

23.10.2024

BITS F464: Machine Learning (1st Sem 2024-25)

NEURAL NETWORKS: PERCEPTRON, MLP, BACKPROPAGATION

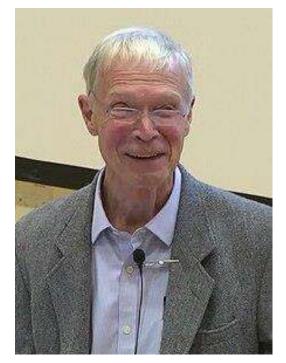
Chittaranjan Hota, Sr. Professor Dept. of Computer Sc. and Information Systems hota@hyderabad.bits-pilani.ac.in

Artificial Neural Networks





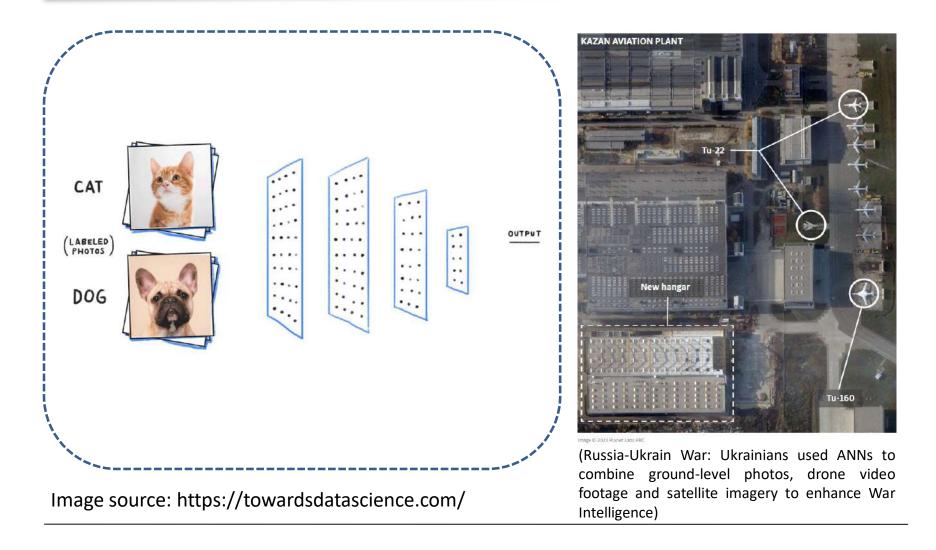
Geoffrey Everest Hinton



John Joseph Hopfield

Who is Godfather of AI?

ANNs: Motivating Examples



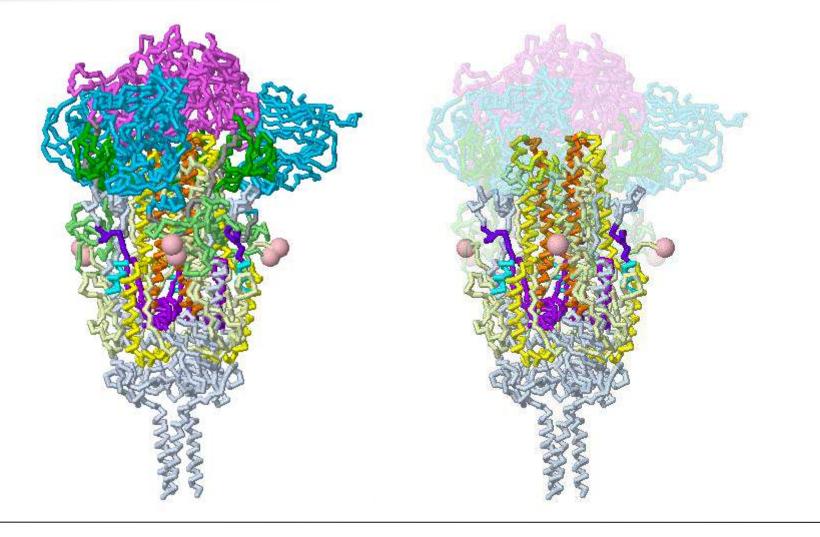


'The machine did it coldly': Israel used AI to identify 37,000 Hamas targets: The Lavender, The Gospel.



Source: https://www.ri.cmu.edu/

Pre-Fusion Spike Protein



https://proteopedia.org/

SARS-CoV-2

Alphafold 2

Learning Rewires the Brain

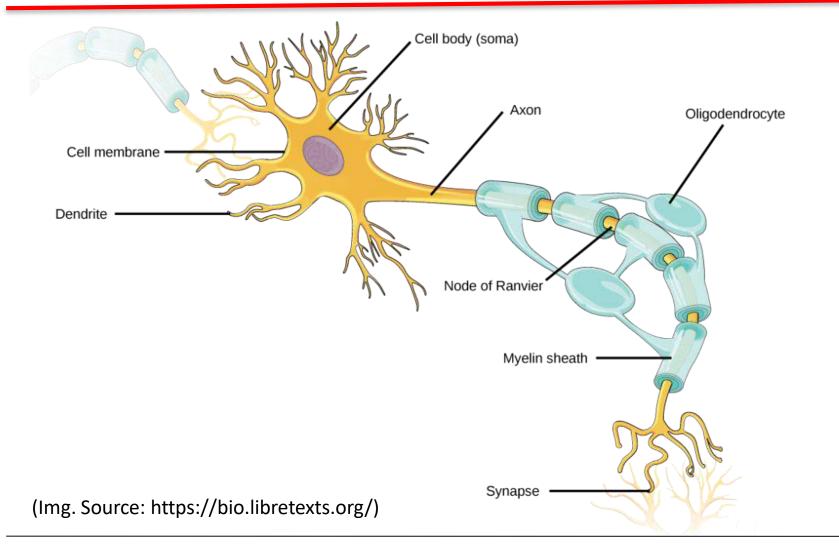


An electrical signal shooting down a nerve cell and then off to others in the brain. Learning strengthens the paths that these signals take, essentially "wiring" certain common paths through the brain.

How many Neurons in a human brain?

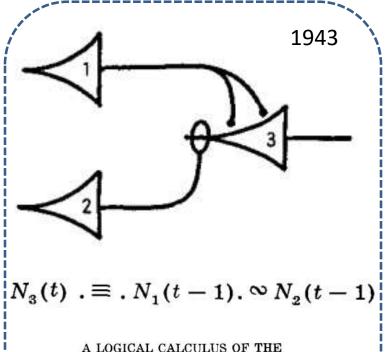
Image Source: <u>https://www.snexplores.org/</u> (imagination)

A Nerve Cell: Neuron



What are their computational abstractions in an Artificial Neural Network?

Perceptron: Modelling the Nerve cell



A LOGICAL CALCULUS OF THE IDEAS IMMANENT IN NERVOUS ACTIVITY

WARREN S. MCCULLOCH AND WALTER PITTS

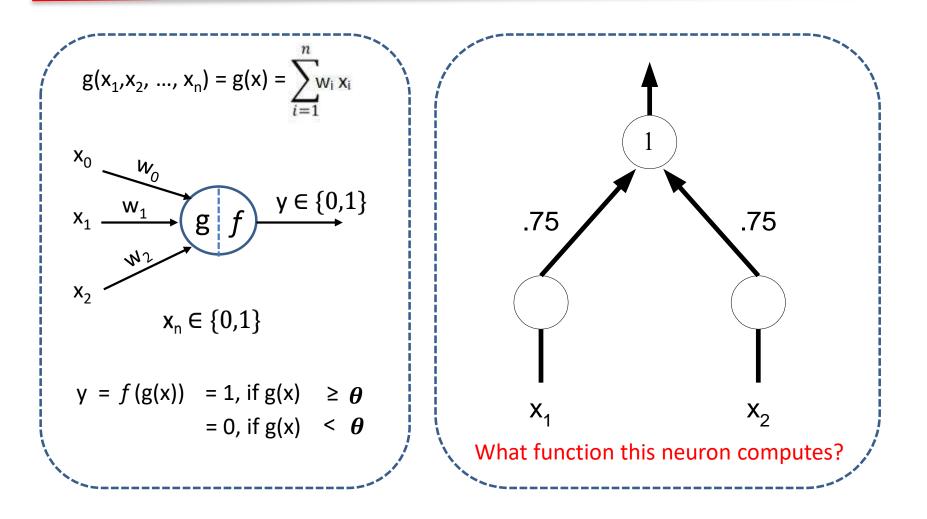
FROM THE UNIVERSITY OF ILLINOIS, COLLEGE OF MEDICINE, DEPARTMENT OF PSYCHIATRY AT THE ILLINOIS NEUROPSYCHIATRIC INSTITUTE, AND THE UNIVERSITY OF CHICAGO



