CS772: Deep Learning for Natural Language Processing (DL-NLP)

Building blocks cntd, Sigmoid, Softmax Pushpak Bhattacharyya Computer Science and Engineering Department IIT Bombay Week 3 of 16th Jan, 2023



The Perceptron Model

A perceptron is a computing element with input lines having associated weights and the cell having a threshold value. The perceptron model is motivated by the biological neuron.



Statement of Convergence of PTA

• Statement:

Whatever be the initial choice of weights and whatever be the vector chosen for testing, PTA converges if the vectors are from a linearly separable function.

To note

- F1: $|G(W_n)|$ is bounded
- IF
- F2: n tends to infinity
- THEN
- F3: $|G(W_n)|$ is unbounded



Sigmoid neuron



$$o^i = \frac{1}{1 + e^{-net^i}}$$

$$net_i = W.X^i = \sum_{j=0}^m w_j x_j^i$$

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Sigmoid function: can saturate

 Brain saving itself from itself, in case of extreme agitation, emotion etc.



Definition: Sigmoid or Logit function



If k tends to infinity, sigmoid tends to the step function

Sigmoid function



$$f(x) = \frac{1}{1+e^{-x}}$$

$$\frac{df(x)}{dx} = \frac{d}{dx} \left(\frac{1}{1+e^{-x}}\right)$$

$$= \frac{e^{-x}}{(1+e^{-x})^{-2}}$$

$$= \frac{1}{1+e^{-x}} \left(1 - \frac{1}{1+e^{-x}}\right)$$

$$= f(x) \cdot (1 - f(x))$$

$$f(x) = \frac{1}{1+e^{-x}}$$

Decision making under sigmoid

• Output of sigmod is between 0-1

• Look upon this value as probability of Class-1 (C_1)

- 1-sigmoid(x) is the probability of Class-2
 (C₂)
- Decide C_1 , if $P(C_1) > P(C_2)$, else C_2

Sigmoid function and multiclass classification

 Why can't we use sigmoid for n-class classification? Have segments on the curve devoted to different classes, just like –infinity to 0.5 is for class 2 and 0.5 to plus infinity is class 2.

• Think about it!!

multiclass: SOFTMAX

- 2-class → multi-class (C classes)
- Sigmoid \rightarrow softmax
- *ith* input, *cth* class (small c), *c* varies over classes
- In softmax, decide for that class which has the highest probability

What is softmax

- Turns a vector of *K* real values into a vector of *K* real values that sum to 1
- Input values can be positive, negative, zero, or greater than one
- But softmax transforms them into values between 0 and 1
- so that they can be interpreted as probabilities.

Mathematical form

$$\sigma(\overline{Z})_i = \frac{e^{Z_i}}{\sum_{j=1}^{K} e^{Z_j}}$$

- σ is the **softmax** function
- *Z* is the input vector of size *K*
- The RHS gives the *ith* component of the output vector
- Input to softmax and output of softmax are of the same dimension

Example



Softmax and Cross Entropy

- Intimate connection between softmax and cross entropy
- Softmax gives a vector of probabilities
- Winner-take-all strategy will give a classification decision

Winner-take-all with softmax

- Consider the softmax vector obtained from the example where the softmax vector is <0.09, 0.24, 0.65>
- These values correspond to 3 classes
 - For example, positive (+), negative (-) and neutral (0) sentiments, given an input sentence like
 - (a) I like the story line of the movie (+). (b)
 However the acting is weak (-). (c) The
 protagonist is a sports coach (0)

Sentence vs. Sentiment

Sentence vs. Sentiment	Positive (a) I like the s (b) However a (c) The protag	Negative tory line of the n the acting is wea gonist is a sports	Neutral novie (+). ak (-). s coach (0)
Sent (a)	1 (P _{max} from softmax)	0	0
Sentence (b)	0	1 (P _{max} from softmax)	0
Sentence (C)	0	0`	1 (Pmax from softmax)

Training data

- (a) I like the story line of the movie (+).
- (b) However the acting is weak (-).
- (c) The protagonist is a sports coach (0)

 Input
 Output

 (a)
 <1,0,0>

 (b)
 <0,1,0>

 (c)
 <0,0,1>

Finding the error

- Difference between target (T) and obtained (Y)
- Difference is called LOSS
- Options:
 - Total Sum Square Loss (TSS)
 - Cross Entropy (measures difference between two probability distributions)
- Softmax goes with cross entropy

Cross Entropy Function

$H(P,Q) = -\sum_{x=1,N} \sum_{k=1,C} P(x,k) \log_2 Q(x,k)$

x varies over *N* data instances, *c* varies over *C* classes *P* is target distribution; *Q* is observed distribution

Cross Entropy Loss

- Can we sum up cross entropies over the instances? Is it allowed?
- Yes, summing up cross entropies (i.e. the total cross entropy loss) is equivalent to multiplying probabilities.
- Minimizing the total cross entropy loss is equivalent to maximizing the likelihood of observed data.

