Data Mining: Artificial Neural Network

Lecture Notes for Chapter 3 Data Mining

https://ml-graph.github.io/winter-2025/

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Course Lecture is very heavily based on "Introduction to Data Mining" by Tan, Steinbach, Karpatne, Kumar

Limitations of Decision-Tree and many other model



Real-world Intuition



Basic Architecture of Perceptron



Artificial Neural Networks (ANN)

- Basic Idea: A complex non-linear function can be learned as a composition of simple processing units
- ANN is a collection of simple processing units (nodes) that are connected by directed links (edges)
 - Every node receives signals from incoming edges, performs computations, and transmits signals to outgoing edges
 - Analogous to *human brain* where nodes are neurons and signals are electrical impulses
 - Weight of an edge determines the strength of connection between the nodes
- Simplest ANN: Perceptron (single neuron)

Basic Architecture of Perceptron



$$y = \sigma(w^{\mathrm{T}}x + b)$$



What happens if there is no nonlinear activation?

• Data -
$$\{(x^{(i)}, y^{(i)})\}_{i=1}^{N}$$
 $f(x) = xw + b$

Regression – Find f that minimizes our uncertainty about y given x

$$y = f(x) + n$$

Minimizing Mean Squared Error = Minimizing Negative Log-Likelihood

$$\underset{f}{\operatorname{argmin}} \frac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - f(x^{(i)}) \right)^2$$

$$\underset{w}{\operatorname{argmir}} \frac{1}{N} \sum_{i=1}^{N} (y^{(i)} - w^T \hat{x}^{(i)})^2 = \underset{w}{\operatorname{argmin}} \frac{1}{N} ||y - Xw||^2$$

$$\operatorname{Loss/Cost Function}$$



Where

•
$$y = [y^{(1)}, ..., y^{(N)}]^T \in \mathbb{R}^{N \times 1}$$
 and
• $X = [\hat{x}^{(1)}, ..., \hat{x}^{(N)}]^T \in \mathbb{R}^{N \times (d+1)}$ (here $d = 1$)
• $w = [w_0, w_1, ..., w_d]^T \in \mathbb{R}^{d+1}$

$$J(w) = rac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - w^T \hat{x}^{(i)}
ight)^2$$

Compute the minimum value? How to do it in Math?

Find points where gradient = 0

$$J(w) = rac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - w^T \hat{x}^{(i)}
ight)^2$$

$$J(W) = rac{1}{N}(Y-XW)^T(Y-XW)$$

https://www.math.uwaterloo.ca/~hwol kowi/matrixcookbook.pdf

$$J(W) = rac{1}{N} \left(Y^TY - 2Y^TXW + W^TX^TXW
ight)$$

$$abla J(W) = rac{\partial}{\partial W} \left[rac{1}{N} (Y^TY - 2Y^TXW + W^TX^TXW)
ight] \qquad X^TXW = X^TY
onumber \ W^* = (X^TX)^{-1}X^TY
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$$J(w) = rac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - w^T \hat{x}^{(i)}
ight)^2$$



If the gradient of a function is nonzero at a point, the direction of the gradient is the direction in which the function increases most quickly

$$J(w) = rac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - w^T \hat{x}^{(i)}
ight)^2$$

$$abla J(w) = rac{\partial J(w)}{\partial w} \qquad \qquad
abla J(w) = -rac{2}{N}\sum_{i=1}^N (y^{(i)} - w^T \hat{x}^{(i)}) \hat{x}^{(i)}$$

$$J(w) = rac{1}{N}\sum_{i=1}^N (y^{(i)} - w^T \hat{x}^{(i)})^2$$

$$w_0:=w_0+rac{2lpha}{N}\sum_{i=1}^N(y^{(i)}-(w_0+w_1x_1^{(i)}))$$

$$w_1:=w_1+rac{2lpha}{N}\sum_{i=1}^N(y^{(i)}-(w_0+w_1x_1^{(i)}))x_1^{(i)}$$

$$egin{aligned} rac{\partial J(w)}{\partial w} &= rac{1}{N}\sum_{i=1}^N 2(y^{(i)}-w^T\hat{x}^{(i)})(-\hat{x}^{(i)}) \ &= -rac{2}{N}\sum_{i=1}^N (y^{(i)}-w^T\hat{x}^{(i)})\hat{x}^{(i)} \end{aligned}$$

Local Minimum vs Global Minimum





$$f(\mathbf{x}) = w_0 x + b$$

Slope

Intercept

Problem of Linear Regression



So far, we have been using a linear function for regression:

$$f(x) = w^T x + w_0 = \sum_{i=0}^d w_i x_i$$
 (Assuming $x_0 = 1$)

• Lets generalize this model:

$$f(x) = \sum_{i=0}^{M} w_i \phi_i(x) = w^T \phi(x)$$

where ϕ_i are fixed "basis" functions.

