can be different
- All weights on edges connecting layers m-1 and m are in matrix $W^{(m)}$, with $W_{ij}^{(m)}$ being the weight connecting output j of layer (m-1) with neuron i of layer m
- Input to network is vector x; output of layer m is vector $y^{(m)}$

$$y_i^{(1)} = \sigma(x_i^{(1)}), \text{ with } x_i^{(1)} = \sum_j W_{ij}^{(1)} x_j + b_i^{(1)}$$

This can be written compactly as:

$$y^{(1)} = \sigma(x^{(1)}) \text{ with } x^{(1)} = W^{(1)} x + b^{(1)}$$

σ applied to each element of $x^{(1)}$

$$y^{(1)} = \sigma(x^{(1)}), \text{ with } x^{(1)} = W^{(1)}x + b^{(1)}$$

Similarly,

$$y^{(2)} = \sigma(x^{(2)}), \text{ with } x^{(2)} = W^{(2)}y^{(1)} + b^{(2)}$$

$$\vdots$$

$$y^{(M)} = \sigma(x^{(M)}), \text{ with } x^{(M)} = W^{(M)}y^{(M-1)} + b^{(M)}$$

Goal is choose the weights $W^{(1)}, \ldots, W^{(M)}, b^{(1)}, \ldots, b^{(M)}$ so that the output of last layer, a.k.a. output of NN approximates some desired function well, i.e., we want

$$\hat{y} = y^{(M)} \approx f^*(x) = y$$

(f^*: unknown; y: possibly multidimensional)

How is the function approximated? Use labelled training data, i.e. inputs for which we know correct output, even though f^* is unknown:

$$(x[1], y[1]), (x[2], y[2]), \ldots (x[N], y[N])$$

Minimize "empirical" loss on training data

$$J = \sum_{n=1}^{N} L(y[n], \hat{y}[n])$$

where $\hat{y}[n]$ is output of NN when input is $x[n]$.

- In case the desired output y is (cont.) scalar, i.e. $f : \mathbb{R}^k \to \mathbb{R}$, then L is often taken to be the square loss : $L(y, \hat{y}) = (y - \hat{y})^2$

  $\hat{y} = y^{(M)}$ means last layer has only one neuron

- $$J = \sum_{n=1}^{N} L(y[n], \hat{y}[n])$$ $\hat{y}[n] = y^{(M)}[n]$

  ↑ assume cont. differentiable

- Note that J is a function of $W^{(1)}, \dots, W^{(M)}, b^{(1)}, \dots, b^{(M)}$
- We wish to minimize J using a gradient descent procedure.
  - Need to compute gradient of J w.r.t. all weights
  - Since J is a sum, we can compute the gradient for each term separately.
    We drop "[n]" for convenience.
  - To compute gradient we need :

    $\frac{\partial L}{\partial W_{ij}^{(l)}}$ for each l, i, j.

    and $\frac{\partial L}{\partial b_i^{(l)}}$ for each l, i.

Back Propagation Algorithm

- Exploit network structure and chain Rule to compute gradient terms efficiently

Layer M Recall $y^{(M)} = \sigma(x^{(M)})$, $x^{(M)} = W^{(M)} y^{(M-1)} + b^{(M)}$

$$\frac{\partial L}{\partial W_{ij}^{(M)}} = \frac{\partial L}{\partial y_i^{(M)}} \cdot \frac{\partial y_i^{(M)}}{\partial W_{ij}^{(M)}} = \frac{\partial L}{\partial y_i^{(M)}} \frac{\partial y_i^{(M)}}{\partial x_i^{(M)}} \frac{\partial x_i^{(M)}}{\partial W_{ij}^{(M)}}$$

$\frac{\partial L}{\partial y_i^{(M)}}$ can easily be computed in practice for each data point $(x[n], y[n])$.

