DES 5002: Designing Robots for Social Good

Autumn 2022



Week 06 | Lecture 07 From Logistic Regression to Neural Networks

Wan Fang

Southern University of Science and Technology

• Statistical Binary Classification

- Logistic Regression
- Stochastic Gradient Descent

• Multi-class Classification

- Loss Function
- Softmax Regression
- Summary of Linear Classifications

Neural Networks

- Multi-Layer Perceptron
- Forward & Backward Propagation
- Exercises

Statistical Binary Classification





AncoraSIR.com

DES5002 Designing Robots for Social Good

Statistical Binary Classification

Recall on linear regression and classification

- Linear Regression
 - A basic linear model for line-fitting
 - $\hat{y} = f_{WeightedSum}(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$





- Linear Classification
 - Vectorized weights for two or multiple classes
 - $\mathbf{s} = f_{WeightedSum}(\mathbf{x}) = \mathbf{W}\mathbf{x} + \mathbf{b}$





Perceptron Algorithm

If data is separable by a large margin, then Perceptron is a good algorithm to use.



- Information lost about the distance to the cutoff value
- Uncertain about the final decision

What if the boundary line is non-linear?



• Unable to classify nonlinear scenarios



By what chances will I get accepted to a University?

Based on my Test and Grade scores ...

• Weighted-sum node

 W_1

 W_2

 W_n

b

• Unchanged as the input data remains the same

Wr ¥×b

Weighted-Sum

Function

• Activation node

 χ_1

 x_2

 x_n

AncoraSIR.com

- Can be changed as we want a new expression of the output as a probability of prediction
- Sigmoid function as a natural choice that transforms the output to a value between 0 and 1 (or within 100%)



Logistic Regression

$$\hat{y} = g_{Activation} [f_{WeightedSum}(\mathbf{x})] = \text{sigmoid}(\mathbf{w}^T \mathbf{x} + b)$$



• Hypothesis Function: $h_w(x) = \text{sigmoid}(\mathbf{w}^T \mathbf{x} + b)$

- Model output with a probability: $P(y \mid x; w) = [h_w(x)]^y [1 h_w(x)]^{1-y}$
 - Yes%: $P(y = 1 | x; w) = h_w(x)$
 - No%: $P(y = 0 | x; w) = 1 h_w(x)$

AncoraSIR.com

Problem statement

- Assume $\hat{y} = g_{Activation} [f_{WeightedSum}(\mathbf{x})] = \frac{1}{1 + e^{-(\mathbf{w}^T \mathbf{x} + b)}}$
- How to minimize the **prediction error/loss** on a single training sample (with a maximum likelihood set of **w**)?



Loss Function for Logistic Regression

It measures how well you are doing on a single training example

- Assume that *m* training examples were generated independently $h_w(x) = \operatorname{sigmoid}(\mathbf{w}^T \mathbf{x} + b)$
- We can write the likelihood of the parameters

•
$$L(w) = p(\vec{y} | X; w)$$

= $\prod_{i=1}^{m} p(y^{(i)} | x^{(i)}; w)$
= $\prod_{i=1}^{m} [h_w(x^{(i)})]^{y^{(i)}} [1 - h_w(x^{(i)})]^{1-y^{(i)}}$

• Take the log expression, we have the **loss function**

$$\ell(w) = \log L(w)$$

= $\sum_{i=1}^{m} y^{(i)} \log h_w(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_w(x^{(i)}))$

• Usually take a "—" sign to indicate loss



Stochastic Gradient Descent

Finding the maximum likelihood of estimation

- Rewrite the weight parameters in vectorized form
 - $w \coloneqq w + \alpha \cdot \nabla_w \cdot \ell(w)$
 - + sign here to **maximize** likelihood
- When working with a single training example (x, y),

•
$$\frac{\partial}{\partial w_j}\ell(w) = \left(y\frac{1}{g(w^Tx)} - (1-y)\frac{1}{1-g(w^Tx)}\right)\frac{\partial}{\partial w_j}g(w^Tx) = \left(y - h_w(x)\right)x_j$$

