SPATIAL ECOLOGY

Neural Nets

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Agenda

1) Perceptron
- Quick recap
- Hands-on tutorial
- Intro to gradient descent and optimizers

2) Feedforward Neural Networks
- The limitations of Perceptrons
- Multi-layer Perceptron
- Training: the forward and back-propagation
- Debugging tips

Linear Regression Optimization

- Add an offset w_0: $f(\boldsymbol{x};\boldsymbol{w}) = \boldsymbol{w}^T\boldsymbol{x} + \mathrm{w}_0$, $\mathcal{D} = \{(\boldsymbol{x}_1, y_1), \ldots (\boldsymbol{x}_n, y_n)\}$

$$\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} \sum_{i=1}^{n} (\boldsymbol{w}^T\boldsymbol{x}_i + w_0 - y_i)^2$$

$$= \arg\min_{\boldsymbol{w}} L(\boldsymbol{w}; \mathcal{D})$$

- Set $\frac{\partial L(\boldsymbol{w};\mathcal{D})}{\partial w_i} = 0$ for each i

Mean squared error loss

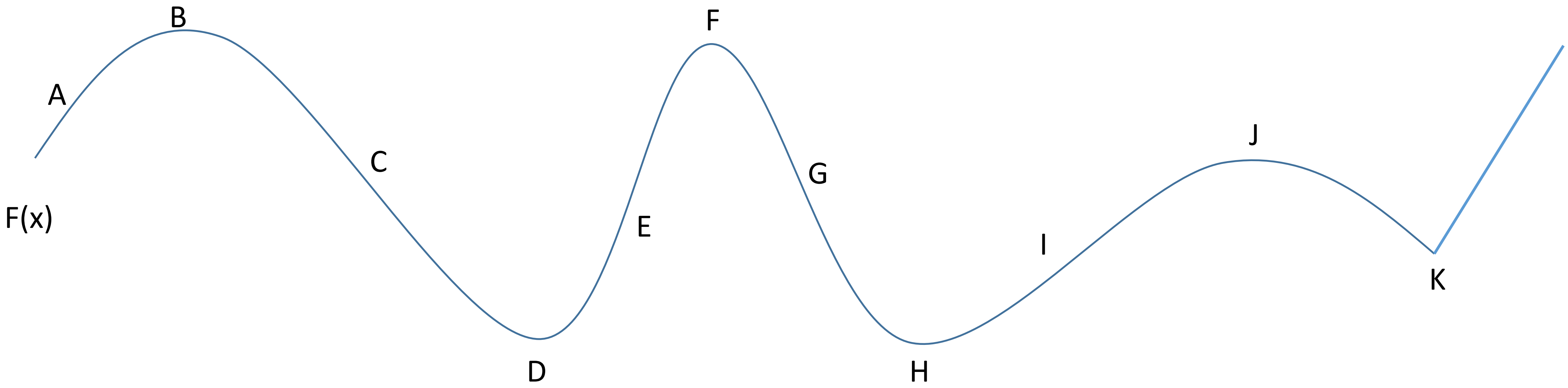
$$\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} \sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i + w_0 - y_i)^2$$

Rewrite:

$$\begin{aligned}
(X\mathbf{w} - \mathbf{y})^T (X\mathbf{w} - \mathbf{y}) &= (\mathbf{w}^T X^T - \mathbf{y}^T)(X\mathbf{w} - \mathbf{y}) \\
&= \mathbf{w}^T X^T X\mathbf{w} - \mathbf{w}^T X^T \mathbf{y} - \mathbf{y}^T X\mathbf{w} + \mathbf{y}^T \mathbf{y} \\
&= \mathbf{w}^T X^T X\mathbf{w} - 2\mathbf{w}^T X^T \mathbf{y} + \mathbf{y}^T \mathbf{y}.
\end{aligned}$$

$$\begin{aligned}
\frac{\partial}{\partial w} \mathbf{w}^T X^T X\mathbf{w} - 2\mathbf{w}^T X^T \mathbf{y} + \mathbf{y}^T \mathbf{y} &= 0 \\
2X^T X\mathbf{w} - 2X^T \mathbf{y} &= 0 \\
X^T X\mathbf{w} &= X^T \mathbf{y} \\
\mathbf{w} &= (X^T X)^{-1} X^T \mathbf{y}
\end{aligned}$$

More on the derivatives



Regularization

- Ridge regression: penalize with L2 norm

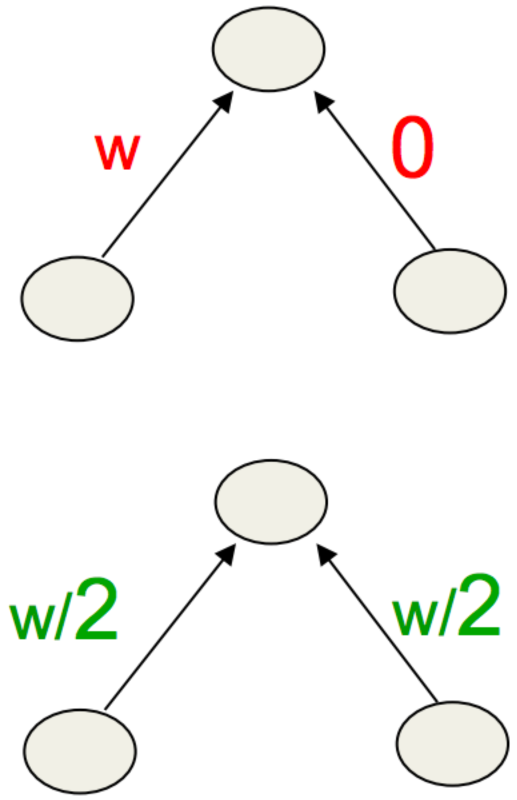
$$\boldsymbol{w}^* = \arg\min \sum_i L(f(\boldsymbol{x}_i; \boldsymbol{w}), y_i) + \lambda \sum_{j=1}^{m} w_j^2$$

  - Closed form solution exists $\boldsymbol{w}^* = (\lambda I + X^T X)^{-1} X^T \boldsymbol{y}$
- LASSO regression: penalize with L1 norm

$$\boldsymbol{w}^* = \arg\min \sum_i L(f(\boldsymbol{x}_i; \boldsymbol{w}), y_i) + \lambda \sum_{j=1}^{m} |w_j|$$

