Deep Learning Architectures for Sequence Processing

Natalie Parde UIC CS 521

Review: Neural Networks Basics



- Earliest and simplest form of neural network
- Data is fed forward from one layer to the next
- Each layer:
 - One or more units
 - A unit in layer *n* receives input from all units in layer *n*-1 and sends output to all units in layer *n*+1
 - A unit in layer n does not communicate with any other units in layer n
- The outputs of all units except for those in the last layer are **hidden** from external viewers







Natalie Parde - UIC CS 521







Natalie Parde - UIC CS 521



Neural networks tend to be more powerful than traditional classification algorithms.

- Traditional classification algorithms usually assume that data is linearly separable
- Neural networks are better equipped to learn complex, nonlinear separations between data classes





Building Blocks for Neural Networks

- At their core, neural networks are comprised of **computational units**
- Computational units:
 - 1. Take real-valued numbers as input
 - 2. Perform some computation on them
 - 3. Produce a single output



Computational Units

- The computation performed by each unit is a weighted sum of inputs
 - Assign a weight to each input
 - Add one additional bias term
- More formally, given a set of inputs x₁, ..., x_n, a unit has a set of corresponding weights w₁, ..., w_n and a bias b, so the weighted sum z can be represented as:

• $z = b + \sum_i w_i x_i$

Computational Units

- The weighted sum of inputs computes a **linear function** of *x*
- We pass this sum through one of many possible nonlinear functions, commonly referred to as **activations**
- The output of a computation unit is thus the **activation value** for the unit, *y*

• $y = f(z) = f(w \cdot x + b)$

There are many different activation functions!



There are many different activation functions!



Computational Unit with Sigmoid Activation











Natalie Parde - UIC CS 521











Particularly Popular Activation Functions

- Tanh:
 - Variant of sigmoid that ranges from -1 to +1
 - $y = \frac{e^z e^{-z}}{e^z + e^{-z}}$
 - Once again differentiable
 - Larger derivatives → generally faster convergence
- ReLU:
 - Ranges from 0 to ∞
 - Simplest activation function:
 - $y = \max(z, 0)$
 - Very close to a linear function!
 - Quick and easy to compute



















Why does this work?

 When computational units are combined, the outputs from each successive layer provide new representations for the input that can better separate the data into the target classes



Why does this work?

 When computational units are combined, the outputs from each successive layer provide new representations for the input that can better separate the data into the target classes



Formalizing Feedforward Neural Networks

+

0

- Let *W*^[n] be the weight matrix for layer n, **b**^[n] be the bias vector for layer n, and so forth
- Let $g(\cdot)$ be an activation function, such as:
 - ReLU
 - tanh
 - softmax
- Let a^[n] be the output from layer n, and z^[n] be the combination of weights and biases W^[n] a^[n-1]+ b^[n]
- Let the input layer be a^[0]
Formalizing Feedforward Neural Networks

- We can represent a two-layer network as:
 - $z^{[1]} = W^{[1]}a^{[0]} + b^{[1]}$
 - $a^{[1]} = g^{[1]}(z^{[1]})$
 - $z^{[2]} = W^{[2]}a^{[1]} + b^{[2]}$
 - $a^{[2]} = g^{[2]}(z^{[2]})$
 - $y' = a^{[2]}$
- We can easily generalize to networks with more layers:
 - For i in 1..*n*
 - $z^{[i]} = W^{[i]}a^{[i-1]} + b^{[i]}$
 - $a^{[i]} = g^{[i]}(z^{[i]})$

$$y' = a^{[n]}$$

Does every layer use the same activation function?

- The activation function $g(\cdot)$ generally differs for the final layer
- Final layers will usually use softmax (for multinomial classification) or sigmoid (for binary classification) activations



Loss function

□Optimization algorithm

□Some way to compute the gradient across all of the network's intermediate layers



Loss function
Optimization algorithm
Some way to compute the gradient across all of the network's intermediate layers

Cross-entropy loss



 \checkmark Loss function

✓ Optimization algorithm ⁴

□Some way to compute the gradient across all of the network's intermediate layers

Gradient descent



 \checkmark Loss function

✓ Optimization algorithm

□Some way to compute the gradient across all of the network's intermediate layers

Recall....



 When we train a logistic regression classifier, we can compute the gradient of our loss function by just taking its derivative:

•
$$\frac{\partial L_{CE}(w,b)}{\partial w_j} = (\hat{y} - y)x_j = (\sigma(w \cdot x + b) - y)x_j$$

Difference between true and estimated *y*

Corresponding input observation

However, we can't do that with a neural network that has multiple weight layers ("hidden" layers).