• Therefore, we can derive the stochastic gradient ascent rule

•
$$w_j \coloneqq w_j + \alpha \left(y^{(i)} - h_w(x^{(i)}) \right) x_j^{(i)}$$



Cost Function

It measures how well you are doing on an entire training set

- We want the loss/error function to be as small as possible
 - If $y^{(i)} = 1$, then
 - LossFunc $(\hat{y}, y) = -\left[y^{(i)}\log h_w(x^{(i)}) + (1 y^{(i)})\log(1 h_w(x^{(i)}))\right] = -\log h_w(x^{(i)}) = -\log \hat{y}$
 - It means that we want $\log \hat{y}$ to be as big as possible, but remember that it is bounded by 1
 - If $y^{(i)} = 0$, then
 - LossFunc $(\hat{y}, y) = -\left[y^{(i)}\log h_w(x^{(i)}) + (1 y^{(i)})\log(1 h_w(x^{(i)}))\right] = -\log(1 \hat{y})$
 - It means that we want $\log \hat{y}$ to be as small as possible, or close to 0
- Cost Function
 - The average of the loss functions of the entire training set, which is to be minimized

$$J(w,b) = -\frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) = -\frac{1}{m} \sum_{i=1}^{m} \left[y^{(i)} \log \hat{y}^{(i)} + (1 - y^{(i)}) \log (1 - \hat{y}^{(i)}) \right]$$



Summary

| | Linear Regression | Perceptron | Logistic Regression |
|------------------------|---|---|---|
| Problem | Value Prediction | Binary Classification with a threshold | Binary Classification with a probability |
| Weighted-Sum | $\mathbf{w}^{\mathrm{T}}\mathbf{x} + b$ | $\mathbf{w}^{\mathrm{T}}\mathbf{x} + b$ | $\mathbf{w}^{\mathrm{T}}\mathbf{x} + b$ |
| Activation Function | NA | Step Function | Sigmoid Function |
| Prediction Outputs | Continuous Value | Discrete Value {0, 1} | Continuous Probability (0, 1) |
| Loss | Squared Loss | Hinge Loss | Log-Loss |

Multi-class Classification





Content University of Storage Automation Storage Automation of Sto

DES5002 Designing Robots for Social Good

Multi-class Classification

 $\hat{\mathbf{y}} = g_{Activation} | f_{WeightedSum}(\mathbf{x}) | = g_{Activation}(\mathbf{W}\mathbf{x} + \mathbf{b})$





1. Define a loss function that quantifies our unhappiness with the scores across the training data.

Come up with a way of efficiently finding the parameters that minimize the loss function. *(optimiz,ation)*

Define a Loss Function

Quantify how good our current classifier is 3 training samples $\{(x_i, y_i)\}_{i=1}^3$ Ground x_i image Truth y_i Labelled \widehat{y}_i label 3.2 1.3 2.2 Cat 3 classes 2.5 5.1 **4.9** Car 2.0 -3.1 Frog -1.7 s_{y_i} s_j

Loss over the dataset is a sum of loss over examples

$$L = \frac{1}{N} \sum_{i} L_i(\widehat{y}_i, y_i)$$

Denote Weighted-Sum score vector as $\mathbf{s} = f_{WeightedSum}(\mathbf{x})$

Let's try with the hinge loss:

$$\begin{split} L_i &= \sum_{j \neq y_i} \begin{cases} 0 & \text{if } s_{y_i} \geq s_j + 1\\ s_j - s_{y_i} + 1 & \text{otherwise} \end{cases} \\ &= \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1) \end{split}$$

Define a Loss Function

| Quantify how good our current classifier is | | | | | | |
|---|-----------------------|------|--------------------|------|--|--|
| | $\{(x, y)\}^{3}$ | | 3 training samples | | $\sum \int 0$ | |
| | Ground Truth | | | | $L_i = \sum_{j \neq y_i} \left\{ s_j - s_j \right\}$ | |
| L P | abelled Prediction | | (111) | | $L_1 = \max(0, 5.1 - 3.2 + \max(0, 2.9) + \max(0, $ | |
| es | Cat | 3.2 | 1.3 | 2.2 | | |
| 3 classe | Car | 5.1 | 4.9 | 2.5 | $L_2 = \max(0, 1.3 - 4.9 + \max(0, -2.6) + \max(0, -$ | |
| | Frog | -1.7 | 2.0 | -3.1 | = 0 + 0 = 0 | |
| Ancor | Loss aSIR.com | 2.9 | 0 | 12.9 | $L_3 = \max(0, 2.2 + 3.1 - 2.4) = \max(0, 6.3) + \max(0, 6.3) + \max(0, 6.3) + 2.4)$ $= 6.3 + 6.6 = 12.9$ | |

