

MAT8034: Machine Learning

Deep Learning

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https://fangkongx.github.io/Teaching/MAT8034/Spring2025/index.html

Part of slide credit: ai.berkeley.edu; SJTU VE445

Outline

- History of artificial neural nets
- Perceptron
- Multilayer perceptron networks
- Activation functions
- Training: backpropagation
- Modules in modern neural networks

History of artificial neural nets

Brief history of artificial neural nets

The First wave

- 1943 McCulloch and Pitts proposed the McCulloch-Pitts neuron model
- 1958 Rosenblatt introduced the simple single layer networks now called Perceptrons
- 1969 Minsky and Papert's book Perceptrons demonstrated the limitation of single layer perceptrons, and almost the whole field went into hibernation

The Second wave

 1986 The Back-Propagation learning algorithm for Multi-Layer Perceptrons was rediscovered and the whole field took off again

The Third wave

- 2006 Deep (neural networks) Learning gains popularity
- 2012 made significant break-through in many applications

Biological neuron structure



Slide credit: Ray Mooney

Biological neural communication

- 细胞膜间的电位表现出的电信号称为动作电位
- 电信号从细胞体中产生,沿着轴突往下传,并且导 致突触末梢释放神经递质介质
- 介质通过化学扩散从突触传递到其他神经元的树突
- 神经递质可以是兴奋的或者是抑制的
- 如果从其他神经元来的神经递质是兴奋的且超过某个阈值,将会触发一个动作电位



McCulloch-Pitts neuron model [1943]

- Model the network as a graph, where the units are nodes, and the synaptic connections are weighted edges from node *i* to node *j*, with the weight as w_{j,i}
- The input of the unit is:

$$\operatorname{net}_j = \sum_i w_{j,i} \cdot o_i$$

- The output of the unit is:
 - 0 if $net_j < T_j$; 1 otherwise
 - T_j is the threshold

Slide credit: Ray Mooney



Single-layer perception by Rosenblatt [1958]



Slide credit: Weinan Zhang

Training perception



□ 训练

$$w_i = w_i + \eta (y - \hat{y}) x_i$$

$$b = b + \eta (y - \hat{y})$$

- 如果输出正确,则不 进行操作
- 如果输出高了,降低 正输入的权重
- 如果输出低了,增加 正输入的权重

Slide credit: Weinan Zhang

Limitation of perception

- Minsky and Papert [1969] showed that some rather elementary computations, such as XOR problem, could not be done by Rosenblatt's one-layer perceptron
- However Rosenblatt believed the limitations could be overcome if more layers of units to be added, but no learning algorithm known to obtain the weights yet



Solution: Add hidden layers

Adding hidden layers to learn more general scenarios



Slide credit: Weinan Zhang

Computation

Single-layer function

•
$$f_{\theta}(x) = \sigma(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

Multi-layer function

•
$$h_1(x) = \sigma(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

•
$$h_2(x) = \sigma(\theta_3 + \theta_4 x_1 + \theta_5 x_2)$$

• $f_{\theta}(x) = \sigma(\theta_6 + \theta_7 h_1 + \theta_8 h_2)$





Non-linear activation functions

- Adding non-linearity allows the network to learn and represent complex patterns in the data
- Common non-linear activation functions







intermediate output $h_1 = \sigma(w_{11}x_1 + w_{21}x_2 + w_{31}x_3)$ $= \frac{1}{1 + e^{-(w_{11}x_1 + w_{21}x_2 + w_{31}x_3)}}$



intermediate output $h_2 = \sigma(w_{12}x_1 + w_{22}x_2 + w_{32}x_3)$ $= \frac{1}{1 + e^{-(w_{12}x_1 + w_{22}x_2 + w_{32}x_3)}}$



$$y = \sigma(w_1h_1 + w_2h_2)$$

= $\frac{1}{1 + e^{-(w_1h_1 + w_2h_2)}}$



 $y = \sigma(w_1h_1 + w_2h_2)$ = $\sigma(w_1\sigma(w_{11}x_1 + w_{21}x_2 + w_{31}x_3) + w_2\sigma(w_{12}x_1 + w_{22}x_2 + w_{32}x_3))$