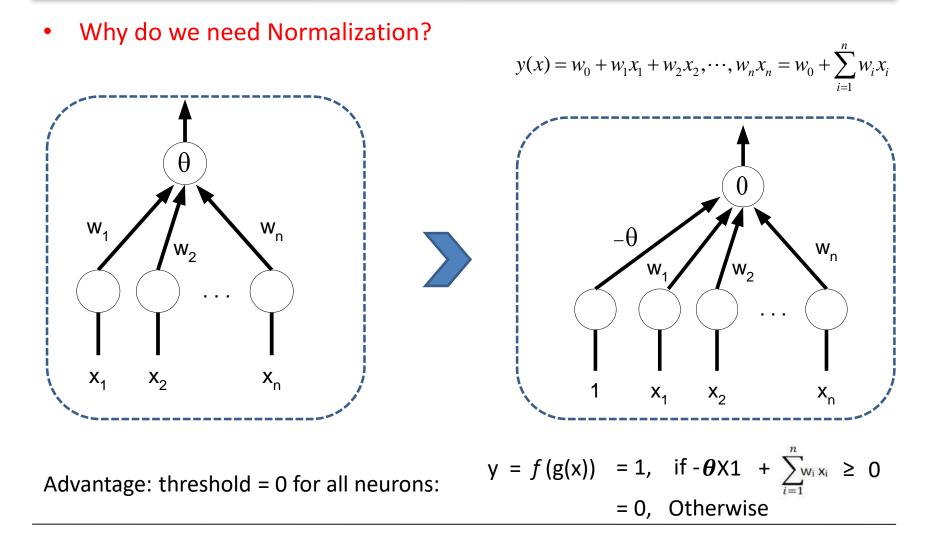
Frank Rosenblatt at IBM 704 (Electronic profile analyzing computer): a precursor to the perceptron, 1958.

(Image source: https://news.cornell.edu)

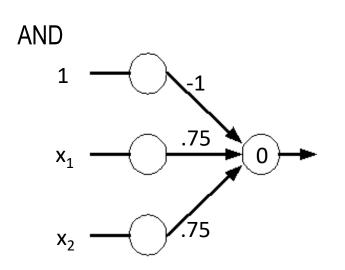
Perceptron: An Example

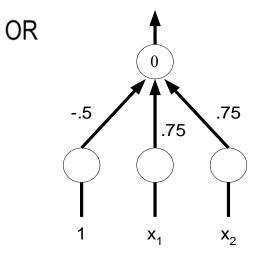


Normalizing thresholds

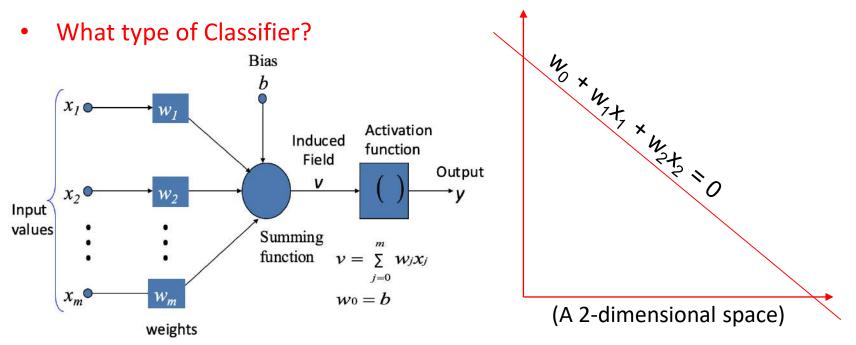


Normalized examples



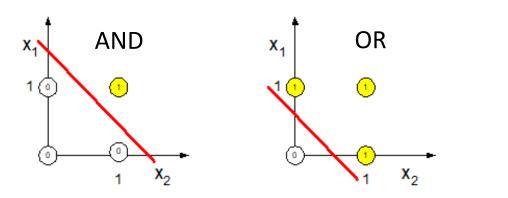


Perceptron as a Decision Surface

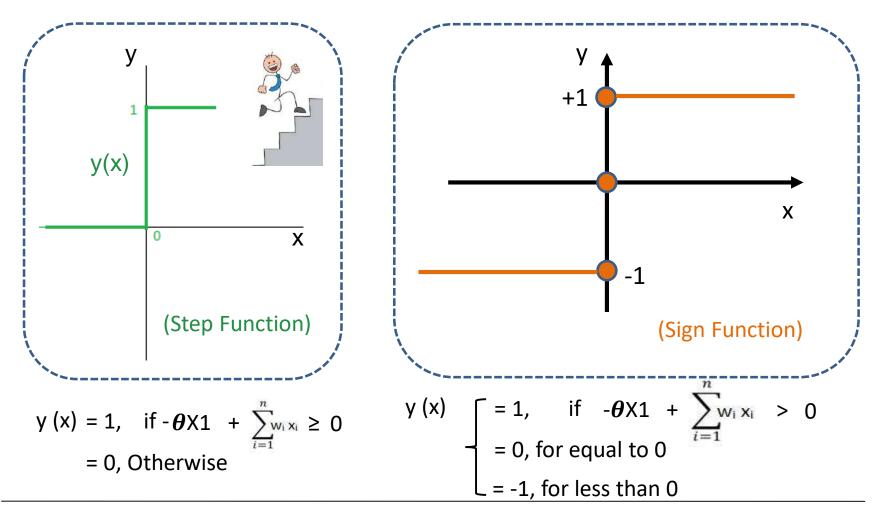


XOR?

• Can it solve Non-linear classification problems?



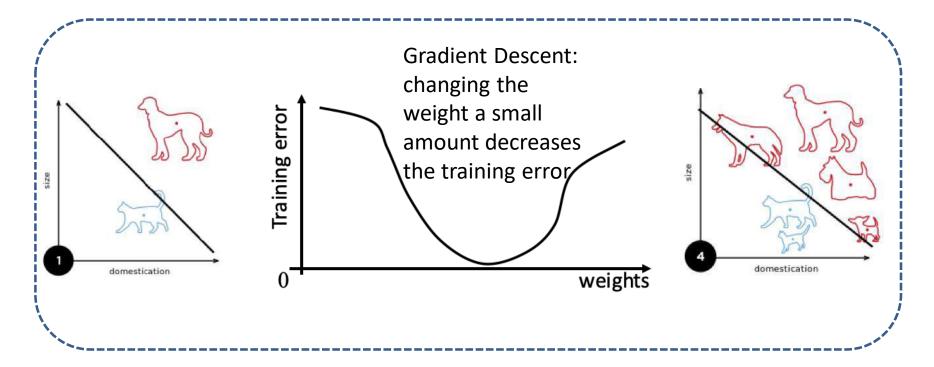
Activation Functions in a Perceptron



What about other activation functions like Sigmoid ?