- Why?
 - Taking the derivative of the loss function only provides the gradient for the final weight layer
- What we need is a way to:
 - Compute the derivative with respect to weight parameters occurring earlier in the network as well
 - Even though we can only compute loss at a single point (the end of the network)

We do this using backward differentiation.

- Usually referred to as backpropagation in the context of neural networks
- Frames neural networks as **computation graphs**
 - Representations of interconnected mathematical operations
 - **Nodes** = Operations
 - Directed edges = connections between output/input of nodes



There are two different ways that we can pass information through our neural network computation graphs.

Forward pass

- Apply operations in the direction of the final layer
- Pass the output of one computation as the input to the next

Backward pass

- Compute partial derivatives in the opposite direction of the final layer
- Multiply them by the partial derivatives passed down from the previous step

Example: Forward Pass

Goal: Represent L(a, b, c) = c(a + 2b)



Example: Forward Pass











To perform a backward pass, how do we get from L all the way back to a, b, and c?

- Chain rule!
 - Given a function f(x) = u(v(x)):
 - Find the derivative of u(x) with respect to v(x)
 - Find the derivative of v(x) with respect to x

 $\frac{\partial \tanh(z)}{\partial z} = 1 - \tanh^2(z)$

Derivatives of popular activation functions:

0 for z < 0

1 for $z \ge 0$

- Multiply the two together
- $\frac{df}{dx} = \frac{du}{dv} * \frac{dv}{dx}$

Natalie Parde - UIC CS 521







Example: Backward Pass









Computation graphs for neural networks involve numerous interconnected units.



What would a computation graph look like for a simple neural network?



What would a computation graph look like for a simple neural network?



Convolutional Neural Networks

- Neural networks that incorporate one or more convolutional layers
- Designed to reflect the inner workings of the visual cortex system
- Require that fewer parameters are learned relative to feedforward networks for equivalent input data

What are convolutional layers?

- Sliding windows that perform matrix operations on subsets of the input
- Compute products between those subsets of input and a corresponding weight matrix





- First layer(s): low-level features
 - Color, gradient orientation
 - N-grams
- Higher layer(s): high-level features
 - Objects
 - Phrases





Convolutional Layers

In NLP, convolutions are typically performed on entire rows of an input matrix, where each row corresponds to a word.



Natalie Parde - UIC CS 521

In NLP, convolutions are typically performed on entire rows of an input matrix, where each row corresponds to a word.



Natalie Parde - UIC CS 521












It's common to extract multiple different feature maps from the same input.



Natalie Parde - UIC CS 521

After extracting feature maps from the input, CNNs utilize pooling layers.

- Pooling layers: Layers that reduce the dimensionality of input feature maps by pooling all of the values in a given region
- Why use pooling layers?
 - Further increase efficiency
 - Improve the model's ability to be invariant to small changes

• • • • • • • • • • • •

Pooling Layers



Common Techniques for Pooling

Max pooling

• Take the maximum of all values computed in a given window





Natalie Parde - UIC CS 521

Common Techniques for Pooling

Max pooling

• Take the maximum of all values computed in a given window

Average pooling

• Take the average of all values computed in a given window





Natalie Parde - UIC CS 521

The output from pooling layers is passed along as input to the rest of the network.



Convolutional neural network architectures can vary greatly!

- Additional hyperparameters:
 - Kernel size
 - Padding
 - Stride size
 - Number of channels
 - Pooling technique

Padding?

- Add empty vectors to the beginning and end of your text input
- Why do this?
 - Allows you to apply a filter to every element of the input matrix



Channels?

For images, generally corresponds to color channels

• Red, green, blue

For text, can mean:

- Different types of word embeddings
 - Word2Vec, GloVe, etc.
- Other feature types
 - POS tags, word length, etc.

Why use CNNs for NLP tasks at all?

- Traditionally for image classification!
- However, offer unique advantages for NLP tasks:
 - CNNs inherently extract meaningful local structures from input
 - In NLP \rightarrow implicitly-learned, useful n-grams!

Summary: Feedforward Neural **Networks** and CNNs

- Neural networks are built from interconnected layers of computing units
- To train the weights across the entire network, loss values are passed backward to earlier layers using backpropagation
- Model design and training procedures for neural networks can be optimized by tuning hyperparameters
- One more specialized neural network architecture is the convolutional neural network
- CNNs can be an efficient way to capture local structure in numerous types of input data

Language is inherently temporal.