Vectorization

$$y = \boldsymbol{\sigma}(w_1h_1 + w_2h_2)$$

= $\boldsymbol{\sigma}(w_1\boldsymbol{\sigma}(w_{11}x_1 + w_{21}x_2 + w_{31}x_3) + w_2\boldsymbol{\sigma}(w_{12}x_1 + w_{22}x_2 + w_{32}x_3))$

The same equation, formatted with matrices:

$$\sigma \left(\begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix} \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \\ w_{31} & w_{32} \end{bmatrix} \right)$$

= $\sigma \left(\begin{bmatrix} w_{11}x_1 + w_{21}x_2 + w_{31}x_3 & w_{12}x_1 + w_{22}x_2 + w_{32}x_3 \end{bmatrix} \right)$
= $\begin{bmatrix} h_1 & h_2 \end{bmatrix}$

$$\boldsymbol{\sigma}\left(\left[\begin{array}{cc}h_1 & h_2\end{array}\right] \left[\begin{array}{c}w_1\\w_2\end{array}\right]\right) = \boldsymbol{\sigma}(w_1h_1 + w_2h_2) = y$$

The same equation, formatted more compactly by introducing variables representing each matrix:

$$\sigma(x \times W_{\text{layer 1}}) = h \qquad \sigma(h \times W_{\text{layer 2}}) = y$$



Multi-Layer Neural Network

- Input to a layer: some *dim(x)*-dimensional input vector
- Output of a layer: some *dim(y)*-dimensional output vector
 - dim(y) is the number of neurons in the layer (1 output per neuron)
- Process of converting input to output:
 - Multiply the (1, dim(x)) input vector with a (dim(x), dim(y)) weight vector.
 The result has shape (1, dim(y)).
 - Apply some non-linear function (e.g. sigmoid) to the result.
 The result still has shape (1, dim(y)).
- Big idea: Chain layers together
 - The input could come from a previous layer's output
 - The output could be used as the input to the next layer

Deep Neural Network



$$z_i^{(k)} = \sigma(\sum_j W_{i,j}^{(k-1,k)} z_j^{(k-1)})$$

 σ = nonlinear activation function

Universal approximation theorem

Theorem (Universal Function Approximators). A two-layer neural network with a sufficient number of neurons can approximate any continuous function to any desired accuracy.



Hornik, Kurt, Maxwell Stinchcombe, and Halbert White. "Multilayer feedforward networks are universal approximators." *Neural networks* 2.5 (1989): 359-366

Increasing power of approximation

 With more neurons, its approximation power increases. The decision boundary covers more details (risk of overfitting)



 Usually in applications, we use more layers with structures to approximate complex functions instead of one hidden layer with many neurons

Connection to the kernel methods

Connection to the kernel methods

Kernel methods

- Design the non-linear feature map function
- The performance significantly depends on the choice of feature map
- Feature engineering: process of choosing the feature maps
- Neural network
 - Automatically learn the right feature map
 - Requires often less feature engineering



Training: Backpropagation

Review: Derivatives and Gradients

• What is the derivative of the function $g(x) = x^2 + 3$?

$$\frac{dg}{dx} = 2x$$

What is the derivative of g(x) at x=5?

$$\frac{dg}{dx}|_{x=5} = 10$$

Review: Derivatives and Gradients

- What is the gradient of the function $g(x, y) = x^2 y$?
 - Recall: Gradient is a vector of partial derivatives with respect to each variable

$$\nabla g = \begin{bmatrix} \frac{\partial f}{\partial x} \\ \\ \frac{\partial f}{\partial y} \end{bmatrix} = \begin{bmatrix} 2xy \\ \\ x^2 \end{bmatrix}$$

What is the derivative of g(x, y) at x=0.5, y=0.5?

$$\nabla g|_{x=0.5,y=0.5} = \begin{bmatrix} 2(0.5)(0.5) \\ (0.5^2) \end{bmatrix} = \begin{bmatrix} 0.5 \\ 0.25 \end{bmatrix}$$

1-D Optimization



• Could evaluate $g(w_0 + h)$ and $g(w_0 - h)$

- Then step in best direction
- Or, evaluate derivative:

$$\frac{\partial g(w_0)}{\partial w} = \lim_{h \to 0} \frac{g(w_0 + h) - g(w_0 - h)}{2h}$$