How to minimize loss

- Gradient descent approach
- Backpropagation Algorithm
- Involves derivative of the input-output function for each neuron
- FFNN with BP is the most important TECHNIQUE for us in the course

Sigmoid and Softmax neurons

Sigmoid neuron



$$o^i = \frac{1}{1 + e^{-net^i}}$$

$$net_i = W.X^i = \sum_{j=0}^m w_j x_j^i$$

- - -

Softmax Neuron



Output for class c (small c), c:1 to C

Notation

- *i*=1...N
- Ni-o pairs, *i* runs over the training data
- *j=0...m*, *m* components in the input vector, *j* runs over the input dimension (also weight vector dimension)
- k=1...C, C classes (C components in the output vector)

Fix Notations: Single Neuron (1/2)



- Capital letter for vectors
- Small letter for scalars (therefore for vector components)
- Xⁱ: *i*th input vector
- *o_i*: output (scalar)
- W: weight vector
 - net_i: W.Xⁱ
- There are *n* input-output observations



W and each X^i has *m* components $W:< W_m, W_{m-1}, ..., W_2, W_0 >$ $X^i:< X^i_m, X^i_{m-1}, ..., X^i_2, X^i_0 >$ Upper suffix *i* indicates *i*th input

Fixing Notations: Multiple neurons in o/p layer



Now, O^i and NET^i are vectors for i^{th} input W_k is the weight vector for c^{th} output neuron, c=1..C

Fixing Notations



Target Vector, $T^{i}: \langle t^{i}_{C}, t^{i}_{C-1}, ..., t^{i}_{2}, t^{i}_{1} \rangle$, $i \rightarrow for i^{th}$ input. Only one of these C componets is 1, rest are 0

Maximum Likelihood and Cross Entropy Loss

Fixing concepts

- The random variable is the class value of the input
- So we are interested in the probability
 P(Oⁱ|Xⁱ), where Oⁱ is the output vector given the input vector Xⁱ
- Each component oⁱ_c of Oⁱ is the probability of Xⁱ belonging to the class c (c=1...C)
- Notice that C components are redundant, since probability(class-c)= 1-Σprobability(class≠c)
- So in case of 2-class, one sigmoid neuron

Interpreting o_i

- oⁱ value is between 0 and 1
- Interpreted as probability
- 2-class situation, oⁱ value is looked upon as probability of class being 1
- That is, $P(Class=1 \text{ for } i^{th} \text{ input})$ = $o^i = 1/(1 + e^{-neti})$
- Each training data instance is labeled as 1 or
 0
- Target value $t^{i}=1/0$, for i^{th} input

Likelihood *L* of observation (2 classes)

For N no. of i - o pairs

$$L = \prod_{i=1}^{N} (o^{i})^{t^{i}} (1 - o^{i})^{(1 - t^{i})}, t^{i} = 1/0$$

log likelihood,
$$LL = \sum_{i=1}^{N} t^{i} \log o^{i} + (1-t^{i}) \log(1-o^{i})$$

$$-LL = -\sum_{i=1}^{N} [t^{i} \log o^{i} + (1-t^{i}) \log(1-o^{i})]$$
Maximize likelihood=Minimize cross entropy

- -LL is called the cross entropy
- Regarded as loss or error
- We give this the notation E
- Minimizing cross entropy brings oⁱ close to tⁱ (Why?)
- Established: equivalence between maximization of likelihood observation and minimization of cross entropy loss

Generalizing 2-class to multiclass: SOFTMAX

$$o_c^i = S(NET^i)_c = \frac{e^{net_c^i}}{\sum_{k=1}^C e^{net_k^i}},$$

- 2-class → multi-class (C classes)
- Sigmoid \rightarrow softmax
- *ith* input, *cth* class (small c), *k* varies over classes