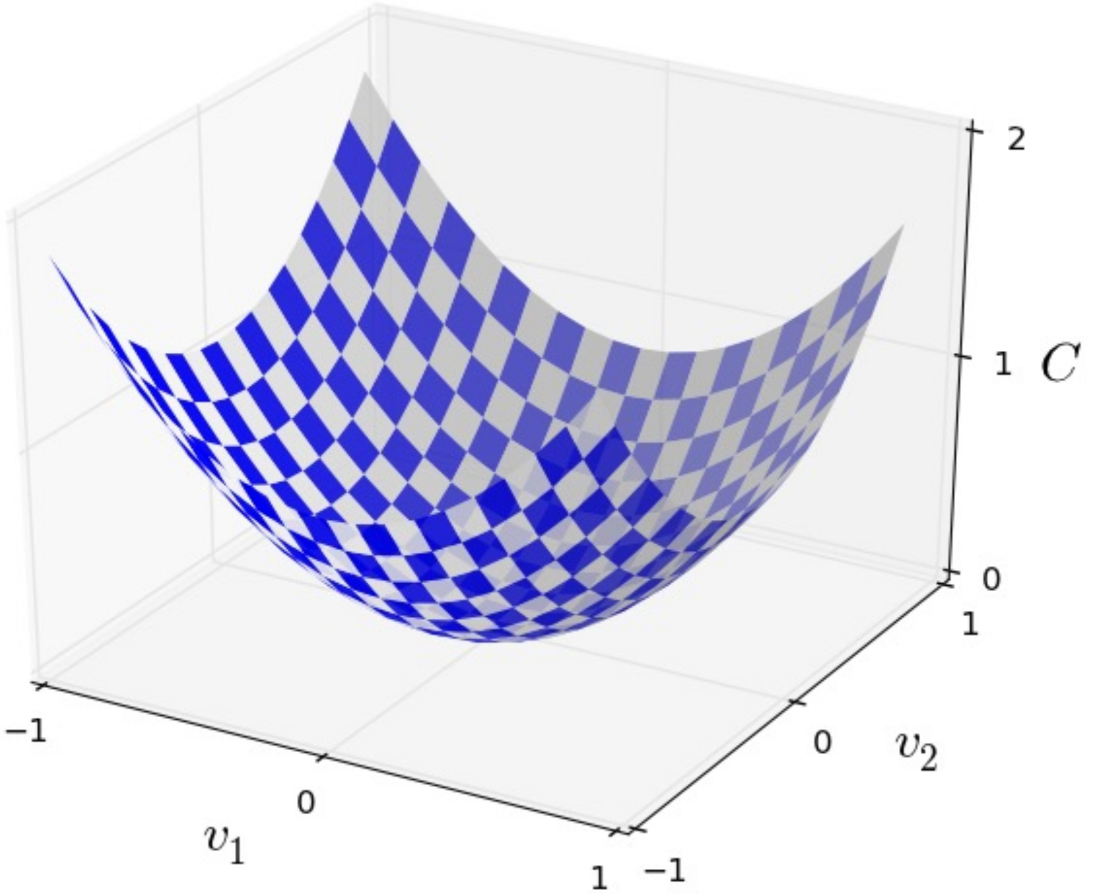
  - No closed form solution but still convex (optimal solution can be found)