Multi-layer Perceptron

Perceptron Training Example



An example: A perceptron updating its linear boundary as more training examples are added. (Image Source: Wiki)

Perceptron Training Algorithm

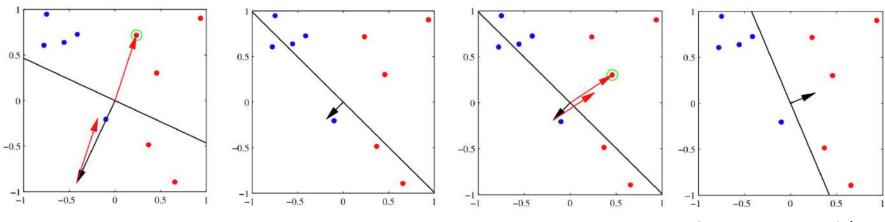


Image Source: PRML, Bishop

| if ($x \in N \&\& w.x \ge 0$) then |
|---|
| $\prod_{x \in \mathbb{N}} \alpha \alpha w.x \ge 0$ (nem |
| W = W - X; |
| endif; |
| |
| endwhile; |
| |
| // Algorithm converges when all th |
| inputs are classified correctly. |
| |

Perceptron Training Rule

$$w_{i} \leftarrow w_{i} + \Delta w_{i} \rightarrow \eta (t - 0) x_{i}$$
Let us see this through an example:
When all $(\eta, (t-0) \text{ and } x_{i})$ are
positive, w_{i} will increase and vice
versa:
 $x_{i} = 0.8, \eta = 0.1, t = 1, 0 = -1:$
 $\Rightarrow \Delta w_{i} = 0.1(1-(-1))0.8 = 0.16$

•o = perceptron output

If t = -1, o = 1, what will happen?

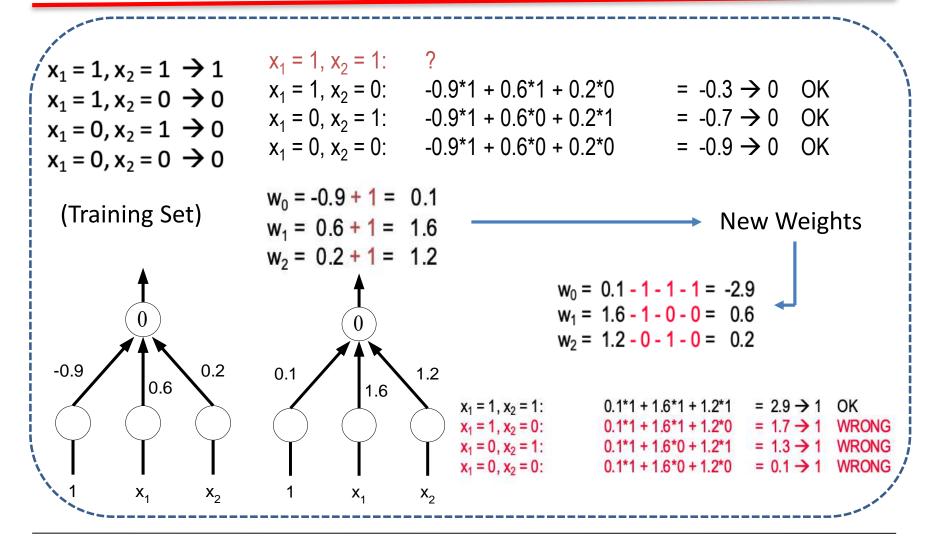
• η a small constant (e.g, 0.1) called the learning rate.

Why should this update rule converge toward successful weight values?

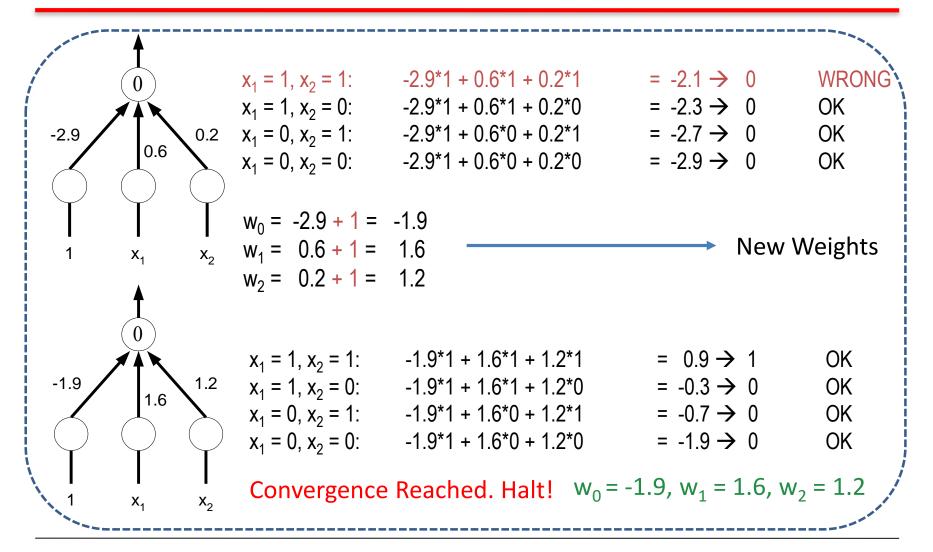
If training data is linearly separable and η is sufficiently small.

It updates the weights only when the predicted class is incorrect. The updates are based on whether the example is misclassified (binary classification).

Run through the algorithm: AND



Continued...



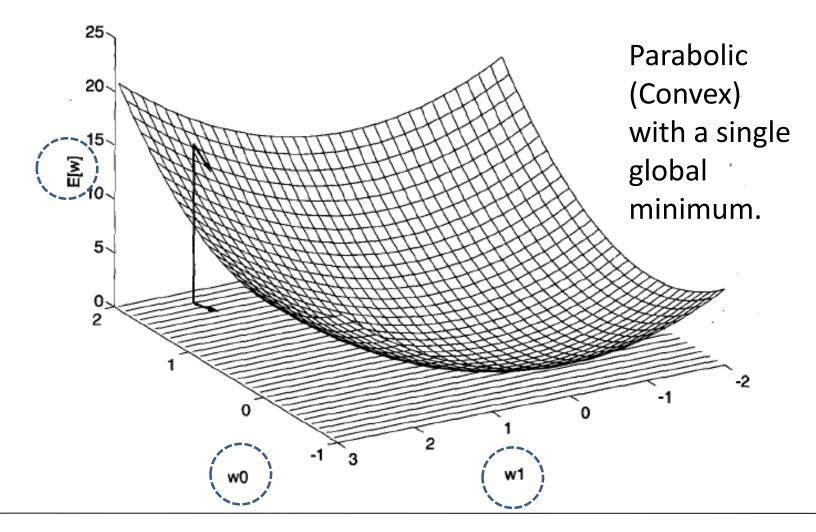
Gradient Descent and the Delta Rule

- If the training examples are NOT linearly separable (which the Perceptron rule cannot handle), the Delta rule converges towards a best-fit approximation to the target concept.
- The key-idea behind the delta rule is to use Gradient descent, a basis for Back-propagation algorithm.
- Delta rule is best understood by considering an un-thresholded Perceptron, i.e. a linear unit without threshold (or activation function).
- Let the linear unit be characterized by: $o = w_0 + w_1x_1 + w_2x_2 + ... + w_nx_n$
- Let us learn w_i's that minimize the squared error: $E[\vec{w}] \equiv \frac{1}{2} \sum_{d \in D} (t_d o_d)^2$

ADALINE: adaptive linear neural network based on MSE. Or Least mean square (LMS) Widrow Hoff

It updates the weights even if the predicted value is close to the correct one but not exactly right. The adjustment is proportional to the error, making it suitable for continuous outputs.

Visualizing Gradient Descent: Recap



 w_0 and w_1 : The two weights of a linear unit and E is the error.