Softmax Neuron



Compare and contrast Sigmoid and Softmax

sigmoid : $o^{i} = \frac{1}{1 + e^{-net^{i}}}$, for i^{th} input soft max : $o_{c}^{i} = \frac{e^{net_{c}^{i}}}{\sum_{k=1}^{C} e^{net_{k}^{i}}}$,

*i*th input, *c*th class (small c), *k* varies over classes 1 to *C*

Interpreting oⁱ_c

- o_c^i value is between 0 and 1
- Interpreted as probability
- Multi-class situation
- oⁱ_c value is the probability of the class being 'c' for the ith input
- That is,

P(Class of ith input=c)=oⁱ_c

Likelihood L of observations in case of softmax

For N no. of i - o pairs

i=1

k=1

$$L = \prod_{i=1}^{N} \prod_{k=1}^{C} (o_k^i)^{t_k^i}, t_k^i = 1/0$$

For a pattern *i*, only one of t_k^i s is 1, rest are 0

$$\log likelihood, LL = \sum_{i=1}^{N} \sum_{k=1}^{C} t_{k}^{i} \log o_{k}^{i}$$
$$-LL = -\sum_{k=1}^{N} \sum_{k=1}^{C} t_{k}^{i} \log o_{k}^{i}$$

For softmax also Maximize likelihood=Minimize cross entropy

- *-LL* is called the cross entropy
- Regarded as loss or error
- Given the notation E
- Established again: equivalence between maximization of likelihood of observation and minimization of cross entropy loss

Derivatives

Derivative of sigmoid



Derivative of Softmax



Derivative of Softmax: Case-1, class c for O and NET same



Derivative of Softmax: Case-2, class c' in $net_{c'}$ different from class c of O $\ln o_c^i = net_c^i - \ln(\sum^C e^{net_k^i})$ k=1 $\frac{1}{o_c^i} \frac{\partial o_c^i}{\partial net_c^i} = 0 - \frac{1}{\sum_{k=1}^C e^{net_k^i}} \cdot e^{net_c^i} = -o_c^i$ $\Rightarrow \frac{\partial O_k^i}{\partial net^i} = -o_c^i o_c^i$

Finding weight change rule

Foundation: Gradient descent

Change is weight Δw_{ji} = - $\eta \delta E / \delta w_{ji}$ η = learning rate, E=loss, w_{ji} = weight of connection from the *i*th neuron to *j*th At A, $\delta E / \delta w_{ji}$ is negative, so Δw_{ji} is positive. At B, $\delta E / \delta w_{ji}$ is positive, so Δw_{ji} is negative. E always decreases. Greedy algo.

F

W_{ii}

B

Gradient Descent is Greedy!

- Gradient Descent is greedy- always moves in the direction of reducing error
- Probabilistically also move in the direction of increasing error, to be able to come out of local minimum
- Nature randomly introduces some variation, and a totally new species emerges
- Darwin's theory of evolution

Genetic Algorithm

- Genetic Algorithms: adaptive heuristic search algorithms
- used to generate high-quality solutions for optimization problems and search problems
- To evolve the generation, genetic algorithms use the following operators, all PROBABILSTICALLY
 - Selection, Cross over, Mutation

Single sigmoid neuron and *cross entropy* loss, derived for single data point, hence dropping upper right suffix *i*



Multiple neurons in the output layer: softmax+*cross entropy* loss (1/2): illustrated with 2 neurons and single training data point



Softmax and Cross Entropy (2/2)

$$E = -t_1 \log o_1 - t_0 \log o_0$$
$$o_1 = \frac{e^{net_1}}{e^{net_1} + e^{net_0}}, \ o_0 = \frac{e^{net_0}}{e^{net_1} + e^{net_0}}$$

 $\frac{\partial E}{\partial w_{11}} = -\frac{t_1}{o_1} \frac{\partial o_1}{\partial w_{11}} - \frac{t_0}{o_0} \frac{\partial o_0}{\partial w_{11}}$

$$\begin{split} \frac{\partial o_1}{\partial w_{11}} &= \frac{\partial o_1}{\partial net_1} \cdot \frac{\partial net_1}{\partial w_{11}} + \frac{\partial o_1}{\partial net_0} \cdot \frac{\partial net_0}{\partial w_{11}} = o_1(1-o_1)x_1 + 0\\ \frac{\partial o_0}{\partial w_{11}} &= \frac{\partial o_0}{\partial net_1} \cdot \frac{\partial net_1}{\partial w_{11}} + \frac{\partial o_0}{\partial net_0} \cdot \frac{\partial net_0}{\partial w_{11}} = -o_1 o_0 x_1 + 0\\ \Rightarrow \frac{\partial E}{\partial w_{11}} &= -t_1(1-o_1)x_1 + t_0 o_1 x_1 = -t_1(1-o_1)x_1 + (1-t_1)o_1 x_1\\ &= [-t_1 + t_1 o_1 + o_1 - t_1 o_1]x_1 = -(t_1 - o_1)x_1\\ \Delta w_{11} &= -\eta \frac{\partial E}{\partial w_{11}} = \eta(t_1 - o_1)x_1 \end{split}$$