$$L_{i} = \sum_{j \neq y_{i}} \begin{cases} 0 & \text{if } s_{y_{i}} \geq s_{j} + 1\\ s_{j} - s_{y_{i}} + 1 & \text{otherwise} \end{cases}$$

$$L_1 = \max(0, 5.1 - 3.2 + 1) + \max(0, -1.7 - 3.2 + 1)$$

= max(0, 2.9) + max(0, - 3.9)
= 2.9 + 0 = 2.9

$$L_2 = \max(0, 1.3 - 4.9 + 1) + \max(0, 2.0 - 4.9 + 1)$$

= max(0, -2.6) + max(0, -1.9)
= 0 + 0 = 0

$$L_3 = \max(0, 2.2 + 3.1 - 1) + \max(0, 2.5 + 3.1 - 1)$$

= max(0, 6.3) + max(0, 6.6)
= 6.3 + 6.6 = 12.9

Define a Loss Function

Quantify how good our current classifier is 3 training samples $\{(x_i, y_i)\}_{i=1}^3$ Ground Truth Labelled Prediction 3.2 1.3 2.2 Cat 5.1 2.5 Car 4.9 -1.72.0 Frog -3.1 12.9 Loss 2.9 0

$L_{i} = \sum_{j \neq y_{i}} \begin{cases} 0 & \text{if } s_{y_{i}} \ge s_{j} + 1\\ s_{j} - s_{y_{i}} + 1 & \text{otherwise} \end{cases}$

Loss over full dataset is average:

 $L = \frac{1}{N} \sum_{i} L_i(\widehat{y}_i, y_i)$ $=\frac{1}{3}(2.9+0+12.9)$ = 5.27

Recall that our goal is to find a set of **W** with minimum loss over full dataset, i.e. the cost = 0

- Suppose that we found a W such that L = 0. Is this W unique?
 - L is still 0 with 2W

• Let's try regularization

- How do we choose between W and 2W?
- SUSTech

3 classes

Regularization

Prevent the model from doing too well on training data



 λ as strength of Regularization (*hyperparameter*)

Data loss Model predictions should match training data

Regularization

Prevent the model from doing too well on training data



Simple examples

L2 regularization: $R(W) = \sum_{k} \sum_{l} W_{k,l}^2$ L1 regularization: $R(W) = \sum_{k} \sum_{l} |W_{k,l}|$ Elastic net (L1 + L2): $R(W) = \sum_{k} \sum_{l} \beta W_{k,l}^2 + |W_{k,l}|$

More complex:

Dropout Batch normalization Stochastic depth, fractional pooling, etc

Why regularize?

- Express preferences over weights
- Make the model simple so it works on test data
- Improve optimization by adding curvature



Softmax Operation

Interpret the outputs of our model as probabilities

 $\hat{y}_i = \operatorname{softmax}(o_i) = \frac{\exp(o_i)}{\sum_j \exp(o_j)} \times 100\%$

- One can interpret outputs \hat{y}_i as the probability that a given item belongs to class *i*.
- Then we can choose the class with the largest output value as our prediction
 - Why using o_i directly, instead of a probability?
 - What if the sum of probability is not 100%?
 - What if when *o_i* becomes negative?



AncoraSIR.com

Softmax Classifier





Kullback–Leibler Divergence

How to quantify the differences between two probability distribution?



| x | 0 | 1 | 2 |
|-------------------|-------|-------|-------|
| Distribution P(x) | 0.36 | 0.48 | 0.16 |
| Distribution Q(x) | 0.333 | 0.333 | 0.333 |

- 4

 $= 0.36 \ln \left(rac{0.36}{0.333}
ight) + 0.48 \ln \left(rac{0.48}{0.333}
ight) + 0.16 \ln \left(rac{0.16}{0.333}
ight)$

$$D_{KL}(P \parallel Q) = \sum_{y \in \mathcal{Y}} P(y) \log \frac{P(y)}{Q(y)}$$
$$= \sum_{y \in \mathcal{Y}} P(y) \log P(y) - \sum_{y \in \mathcal{Y}} P(y) \log Q(y)$$
$$= \left[-\sum_{y \in \mathcal{Y}} P(y) \log Q(y) \right] - \left[-\sum_{y \in \mathcal{Y}} P(y) \log P(y) \right]$$
$$= H(P, Q) - H(P)$$