- Continuous input streams of indefinite length that unfold over time
- Even clear from the metaphors we use to describe language:
 - Conversation flow
 - News feed
 - Twitter stream



Aren't neural network models (e.g., feedforward networks) already able to capture temporal information?

- In a sense, yes
- How?
 - Sliding window approach

Sliding Window Approach



Sliding Window Approach



Sliding Window Approach



However, this method has some limitations.

- Constrains the context from which information can be extracted
 - Only items within the predetermined context window can impact the model's decision
- Makes it difficult to learn systematic patterns
 - Particularly problematic when learning grammatical information (e.g., constituent parses)



However, this method has some limitations.

- Constrains the context from which information can be extracted
 - Only items within the predetermined context window can impact the model's decision
- Makes it difficult to learn systematic patterns
 - Particularly problematic when learning grammatical information (e.g., constituent parses)



Recurrent neural networks (RNNs) are designed to overcome these limitations.

Built-in capacity to handle temporal information

 Contain cycles within their connections, where the value of a unit is dependent upon outputs from previous timesteps

Can accept variable length inputs without the use of fixed-size windows

Many varieties exist

- "Vanilla" RNNs
- Long short-term memory networks (LSTMs)
- Gated recurrent units (GRUs)









Although they are more complex, computation units in RNNs still perform the same core actions.



Biggest change....

- New set of weights that connect the hidden layer from the previous timestep to the current hidden layer
- These weights determine how the network should make use of prior context

Formal Equations

- Recall the basic set of equations for a feedforward neural network:
 - $\mathbf{h} = \sigma(W\mathbf{x} + \mathbf{b})$
 - $\mathbf{z} = V\mathbf{h}$
 - $y = \operatorname{softmax}(\mathbf{z})$
- Just add (weights X activation values from previous timestep) product to the current (weights X inputs) product
 - $\mathbf{h_t} = \sigma(W\mathbf{x_t} + U\mathbf{h_{t-1}} + \mathbf{b})$
 - $\mathbf{z_t} = V\mathbf{h_t}$
 - $y_t = \operatorname{softmax}(\mathbf{z})$
- *W*, *U*, and *V* are shared across all timesteps

Formal Algorithm

 $h_0 \leftarrow 0$ # Initialize activations from the hidden layer to 0



Earlier Example: RNN Edition



Earlier Example: RNN Edition



Earlier Example: RNN Edition



Training RNNs

- Same core elements:
 - Loss function
 - Optimization function
 - Backpropagation
- One extra set of weights to update
 - Hidden layer from *t-1* to current hidden layer at *t*
- For forward inference:
 - Compute h_t and y_t at each step in time
 - Compute the loss at each step in time
- For backward inference:
 - Process the sequence in reverse
 - Compute the required error gradients at each step backward in time









Natalie Parde - UIC CS 521









####




Updated Backpropagation Equations

- Now we have three sets of weights we need to update
 - *w*, the weights from the input layer to the hidden layer
 - U, the weights from the previous hidden layer to the current hidden layer
 - V, the weights from the hidden layer to the output layer





Updated Backpropagation Equations

- Now we have three sets of weights we need to update:
 - *W*, the weights from the input layer to the hidden layer
 - *U*, the weights from the previous hidden layer to the current hidden layer
 - V, the weights from the hidden layer to the output layer





Updated Backpropagation Equations

- Now we have three sets of weights we need to update:
 - *W*, the weights from the input layer to the hidden layer
 - *U*, the weights from the previous hidden layer to the current hidden layer
 - V, the weights from the hidden layer to the output layer



Weight Update Equations

- Updating the weights for V works no differently from feedforward networks
- When updating the other weights, remember that a hidden layer, δ_h , must be the sum of the error term from the current output and the error term from the next timestep
 - $\delta_h = g'(z)V\delta_t + \delta_{t+1}$
- Once we have this updated error term for the hidden layer, we can proceed as usual to compute the gradients for *U* and *W*
 - $\frac{\partial L}{\partial W} = \frac{\partial L}{\partial z} \frac{\partial z}{\partial a} \frac{\partial a}{\partial W} = \delta_h x_t$ • $\frac{\partial L}{\partial U} = \frac{\partial L}{\partial z} \frac{\partial z}{\partial a} \frac{\partial a}{\partial U} = \delta_h h_{t-1}$
- Backpropagate the error from δ_h to h_{t-1} based on the weights in U
 - $\delta_{t+1} = g'(z)U\delta_h$
- At this point, we have all of the necessary gradients to update U, V, and W!

Earlier language models (e.g., n-gram language models or those using feedforward neural networks) attempted to predict the next word in a sequence given a prior context of fixed length.