Can be generalized

When E is Cross Entropy Loss

• The change in any weight is

learning rate * *diff between target and observed outputs* * *input at the connection*

Weight change rule with TSS

Single neuron: *sigmoid+total sum* square (tss) loss



Lets consider wlg w_1 . Change is weight $\Delta w_1 = -\eta \delta L / \delta w_1$ $\eta = learning rate,$

 $L = loss = \frac{1}{2}(t-0)^2,$ t=target, o=observed output

$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial o} \cdot \frac{\partial o}{\partial net} \cdot \frac{\partial net}{\partial w_1}$$

$$L = \frac{1}{2} (t - o)^2 \implies \frac{\partial L}{\partial o} = -(t - o) \quad (1)$$

$$o = \frac{1}{1 + e^{-net}} (sigmoid) \implies \frac{\partial o}{\partial net} = o(1 - o) \quad (2)$$

$$net = \sum_{i=0}^n w_i x_i \implies \frac{\partial net}{\partial w_1} = x_1 \quad (3)$$

$$\implies \Delta w_1 = \eta (t - o) o(1 - o) x_1$$



 $\Delta w_1 = \eta(t-0)o(1-0)x_1$

Multiple neurons in the output layer: sigmoid+total sum square (tss) loss



CE Loss and TSS Loss

- Can we sum up cross entropies over the instances? Is it allowed?
- Yes, summing up cross entropies (i.e. the total cross entropy loss) is equivalent to multiplying probabilities.
- Minimizing the total cross entropy loss is equivalent to maximizing the likelihood of observed data.

Backpropagation

With total sum square loss (TSS)

Backpropagation algorithm



- Fully connected feed forward network
- Pure FF network (no jumping of connections over layers)

Gradient Descent Equations



Backpropagation – for outermost layer

$$\delta j = -\frac{\delta E}{\delta n e t_j} = -\frac{\delta E}{\delta o_j} \times \frac{\delta o_j}{\delta n e t_j} (n e t_j = \text{input at the } j^{th} \text{ layer})$$
$$E = \frac{1}{2} \sum_{i=1}^{N} (t_j - o_j)^2$$

Hence, $\delta j = -(-(t_j - o_j)o_j(1 - o_j))$

$$\Delta w_{ji} = \eta (t_j - o_j) o_j (1 - o_j) o_i$$

Observations from ΔW_{jj}

$$\Delta w_{ji} = \eta (t_j - o_j) o_j (1 - o_j) o_i$$

 $\Delta w_{ji} \rightarrow 0$ if,

 $1.o_i \rightarrow t_i$ and/or

 $2.o_j \rightarrow 1$ and/or

 $3.o_j \rightarrow 0$ and/or

 $4.o_i \rightarrow 0$

Saturation behaviour

}Credit/Blame assignment

Backpropagation for hidden layers



 δ_k is propagated backwards to find value of δ_i

Backpropagation – for hidden layers



Back-propagation- for hidden layers: Impact on net input on a neuron



 O_j affects the net input coming to all the neurons in next layer

General Backpropagation Rule

- General weight updating rule: $\Delta w_{ji} = \eta \delta j o_i$
- Where

$$\delta_j = (t_j - o_j)o_j(1 - o_j)$$
 for outermost layer

 $= \sum_{k \in \text{next layer}} (w_{kj} \delta_k) o_j (1 - o_j) \text{ for hidden layers}$

Why Symbolic AI community did not see the merit of backpropagation

- Symbolic AI is theory and modelling driven; Connectionist AI is data and experimentation driven
- Rationalism and empiricism have been competing approaches
- Symbolic AI people did not see the possibility of arrival of huge amount of data and exploiting the inherent regularities data to train the humongous number of parameters of neural net

Project ideas

1. Interpretation of word vector components.

 Inconsistency detection - Given a set of sentences in a system, detect if there is internal inconsistency (using sentence vectors)