Derivation of Gradient Descent: Recap

- How can we calculate the direction of $\frac{\partial I}{\partial u}$ surface?
- Gradient:

 $\nabla E[\vec{w}] \equiv \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \cdots, \frac{\partial E}{\partial w_n}\right]$

- When interpreted as a vector in weig the direction that produces the steepes
- The negative of this vector therefore decrease.
- The training rule: $\vec{w} \leftarrow \vec{w} + \Delta \vec{w}$ Where:

$$\begin{aligned} \frac{\partial E}{\partial w_i} &= \frac{\partial}{\partial w_i} \frac{1}{2} \sum_{d} (t_d - o_d)^2 \\ &= \frac{1}{2} \sum_{d} \frac{\partial}{\partial w_i} (t_d - o_d)^2 \\ &= \frac{1}{2} \sum_{d} 2(t_d - o_d) \frac{\partial}{\partial w_i} (t_d - o_d) \\ &= \sum_{d} (t_d - o_d) \frac{\partial}{\partial w_i} (t_d - \vec{w} \cdot \vec{x_d}) \\ \frac{\partial E}{\partial w_i} &= \sum_{d} (t_d - o_d) (-x_{i,d}) \end{aligned}$$

Substituting (2) in (1):

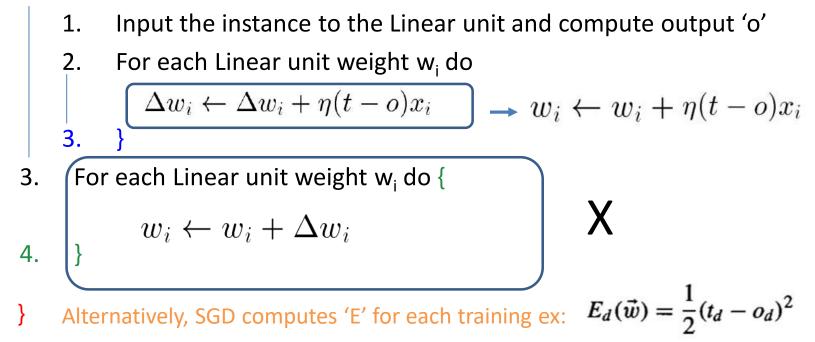
$$\Delta \vec{w} = -\eta \nabla E[\vec{w}] \sum \Delta w_i = -\eta \frac{\partial E}{\partial w_i} \quad (1) \qquad \Delta w_i = \eta \sum_{d \in D} (t_d - o_d) x_{id}$$

Gradient Descent & Stochastic Gradient Descent

- 1. Initialize each w_i to some small random value
- 2. Until the termination condition is met {
 - 1. Initialize each Δw_i to 0

3.

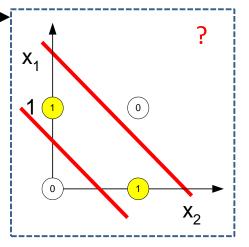
2. For each training example do {

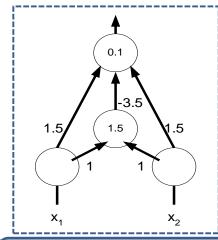


GD: the error is summed over all examples before updating weights. It might miss global minima when multiple local minima are present. In SGD/Incremental GD, weights are updated upon examining each training example.

Inadequacy of Perceptron

- Many simple problems are NOT linearly separable.
- Output is in the form of binary (0 or 1), NOT in the form of continuous values or probabilities.
- No memory and hence treat each input independently. Hence, limited ability to understand sequential or temporal patterns in data.





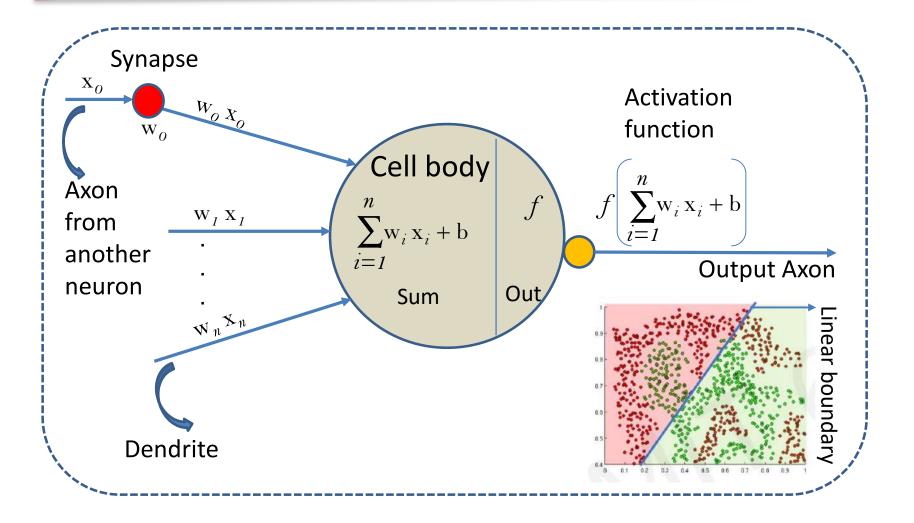
However, you can compute XOR by introducing a new, hidden unit as shown in the left.

Every classification problem has a Perceptron solution if enough hidden layers are used.

How to build such a multi-layer network?

Minsky & Papert's paper: Pretty much killed ANN research in 1970. Rebirth in 1980: faster parallel computers, newer algorithms (BPN,...), newer architectures (Hopfield nets).

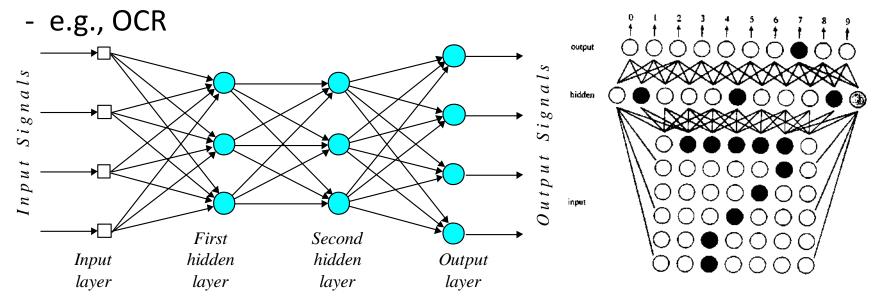
Recap: A Perceptron



Modelling Mathematically a Neuron

Hidden units in a Multi-layer Perceptron (MLP)

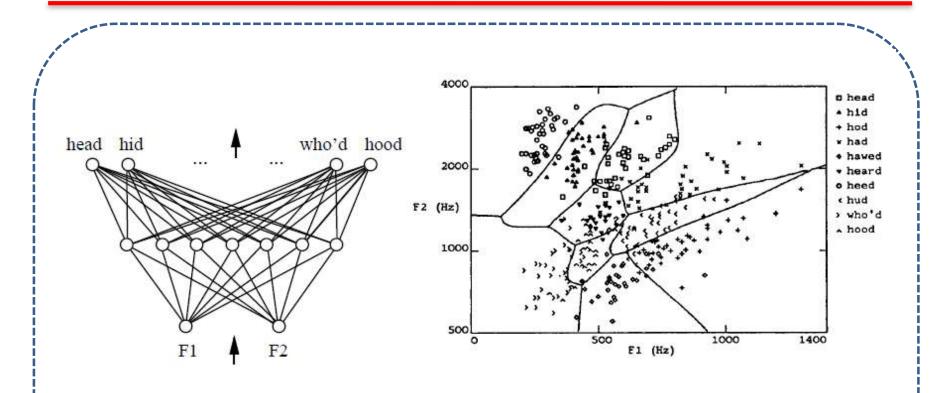
- The addition of hidden units allows the network to develop complex feature detectors (i.e., internal representations)



What does a hidden layer hide?

No. of nodes in a layer and no. of layers? Nodes too few: can't learn, Too many: poor generalization Expt. & tuning.

Decision Surface in a Multilayer Network: An Ex.