- What's challenging about this approach?
 - Model quality is dependent on context size
 - Anything outside the fixed context window has no impact on the model's decision
- Recurrent neural language models
 address many of these challenges

- At each timestep:
 - Retrieve an embedding for the current input word
 - 2. Combine the weighted sums of (a) the input embedding values and (b) the activations of the hidden layer from the previous step, to compute a new set of activation values from the hidden layer
 - 3. Generate a set of outputs based on the activations from the hidden layer
 - 4. Pass the outputs through a softmax function to generate a probability distribution over the entire vocabulary

- At each timestep:
 - 1. Retrieve an embedding for the current input word
 - 2. Combine the weighted sums of (a) the input embedding values and (b) the activations of the hidden layer from the previous step, to compute a new set of activation values from the hidden layer
 - 3. Generate a set of outputs based on the activations from the hidden layer
 - 4. Pass the outputs through a softmax function to generate a probability distribution over the entire vocabulary

- At each timestep:
 - 1. Retrieve an embedding for the current input word
 - 2. Combine the weighted sums of (a) the input embedding values and (b) the activations of the hidden layer from the previous step, to compute a new set of activation values from the hidden layer
 - 3. Generate a set of outputs based on the activations from the hidden layer
 - 4. Pass the outputs through a softmax function to generate a probability distribution over the entire vocabulary

- At each timestep:
 - 1. Retrieve an embedding for the current input word
 - 2. Combine the weighted sums of (a) the input embedding values and (b) the activations of the hidden layer from the previous step, to compute a new set of activation values from the hidden layer
 - 3. Generate a set of outputs based on the activations from the hidden layer
 - 4. Pass the outputs through a softmax function to generate a probability distribution over the entire vocabulary

Generation with Neural Language Models

- Sample the first word in the output from the softmax distribution that results from using the beginning of sentence marker (<s>) as input
- 2. Get the embedding for that word
- 3. Use it as input to the network at the next time step, and sample the following word as in (1)
- Repeat until the end of sentence marker (</s>) is sampled, or a fixed length limit is reached

- This technique is referred to as
 autoregressive generation
 - Word generated at each timestep is conditioned on the word generated previously by the model









Key to successful autoregressive generation?

Prime the generation component with **appropriate context** (e.g., something more useful than <s>)



Sequence processing models like **RNNs** are also useful for many classification problems.

- Sequence Labeling Tasks: Given a fixed set of labels, assign a label to each element of a sequence
 - Example: Part-of-speech tagging
- Inputs \rightarrow word embeddings
- Outputs → label probabilities generated by the softmax (or other activation) function over the set of all labels
- Sequence Classification Tasks: Given an input sequence, assign the entire sequence to a class (rather than the individual tokens within it)

Sequence Labeling



Sequence Labeling





How to use RNNs for sequence classification?



Sequence Classification



Sequence Classification



Natalie Parde - UIC CS 521

Notes about Sequence Classification

- Loss function is based entirely on the final classification task (not with intermediate outputs)
- Errors are still backpropagated all the way through the RNN
- The process of adjusting weights the entire way through the network based on the loss from a downstream application is often referred to as end-to-end training

Where do we go from here?

- So far, we've discussed "vanilla" RNNs
- Many additional varieties exist!
- Extensions to the vanilla RNN model:
 RNN + Feedforward layers
 Stacked RNNs
 - Bidirectional RNNs



Stacked RNNs



- Use the entire sequence of outputs from one RNN as the input sequence to another
- Capable of outperforming single-layer networks
- Why?
 - Having more layers allows the network to learn representations at differing levels of abstraction across layers
 - Early layers → more fundamental properties
 - Later layers → more meaningful groups of fundamental properties
- Optimal number of RNNs to stack together?
 - Depends on application and training set
- More RNNs in the stack \rightarrow increased training costs

 Standard RNNs only consider the information in a sequence leading up to the current timestep

•
$$h_t^f = RNN_{forward}(x_1^t)$$

• h_t^f corresponds to the normal hidden state at time t



- However, in many cases the context after the current timestep could be useful as well!
- In many applications we also have access to the entire input sequence anyway



- How can we make use of information both before and after the current timestep?
 - Train an RNN on an input sequence in
 reverse
 - $h_t^b = RNN_{backward}(x_t^n)$
 - *h*^b_t corresponds to information from the current timestep to the end of the sequence
 - Combine the forward and backward networks

- Two independent RNNs
 - One where the input is processed from start to end
 - One where the input is processed from end to start
- Outputs combined into a single representation that captures both the prior and future contexts of an input at each timestep
 - $h_t = h_t^f \oplus h_t^b$
- How to combine the contexts?
 - Concatenation
 - Element-wise addition, multiplication, etc.







