

# Natural Language Processing Neural Networks

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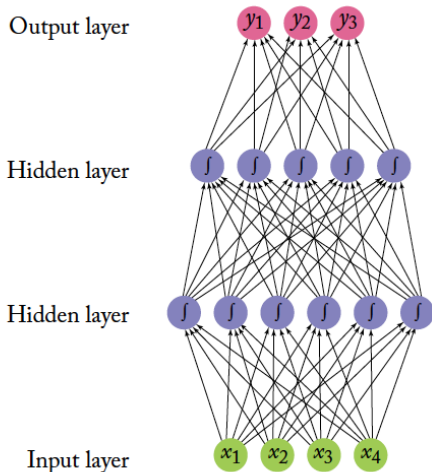
# Introduction to Neural Networks

- Very popular machine learning models formed by units called **neurons**.
- A neuron is a computational unit that has scalar inputs and outputs.
- Each input has an associated weight  $w$ .
- The neuron multiplies each input by its weight, and then sums them (other functions such as **max** are also possible).
- It applies an activation function  $g$  (usually non-linear) to the result, and passes it to its output.
- Multiple layers can be stacked.

# Activation Functions

- The nonlinear activation function  $g$  has a crucial role in the network's ability to represent complex functions.
- Without the nonlinearity in  $g$ , the neural network can only represent linear transformations of the input.

# Feedforward Network with two Layers



# Feedforward Network Neural Networks

- The feedforward network from the picture is a stack of linear models separated by nonlinear functions.
- The values of each row of neurons in the network can be thought of as a vector.
- The input layer is a 4-dimensional vector ( $\vec{x}$ ), and the layer above it is a 6-dimensional vector ( $\vec{h}^1$ ).
- The fully connected layer can be thought of as a linear transformation from 4 dimensions to 6 dimensions.
- A fully connected layer implements a vector-matrix multiplication,  $\vec{h} = \vec{x}W$ .
- The weight of the connection from the  $i$ -th neuron in the input row to the  $j$ -th neuron in the output row is  $W_{[i,j]}$ .
- The values of  $\vec{h}$  are transformed by a nonlinear function  $g$  that is applied to each value before being passed on as input to the next layer.

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<sup>0</sup>Vectors are assumed to be row vectors and superscript indices correspond to network layers.

# Neural Networks as Mathematical Functions

- The Multilayer Perceptron (MLP) from the figure is called MLP2 because it has two hidden layers.
- A simpler model would be MLP1, a multilayer perceptron of one hidden layer:

$$\vec{y} = NN_{MLP1}(\vec{x}) = g(\vec{x}W^1 + \vec{b}^1)W^2 + \vec{b}^2 \quad (1)$$
$$\vec{x} \in \mathcal{R}^{in}, W^1 \in \mathcal{R}^{d_{in} \times d_1}, \vec{b}^1 \in \mathcal{R}^{d_{in}}, W^2 \in \mathcal{R}^{d_1 \times d_{out}}, \vec{b}^2 \in \mathcal{R}^{d_{out}}, \vec{y} \in \mathcal{R}^{d_{out}}$$

- Here  $W^1$  and  $\vec{b}^1$  are a matrix and a bias term for the first linear transformation of the input.
- The function  $g$  is a nonlinear function that is applied element-wise (also called a nonlinearity or an activation function).
- $W^2$  and  $\vec{b}^2$  are the matrix and bias term for a second linear transform.
- When describing a neural network, one should specify the dimensions of the layers ( $d_1$ ), the input ( $d_{in}$ ), and the output ( $d_{out}$ ).

# Neural Networks as Mathematical Functions

- MLP2 can be written as the following mathematical function:

$$\begin{aligned} NN_{MLP2}(\vec{x}) &= \vec{\hat{y}} \\ \vec{h}^1 &= g^1(\vec{x}W^1 + \vec{b}^1) \\ \vec{h}^2 &= g^2(\vec{h}^1W^2 + \vec{b}^2) \\ \vec{y} &= \vec{h}^2W^3 \\ \vec{y} &= (g^2(g^1(\vec{x}W^1 + \vec{b}^1)W^2 + \vec{b}^2))W^3. \end{aligned} \tag{2}$$

- The matrices and the bias terms that define the linear transformations are the parameters of the network.
- Like in linear models, it is common to refer to the collection of all parameters as  $\Theta$ .