Regularization

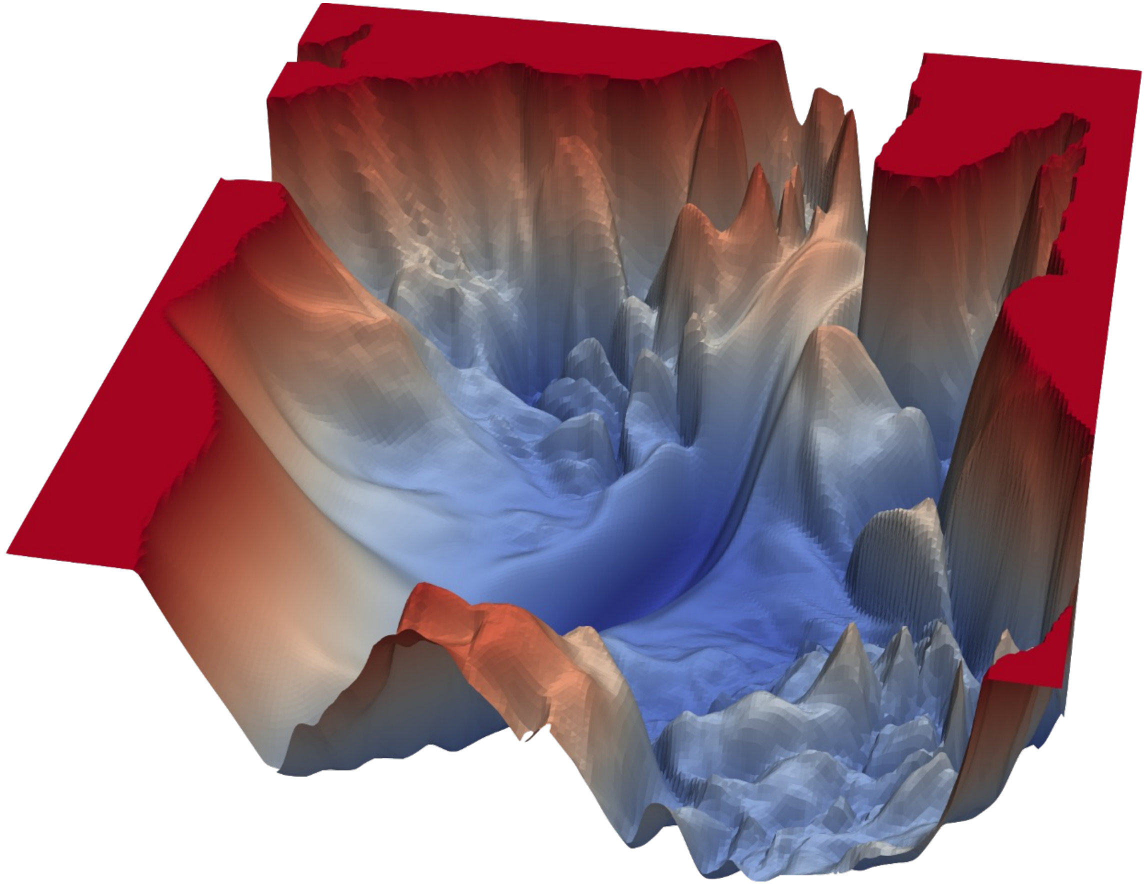


- Prefers to share smaller weights
- Makes model smoother
- More Convex

Expectation

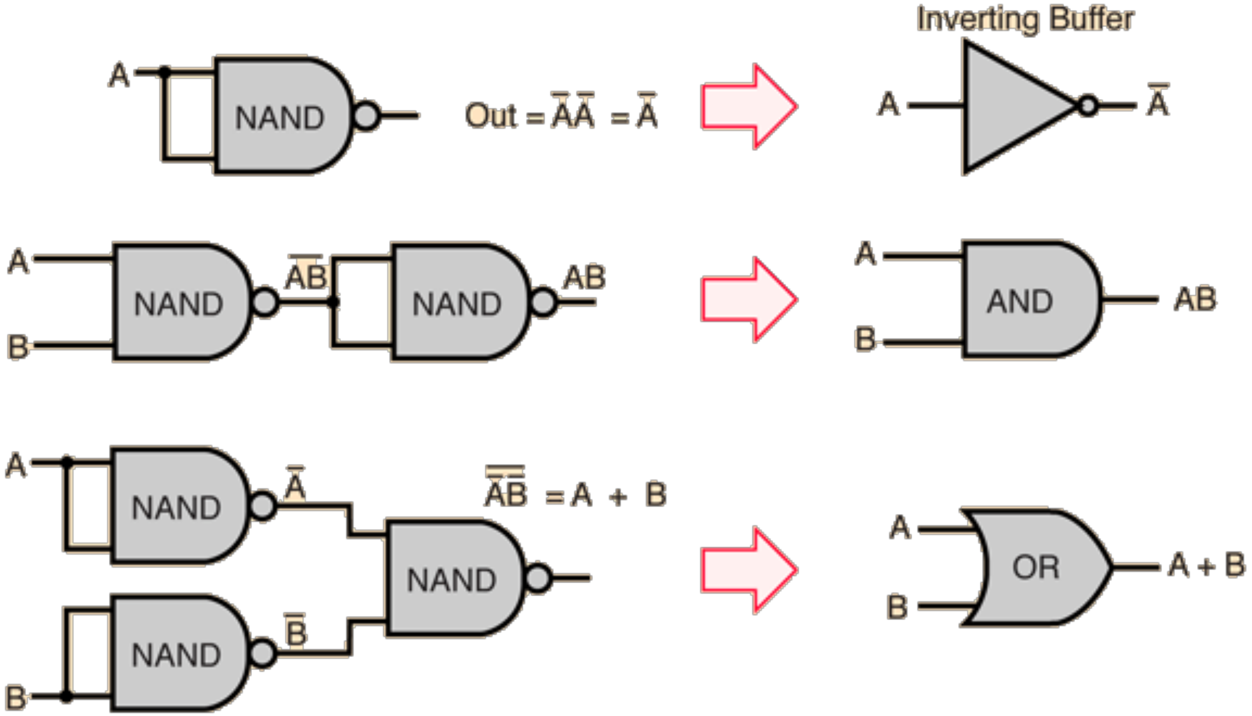


Reality



Logic circuits with perceptrons

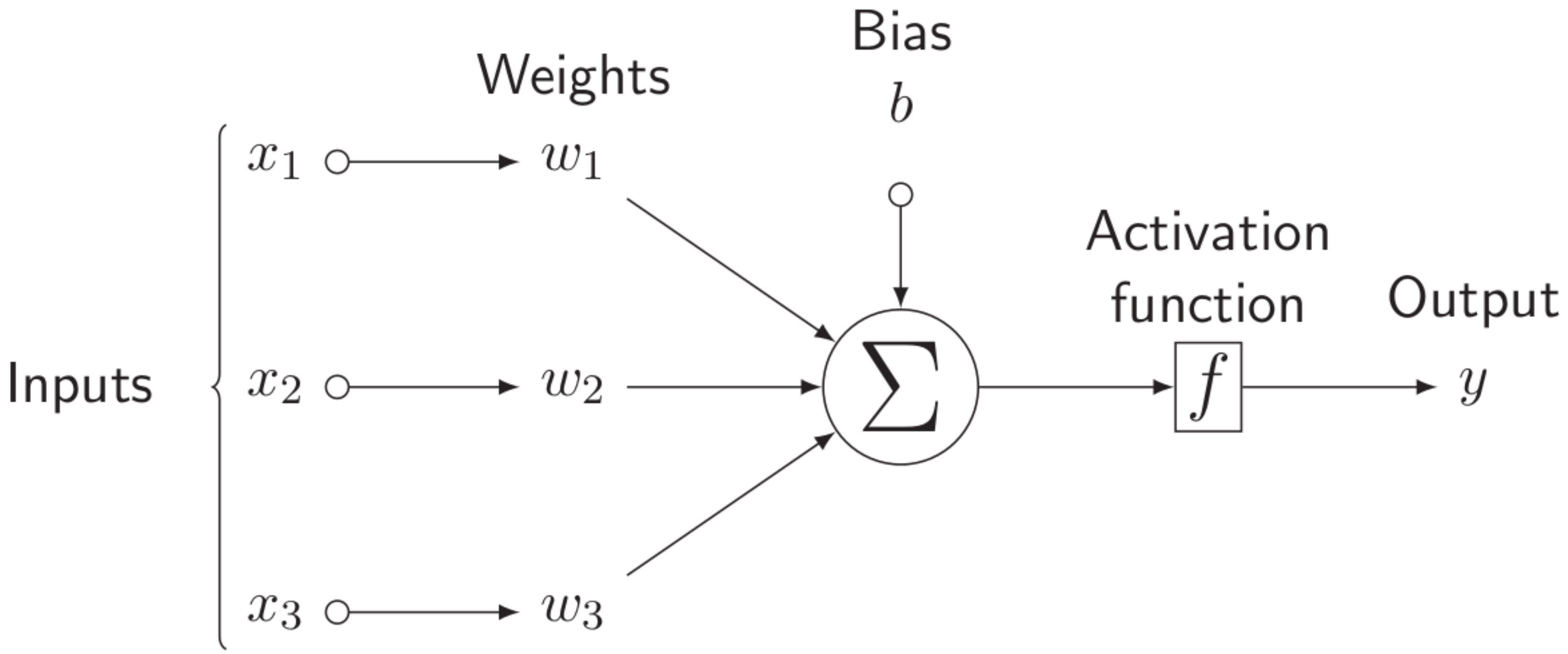
- NAND gates can be constructed from perceptrons
- NAND gates are universal for computation
  - Any computation can be built from NAND gates
  - Therefore, perceptrons are universal for computation



Nielsen, 2015

Perceptron: Threshold Logic

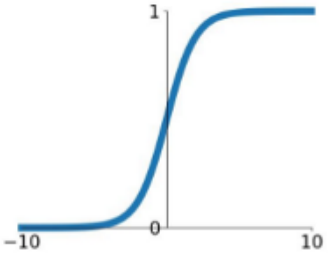
$$\mathcal{L}_{\text{perc}}(\mathbf{x}, y) = \begin{cases} 0 & \text{if } y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) > 0 \\ -y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) & \text{if } y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) \leq 0 \end{cases}$$



Activation functions

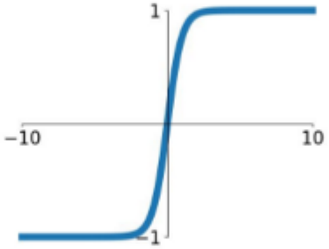
Sigmoid

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



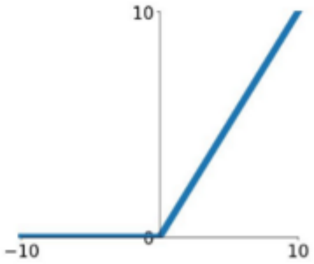
tanh

$\tanh(x)$



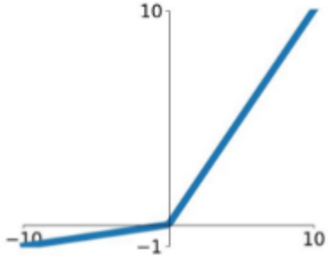
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

