COMP9414/9814/3411: Artificial Intelligence

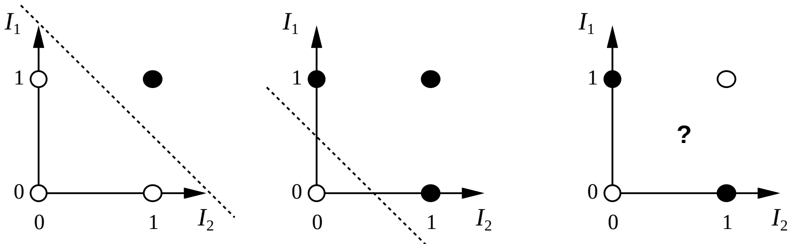
11. Neural Networks

Outline

- Multi-Layer Neural Networks
- Backpropagation
- Application - ALVINN
- Variations on Backprop
  - Cross Entropy, Weight Decay, Momentum
- Training Tips

Recall: Limitations of Perceptrons

Problem: many useful functions are not linearly separable (e.g. XOR)



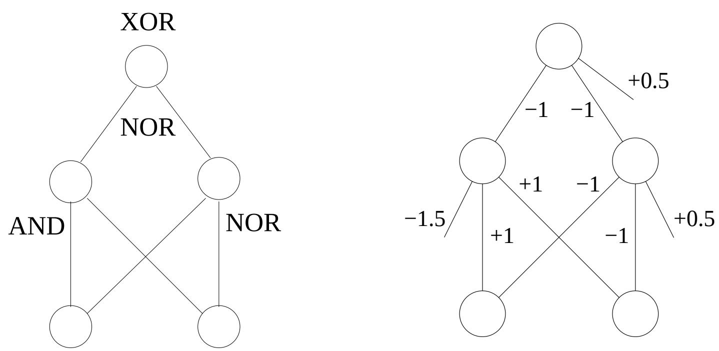
(a) I_1 **and** I_2 **(b)** I_1 **or** I_2 **(c)** I_1 **xor** I_2

Possible solution:

x_1 XOR x_2 can be written as: (x_1 AND x_2) NOR (x_1 NOR x_2)

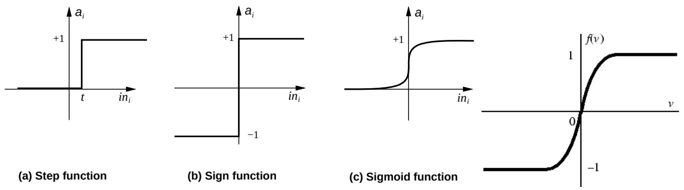
Recall that AND, OR and NOR can be implemented by perceptrons.

Multi-Layer Neural Networks



Problem: How can we train it to learn a new function? (credit assignment)

Key Idea



(a) Step function (b) Sign function (c) Sigmoid function

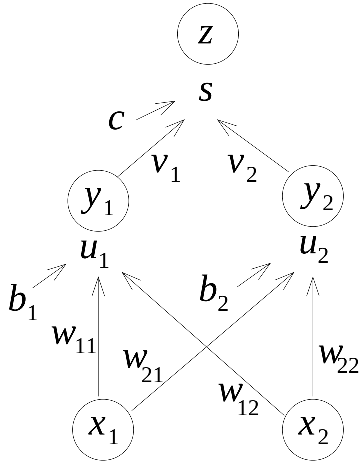
Replace the (discontinuous) step function with a differentiable function, such as the sigmoid:

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

or hyperbolic tangent

$$g(s) = \tanh(s) = \frac{e^s - e^{-s}}{e^s + e^{-s}} = 2\Big(\frac{1}{1+e^{-2s}}\Big) - 1$$

Forward Pass



$$\begin{aligned}
u_1 &= b_1 + w_{11}x_1 + w_{12}x_2 \\
y_1 &= g(u_1) \\
s &= c + v_1 y_1 + v_2 y_2 \\
z &= g(s) \\
E &= \frac{1}{2}\sum (z-t)^2
\end{aligned}$$