# Representation Power

- [Hornik et al., 1989] and [Cybenko, 1989] showed that a multilayer perceptron of one hidden layer (MLP1) is a universal approximator.
- MLP1 can approximate all continuous functions on a closed and bounded subset of  $\mathcal{R}^n$ .
- This may suggest there is no reason to go beyond MLP1 to more complex architectures.
- The result does not say how easy or hard it is to set the parameters based on training data and a specific learning algorithm.
- It also does not guarantee that a training algorithm will find the correct function generating our training data.
- Finally, it does not state how large the hidden layer should be.



# Representation Power

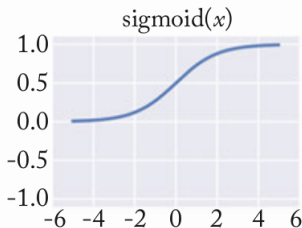
- In practice, we train neural networks on relatively small amounts of data using local search methods.
- We also use hidden layers of relatively modest sizes (up to several thousands).
- The universal approximation theorem does not give any guarantees under these conditions.
- However, there is definitely benefit in trying out more complex architectures than MLP1.
- In many cases, however, MLP1 does indeed provide strong results.

# Activation Functions

- The nonlinearity  $g$  can take many forms.
- There is currently no good theory as to which nonlinearity to apply in which conditions.
- Choosing the correct nonlinearity for a given task is for the most part an empirical question.

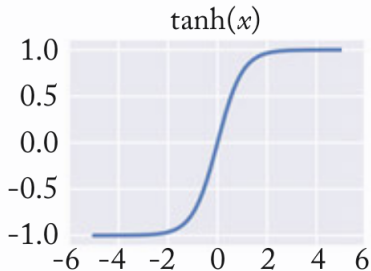
# Sigmoid

- The sigmoid activation function  $\sigma(x) = \frac{1}{1+e^{-x}}$  is an S-shaped function, transforming each value  $x$  into the range  $[0, 1]$ .
- The sigmoid was the canonical nonlinearity for neural networks since their inception.
- Is currently considered to be deprecated for use in internal layers of neural networks, as the choices listed next prove to work much better empirically.



# Hyperbolic tangent (tanh)

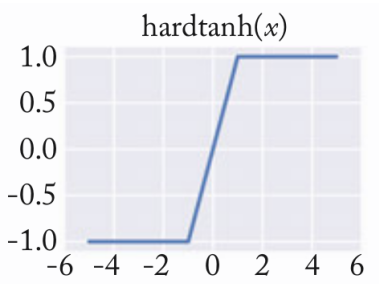
- The hyperbolic tangent  $\tanh(x) = \frac{e^{2x}-1}{e^{2x}+1}$  activation function is an S-shaped function, transforming the values  $x$  into the range  $[-1, 1]$ .



# Hard tanh

- The hard-tanh activation function is an approximation of the tanh function which is faster to compute and to find derivatives thereof:

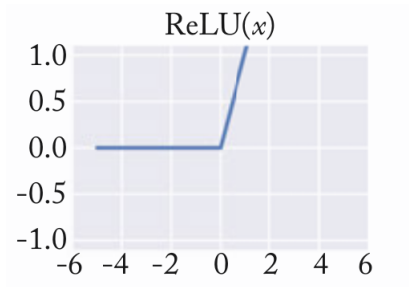
$$\text{hardtanh}(x) = \begin{cases} -1 & x < -1 \\ 1 & x > 1 \\ x & \text{otherwise.} \end{cases}$$



# ReLU

- The rectifier activation function [Glorot et al., 2011], also known as the rectified linear unit is a very simple activation function.
- It is easy to work with and was shown many times to produce excellent results.
- The ReLU unit clips each value  $x < 0$  at 0.

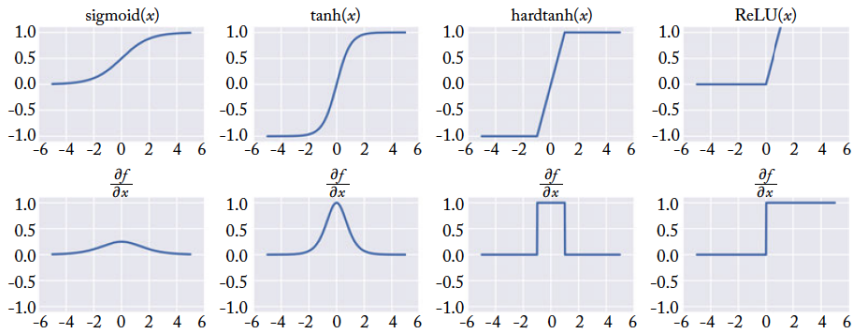
$$\text{ReLU}(x) = \max(0, x)$$



- It performs well for many tasks, especially when combined with the dropout regularization technique (to be explained later).