Tells which direction to step into

2-D Optimization



https://machinelearningmastery.com/2d-test-functions-for-function-optimization/

Gradient descent

- Perform update in downhill direction for each coordinate
- The steeper the slope (i.e. the higher the derivative) the bigger the step for that coordinate
- E.g., consider: $g(w_1, w_2)$
 - Updates:

$$w_{1} \leftarrow w_{1} - \alpha * \frac{\partial g}{\partial w_{1}}(w_{1}, w_{2})$$
$$w_{2} \leftarrow w_{2} - \alpha * \frac{\partial g}{\partial w_{2}}(w_{1}, w_{2})$$

Updates in vector notation:

$$w \leftarrow w - \alpha * \nabla_w g(w)$$

with:
$$\nabla_w g(w) = \begin{bmatrix} \frac{\partial g}{\partial w_1}(w) \\ \frac{\partial g}{\partial w_2}(w) \end{bmatrix}$$

= gradient

Gradient descent

- Idea:
 - Start somewhere
 - Repeat: Take a step in the gradient direction



https://ludovicarnold.com/teaching/optimization/gradient-descent/

Gradient in n dimensions

$$\nabla g = \begin{bmatrix} \frac{\partial g}{\partial w_1} \\ \frac{\partial g}{\partial w_2} \\ \cdots \\ \frac{\partial g}{\partial w_n} \end{bmatrix}$$

Optimization procedure: Gradient descent

• init
$$w$$

$$w \leftarrow w - \alpha * \nabla g(w)$$

• \alpha: learning rate --- tweaking parameter that needs to be chosen carefully

Training Neural Networks

 Step 1: For each input in the training (sub)set x, predict a classification y using the current weights

$$\sigma(x \times W_{\text{layer 1}}) = h \qquad \qquad \sigma(h \times W_{\text{layer 2}}) = y$$

- Step 2: Compare predictions with the true y values, using a loss function
 - Higher value of loss function = bad model
 - Lower value of loss function = good model
 - Example: zero-one loss: count the number of misclassified inputs
 - Example: log loss (derived from maximum likelihood)
 - Example: **sum of squared errors** (more on this soon)
- Step 3: Use numerical method (e.g. gradient descent) to minimize loss
 - Loss is a function of the weights. Optimization goal: find weights that minimize loss

Optimization Procedure: Gradient Descent



• \(\alpha\): learning rate --- tweaking parameter that needs to be chosen carefully

Computing Gradients

- How do we compute gradients of these loss functions?
 - Repeated application of the chain rule:

If
$$f(x) = g(h(x))$$

Then
$$f'(x) = g'(h(x))h'(x)$$

→ Derivatives can be computed by following well-defined procedures

Feed forward vs. Backpropagation



Backpropagation - demo

Backpropagation demo

Make a prediction



$$\begin{array}{c} h_{j}^{(1)} = f_{(1)}(net_{j}^{(1)}) = f_{(1)}(\sum_{m} w_{j,m}^{(1)} x_{m}) \quad y_{k} = f_{(2)}(net_{k}^{(2)}) = f_{(2)}(\sum_{j} w_{k,j}^{(1)} h_{j}^{(1)}) \\ \hline x = (x_{1}, \dots, x_{m}) \xrightarrow{\qquad \qquad } h_{j}^{(1)} \xrightarrow{\qquad \qquad } h_{j}^{(1)} \xrightarrow{\qquad \qquad } h_{j}^{(1)} \xrightarrow{\qquad \qquad } y_{k} \\ \hline \text{where} \qquad net_{j}^{(1)} = \sum_{m} w_{j,m}^{(1)} x_{m} \qquad \qquad net_{k}^{(2)} = \sum_{j} w_{k,j}^{(2)} h_{j}^{(1)} \end{array}$$

Make a prediction (cont.)