Gradient Descent

We define an **error function** E to be (half) the sum over all input patterns of the square of the difference between actual output and desired output

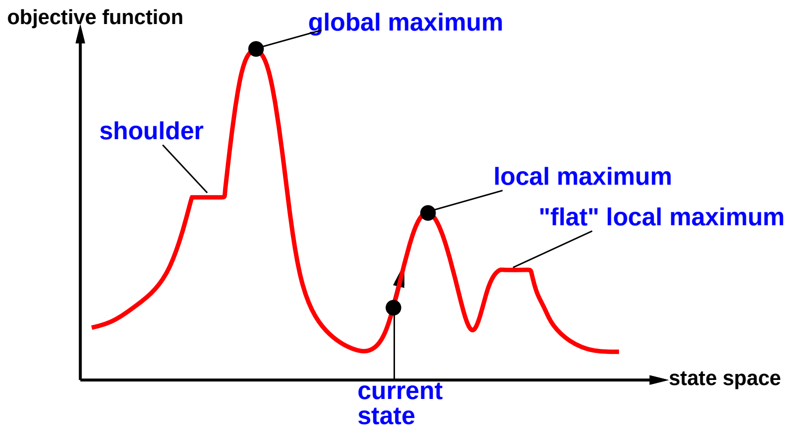
$$E = \frac{1}{2}\sum (z-t)^2$$

If we think of E as height, it defines an error **landscape** on the weight space. The aim is to find a set of weights for which E is very low. This is done by moving in the steepest downhill direction.

$$w \leftarrow w - \eta\,\frac{\partial E}{\partial w}$$

Parameter η is called the learning rate.

Local Search in Weight Space



Chain Rule

If, say

$$y = y(u)$$

$$u = u(x)$$

Then

$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial u}\,\frac{\partial u}{\partial x}$$

This principle can be used to compute the partial derivatives in an efficient and localized manner. Note that the transfer function must be differentiable (usually sigmoid, or tanh).

Note: if $z(s) = \frac{1}{1+e^{-s}}, \qquad z'(s) = z(1-z).$

if $z(s) = \tanh(s), \qquad z'(s) = 1 - z^2.$

Backpropagation

Partial Derivatives

$$\begin{aligned}
\frac{\partial E}{\partial z} &= z - t \\
\frac{dz}{ds} &= g'(s) = z(1-z) \\
\frac{\partial s}{\partial y_1} &= v_1 \\
\frac{dy_1}{du_1} &= y_1(1-y_1)
\end{aligned}$$

Useful notation

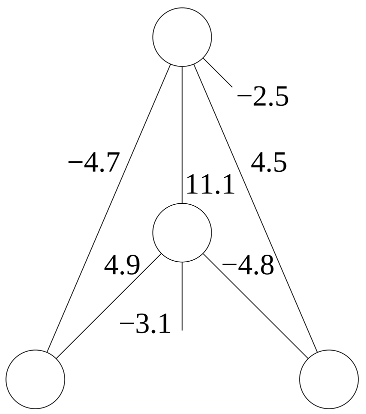
$$\delta_{\text{out}} = \frac{\partial E}{\partial s} \qquad \delta_1 = \frac{\partial E}{\partial u_1} \qquad \delta_2 = \frac{\partial E}{\partial u_2}$$

Then

$$\begin{aligned}
\delta_{\text{out}} &= (z-t)\, z\, (1-z) \\
\frac{\partial E}{\partial v_1} &= \delta_{\text{out}}\, y_1 \\
\delta_1 &= \delta_{\text{out}}\, v_1\, y_1\, (1-y_1) \\
\frac{\partial E}{\partial w_{11}} &= \delta_1\, x_1
\end{aligned}$$

Partial derivatives can be calculated efficiently by packpropagating deltas through the network.