# Activation Functions

- As a rule of thumb, both ReLU and tanh units work well, and significantly outperform the sigmoid.
- You may want to experiment with both tanh and ReLU activations, as each one may perform better in different settings.
- The figure from below shows the shapes of the different activations functions, together with the shapes of their derivatives.



# Embedding Layers

- In NLP the input to the neural network contains symbolic categorical features (e.g., words from a closed vocabulary, character n-grams, POS tags).
- In linear models we usually represent the input with sparse vectors e.g., as the sum or the concatenation of one-hot encoded vectors (the sum is equivalent to a bag-of words representation).
- In neural networks, it is common to associate each possible feature value (i.e., each word in the vocabulary, each POS tag category) with a  $d$ -dimensional vector for some  $d$ .
- These vectors are then considered parameters of the model, and are trained jointly with the other parameters.
- The mapping from a symbolic feature values such as “word number 1249” to  $d$ -dimensional vectors is performed by an embedding layer (also called a lookup layer ).



# Embedding Layers

- The parameters in an embedding layer are simply a matrix  $E \in \mathcal{R}^{|vocab| \times d}$  where each row corresponds to a different word in the vocabulary.
- The lookup operation is then simply indexing:  $v_{1249} = E_{[1249, :]}$ .
- If the symbolic feature is encoded as a one-hot vector  $\vec{x}$ , the lookup operation can be implemented as a vector-matrix multiplication  $\vec{x}E$ .
- The word vectors are often concatenated to each other before being passed on to the next layer.
- The embeddings matrix  $E$  can be initialized with pre-trained word vectors trained from unlabeled documents using specific methods based on the distributional hypothesis such as the ones implemented in Word2Vec (to be discussed later in the course).

# Dense Vectors vs. One-hot representations

- What are the benefits of representing our features as vectors instead of as unique IDs?
- Should we always represent features as dense vectors?
- Let's consider the two kinds of representations.
- 1) **One Hot**: each feature is its own dimension.
  - Dimensionality of one-hot vector is same as number of distinct features.
  - Features are completely independent from one another. The feature “word is ‘dog’ ” is as dissimilar to “word is ‘thinking’ ” than it is to “word is ‘cat’ ”.
- 2) **Dense**: each feature is a  $d$ -dimensional vector.
  - Dimensionality of vector is  $d$ .
  - Model training will cause similar features to have similar vectors: information is shared between similar features.

# Example: Dense Vectors vs. One-hot representations

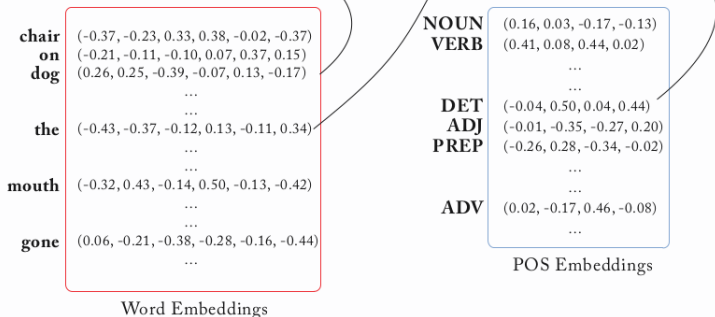
(a)

$x = (0, \dots, 0, 1, 0, \dots, 0, 1, 0, \dots, 0, 1, 0, \dots, 0, 1, 0, \dots, 0, 1, 0, \dots, 0, 0, 0, \dots, 0)$

w=dog      pw=the      pt=NOUN      pt=DET      w=dog&pt=DET      w=dog&pw=the      w=chair&pt=DET

(b)

$x = (0.26, 0.25, -0.39, -0.07, 0.13, -0.17) (-0.43, -0.37, -0.12, 0.13, -0.11, 0.34) (-0.04, 0.50, 0.04, 0.44)$



# Example: Dense Vectors vs. One-hot representations

- Previous figure shows two encodings of the information: current word is “dog;” previous word is “the;” previous pos-tag is “DET.”
- (a) Sparse feature vector.
  - Each dimension represents a feature.
  - Feature combinations receive their own dimensions.
  - Feature values are binary.
  - Dimensionality is very high.
- (b) Dense, embeddings-based feature vector.
  - Each core feature is represented as a vector.
  - Each feature corresponds to several input vector entries.
  - No explicit encoding of feature combinations.
  - Dimensionality is low.
  - The feature-to-vector mappings come from an embedding table.