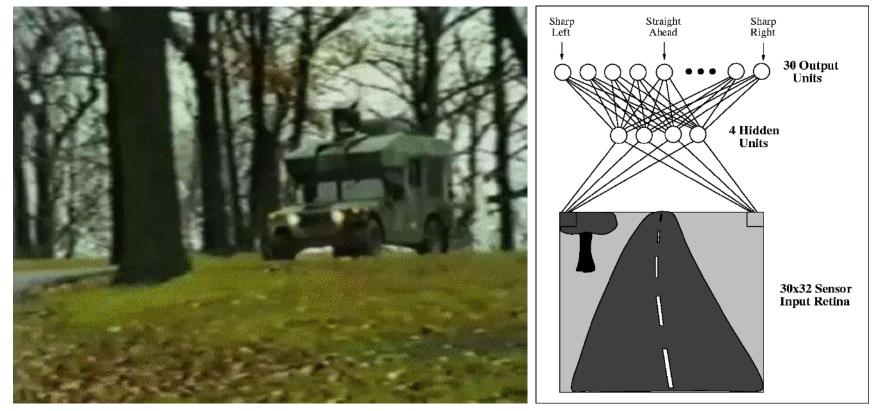


Input to the Network: two features from spectral analysis of a spoken sound

Output: vowel sound occurring in the context "h___d"

Image source: Tom Mitchell's Text

ALVINN: An Autonomous Land Vehicle In a Neural Network

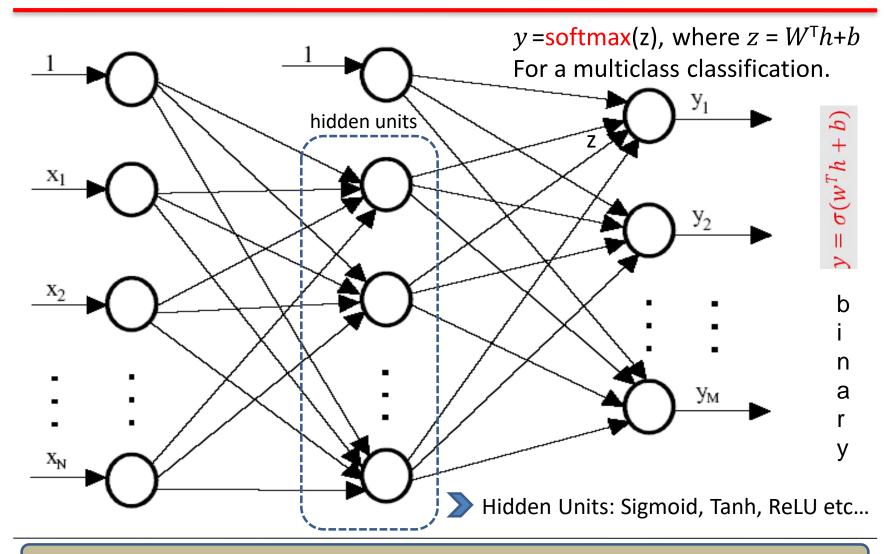


Source: https://www.ri.cmu.edu/

(1989: 3-layer Network)

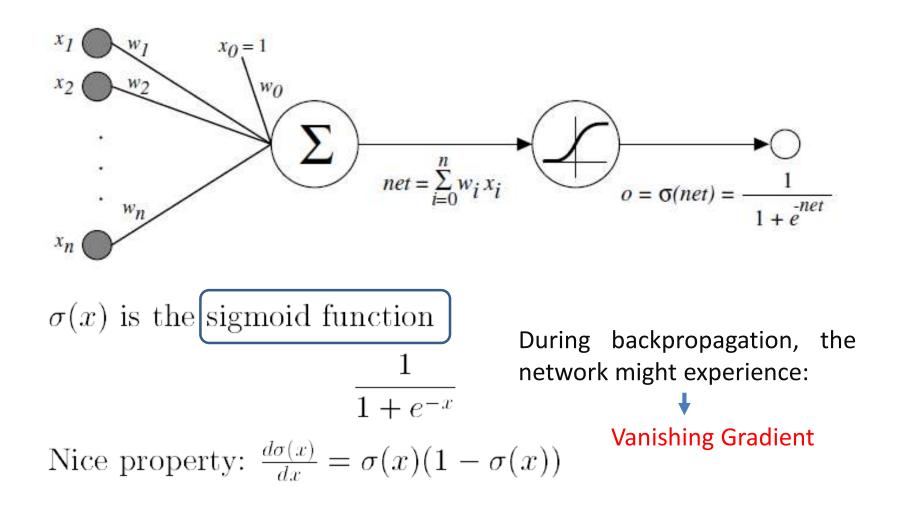
An application of a Backpropagation Neural Network in smart driving

An Example 3-layer Perceptron



What is Sparse Connectivity and what are its' Pros and Cons? Leaving out some links.

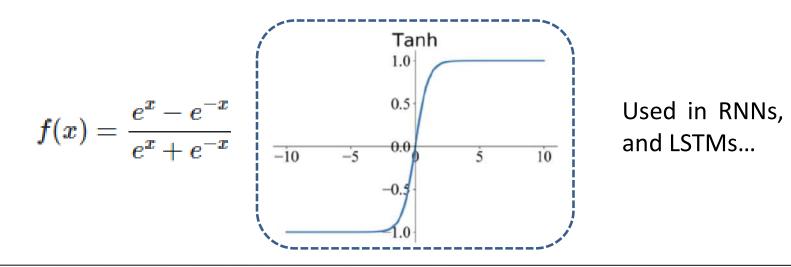
Activation Function: Sigmoid



Where should you worry much? Shallow or Deep NNs?

Activation Function: Tanh

- The hyperbolic tangent (tanh) activation function is another commonly used non-linear activation function in neural networks.
- The tanh function squashes the input values to the range [-1, 1]. It is similar to the sigmoid function, but its output is zero-centered, meaning that its output is centered around zero, unlike the sigmoid function which outputs values between 0 and 1.



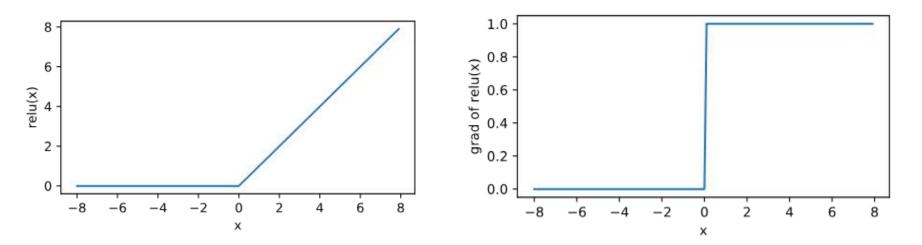
Does it suffer from Vanishing gradient problem?

Activation Functions: ReLU

Rectified linear unit function (ReLU) provides a very simple nonlinear transformation:

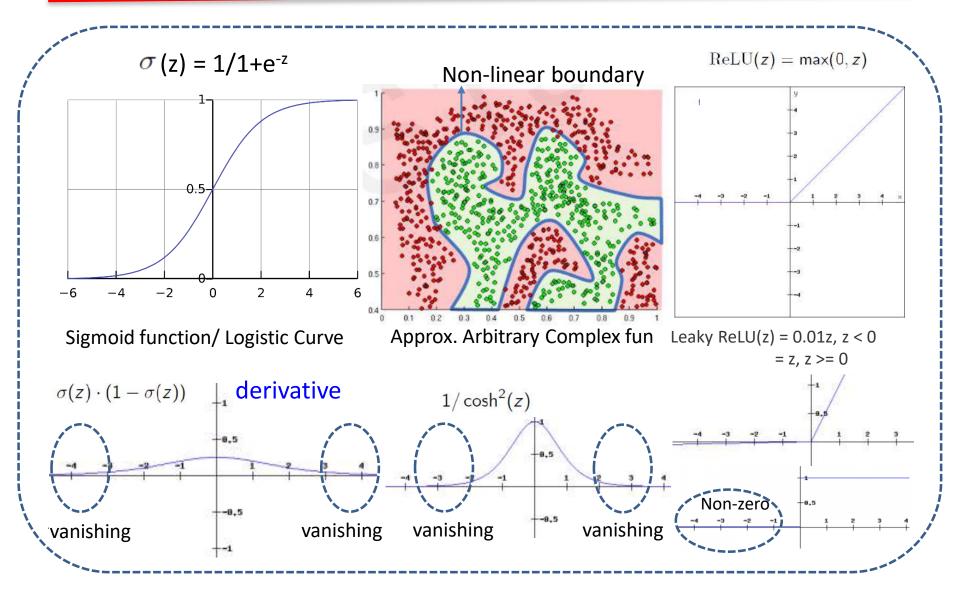
$$\mathsf{ReLU}(x) = \begin{cases} x, if \ x > 0 \\ o, if \ x \le 0 \end{cases}$$

What is ReLU'(x)?