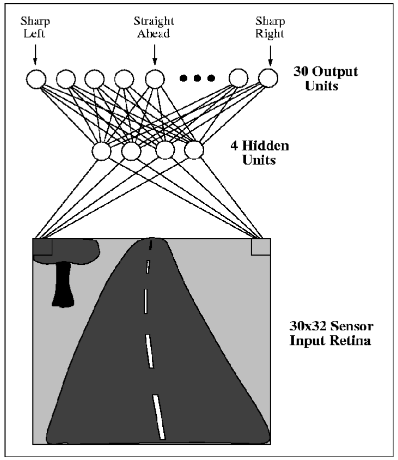
Trained XOR Network

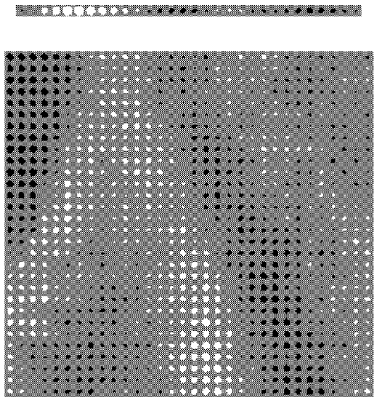


Neural Network – Applications

- Autonomous Driving
- Game Playing
- Credit Card Fraud Detection
- Handwriting Recognition
- Financial Prediction

ALVINN





ALVINN

- Autonomous Land Vehicle In a Neural Network
- later version included a sonar range finder
  - 8×32 range finder input retina
  - 29 hidden units
  - 45 output units
- Supervised Learning, from human actions (Behavioral Cloning)
  - additional “transformed” training items to cover emergency situations
- drove autonomously from coast to coast

Variations on Backprop

- Cross Entropy
  - problem: least squares error function unsuitable for classification, where target = 0 or 1
  - mathematical theory: maximum likelihood
  - solution: replace with cross entropy error function
- Weight Decay
  - problem: weights “blow up”, and inhibit further learning
  - mathematical theory: Bayes’ rule
  - solution: add weight decay term to error function
- Momentum
  - problem: weights oscillate in a “rain gutter”
  - solution: weighted average of gradient over time

Cross Entropy

For classification tasks, target t is either 0 or 1, so better to use

$$E = -t\log(z) - (1-t)\log(1-z)$$

This can be justified mathematically, and works well in practice – especially when negative examples vastly outweigh positive ones.
It also makes the backprop computations simpler

$$\frac{\partial E}{\partial z} = \frac{z-t}{z(1-z)}$$

$$\text{if} \quad z = \frac{1}{1+e^{-s}},$$

$$\frac{\partial E}{\partial s} = \frac{\partial E}{\partial z}\frac{\partial z}{\partial s} = z - t$$

Maximum Likelihood

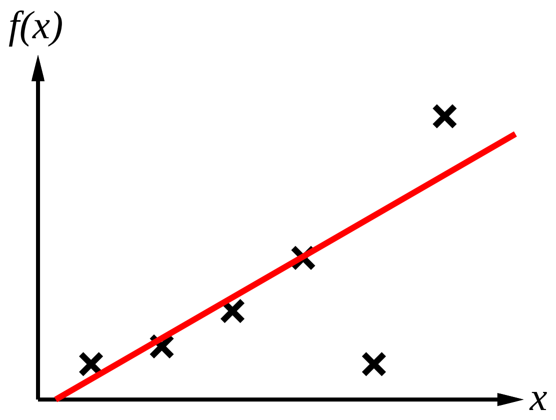
H is a class of hypotheses

$P(D|h)$ = probability of data D being generated under hypothesis $h \in H$.

$\log P(D|h)$ is called the likelihood.