# Dense Vectors vs. One-hot representations

- One benefit of using dense and low-dimensional vectors is computational: the majority of neural network toolkits do not play well with very high-dimensional, sparse vectors.
- However, this is just a technical obstacle, which can be resolved with some engineering effort.
- The main benefit of the dense representations is in generalization power.
- If we believe some features may provide similar clues, it is worthwhile to provide a representation that is able to capture these similarities.

# Dense Vectors vs. One-hot representations

- Let's assume we have observed the word dog many times during training, but only observed the word cat a handful of times.
- If each of the words is associated with its own dimension (one-hot), occurrences of dog will not tell us anything about the occurrences of cat.
- However, in the dense vectors representation the learned vector for dog may be similar to the learned vector for cat.
- This will allow the model to share statistical strength between the two events.
- This argument assumes that we saw enough occurrences of the word cat such that its vector will be similar to that of dog.
- Pre-trained word embeddings (e.g., Word2Vec, Glove) to be discussed later in the course can be used to obtain dense vectors from unannotated text.

# Neural Network Training

- Neural networks are trained in the same way as linear models.
- The network's output is used to compute a loss function  $L(\hat{y}, y)$  that is minimized across the training examples using gradient descent.
- Backpropagation is an efficient technique for evaluating the gradient of a loss function  $L$  for a feed-forward neural network with respect to all its parameters [Bishop, 2006].<sup>1</sup>
- Those parameters are:  $W^1, \vec{b}^1, \dots, W^m, \vec{b}^m$ , for a network of  $m$  layers.
- Recall that superscripts are used to denote layer indexes (not exponentiations).
- For simplicity, we will assume that  $L$  is calculated over a single example.
- Challenge: in neural networks the number of parameters can be huge and we need an efficient way to calculate the gradients.
- Idea: apply the derivative chain rule wisely.

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<sup>1</sup>The following slides on backpropagation are based on [Bishop, 2006], we adapted the notation to be consistent with [Goldberg, 2017].

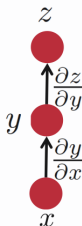
# Derivative Chain Rule Recap

- Simple chain rule: let  $z = f(y)$ ,  $y = g(x)$ ,

$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y} \times \frac{\partial y}{\partial x}$$

- Example:  $z = e^y$ ,  $y = 2x$

$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y} \times \frac{\partial y}{\partial x} = e^y \times 2 = 2e^{2x}$$



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<sup>1</sup>Figure taken from:



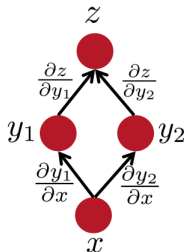
## Derivative Chain Rule Recap

- Multiple path chain rule: let  $z = f(y_1, y_2)$ ,  $y_1 = g_1(x)$ ,  $y_2 = g_2(x)$

$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y_1} \times \frac{\partial y_1}{\partial x} + \frac{\partial z}{\partial y_2} \times \frac{\partial y_2}{\partial x}$$

- Example:  $z = e^{y_1 \times y_2}$ ,  $y_1 = 2x$ ,  $y_2 = x^2$

$$\frac{\partial z}{\partial x} = (e^{y_1 \times y_2} \times y_2) \times 2 + (e^{y_1 \times y_2} \times y_1) \times 2x = e^{2x^3} \times 6x^2$$



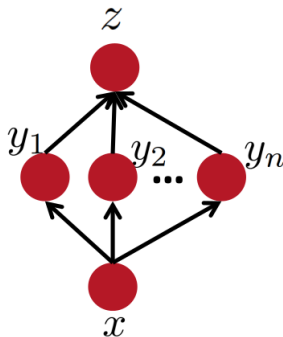
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<sup>1</sup>Figure taken from:

## Derivative Chain Rule Recap

The general version of the multiple path chain rule would be:

$$\frac{\partial z}{\partial x} = \sum_{i=1}^n \frac{\partial z}{\partial y_i} \times \frac{\partial y_i}{\partial x}$$



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<sup>1</sup>Figure taken from:

# Backpropagation

- In a general feed-forward network, each unit computes a weighted sum of its inputs in the form:

$$\vec{h}_{[j]}^l = \left( \sum_i w_{[i,j]}^l \times \vec{z}_{[i]}^{(l-1)} \right) + \vec{b}_{[j]}^l \quad (3)$$

- The variable  $\vec{z}_{[i]}^{(l-1)}$  is an input that sends a connection to unit  $\vec{h}_{[j]}^l$ ,  $w_{[i,j]}^l$  is the weight associated with that connection, and  $l$  is the layer index.
- The biases vectors  $\vec{b}_{[j]}^l$  can be excluded from (eq.3) and included to the weight matrix  $w_{[i,j]}^l$  by introducing an extra unit, or input, with activation fixed at +1.