Does it suffer from Vanishing gradient problem?

Vanishing Gradient in MLPs/BPNs



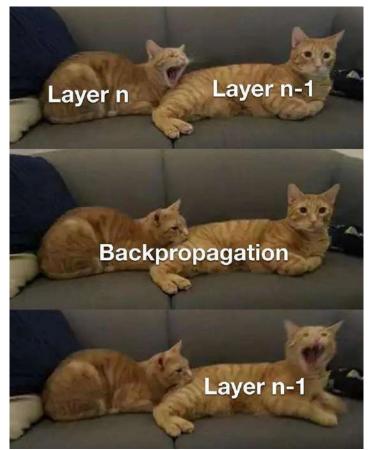
Gradient Descent for Sigmoid Unit

$$\begin{aligned} \frac{\partial E}{\partial w_i} &= \frac{\partial}{\partial w_i} \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2 \\ &= \frac{1}{2} \sum_d \frac{\partial}{\partial w_i} (t_d - o_d)^2 \\ &= \frac{1}{2} \sum_d 2(t_d - o_d) \frac{\partial}{\partial w_i} (t_d - o_d) \\ &= \sum_d (t_d - o_d) \left(-\frac{\partial o_d}{\partial w_i} \right) \\ &= -\sum_d (t_d - o_d) \frac{\partial o_d}{\partial net_d} \frac{\partial net_d}{\partial w_i} \end{aligned}$$

But we know: But we know: $\frac{\partial o_d}{\partial net_d} = \frac{\partial \sigma(net_d)}{\partial net_d} = o_d(1 - o_d)$ $\frac{\partial net_d}{\partial w_i} = \frac{\partial(\vec{w} \cdot \vec{x}_d)}{\partial w_i} = x_{i,d}$ $\sum_{d=1}^{N} \frac{\partial E}{\partial w_i} = -\sum_{d \in D} (t_d - o_d) o_d(1 - o_d) x_{i,d}$

Backpropagation Training Algorithm (BPN)

- Initialize weights (typically random!)
- Keep doing epochs
 - For each example 'e' in the training set do
 - forward pass to compute
 - O = neural-net-output (network, e)
 - miss = (T-O) at each output unit
 - backward pass to calculate deltas to weights
 - update all weights
 - end
- until tuning set error stops improving



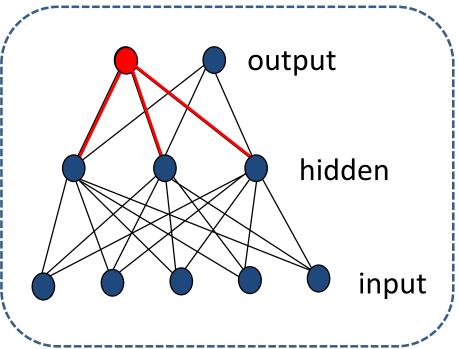
Error Backpropagation

• First calculate error of output units and use this to change the top layer of weights.

Current output: o_j =0.2 Correct output: t_j =1.0 Error $\delta_j = o_j(1-o_j)(t_j-o_j)$ 0.2(1-0.2)(1-0.2)=0.128

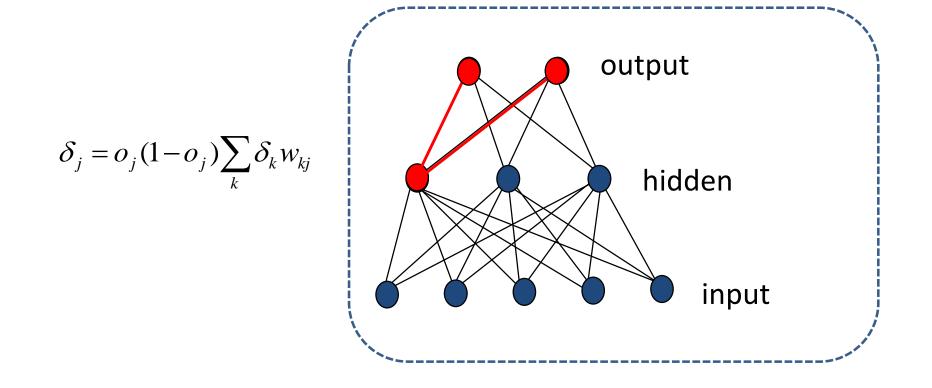
Update weights into j

$$\Delta w_{ji} = \eta \delta_j o_i$$



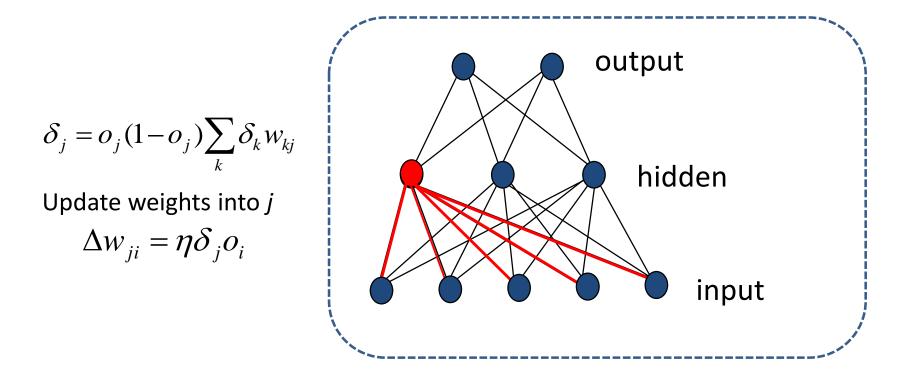
Error Backpropagation continued...

• Next calculate error for hidden units based on errors on the output units it feeds into.



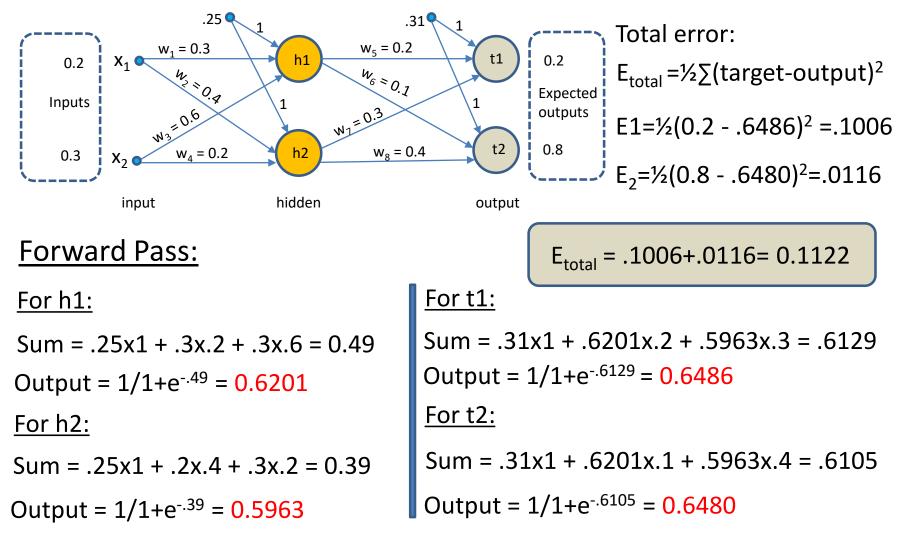
Error Backpropagation continued...

• Finally update bottom layer of weights based on errors calculated for hidden units.