Make a prediction (cont.)



$$\begin{aligned} & h_{j}^{(1)} = f_{(1)}(net_{j}^{(1)}) = f_{(1)}(\sum_{m} w_{j,m}^{(1)} x_{m}) \quad y_{k} = f_{(2)}(net_{k}^{(2)}) = f_{(2)}(\sum_{j} w_{k,j}^{(1)} h_{j}^{(1)}) \\ & \longrightarrow h_{j}^{(1)} \longrightarrow h_{j}^{(1)} \longrightarrow y_{k} \end{aligned} \\ & \text{where} \qquad net_{j}^{(1)} = \sum_{m} w_{j,m}^{(1)} x_{m} \qquad \qquad net_{k}^{(2)} = \sum_{j} w_{k,j}^{(2)} h_{j}^{(1)} \end{aligned}$$

Backpropagation



• Assume all the activation functions are sigmoid
• Error function
$$E = \frac{1}{2} \sum_{k} (y_k - d_k)^2$$

• $\frac{\partial E}{\partial y_k} = y_k - d_k$
• $\frac{\partial y_k}{\partial w_{k,j}^{(2)}} = f'_{(2)} (net_k^{(2)}) h_j^{(1)} = y_k (1 - y_k) h_j^{(1)}$
• $\Rightarrow \frac{\partial E}{\partial w_{k,j}^{(2)}} = (y_k - d_k) y_k (1 - y_k) h_j^{(1)}$
• $\Rightarrow w_{k,j}^{(2)} \leftarrow w_{k,j}^{(2)} - \eta (y_k - d_k) y_k (1 - y_k) h_j^{(1)}$

$$x = (x_1, \dots, x_m) \xrightarrow{h_j^{(1)} = f_{(1)}(net_j^{(1)}) = f_{(1)}(\sum_m w_{j,m}^{(1)} x_m)}_{m} y_k = f_{(2)}(net_k^{(2)}) = f_{(2)}(\sum_j w_{k,j}^{(2)} h_j^{(1)}) }_{j} \xrightarrow{y_k} y_k$$
where $net_j^{(1)} = \sum_m w_{j,m}^{(1)} x_m$ $net_k^{(2)} = \sum_j w_{k,j}^{(2)} h_j^{(1)}$

Backpropagation (cont.)



$$x = (x_1, \dots, x_m) \xrightarrow{h_j^{(1)} = f_{(1)}(net_j^{(1)}) = f_{(1)}(\sum_m w_{j,m}^{(1)} x_m)}_{m} y_k} = f_{(2)}(net_k^{(2)}) = f_{(2)}(\sum_j w_{k,j}^{(1)} h_j^{(1)}) } \xrightarrow{y_k} y_k$$
where $net_j^{(1)} = \sum_m w_{j,m}^{(1)} x_m$ $net_k^{(2)} = \sum_j w_{k,j}^{(2)} h_j^{(1)}$

Backpropagation - example

Consider the simple network below:



- Assume that the neurons have sigmoid activation function
 - Perform a forward pass on the network and find the predicted output
 - Perform a reverse pass (training) once (target = 0.5) with $\eta = 1$
 - Perform a further forward pass and comment on the result

Backpropagation – example (cont.)

(i)

Input to top neuron = $(0.35 \times 0.1) + (0.9 \times 0.8) = 0.755$. Out = 0.68. Input to bottom neuron = $(0.9 \times 0.6) + (0.35 \times 0.4) = 0.68$. Out = 0.6637. Input to final neuron = $(0.3 \times 0.68) + (0.9 \times 0.6637) = 0.80133$. Out = 0.69.

(ii) New weights for output layer:

$$w1^{+} = w1 - (y - t)y(1 - y)h_{1}$$

= 0.3 - (0.69 - 0.5) × 0.69 × (1 - 0.69) × 0.68) = 0.272392.
$$w2^{+} = w2 - (y - t)y(1 - y)h_{2}$$

= 0.9 - (0.69 - 0.5) × 0.69 × (1 - 0.69) × 0.6637) = 0.87305.

New weights for hidden layer:

$$w3^+ = w3 - (y - t)y(1 - y)w_1h_1(1 - h_1)A$$

=?
 $w4^+ =$?
 $w5^+ =$?
 $w6^+ =$?