# Backpropagation

- The inputs at layer  $l$ ,  $\vec{z}_{[l]}^{(l-1)}$  are the result of applying the activation function  $g$  to units from the previous layer:

$$\vec{z}_{[l]}^l = g(\vec{h}_{[l]}^l) \quad (4)$$

- For the input layer ( $l = 0$ ),  $\vec{z}$  corresponds to the input vector  $\vec{z} = \vec{x}$

$$\vec{z}_{[l]}^0 = \vec{x}_{[l]} \quad (5)$$

- For each instance in the training set, we supply the corresponding input vector  $\vec{x}$  to the network.
- Next we calculate the activations of all of the hidden and output units in the network by successive application of (eq.3) and (eq.4).
- This process is often called forward propagation because it can be regarded as a forward flow of information through the network.

# Backpropagation

- Now consider the evaluation of the derivative of  $L$  with respect to a weight  $W_{[i,j]}^l$ .
- Assuming that the loss  $L$  is calculated over a single example, we can note that  $L$  depends on the weight  $W_{[i,j]}^l$  only via the summed input  $\vec{h}_{[j]}^l$ .
- We can therefore apply the chain rule for partial derivatives to give

$$\frac{\partial L}{\partial W_{[i,j]}^l} = \frac{\partial L}{\partial \vec{h}_{[j]}^l} \times \frac{\partial \vec{h}_{[j]}^l}{\partial W_{[i,j]}^l} \quad (6)$$

# Backpropagation

- We now introduce a useful notation:

$$\vec{\delta}_{[l]}^l \equiv \frac{\partial L}{\partial \vec{h}_{[l]}^l} \quad (7)$$

- Using (3), we can write

$$\frac{\partial \vec{h}_{[l]}^l}{\partial \mathbf{W}_{[i,j]}^l} = \vec{z}_{[i]}^{(l-1)} \quad (8)$$

- Substituting (7) and (8) into (6), we then obtain

$$\frac{\partial L}{\partial \mathbf{W}_{[i,j]}^l} = \vec{\delta}_{[l]}^l \times \vec{z}_{[i]}^{(l-1)} \quad (9)$$

# Backpropagation

- Equation (9) tells us that the required derivative is obtained simply by multiplying the value of  $\vec{\delta}_{[j]}^l$  by the value of  $\vec{z}_{[j]}^{(l-1)}$ .
- Thus, in order to evaluate the derivatives, we need only to calculate the value of  $\vec{\delta}_{[j]}^l$  for each hidden and output unit in the network, and then apply (9).
- Calculating  $\vec{\delta}_{[j]}^m$  for output units ( $l = m$ ), is usually straightforward, since activation units  $\vec{h}_{[j]}^m$  are directly observed in the loss expression.
- The same applies for shallow linear models.

# Backpropagation

- To evaluate the  $\vec{\delta}_{[l]}^l$  for hidden units, we again make use of the chain rule for partial derivatives:

$$\vec{\delta}_{[l]}^l \equiv \frac{\partial L}{\partial \vec{h}_{[l]}^l} = \sum_k \left( \frac{\partial L}{\partial \vec{h}_{[k]}^{l+1}} \times \frac{\partial \vec{h}_{[k]}^{l+1}}{\partial \vec{h}_{[l]}^l} \right) \quad (10)$$

- The sum runs over all units  $\vec{h}_{[k]}^{l+1}$  to which unit  $\vec{h}_{[l]}^l$  sends connections.
- We assume that connections go only to consecutive layers in the network (from layer  $l$  to layer  $(l + 1)$ ).
- The units  $\vec{h}_{[k]}^{l+1}$  could include other hidden units and/or output units.
- If we now substitute the definition of  $\vec{\delta}_{[l]}^l$  given by (eq.7) into (eq.10), we get

$$\vec{\delta}_{[l]}^l \equiv \frac{\partial L}{\partial \vec{h}_{[l]}^l} = \sum_k \left( \vec{\delta}_{[k]}^{l+1} \times \frac{\partial \vec{h}_{[k]}^{l+1}}{\partial \vec{h}_{[l]}^l} \right) \quad (11)$$