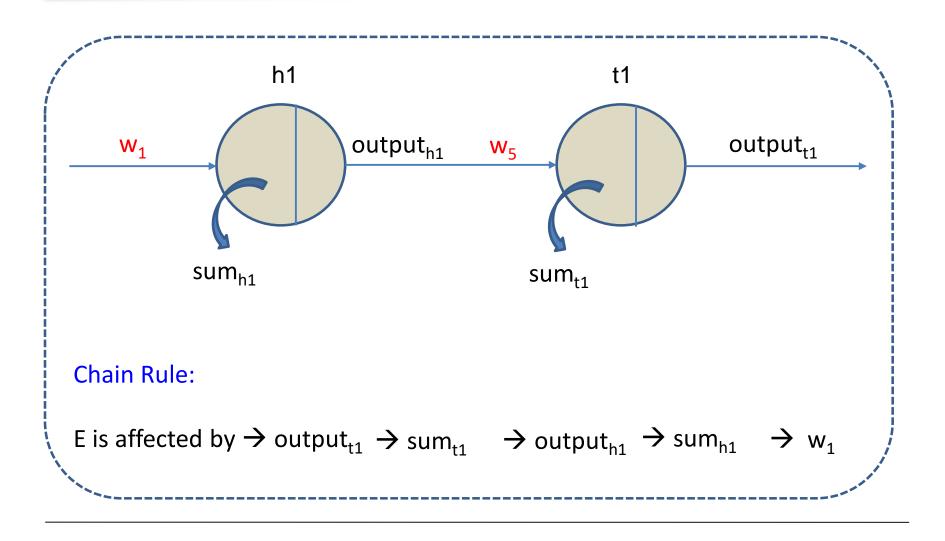


Example Backpropagation Neural Networks

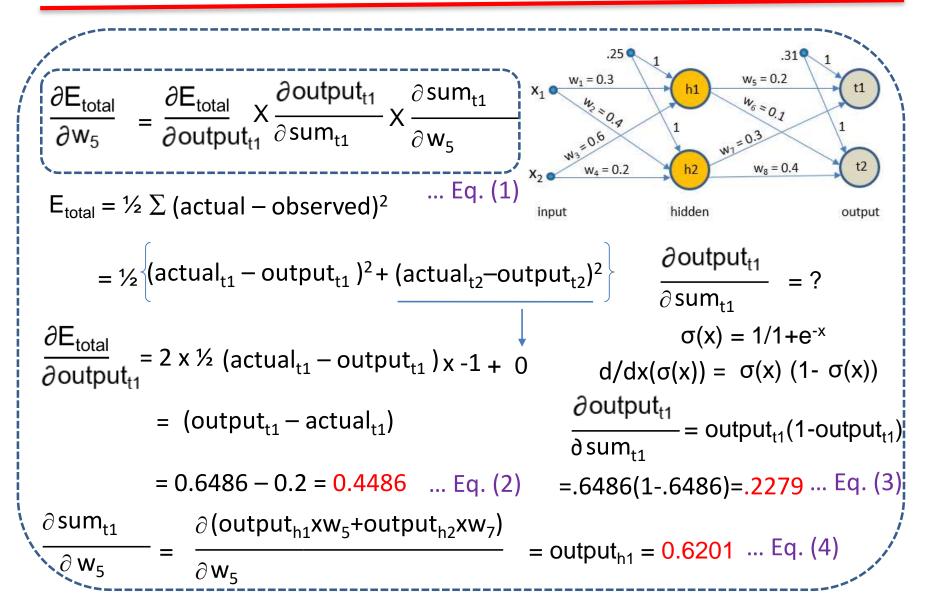
Learning rate: $\eta = 0.4$



Example Chain Rule



Backward Pass

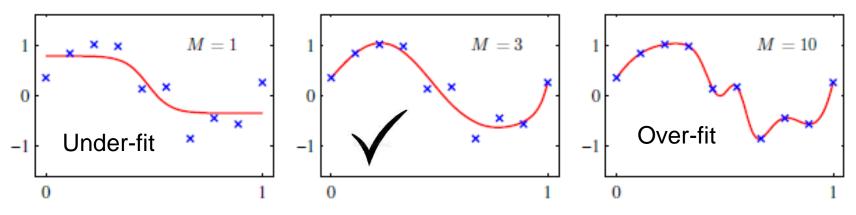


Expected Inputs outputs Continued... $w_{g} = 0.4$ 0.8 Eq. (1): $\frac{\partial E_{\text{total}}}{\partial w_5}$ = Eq.(1) x Eq.(2) x Eq.(3) = .4486 x .2279 x .6201 = .0634 > $w_5 = w_5 - \eta \frac{\partial E_{\text{total}}}{\partial w_5} = .2 - .4 \times .0634 =$.1746 $\frac{\partial \mathsf{E}_{\text{total}}}{\partial \mathsf{w}_6} = \frac{\partial \mathsf{E}_{\text{total}}}{\partial \text{output}_{t_2}} X \frac{\partial \text{output}_{t_2}}{\partial \text{sum}_{t_2}} X \frac{\partial \text{sum}_{t_2}}{\partial \mathsf{w}_6} = (.6480 - .8) \times (.6480 \times (1 - .6480)) \times .6201$ =-.152x.2281x.6201 = -.0215 $\gg w_6 = w_6 - \eta \frac{\partial E_{\text{total}}}{\partial w_6} = .1 - (.4x - .0215) = .1086$ $\frac{\partial E_{total}}{\partial w_7} = \frac{\partial E_{total}}{\partial output_{t1}} X \frac{\partial output_{t1}}{\partial sum_{t1}} X \frac{\partial sum_{t1}}{\partial w_7} = Eq.(2) \times Eq.(3) \times output_{h2}$ $= 0.4486 \times 0.2279 \times 0.5963 = 0.0609$ $w_7 = w_7 - \eta \frac{\partial E_{\text{total}}}{\partial w_7} = .3 - .4 \times .0609 = 0.3 - 0.02436 = 0.2756$

$w_5 = 0.2$ Expected Inputs outputs Continued... $w_{g} = 0.4$.5963 $\frac{\partial E_{\text{total}}}{\partial w_8} = \frac{\partial E_{\text{total}}}{\partial \text{output}_{t_2}} X \frac{\partial \text{output}_{t_2}}{\partial \text{sum}_{t_2}} X \frac{\partial \text{sum}_{t_2}}{\partial w_8} = (-.152) \text{x} .2281 \text{xoutput}_{h_2} = -0.0207$ Similarly, > $w_8 = w_8 - \eta \frac{\partial E_{\text{total}}}{\partial w_8} = 0.4 + 0.4 \times 0.0207 = 0.4 + 0.0083 = .4083$ $w_2 = .4007$... for you ... for you Now Compute Weights in the Hidden Layer (w_1 , w_2 , w_3 , and w_4): Chain becomes longer or <u>shorter</u>? For w₁: Where, $\frac{\partial E_1}{\partial w_1} = \frac{\partial E_1}{\partial \text{output}_{t1}} \times \frac{\partial \text{output}_{t1}}{\partial \text{sum}_{t1}} \times \frac{\partial \text{sum}_{t1}}{\partial \text{output}_{h1}} \times \frac{\partial \text{sum}_{t1}}{\partial \text{sum}_{h1}} \times \frac{\partial \text{sum}_{h1}}{\partial \text{sum}_{h1}} \times \frac{\partial \text{sum}_{h1}}{\partial w_1}$ $\frac{\partial E_1}{\partial w_1} = .4486 \text{ x } .2279 \text{ x } w5 \text{ x } (\text{output}_{h1} \text{ x } (1 - \text{output}_{h1})) \text{ x } 0.2 = 0.00096$ Now, $\frac{\partial E_2}{\partial w_1} = \frac{\partial E_2}{\partial \text{output}_{t2}} \times \frac{\partial \text{output}_{t2}}{\partial \text{sum}_{t2}} \times \frac{\partial \text{sum}_{t2}}{\partial \text{output}_{h1}} \times \frac{\partial \text{output}_{h1}}{\partial \text{sum}_{h1}} \times \frac{\partial \text{output}_{h1}}{\partial w_1}$ \sim = -.1520 x .2281 x w6 x .2356 x .2 = -.00016 $\ge \partial E_{total} / \partial w_1$ =.00096 - .00016=.0008

Regularization in Neural Networks

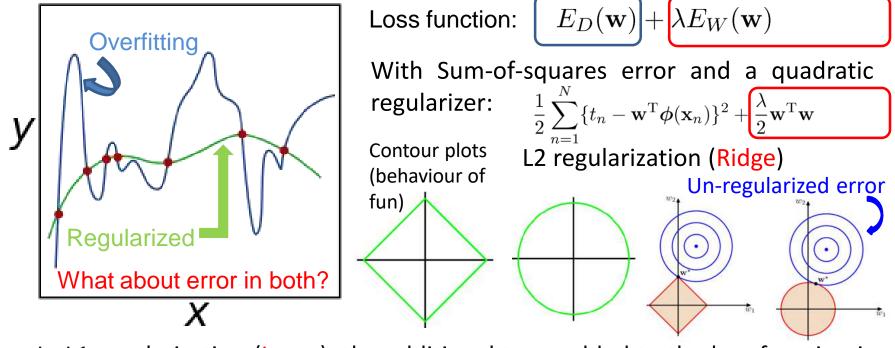
- Which one is a free parameter in a Neural network?
 - Input Output or Number of units in the hidden layer (M)
- Why Regularization is needed in Neural Networks?
 - To improve the generalization/learning outcome. To control impact of noise and fluctuations on the dataset. Alternatively, to avoid over-fitting.