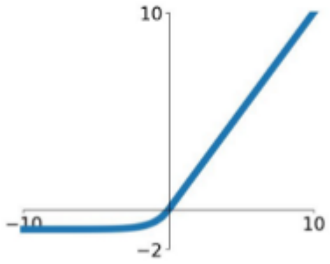


Maxout

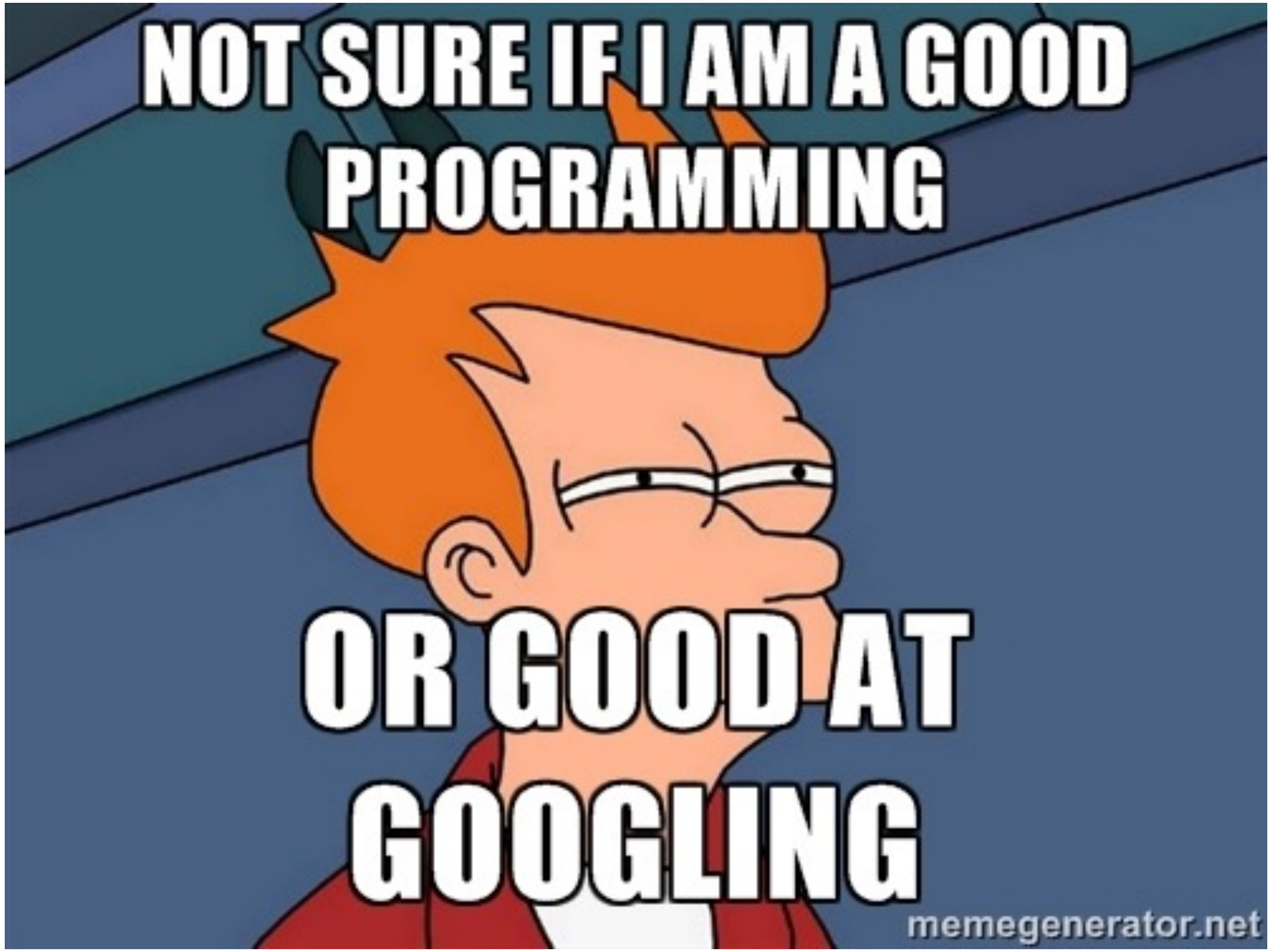
$\max(w_1^T x + b_1, w_2^T x + b_2)$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Now let’s get our hand dirty!



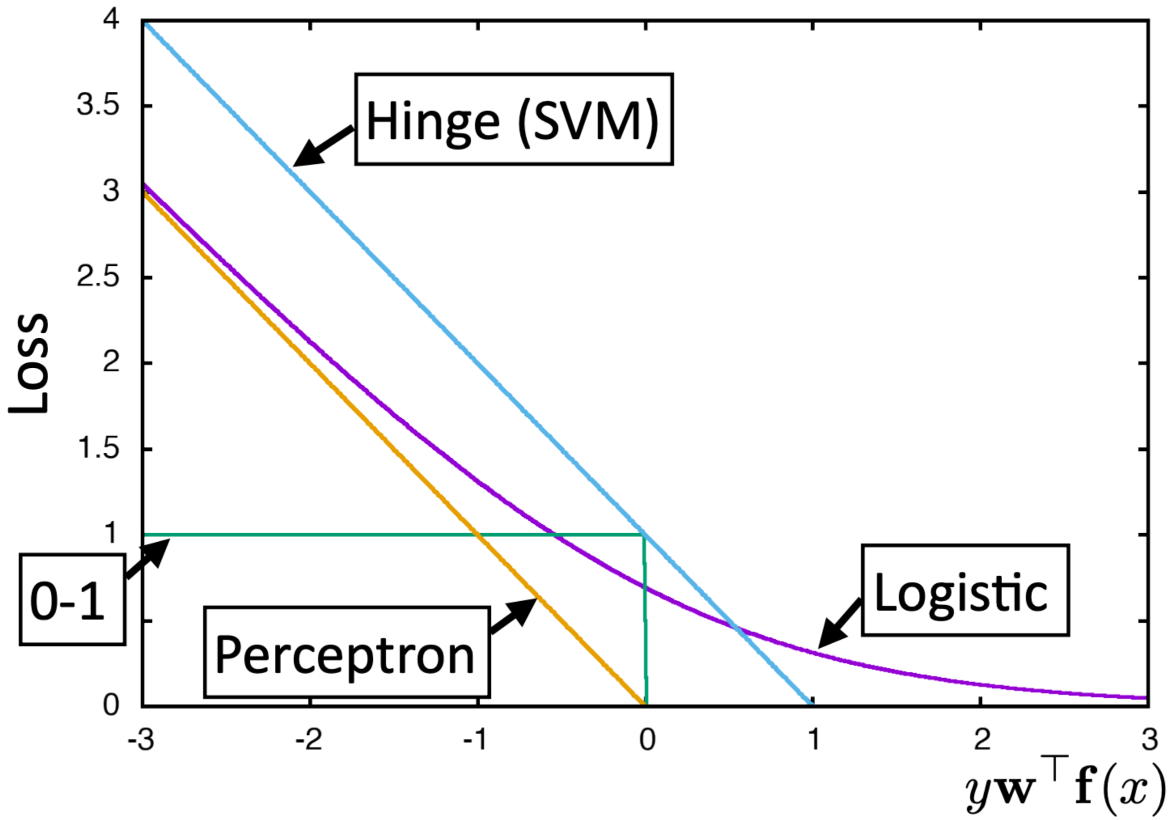
(Putting things in perspective)