# Backpropagation

- Now, for expression  $\vec{h}_{[k]}^{l+1}$  we can go to its definition (eq.3):

$$\vec{h}_{[k]}^{(l+1)} = \left( \sum_i w_{[i,k]}^{l+1} \times \vec{z}_{[i]}^l \right) + \vec{b}_{[k]}^{(l+1)}$$

- Now, we replace (eq.4) ( $\vec{z}_{[i]}^l = g(\vec{h}_{[i]}^l)$ ) into previous equation and we obtain:

$$\vec{h}_{[k]}^{(l+1)} = \left( \sum_i w_{[i,k]}^{l+1} \times g(\vec{h}_{[i]}^l) \right) + \vec{b}_{[k]}^{(l+1)}$$

- Now when calculating  $\frac{\partial \vec{h}_{[k]}^{l+1}}{\partial \vec{h}_{[j]}^l}$  all the terms in the summation where  $i \neq j$  get canceled out.
- Hence:

$$\frac{\partial \vec{h}_{[k]}^{l+1}}{\partial \vec{h}_{[j]}^l} = w_{[j,k]}^{l+1} \times g'(\vec{h}_{[j]}^l) \quad (12)$$

# Backpropagation

- Now, if we substitute (eq.12) into (eq.11)

$$\vec{\delta}_{[j]}^l \equiv \frac{\partial L}{\partial \vec{h}_{[j]}^l} = \sum_k \left( \vec{\delta}_{[k]}^{l+1} \times w_{[j,k]}^{l+1} \times g'(\vec{h}_{[j]}^l) \right) \quad (13)$$

- Since  $g'(\vec{h}_{[j]}^l)$  doesn't depend on  $k$  we can obtain the following backpropagation formula:

$$\vec{\delta}_{[j]}^l = g'(\vec{h}_{[j]}^l) \times \sum_k \left( \vec{\delta}_{[k]}^{l+1} \times w_{[j,k]}^{l+1} \right) \quad (14)$$

- Which tells us that the value of  $\delta$  for a particular hidden unit can be obtained by propagating the  $\delta$ 's backwards from units higher up in the network.  
[Bishop, 2006].

# Backpropagation

The backpropagation procedure can be summarized as follows.

1. Apply an input vector  $\vec{x}$  to the network and forward propagate through the network using (eq.3) and (eq.4) to find the activations of all the hidden and output units.
2. Evaluate the  $\vec{\delta}_{[j]}^m$  for all the output units (recall that the derivatives involved here are easy to calculate).
3. Backpropagate the  $\vec{\delta}_{[k]}^{(l+1)}$  using (eq.14) to obtain  $\vec{\delta}_{[j]}^l$  for each hidden unit in the network. We go from higher to lower layers in the network.
4. Use (eq.9) ( $\frac{\partial L}{\partial w_{[i,j]}^l} = \vec{\delta}_{[j]}^l \times \vec{z}_{[i]}^{(l-1)}$ ) to evaluate the required derivatives.

# The Computation Graph Abstraction

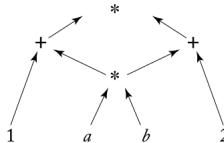
- One can compute the gradients of the various parameters of a network by hand and implement them in code.
- This procedure is cumbersome and error prone.
- For most purposes, it is preferable to use automatic tools for gradient computation [Bengio, 2012].
- A computation graph is a representation of an arbitrary mathematical computation (e.g., a neural network) as a graph.
- This abstraction will allow us computing the gradients from any kind of neural network architecture using the backpropagation algorithm.
- Previous formulation was restricted to feedforward networks.

# The Computation Graph Abstraction

- A computation graph is a directed acyclic graph (DAG).
- Nodes correspond to mathematical operations or (bound) variables.
- Edges correspond to the flow of intermediary values between the nodes.
- The graph structure defines the order of the computation in terms of the dependencies between the different components.
- The graph is a DAG and not a tree, as the result of one operation can be the input of several continuations.

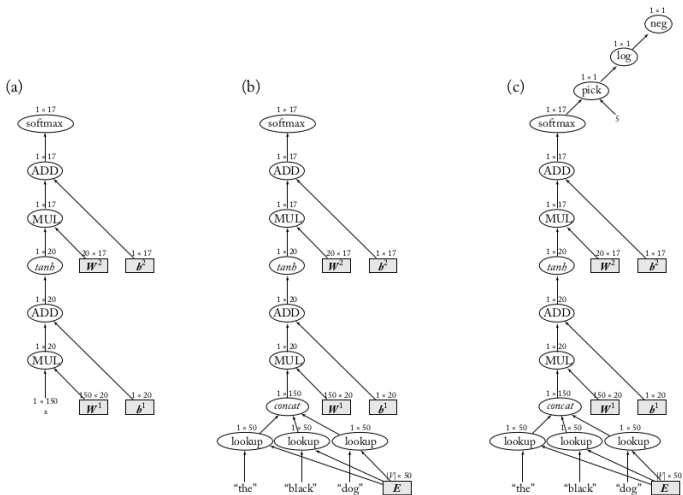
# The Computation Graph Abstraction

- Consider for example a graph for the computation of  $(a * b + 1) * (a * b + 2)$ :