• For linear regression M = d, $\phi_i(x) = x_i$.

$$f(x) = \sum_{i=0}^{M} w_i \phi_i(x) = w^T \phi(x)$$

E.g., Polynomial Regression:

• 1D Polynomial Regression, $\phi(x) = [1, x, x^2, x^3]$:

$$\underset{w}{\operatorname{argmin}} \frac{1}{N} \sum_{n=1}^{N} \left(w^{T} \phi(x^{(i)}) - y^{(i)} \right)^{2}$$

To avoid confusion, note that: $\phi(x^{(i)}) = [1, x^{(i)}, (x^{(i)})^2, (x^{(i)})^3]$

$$f(x^{(i)}) = w_0 + w_1 x^{(i)} + w_2 (x^{(i)})^2 + w_3 (x^{(i)})^3$$



OSS:

$$\operatorname{argmin}_{w} \frac{1}{N} \sum_{n=1}^{N} \left(w^{T} \phi(x^{(i)}) - y^{(i)} \right)^{2} = \operatorname{argmin}_{w} \|\Phi w - y\|^{2}$$
Where $\Phi = \left[\phi(x^{(1)}), \dots, \phi(x^{(N)}) \right]^{T} \in \mathbb{R}^{N \times M}$ and $w \in \mathbb{R}^{M}$.

Optimization:

- 1. Closed form solution: $w^* = (\Phi^T \Phi)^{-1} \Phi^T y$
- 2. Gradient descent: $w^{(t)} = w^{(t-1)} \epsilon \nabla_w Loss(w^{(t-1)})$

 $J(w) = rac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - w^T \hat{x}^{(i)}
ight)^2$

What is the problem of Nonlinear Regression?

 $W^* = (X^T X)^{-1} X^T Y$



The basis function is all fixed! Can we learn the basis function?

• Lets first look at what the learning problem might look like:

$$\underset{w}{\operatorname{argmin}} \sum_{i} \left(\left(\sum_{j} w_{j} \phi_{j}(x^{(i)}) \right) - y^{(i)} \right)^{2}$$

Neural Networks do this for us!

What things are learned here? What things are fixed here?

1-layer Multi-layer Perceptron







Lets first look at what the learning problem might look like:

$$\underset{w_{\{\phi_{j}\}_{j=1}^{M}}{\operatorname{argmin}}}{\operatorname{argmin}} \sum_{i} \left(\left(\sum_{j} w_{j} \phi_{j}(x^{(i)}) \right) - y^{(i)} \right)^{2}$$

Neural Networks do this for us!

What things are learned here? What things are fixed here?

1-hidden layer Multi-layer Perceptron



1-hidden layer Multi-layer Perceptron



Example

- Activations at hidden layers can be viewed as features extracted as functions of inputs
- Every hidden layer represents a level of abstraction
 - Complex features are compositions of simpler features



- Number of layers is known as depth of ANN
 - Deeper networks express complex hierarchy of features

Question?



- 1. "Judge a man by his questions rather than by his answers."
 - Voltaire
- "If I had an hour to solve a problem, I'd spend 55 minutes thinking about the problem and 5 minutes thinking about solutions."
 - Albert Einstein
- 3. "The art and science of asking questions is the source of all knowledge."
 - Thomas Berger
- 4. "Asking the right questions takes as much skill as giving the right answers."
 Robert Half
- 5. "The wise man doesn't give the right answers, he poses the right questions."
 - Claude Lévi-Strauss
- 6. "Great questions make great companies."
 - Peter Drucker

100

500

1000

1500

Living Area (Square Feet)