$$\mathcal{L}_{\mathrm{lr}}(\mathbf{x}, y) = \begin{cases} -y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) + \log\left(1 + \exp\left(y\mathbf{w}^\top \mathbf{f}(\mathbf{x})\right)\right) & \text{if } y = +1 \text{ (positive)} \\ \log\left(1 + \exp\left(-y\mathbf{w}^\top \mathbf{f}(\mathbf{x})\right)\right) & \text{if } y = -1 \text{ (negative)} \end{cases}$$

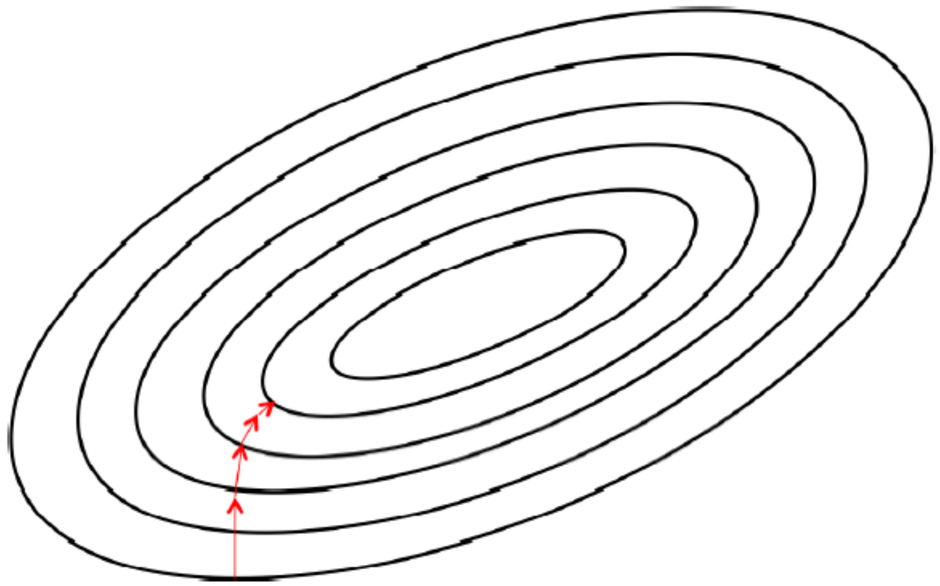
$$\mathcal{L}_{\mathrm{perc}}(\mathbf{x}, y) = \begin{cases} 0 & \text{if } y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) > 0 \\ -y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) & \text{if } y\mathbf{w}^\top \mathbf{f}(\mathbf{x}) \leq 0 \end{cases}$$

Main differences:

- Perceptron: gradient-based optimization
- LR: probabilistic model
- Perceptron: if the data are linearly separable, perceptron is guaranteed to converge.
- LR: likelihood can never truly be maximized with a finite w vector.



Optimizers

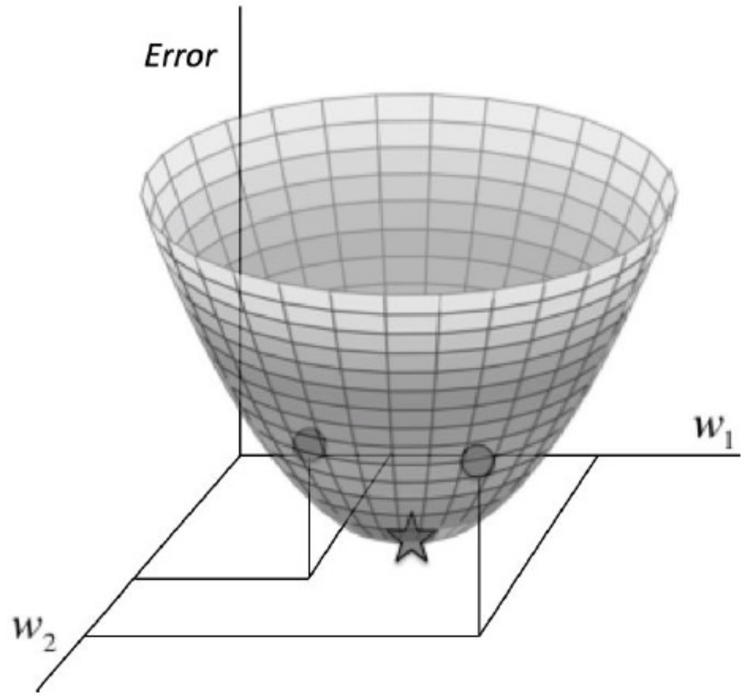


Gradient

$$\Delta w_k = -\frac{\partial E}{\partial w_k}$$

$$= -\frac{\partial}{\partial w_k}\left(\frac{1}{m}\sum_i (w^T X_i - y_i)_i^2\right)$$

$$w_{i+1} = w_i + \Delta w_k$$



Stochastic gradient descent (**SGD**)

Optimizers

Practical test:
lr_val = [1; 0.1; 0.01]
momentum_val = 0
nesterov_val = ‘False'
decay_val = 1e-6

Hyperparameters

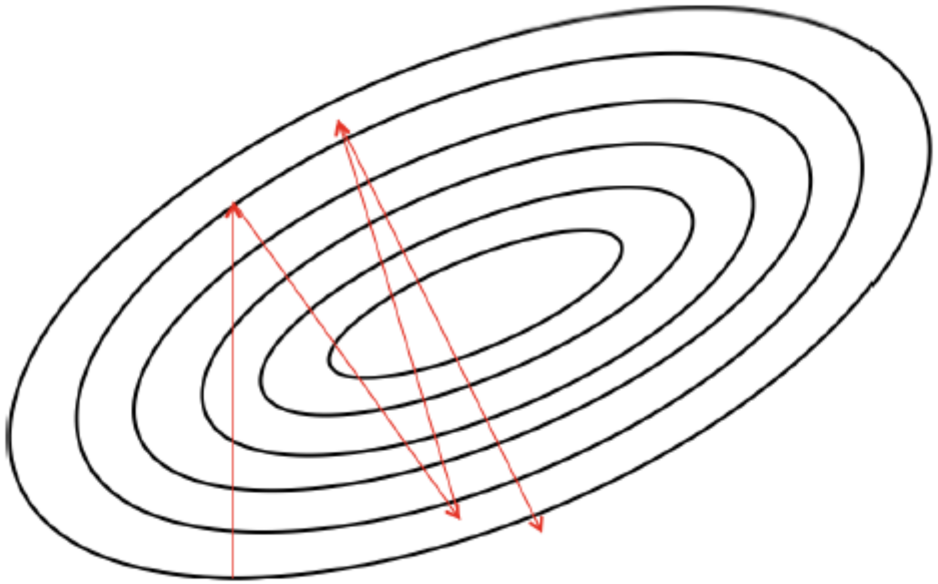
- Learning rate (α)