- The computation of  $a * b$  is shared.
- Since a neural network is essentially a mathematical expression, it can be represented as a computation graph.

# The Computation Graph Abstraction



**Figure 5.1:** (a) Graph with unbound input. (b) Graph with concrete input. (c) Graph with concrete input, expected output, and a final loss node.

# The Computation Graph Abstraction

- The presents the computation graph for an MLP with one hidden-layer and a softmax output transformation.
- Oval nodes represent mathematical operations or functions, and shaded rectangle nodes represent parameters (bound variables).
- Network inputs are treated as constants, and drawn without a surrounding node.
- Input and parameter nodes have no incoming arcs, and output nodes have no outgoing arcs.
- The output of each node is a matrix, the dimensionality of which is indicated above the node.



# The Computation Graph Abstraction

- This graph is incomplete: without specifying the inputs, we cannot compute an output.
- Figure 5.1b shows a complete graph for an MLP that takes three words as inputs, and predicts the distribution over part-of-speech tags for the third word.
- This graph can be used for prediction, but not for training, as the output is a vector (not a scalar) and the graph does not take into account the correct answer or the loss term.
- Finally, the graph in Figure 5.1c shows the computation graph for a specific training example, in which the inputs are the (embeddings of ) the words “the,” “black,” “dog,” and the expected output is “NOUN” (whose index is 5).
- The pick node implements an indexing operation, receiving a vector and an index (in this case, 5) and returning the corresponding entry in the vector.

# Forward Computation

- The forward pass computes the outputs of the nodes in the graph.
- Since each node's output depends only on itself and on its incoming edges, it is trivial to compute the outputs of all nodes.
- This is done by traversing the nodes in a topological order and computing the output of each node given the already computed outputs of its predecessors.
- More formally, in a graph of  $N$  nodes, we associate each node with an index  $i$  according to their topological ordering.
- Let  $f_i$  be the function computed by node  $i$  (e.g., multiplication, addition , etc.).

# Forward Computation

- Let  $\pi(i)$  be the parent nodes of node  $i$ , and  $\pi^{-1}(i) = \{j | i \in \pi(j)\}$  the children nodes of node  $i$  (these are the arguments of  $f_i$ ).
- Denote by  $v(i)$  the output of node  $i$ , that is, the application of  $f_i$  to the output values of its arguments  $\pi^{-1}(i)$ .
- For variable and input nodes,  $f_i$  is a constant function and  $\pi^{-1}(i)$  is empty.
- The computation-graph forward pass computes the values  $v(i)$  for all  $i \in [1, N]$ .

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**Algorithm 5.3** Computation graph forward pass.