A good candidate of loss function for softmax Can be minimized to update the weights

$$H(P,Q) = -\sum_{y \in \mathcal{Y}} P(y) \log Q(y) \quad H(P) = -\sum_{y \in \mathcal{Y}} P(y) \log P(y)$$

the cross-entropy of P and Q the cross-entropy of P with itself (or the entropy of P)



AncoraSIR.com

= 0.0852996

 $D_{ ext{KL}}(P \parallel Q) = \sum_{x \in \mathcal{V}} P(x) \ln \left(rac{P(x)}{Q(x)}
ight)$

Loss Function

Log-Likelihood expressed in cross-entropy

• The **likelihood** of the actual classes according to our model is

$$P(Y \mid X) = \prod_{i=1}^{n} P(y^{(i)} \mid x^{(i)}) \qquad -\log P(Y \mid X) = \sum_{i=1}^{n} -\log P(y^{(i)} \mid x^{(i)})$$

- Maximizing the likelihood is equivalent to minimizing the log-likelihood.
- **Cross-entropy** loss for a single example (dropped superscript *i*)

$$l = -\log P(y \mid x) = -\sum_{j} y_j \log \hat{y}_j$$

• As \hat{y} is a discrete probability distribution and y is a one-hot vector, the sum over all j vanishes for all but one term.



Cross-Entropy Loss and its Derivative

Also called softmax loss

• Plugging **o** into the definition of the cross-entropy loss, we obtain:

$$l = -\sum_{j} y_j \log \hat{y}_j = \sum_{j} y_j \log \sum_{k} \exp(o_k) - \sum_{j} y_j o_j = \log \sum_{k} \exp(o_k) - \sum_{j} y_j o_j$$

• The derivative with respect to **o** is

$$\partial_{o_j} l = \frac{\exp(o_j)}{\sum_k \exp(o_k)} - y_j = \operatorname{softmax}(\mathbf{0})_j - y_j = P(y = j \mid x) - y_j$$

- The gradient is $P(y = j | x) y_j$
 - The difference between the probability predicted by our model P(y = j | x) and the true label y.
- Similar to regression where the gradient is $\hat{y} y$
 - The difference between the true label y and the estimation \hat{y}

Vectorization for Minibatches

We typically carry out vector calculations for minibatches of data for efficiency

$$\hat{y}_i = \operatorname{softmax}(o_i) = \frac{\exp(o_i)}{\sum_j \exp(o_j)} \times 100\%$$

$$\hat{\mathbf{y}} = \operatorname{softmax}(\mathbf{o}) \text{ where } \hat{y}_i = \frac{\exp(o_i)}{\sum_j \exp(o_j)} \times 100\%$$



minibatch features **X** are in $\mathbb{R}^{n \times d}$, weights $\mathbf{W} \in \mathbb{R}^{d \times q}$, and the bias satisfies $\mathbf{b} \in \mathbb{R}^{q}$

 $\mathbf{O} = \mathbf{X}\mathbf{W} + \mathbf{b},$ $\hat{\mathbf{Y}} = \operatorname{softmax}(\mathbf{O})$

A minibatch **X** of examples

• dimensionality *d* and batch size *n* Assume that we have *q* categories (outputs)

More efficient matrix-matrix computation **XW** Exponentiating all entries in **O** then sum



Understanding of Softmax Regression

• When there are two classes, softmax regression reduces to logistic regression.