2000

2500



$$\sigma(w^{\mathrm{T}}x+b)$$

$$\underset{w}{\operatorname{argmir}} \frac{1}{N} \sum_{i=1}^{N} (y^{(i)} - w^T \hat{x}^{(i)})^2 = \underset{w}{\operatorname{argmin}} \frac{1}{N} \|y - Xw\|^2$$

Loss/Cost Function

Gradient Descent

 $abla J(W) = -rac{2}{N}X^TY + rac{2}{N}X^TXW \quad W^* = (X^TX)^{-1}X^TY$





$$y = \sigma(w^{T}x + b)$$

$$y = \sigma(w^{\mathrm{T}}\phi(x) + b)$$

$$abla J(W) = -rac{2}{N}X^TY + rac{2}{N}X^TXW$$

 $W^* = (X^T X)^{-1} X^T Y$

$$\nabla J(W) = -\frac{2}{N}\phi(X)^{\mathrm{T}}Y + \frac{2}{N}\phi(X)^{\mathrm{T}}\phi(X)W$$

$$W^* = (\phi(X)^T \phi(X))^{-1} \phi(X)^T Y$$

$$J(w) = rac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - w^T \hat{x}^{(i)}
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$$y = w_1 x + w_0$$

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$$y = \sigma(w^{T}x + b)$$

$$y = \sigma(w^{\mathrm{T}}\phi(x) + b)$$

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$$\nabla J(W) = -\frac{2}{N}\phi(X)^{\mathrm{T}}Y + \frac{2}{N}\phi(X)^{T}\phi(X)W$$

$$W^* = (X^T X)^{-1} X^T Y$$

$$W^* = (\phi(X)^T \phi(X))^{-1} \phi(X)^T Y$$

Multi-NonLinear Regression

1-hidden layer Multi-layer Perceptron



Multi-NonLinear Regression

1-hidden layer Multi-layer Perceptron



Classification



Classification



$$\mathcal{L}(w) = -\sum_{i=1}^{N} y^{(i)} \log \left(f(x^{(i)}) \right) + (1 - y^{(i)}) \log(1 - f(x_i))$$



A 256x256 (RGB) image \implies ~200K dimensional input x
MLP for MINIST



A fully connected network would need a very large number of parameters, very likely to overfit the data





- The features of these classes are spatially local.
- Translation does not change the identity of the classes, i.e., we require a translation equivariant model.
- MLP is not a good match to this problem

Can represent a small region with fewer parameters







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- Translation does not change the identity of the classes, i.e., we require a translation equivariant model.
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Can represent a small region with fewer parameters







What about training a lot of such "small" detectors and each detector must "move around".

Convolution Layer





For example, if we had 6 5x5 filters, we'll get 6 separate activation maps:



We stack these up to get a "new image" of size 28x28x6!

1	0	0	0	0	1
0	1	0	0	1	0
0	0	1	1	0	0
1	0	0	0	1	0
0	1	0	0	1	0
0	0	1	0	1	0

6 x 6 image



Filter 1



: :

Each filter detects a small pattern (3 x 3).

stride=1 Dot product -1 -1 -1 Filter 1 -1 -1 -1 -1

6 x 6 image



6 x 6 image



Convolutions (typically with *prespecified* filters) are a common operation in many computer vision applications







Convolution is a linear operator

We need to follow convolution with a nonlinearity (e.g., ReLU) to get nonlinear functions.

bird



1	-1	-1	
-1	1	-1	Filter 1
-1	-1	1	





bird









Equivariant and Invariant



Equivariant and Invariant



must learn shift invariance from data!

Code Demo

Equivariant and Invariant

G-invariance $f(\rho(g)x) = f(x)$



Gequivariance $f(\rho(g)x) = \rho(g)f(x)$



Equivariant and Invariant



Image Convolution is ?



Deep Neural Networks

20th Century Zoo of Neural Network Architectures



DNNs

IM GENET



Speech data

Grid games



Deep neural nets that exploit:

- translation equivariance (weight sharing)
- hierarchical compositionality







The teacher told the student that he was brilliant.

The student told the teacher that he was brilliant.

You read this sentence from left to right and understand the sentence What if we have sequences of variable lengths, like sentences or videos that we would like to analyze?



Time or Progression



Token embedding – DNA of the Token





What if we have sequences of variable lengths, like sentences or videos that we would like to analyze?