$$\Delta w_k = -\alpha \frac{\partial E}{\partial w_k}$$

$$= -\alpha \frac{\partial}{\partial w_k}\left(\frac{1}{m}\sum_i (w^T X_i - y_i)_i^2\right)$$

$$w_{i+1} = w_i + \Delta w_k$$

Stochastic gradient descent (**SGD**)



Result of a large learning rate α

Optimizers

Watch out for local minimal areas

Hyperparameters

- Learning rate (α)

$$\Delta w_k = -\alpha \frac{\partial E}{\partial w_k}$$

$$= -\alpha \frac{\partial}{\partial w_k}\left(\frac{1}{m}\sum_i (w^T X_i - y_i)_i^2\right)$$

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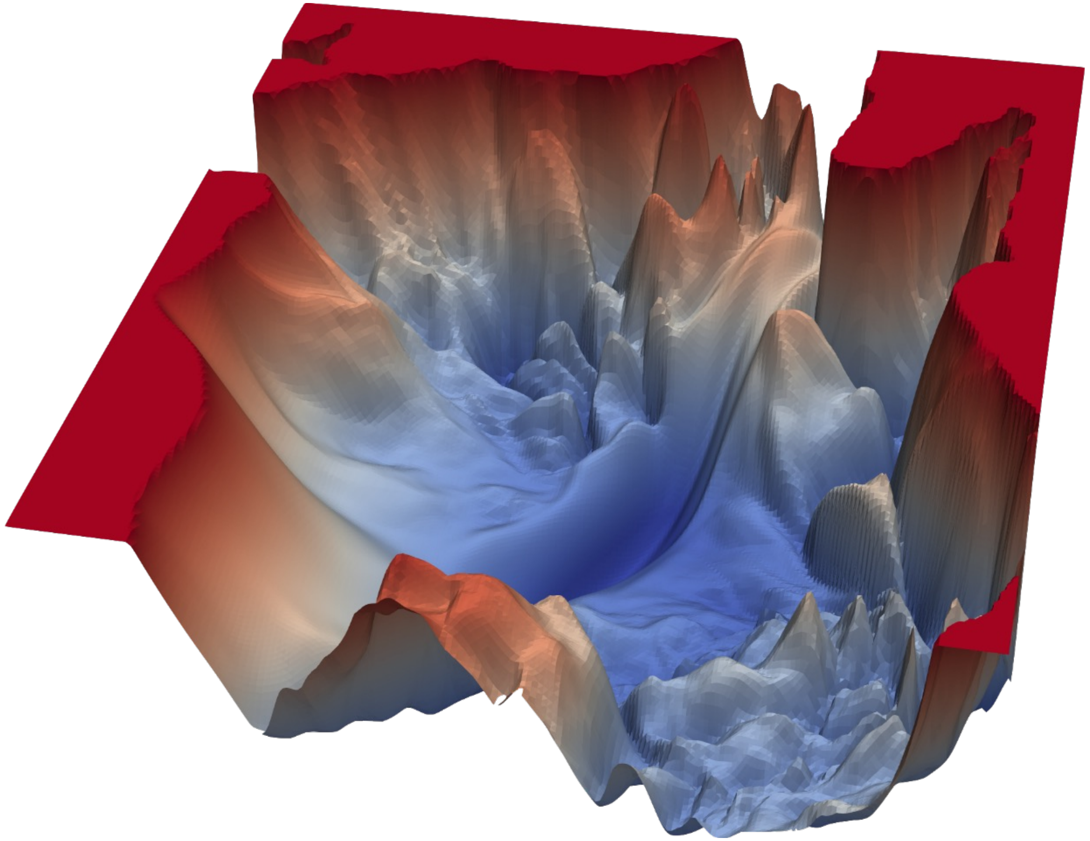


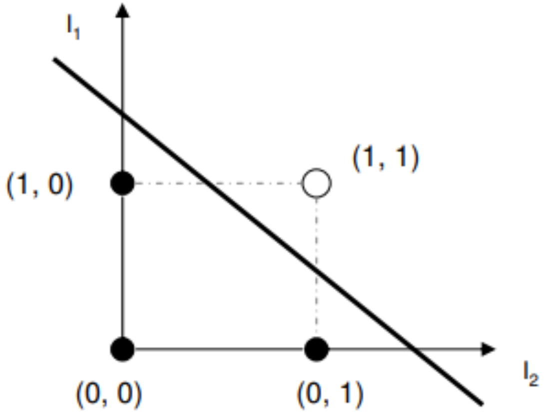
Stochastic gradient descent (**SGD**)

Gradient Descent

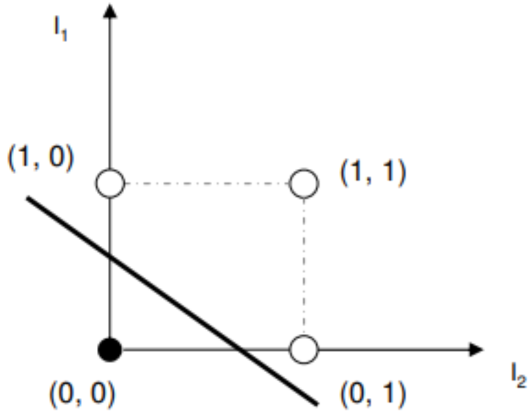
- Gradient descent refers to taking a step in the direction of the ***gradient (partial derivative)*** of a weight or bias with respect to the cost function
- Gradients are propagated backwards through the network in a process known as ***backpropagation***
- The size of the step taken in the direction of the gradient is called the ***learning rate***