SoftmaxBinary ClassesLogistic
$$\hat{y}_j = \frac{\exp(o_j)}{\sum_j \exp(o_j)}$$
Activation $\hat{y} = \frac{\exp(o)}{\exp(o) + 1}$ • Softmax when $j=2$ $\hat{y}_0 = \frac{\exp(o_0)}{\sum_j \exp(o_j)}$ Activation $\hat{y} = \frac{\exp(o)}{\exp(o) + 1}$ $\hat{y}_0 = \frac{\exp(o_0)}{\exp(o_0) + \exp(o_1)}$ $\frac{1}{2}\sum_{i=1}^n y_i \log(\hat{y}_i) + (1 - y_i)\log(1 - \hat{y}_i)$ Loss $-\sum_{i=1}^n \sum_j y_j^{(i)} \log \hat{y}_j^{(i)}$ $= \frac{\exp(o_0 - o_1)}{\exp(o_0 - o_1) + 1}$

- The cross-entropy classification can be thought in two ways
 - 1. As maximizing the likelihood of the observed data.
 - 2. As minimizing out surprise required to communicate the labels.



Summary & Comparison

Linear Neural Network

| | Linear Regression | Perceptron | Logistic Regression | Softmax Regression |
|------------------------|-------------------|--------------------------|------------------------------------|---|
| Problem | Value Prediction | Binary Classification | Binary Classification | Multi-Class Classification |
| Weights | wx + b | wx + b | wx + b | Wx + B |
| Activation Function | NA | Step Function | Sigmoid Function | Softmax |
| Prediction Outputs | Continuous Value | Discrete Value 0, 1 | Continuous Probability in (0,1) | A vector of Continuous Probabilities |
| Loss | Squared Loss | Hinge Loss | Log Loss (Binary cross entropy) | Cross Entropy |
| Decision Boundary | | | Linear | |

Neural Network





Subar Deversity of States

DES5002 Designing Robots for Social Good

What is a Neural Network?

From biological inspiration to mathematical modeling



Wan Fang

SUSTech

A Perceptron as an Artificial Neuron



Multi-Layer Perceptrons

Artificial Neural Networks



Forward Propogation

Accept inputs to train a Multi-layer Neural Network



Backward Propogation

Calculate the prediction error node-by-node



AncoraSIR.com

nern University

Backward Propogation



 $rac{\partial E}{\partial w_{ij}}=o_i\delta_j$

with

$$\delta_j = rac{\partial E}{\partial o_j} rac{\partial o_j}{\partial \mathrm{net}_j} = \left\{egin{array}{c} rac{\partial L(o_j,t)}{\partial o_j} rac{darphi(\mathrm{net}_j)}{d\mathrm{net}_j} & ext{if j is an output neuron,} \ (\sum_{\ell \in L} w_{j\ell} \delta_\ell) rac{darphi(\mathrm{net}_j)}{d\mathrm{net}_j} & ext{if j is an inner neuron.} \end{array}
ight.$$

https://en.wikipedia.org/wiki/Backpropagation

$$\Delta w_{ij} = -\eta rac{\partial E}{\partial w_{ij}} = -\eta o_i \delta_j$$
 .

Suthern University el cience and Technology



Exercise I

Neural Networks Playground from Google

- Build your first neural networks on the website
 - https://playground.tensorflow.org/
- Play with different data types, features, network structures. Can Neural networks separate nonlinear features?
- Try different hyperparameters.



Exercise II

"Hello, MNIST!"

Hello World: handwritten digits classification - MNIST S Ø ዮ a <u>ـ</u>۲ D



AncoraSIR.com



MNIST = Mixed National Institute of Standards and Technology - Download the dataset at http://yann.lecun.com/exdb/mnist/

A Toy Example of Training a Neural Network

Training => Validation => Regularization => Testing => Optimization



A Single-layer Network of Image Classification

Modified National Institute of Standards and Technology database



DES5002 Designing Robots for Social Good

Softmax on a Batch of Images

Output with a distribution of computed probabilities







б





Training digits

Test digits



Adding Layers

Simply adding more layers with sigmoid activations does not give us the expected results ...





Getting flat

• The gradient can become very small and training get slower and slower.





DES5002 Designing Robots for Social Good

Special Care for Deep Networks



HANDS ON:

Replace all activation='sigmoid' with activation='relu' in your layers and train again.



HANDS ON:

Replace the 'sgd' optimizer with a better one, for example 'adam' and train again.





AncoraSIR.com

https://github.com/GoogleCloudPlatform/tensorflow-without-a-phd/blob/master/tensorflow-mnist-tutorial/keras 02 mnist dense.ipynb



DES 5002: Designing Robots for Social Good

Autumn 2022

Thank you~

Wan Fang Southern University of Science and Technology