ML Principle: Choose $h \in H$ which maximizes the likelihood,
i.e. maximizes $P(D|h)$ [or, maximizes $\log P(D|h)$]

Least Squares Line Fitting



Derivation of Least Squares

Suppose data generated by a linear function h, plus Gaussian noise with standard deviation σ.

$$\begin{aligned}
P(D|h) &= \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{1}{2\sigma^2}(d_i - h(x_i))^2} \\
\log P(D|h) &= \sum_{i=1}^{m} -\frac{1}{2\sigma^2}(d_i - h(x_i))^2 - \log(\sigma) - \frac{1}{2}\log(2\pi) \\
h_{ML} &= \mathrm{argmax}_{h\in H}\ \log P(D|h) \\
&= \mathrm{argmin}_{h\in H} \sum_{i=1}^{m} (d_i - h(x_i))^2
\end{aligned}$$

(Note: we do not need to know σ)

Derivation of Cross Entropy

For classification tasks, d is either 0 or 1.
Assume D generated by hypothesis h as follows:

$$\begin{aligned}
P(1|h(x_i)) &= h(x_i) \\
P(0|h(x_i)) &= (1 - h(x_i)) \\
\text{i.e.} \quad P(d_i|h(x_i)) &= h(x_i)^{d_i}(1 - h(x_i))^{1-d_i}
\end{aligned}$$

then

$$\begin{aligned}
\log P(D|h) &= \sum_{i=1}^{m} d_i \log h(x_i) + (1 - d_i)\log(1 - h(x_i)) \\
h_{ML} &= \mathrm{argmax}_{h\in H} \sum_{i=1}^{m} d_i \log h(x_i) + (1 - d_i)\log(1 - h(x_i))
\end{aligned}$$

(Can be generalized to multiple classes.)

Bayes Rule

H is a class of hypotheses

$P(D|h)$ = probability of data D being generated under hypothesis $h \in H$.

$P(h|D)$ = probability that h is correct, given that data D were observed.

Bayes' Theorem:

$$\begin{aligned} P(h|D)P(D) &= P(D|h)P(h) \\ P(h|D) &= \frac{P(D|h)P(h)}{P(D)} \end{aligned}$$

$P(h)$ is called the prior.

Example: Medical Diagnosis

Suppose we have a 98% accurate test for a type of cancer which occurs in 1% of patients. If a patient tests positive, what is the probability that they have the cancer?

Weight Decay

Assume that small weights are more likely to occur than large weights, i.e.

$$P(w) = \frac{1}{Z} e^{-\frac{\lambda}{2}\sum_j w_j^2}$$

where Z is a normalizing constant. Then the cost function becomes:

$$E = \frac{1}{2}\sum_i (z_i - t_i)^2 + \frac{\lambda}{2}\sum_j w_j^2$$

This can prevent the weights from "saturating" to very high values.

Problem: need to determine λ from experience, or empirically.

Momentum

If landscape is shaped like a "rain gutter", weights will tend to oscillate without much improvement.

Solution: add a momentum factor

$$\begin{aligned} \delta w &\leftarrow \alpha\,\delta w + (1-\alpha)\frac{\partial E}{\partial w} \\ w &\leftarrow w - \eta\,\delta w \end{aligned}$$

Hopefully, this will dampen sideways oscillations but amplify downhill motion by $\frac{1}{1-\alpha}$.

Conjugate Gradients

Compute matrix of second derivatives $\frac{\partial^2 E}{\partial w_i \partial w_j}$ (called the Hessian).

Approximate the landscape with a quadratic function (paraboloid).

Jump to the minimum of this quadratic function.

Natural Gradients (Amari, 1995)

Use methods from information geometry to find a "natural" re-scaling of the partial derivatives.

Training Tips

- re-scale inputs and outputs to be in the range 0 to 1 or -1 to 1
- initialize weights to very small random values
- on-line or batch learning
- three different ways to prevent overfitting:
  - limit the number of hidden nodes or connections
  - limit the training time, using a validation set
  - weight decay
- adjust learning rate and momentum to suit the particular task