Limitations of the Perceptron

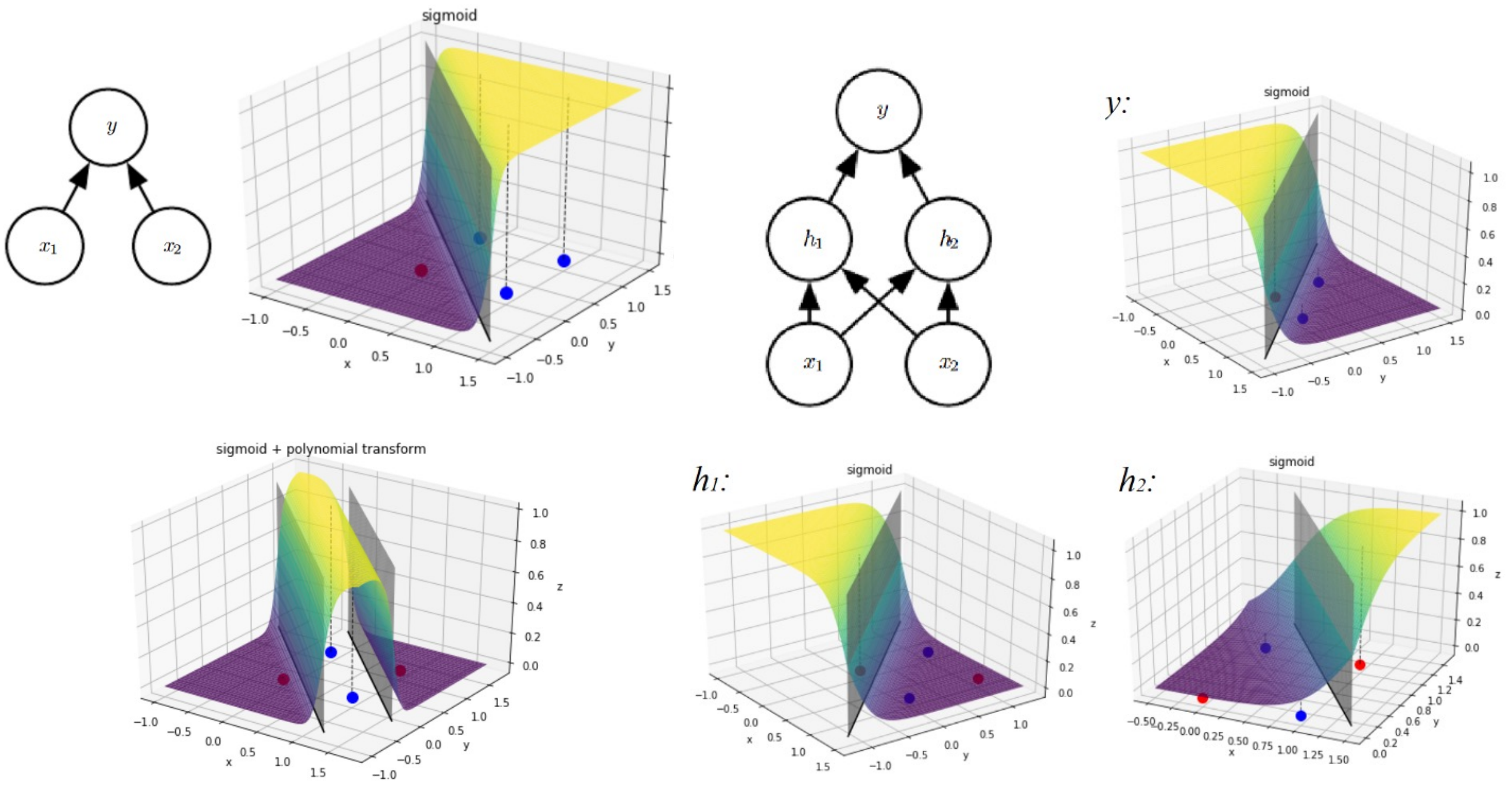
AND		
I_1	I_2	out
0	0	0
0	1	0
1	0	0
1	1	1



OR		
I_1	I_2	out
0	0	0
0	1	1
1	0	1
1	1	1

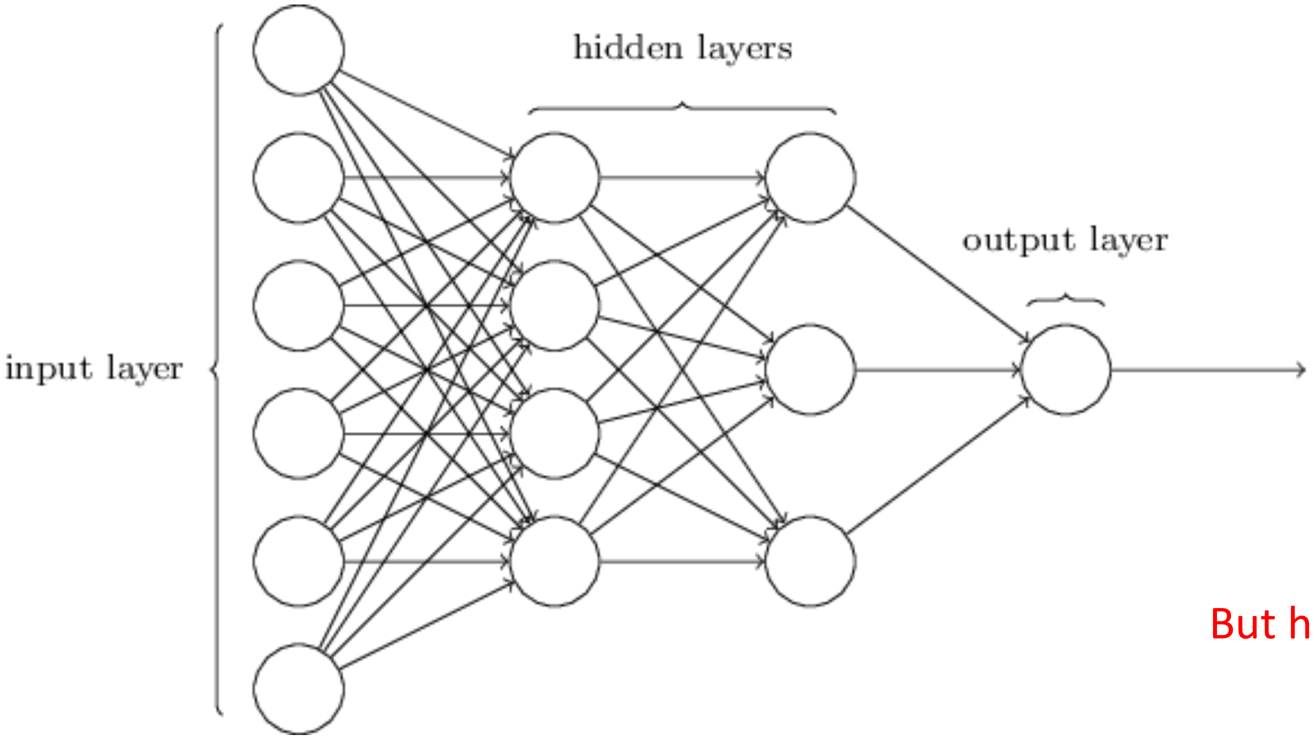


Perceptron



y
x1
x2
sigmoid
h1
h2
y:
sigmoid
sigmoid + polynomial transform
h1:
sigmoid
h2:
sigmoid