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```
1: for  $i = 1$  to  $N$  do  
2:   Let  $a_1, \dots, a_m = \pi^{-1}(i)$   
3:    $v(i) \leftarrow f_i(v(a_1), \dots, v(a_m))$ 
```

---

# Backward Computation (Backprop)

- The backward pass begins by designating a node  $N$  with scalar ( $1 \times 1$ ) output as a loss-node, and running forward computation up to that node.
- The backward computation computes the gradients of the parameters with respect to that node's value.
- Denote by  $d(i)$  the quantity  $\frac{\partial N}{\partial i}$ .
- The backpropagation algorithm is used to compute the values  $d(i)$  for all nodes  $i$ .
- The backward pass fills a table of values  $d(1), \dots, d(N)$  as shown in the following algorithm.

---

**Algorithm 5.4** Computation graph backward pass (backpropagation).

---

1: $d(N) \leftarrow 1$	$\triangleright \frac{\partial N}{\partial N} = 1$
2: <b>for</b> $i = N-1$ <b>to</b> $1$ <b>do</b>	
3: $d(i) \leftarrow \sum_{j \in \pi(i)} d(j) \cdot \frac{\partial f_j}{\partial i}$	$\triangleright \frac{\partial N}{\partial i} = \sum_{j \in \pi(i)} \frac{\partial N}{\partial j} \frac{\partial j}{\partial i}$

---

# Backward Computation (Backprop)

- The backpropagation algorithm is essentially following the chain-rule of differentiation.
- The quantity  $\frac{\partial f_j}{\partial i}$  is the partial derivative of  $f_j(\pi^{-1}(j))$  w.r.t the argument  $i \in \pi^{-1}(j)$ .
- This value depends on the function  $f_j$  and the values  $v(a_1), \dots, v(a_m)$  (where  $a_1, \dots, a_m = \pi^{-1}(j)$ ) of its arguments, which were computed in the forward pass.
- Thus, in order to define a new kind of node, one needs to define two methods: one for calculating the forward value  $v(i)$  based on the node's inputs, and the another for calculating  $\frac{\partial f_j}{\partial i}$  for each  $x \in \pi^{-1}(i)$ .

# Summary of the Computation Graph Abstraction

- Notice that the above formulation of backpropagation is equivalent to one given earlier in the class.
- The computation graph abstraction allows us to:
  1. Easily construct arbitrary networks.
  2. Evaluate their predictions for given inputs (forward pass)
  3. Compute gradients for their parameters with respect to arbitrary scalar losses (backward pass or backpropagation).
- A nice property of the computation graph abstraction is that it allows computing the gradients for arbitrary networks (e.g., networks with skip-connections, shared weights, special loss functions, etc.)

---

<sup>1</sup>A comprehensive tutorial on the backpropagation algorithm over the computational graph abstraction can be found here:

<https://colah.github.io/posts/2015-08-Backprop/>.

# Derivatives of “non-mathematical” functions

- Defining  $\frac{\partial f_j}{\partial i}$  for mathematical functions such as  $\log$  or  $+$  is straightforward.
- It may be challenging to think about the derivative of operations as as  $\text{pick}(\vec{x}, 5)$  that selects the fifth element of a vector.
- The answer is to think in terms of the contribution to the computation.
- After picking the  $i$ -th element of a vector, only that element participates in the remainder of the computation.
- Thus, the gradient of  $\text{pick}(\vec{x}, 5)$  is a vector  $\vec{v}$  with the dimensionality of  $\vec{x}$  where  $\vec{v}_{[5]} = 1$  and  $\vec{v}_{[i \neq 5]} = 0$ .
- Similarly, for the function  $\max(0, x)$  the value of the gradient is 1 for  $x > 0$  and 0 otherwise.

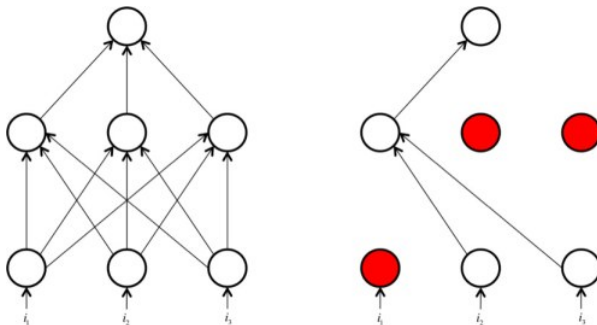
# Regularization and Dropout

- Multi-layer networks can be large and have many parameters, making them especially prone to overfitting.
- Model regularization is just as important in deep neural networks as it is in linear models, and perhaps even more so.
- The regularizers discussed for linear models, namely  $L_2$ ,  $L_1$ , and the elastic-net, are also relevant for neural networks.
- Another effective technique for preventing neural networks from overfitting the training data is **dropout training** [Hinton et al., 2012].



# Regularization and Dropout

- The dropout method is designed to prevent the network from learning to rely on specific weights.
- It works by randomly dropping (setting to 0) half of the neurons in the network (or in a specific layer) in each training example in the stochastic-gradient training.



---

<sup>1</sup>Figure taken from: <https://www.kdnuggets.com/wp-content/uploads/drop-out-in-neural-networks.jpg>

# Deep Learning Frameworks

Several software packages implement the computation-graph model. All these packages support all the essential components (node types) for defining a wide range of neural network architectures.

- TensorFlow (<https://www.tensorflow.org/>): an open source software library for numerical computation using data-flow graphs originally developed by the Google Brain Team.
- Keras: High-level neural network API that runs on top of Tensorflow as well as other backends (<https://keras.io/>).
- PyTorch: open source machine learning library for Python, based on Torch, developed by Facebook's artificial-intelligence research group. It supports dynamic graph construction, a different computation graph is created from scratch for each training sample. (<https://pytorch.org/>)

Questions?

Thanks for your Attention!

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