(Fitting a Sinusoidal dataset with different number of hidden units and Sum-of-Squares error function optimized by Gradient descent)

Regularization: Weight Decay (L1/L2)

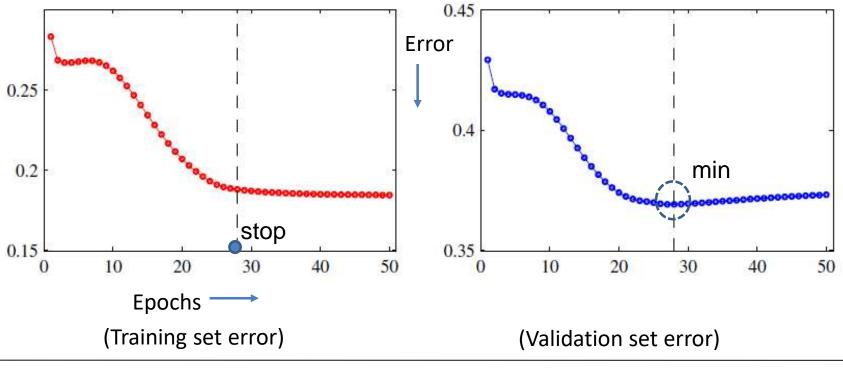
Control model complexity by the addition of a regularization term to the error function.



In L1 regularization (Lasso), the additional term added to the loss function is the sum of the absolute values of the weights. This encourages sparsity in the weights, effectively shrinking some of them to zero. $J_{L1}(\theta) = J(\theta) + \lambda \sum_{i=1}^{n} |\theta_i|$ *Where*, λ as the regularization parameter, ϑ as the vector of weights of the Network.

Regularization: Early Stopping

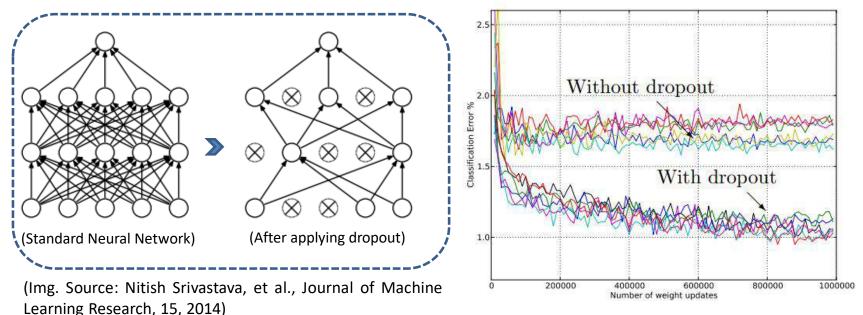
- Early stopping monitors the performance of the model on a validation set and stops training when the performance starts to degrade, thus preventing the model from overfitting to the training data.
- Example sinusoidal dataset



Img. Source: Bishop text

Stochastic Regularization: Dropout

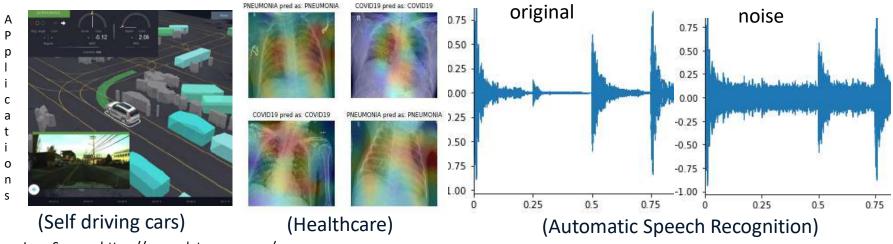
- Drop out each individual unit with some probability ρ (usually $\rho = 1/2$) by setting its activation to '0'.
- The key idea behind dropout is to prevent overfitting by adding noise to the network during training.



During inference (testing or prediction), dropout is typically turned off, and the full network is used. However, the weights are usually scaled by '1- ρ ' during inference to account for the fact that more units were active during training.

Regularization: Data Augmentation

- Data augmentation acts as a form of regularization by introducing additional variations and diversity into the training dataset.
- A technique used to artificially increase the size of a training dataset by applying various transformations to the existing data samples.
- Random rotation, Random scaling, Random cropping, Horizontal or vertical flipping, Adding noise (e.g., Gaussian noise), Changing brightness, contrast, or saturation



Img. Source: https://www.datacamp.com/

resize_and_rescale=keras.Sequential([layers.Resizing(IMG_SIZE, IMG_SIZE), layers.Rescaling(1./255)])













PyTorch Ex: BPNs for Predicting Age of Abalones

import pandas as pd import numpy as np from sklearn.model_selection import train_test_split from sklearn.preprocessing import StandardScaler import torch import torch.nn as nn import torch.optim as optim



| | Longth | Diamoton | Hojaht | Whole weight | Shucked_weight | Viccona woight | Shall waight | Pinge | |
|-----|------------------|---------------------------------------|------------------------|--------------|---|----------------|--------------|----------------------------------|--|
| | Length | Diameter | nergire | whore wergin | Shucked_weight | viscena_weight | SHEIT_WEIGHT | Kings | e |
| 0 | 0.455 | 0.365 | 0.095 | 0.5140 | 0.2245 | 0.1010 | 0.150 | 15 | rings he ag |
| 1 | 0.350 | 0.265 | 0.090 | 0.2255 | 0.0995 | 0.0485 | 0.070 | 7 | of rin e the |
| 2 | 0.530 | 0.420 | 0.135 | 0.6770 | 0.2565 | 0.1415 | 0.210 | 9 | (no ecide |
| 3 | 0.440 | 0.365 | 0.125 | 0.5160 | 0.2155 | 0.1140 | 0.155 | 10 | will de |
| 4 | 0.330 | 0.255 | 0.080 | 0.2050 | 0.0895 | 0.0395 | 0.055 | 7 | , Ea |
| cla | self.f self.f | · · · · · · · · · · · · · · · · · · · | r(10, 64) r(64, 32) | | <pre>train(model, criterion, optimizer, X_train_tensor, y_train_ten def evaluate(model, X_test, y_test): model.eval() with torch.no_grad(): outputs = model(X_test)</pre> | | | Epoch 30 Epoch 40 Epoch 50 | <pre>), Loss: 1110.1275), Loss: 1110.1275</pre> |

def forward(self, x): x = torch.relu(self.fc1(x))

x = torch.relu(self.fc2(x))
x = self.fc3(x)

return x

evaluate(model, X_test_tensor, y_test_tensor)

loss = mse(outputs, y test)

print(f"Test Loss: {loss.item()}")

mse = nn.MSELoss()

``-----

Epoch 70, Loss: 1110.1275.

Epoch 90, Loss: 1110.1275

Test Loss: 13.29509258270

Epoch 80, Loss: 1110.1275

Epoch 100, Loss: 1110.127

Thank You!