Fun Neural Net Demo Site

- Demo-site:
 - http://playground.tensorflow.org/

Modules in modern neural networks

Multi-layer perceptron (MLP)

- Denote the matrix multiplication operation with (W, b) as
 - $MM_{W,b}(x) = Wx + b$



- Denote $W^{[r]}$, $b^{[r]}$ as the weight/bias of the r-th layer
- Then the MLP can be represented as

 $MLP(x) = MM_{W^{[r]}, b^{[r]}}(\sigma(MM_{W^{[r-1]}, b^{[r-1]}}(\sigma(\cdots MM_{W^{[1]}, b^{[1]}}(x))))$



Residual connections

An important network structure in CV: ResNet



Residual connections

 $\operatorname{Res}(z) = z + \sigma(\operatorname{MM}(\sigma(\operatorname{MM}(z))))$

- A much simplified ResNet (not the classic one)
 - Composition of many residual blocks followed by a matrix multiplication

 $\operatorname{ResNet-S}(x) = \operatorname{MM}(\operatorname{Res}(\operatorname{Res}(\cdots \operatorname{Res}(x))))$

Classic ResNet uses convolution layers instead of vanilla matrix multiplication, and adds batch normalization between convolutions and activations.

Residual connections (cont'd)

Advantages of residual connections

- Enable identity mapping, Improve the ability of model expression
- Mitigate gradient disappearance, Ease training of deep networks
- Applications
 - Computer Vision (ResNet)
 - Natural Language Processing (Transformer encoder/decoder block)
 - Reinforcement Learning (policy/value networks)

Layer normalization

- A sub-module of the layer normalization \longrightarrow LN-S(z) = $\begin{bmatrix} \frac{z_1 \hat{\mu}}{\hat{\sigma}} \\ \frac{z_2 \hat{\mu}}{\hat{\sigma}} \\ \vdots \\ \frac{z_1 \hat{\mu}}{\hat{\sigma}} \end{bmatrix}$

•
$$\hat{\sigma} = \sqrt{\frac{\sum_{i=1}^{m} (z_i - \hat{\mu}^2)}{m}}$$
 is the empirical standard deviation

Intuition: normalized to having empirical mean zero and empirical standard deviation 1

Layer normalization (cont'd)

More general mean and variance

$$ext{LN}(z) = eta + \gamma \cdot ext{LN-S}(z) = egin{bmatrix} eta + \gamma \left(rac{z_1 - \mu}{\hat{\sigma}}
ight) \ eta + \gamma \left(rac{z_2 - \hat{\mu}}{\hat{\sigma}}
ight) \ dots \ dots \ eta + \gamma \left(rac{z_2 - \hat{\mu}}{\hat{\sigma}}
ight) \ dots \ eta + \gamma \left(rac{z_m - \hat{\mu}}{\hat{\sigma}}
ight) \end{bmatrix}$$

- β , γ are learnable parameters
- Properties: Scaling-invariant

 $LN(MM_{\alpha W,\alpha b}(z)) = LN(MM_{W,b}(z)), \forall \alpha > 0.$

- Applications
 - Transformer / BERT / GPT / RL policy networks

Convolutional layers

Intuition

- Given an input matrix (e.g. an image)
- Use a small matrix (called filter or kernel) to screening the input at every position of the input matrix
- Put the convolution results at corresponding positions



Convolutional layers (cont'd)

- Advantage
 - Sparse connections
 - Weight sharing



MLP Edges: 5*5 Parameters: 5*5

Convolution Edges: 3*3+2*2 Parameters: 3

Interpretation of convolution

- Convolution can be used to find an area with particular patterns
- Example
 - The filter in the left represents the edge in the right, which is the back of a mouse

0	0	0	0	0	30	0	
0	0	0	0	30	0	0	
0	0	0	30	0	0	0	
0	0	0	30	0	0	0	
0	0	0	30	0	0	0	
0	0	0	30	0	0	0	
0	0	0	0	0	0	0	
		(4	Ś	<u> </u>
	(1	
	Or	iginal ima	ge				Visualization of the filter on the image

Interpretation of convolution (cont'd)

When the filter moves to the back of the mouse, the convolution operation will generate a very large value



Multiplication and Summation = (50*30)+(50*30)+(50*30)+(20*30)+(50*30) = 6600 (A large number!)

Otherwise, it generates a very small value



	0	0	0	0	0	30	0
Ì	0	0	0	0	30	0	0
I	0	0	0	30	0	0	0
Ì	0	0	0	30	0	0	0
I	0	0	0	30	0	0	0
Ì	0	0	0	30	0	0	0
Ì	0	0	0	0	0	0	0

Pixel representation of filter

Multiplication and Summation = 0

Summary

- History of artificial neural nets
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- Activation functions
- Training: backpropagation
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