For example if $y^{(M)}, y$ are scalar, and $L(y, y^{(M)}) = (y - y^{(M)})^2$. Then, for $(x[n], y[n])$,

$$\frac{\partial L}{\partial y_{[n]}^{(M)}}(y[n], y^{(M)}[n]) = 2\left(y^{(M)}[n] - y[n]\right).$$

$$\frac{\partial y_i^{(M)}}{\partial x_i^{(M)}} = \frac{d\,\sigma(x_i^{(M)})}{d\,x_i^{(M)}} = \sigma'(x_i^{(M)})$$

(assuming σ cont. diff.)

$$x_i^{(M)} = \sum_k W_{ik}^{(M)} y_k^{(M-1)} + b_i^{(M)}$$

$$\Rightarrow \frac{\partial x_i^{(M)}}{\partial W_{ij}^{(M)}} = y_j^{(M-1)}$$

Thus, $$\frac{\partial L}{\partial W_{ij}^{(M)}} = \frac{\partial L}{\partial y_i^{(M)}} \cdot \sigma'(x_i^{(M)})\, y_j^{(M-1)}$$

Similarly, $\frac{\partial L}{\partial b_i^{(M)}} = \frac{\partial L}{\partial y_i^{(M)}} \cdot \frac{\partial y_i^{(M)}}{\partial x_i^{(M)}} \cdot \underbrace{\frac{\partial x_i^{(M)}}{\partial b_i^{(M)}}}_{=1}$

$$= \frac{\partial L}{\partial y_i^{(M)}} \cdot \sigma'(x_i^{(M)})$$

Layer m, $1 \leq m \leq M$

Recall that $y^{(m)} = \sigma(x^{(m)})$ with $x^{(m)} = W^{(m)} y^{(m-1)} + b^{(m)}$

$$\frac{\partial L}{\partial W_{ij}^{(m)}} = \frac{\partial L}{\partial y_i^{(m)}} \cdot \underbrace{\frac{\partial y_i^{(m)}}{\partial x_i^{(m)}}}_{\sigma'(x_i^{(m)})} \cdot \underbrace{\frac{\partial x_i^{(m)}}{\partial W_{ij}^{(m)}}}_{y_j^{(m-1)}}$$

just as in layer M

Note that $y^{(m)}$ is related to $x^{(m+1)} = W^{(m+1)} y^{(m)} + b^{(m+1)}$

$$\Rightarrow \frac{\partial L}{\partial y_i^{(m)}} = \sum_k \frac{\partial L}{\partial x_k^{(m+1)}} \frac{\partial x_k^{(m+1)}}{\partial y_i^{(m)}}$$

$$= \sum_k \underbrace{\frac{\partial L}{\partial y_k^{(m+1)}}}_{\text{computed in previous step}} \cdot \underbrace{\frac{\partial y_k^{(m+1)}}{\partial x_k^{(m+1)}}}_{\sigma'(x_k^{(m+1)})} \cdot \underbrace{\frac{\partial x_k^{(m+1)}}{\partial y_i^{(m)}}}_{W_{ki}^{(m+1)}}$$

$$= \sum_k \frac{\partial L}{\partial y_k^{(m+1)}} \sigma'(x_k^{(m+1)}) W_{ki}^{(m+1)}$$

Similarly,

$$\frac{\partial L}{\partial b_i^{(m)}} = \underbrace{\frac{\partial L}{\partial y_i^{(m)}}}_{\text{above}} \cdot \underbrace{\frac{\partial y_i^{(m)}}{\partial x_i^{(m)}}}_{\sigma'(x_i^{(m)})} \cdot \underbrace{\frac{\partial x_i^{(m)}}{\partial b_i^{(m)}}}_{1}$$

Back Propagation Summary

(1) Compute $\frac{\partial L}{\partial y_i^{(M)}}$ for all i

(2) For $m = M$ down to 1.

$$\frac{\partial L}{\partial W_{ij}^{(m)}} = \frac{\partial L}{\partial y_i^{(m)}} \sigma'(x_i^{(m)}) \, y_j^{(m-1)}$$

$$\frac{\partial L}{\partial b_i^{(m)}} = \frac{\partial L}{\partial y_i^{(m)}} \sigma'(x_i^{(m)})$$

Where $$\frac{\partial L}{\partial y_i^{(m)}} = \sum_k \frac{\partial L}{\partial y_k^{(m+1)}} \sigma'(x_k^{(m+1)}) \, W_{ki}^{(m+1)}$$

Remarks

1. Gradient computation can be performed in parallel for different data points

2. In practice iterates are generated using gradients of only subset of data points for each iteration:

(Batch) Stochastic Gradient Descent (SGD)