Architecture of Neural Networks

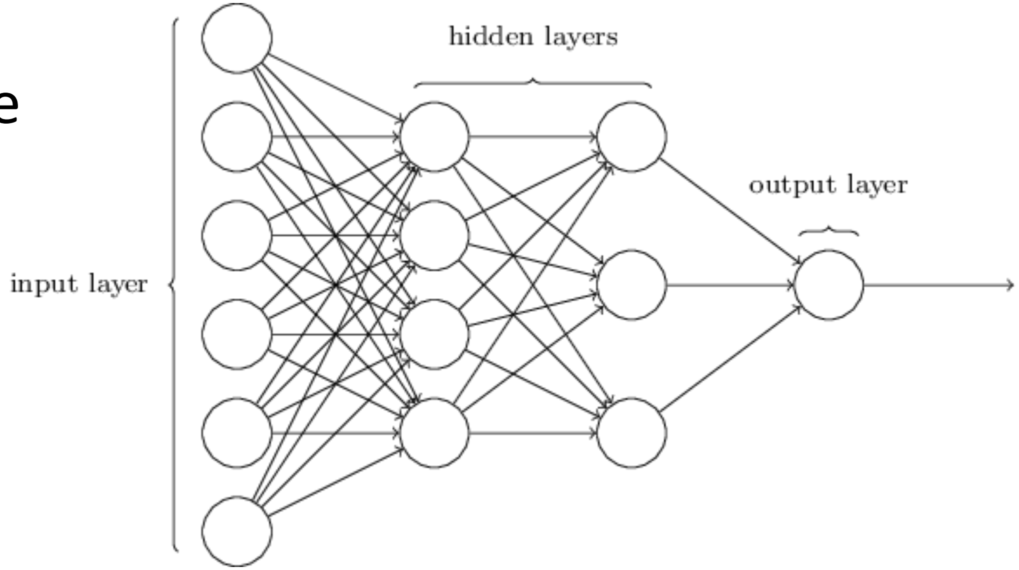


But how do we train it?

- Sometimes called multi-layer perceptron (MLP)
- Output from one layer is used as input for the next (Feedforward network)

Forward Propagation

- Store weights and biases as matrices
- Suppose we are considering the weights from the second (hidden) layer to the third (output) layer
  - w is the weight matrix with w_{ji} the weight for the connection between the ith neuron in the second layer and the jth neuron in the third layer
  - b is the vector of biases in the third layer
  - a is the vector of activations (output) of the 2nd layer
  - a' the vector of activations (output) of the third layer



$$\boldsymbol{a}' = \boldsymbol{\sigma}(\boldsymbol{w}\boldsymbol{a} + \boldsymbol{b})$$

Backpropagation

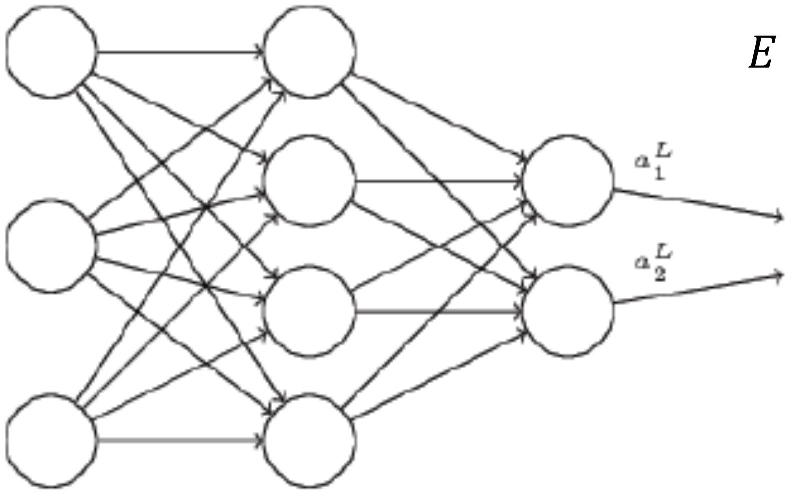
1. **Input x:** Set the corresponding activation a^1 for the input layer.

2. **Feedforward:** For each $l = 2, 3, \ldots, L$ compute $z^l = w^l a^{l-1} + b^l$ and $a^l = \sigma(z^l)$.

3. **Output error δ^L:** Compute the vector $\delta^L = \nabla_a C \odot \sigma'(z^L)$.

4. **Backpropagate the error:** For each $l = L-1, L-2, \ldots, 2$ compute $\delta^l = ((w^{l+1})^T \delta^{l+1}) \odot \sigma'(z^l)$.

5. **Output:** The gradient of the cost function is given by $\frac{\partial C}{\partial w^l_{jk}} = a^{l-1}_k \delta^l_j$ and $\frac{\partial C}{\partial b^l_j} = \delta^l_j$.



$$E = \frac{1}{2}\sum_i \left(a_i^L - y_i\right)^2$$

$$cost\ E = E(a^L)$$

$$z_j^l = \sum_i w_{ji}^l a_i^{l-1} + b_j^l \qquad a_j^l = \sigma\left(\sum_i w_{ji}^l a_i^{l-1} + b_j^l\right) = \sigma(z_j^l)$$

$$\delta_j^L \equiv \frac{\partial E}{\partial z_j^L} = \frac{\partial E}{\partial a_i^L}\frac{\partial a_i^L}{\partial z_j^L} = \frac{\partial E}{\partial a_j^L}\sigma'(z_j^L) \qquad (1)$$

$$\delta_j^l \equiv \frac{\partial E}{\partial z_j^l} = \frac{\partial E}{\partial z_i^{l+1}}\frac{\partial z_i^{l+1}}{\partial z_j^l} = \frac{\partial z_i^{l+1}}{\partial z_j^l}\delta_i^{l+1}$$

$$= \frac{\partial\left(\sum_i w_{ij}^{l+1} a_j^l + b_i^{l+1}\right)}{\partial z_j^l}\delta_j^{l+1} = \sum_i w_{ij}^{l+1}\delta_i^{l+1}\sigma'(z_j^l) \qquad (2)$$

$$\frac{\partial E}{\partial w_{ji}^l} = \frac{\partial E}{\partial a_i^l}\frac{\partial a_i^l}{\partial z_j^l}\frac{\partial(w_{ji}^l a_i^{l-1})}{\partial w_{ji}^l}$$

Back to the code (Feedforward networks)

When people want to use Machine Learning without math

How training works

1. In each ***epoch***, randomly shuffle the training data
2. Partition the shuffled training data into ***mini-batches***
3. For each mini-batch, apply a single step of **gradient descent**
   - **Gradients** are calculated via ***backpropagation*** (the next topic)
4. Train for multiple epochs

Debugging a neural network

- What can we do?
  - Should we change the learning rate?
  - Should we initialize differently?
  - Do we need more training data?
  - Should we change the architecture?
  - Should we run for more epochs?
  - Are the features relevant for the problem?
- Debugging is an art
  - We'll develop good heuristics for choosing good architectures and hyper parameters