Image Captioning

- Given an image, produce a sentence describing its contents
- Inputs: Image feature (from a CNN)
- Outputs: Multiple words (let's consider one sentence)



: The dog is hiding

Image Captioning



Input – Output Scenarios





$$y_{1} = f_{1}(x; W_{1})$$

$$y_{2} = f_{2}(y_{1}; W_{2})$$

$$C = \text{Loss}(y_{2}, y_{GT})$$
Find $\frac{\partial C}{\partial W_{1}}, \frac{\partial C}{\partial W_{2}}$

$$\frac{\partial C}{\partial W_{2}} = \left(\frac{\partial C}{\partial y_{2}}\right) \left(\frac{\partial y_{2}}{\partial W_{2}}\right)$$

$$\frac{\partial C}{\partial W_{1}} = \left(\frac{\partial C}{\partial y_{1}}\right) \left(\frac{\partial y_{1}}{\partial W_{1}}\right)$$

$$= \left(\frac{\partial C}{\partial y_{2}}\right) \left(\frac{\partial y_{2}}{\partial y_{1}}\right) \left(\frac{\partial y_{1}}{\partial W_{1}}\right)$$

$$h_t = f(Wh_{t-1} + b) \qquad \qquad \|rac{\partial L}{\partial h_0}\| pprox \sigma_{ ext{max}}^T \|rac{\partial L}{\partial h_T}\|$$

 $\sim \pi$

- Largest singular value > 1 → Exploding gradients
 - Slight error in the late time steps causes drastic updates in the early time steps → Unstable learning
- Largest singular value < 1 → Vanishing gradients
 - Gradients passed to the early time steps is close to 0. → Uninformed correction

Any other problem with RNN?

Sequential Data - Transformer



Key Value Query

Sequential Data - Transformer

Think of YouTube.

First you enter your **Query** in the search bar. Then your **Query** is compared against a set of **Keys** (in this case, video titles, tags and descriptions etc. within the YouTube database). After this, YouTube proceeds to retrieve the videos that best match your **Query**. These video results are referred to as **Values**.

Key Value Query

I would like to taste the local food in France.
I would like to taste the local food in France.

$$Q = XW_Q \quad K = XW_K \quad V = XW_V$$



$$softmax\left(\frac{Q_{i}K^{T}}{\sqrt{d_{k}}}\right) = \frac{e^{\left(\frac{Q_{i}K^{T}}{\sqrt{d_{k}}}\right)}}{\sum_{j=1}^{d_{k}} e^{\left(\frac{Q_{j}K^{T}}{\sqrt{d_{k}}}\right)}}$$



I would like to taste the local food in France.

$Q = XW_Q \quad K = XW_K \quad V = XW_V$







I would like to taste the local food in France.

$Q = XW_Q \quad K = XW_K \quad V = XW_V$

Life

is

short

eat

Self-Attention

Causal-Attention

Attention weight between the tokens corresponding to "Life" and "short"



In the row for corresponding to "Life", mask out all words that come after "Life"

aat

0.17 0.13 0.18 0.16 0.15

0.03 0.68 0.82 0.08 0.14 0.02

0.19 0.06 0.25 0.4 0.11 0.23

0.15 0.21 0.14 0.16 0.7 0.14

desert 0.13 0.27 0.11 0.16 0.18 0

first 0.19 0.02 0.31 0.11 0.07 0.27

deser

first

Cross-attention



Multi-Attention





The teacher told the student that he was brilliant.

The student told the teacher that he was brilliant.

Two sentences using exactly the same tokens but end up with very different meaning

- 0: 0 0 0 0
- 1: 0 0 0 1
- 2: 0 0 1 0
- 3: 0 0 **1 1**
- 4: 0100
- 5: 0 1 0 1
- 6: 0 1 1 0
- 7: 0111

- 8: 1000
- 9: 1001
- 10: **1** 0 **1** 0
- 11: **1** 0 **1 1**
- 12: **1 1 0 0**
- 13: 1 1 0 1
- 14:
 1
 1
 0

 15:
 1
 1
 1
 1

$$P(k,2i) = \sin\left(\frac{k}{n^{2i/d}}\right)$$
$$P(k,2i+1) = \cos\left(\frac{k}{n^{2i/d}}\right)$$

k: Position of an object in the input sequence, $0 \le k < L/2$

d: Dimension of the output embedding space