Sequence Classification with a Bidirectional RNN



Natalie Parde - UIC CS 521

Despite the advantages we've seen compared to feedforward neural networks, RNNs may still struggle with managing context.

- In a standard RNN, the final state tends to reflect more information about recent items than those at the beginning of the sequence
- Distant timesteps \rightarrow less information



This long-distance information can be critical to many tasks!
Why is it so hard to maintain longdistance context?

- Hidden layers must perform two tasks simultaneously:
 - Provide information useful for the current decision (input at *t*)
 - Update and carry forward information required for future decisions (input at time *t*+1 and beyond)
- These tasks may not always be perfectly aligned with one another

There's also the issue of "vanishing gradients"....

- When small derivatives are repeatedly multiplied together, the products can become extremely small
- This means that when backpropagating through time for a long sequence, gradients can become so close to zero that they are no longer effective for model training!



How can we address this?

- Design more complex RNNs that learn to:
 - Forget information that is no longer needed
 - **Remember** information still required for future decisions

Long Short-Term Memory Networks (LSTMs)

- Remove information no longer needed from the context, and add information likely to be needed later
- Do this by:
 - Adding an explicit context layer to the architecture
 - This layer controls the flow of information into and out of network layers using specialized neural units called gates

LSTM Gates

- Feedforward layer + sigmoid activation + pointwise
 multiplication with the layer being gated
- Combination of sigmoid activation and pointwise multiplication essentially creates a **binary mask**
 - Values near 1 in the mask are passed through nearly unchanged
 - Values near 0 are nearly erased
- Three main gates:
 - Forget gate: Should we erase this existing information from the context?
 - Add gate: Should we write this new information to the context?
 - **Output gate:** What information should be leveraged for the current hidden state?



Forget Gate

• Goal: Delete information from the context that is no longer needed

•
$$f_t = \sigma(U_f h_{t-1} + W_f x_t)$$

• $k_t = c_{t-1} \odot f_t$
Weighted sum of:
• Hidden layer at the previous timestep
• Current input

Add Gate

 Goal: Select the information to add to the current context



Add Gate

 Goal: Select the information to add to the current context • $g_t = \tanh(U_g h_{t-1} + W_g x_t)$ • $i_t = \sigma(U_i h_{t-1} + W_i x_t)$ • $j_t = g_t \odot i_t$ New information to be added • $c_t = j_t + k_t$ Updated context vector contains: New information to be added • Existing information from context vector that was not removed by the forget gate

Output Gate

 Goal: Decide what information is required for the *current* hidden state

•
$$o_t = \sigma(U_o h_{t-1} + W_o x_t)$$

• $h_t = o_t \odot tanh(c_t)$
Weighted sum of:
• Hidden layer at the previous timestep
• Current input













Gated Recurrent Units (GRUs)

- Also manage the context that is passed through to the next timestep, but do so using a simpler architecture than LSTMs
 - No separate context vector
 - Only two gates
 - Reset gate
 - Update gate
- Gates still use a similar design to that seen in LSTMs
 - Feedforward layer + sigmoid activation + pointwise multiplication with the layer being gated, resulting in a binary-like mask

Reset Gate

• Goal: Decide which aspects of the previous hidden state are relevant to the current context

•
$$r_t = \sigma(U_r h_{t-1} + W_r x_t)$$

• $\tilde{h_t} = \tanh(U(r_t \odot h_{t-1}) + W x_t)$
Weighted sum of:
• Hidden layer at
the previous
timestep
• Current input

Hidden layer at

the previous

Current input

timestep

•

Update Gate

 Goal: Decide which aspects of the intermediate hidden state and which aspects of the previous hidden state need to be preserved for future use

•
$$z_t = \sigma(U_z h_{t-1} + W_z x_t)$$

• $h_t = (1 - z_t)h_{t-1} + z_t \tilde{h_t}$

Updated hidden layer output

Weighted sum of:

- Hidden layer at the previous timestep
- Current input











Overall, comparing inputs and outputs for some different types of neural units....



When to use LSTMs vs. GRUs?

Why use GRUs instead of LSTMs?

 Computational efficiency: Good for scenarios in which you need to train your model quickly and don't have access to highperformance computing resources

Why use LSTMs instead of GRUs?

• Performance: LSTMs generally outperform GRUs at the same tasks

Summary: Recurrent Neural Networks

- Recurrent neural networks incorporate prior context into their design by leveraging weighted temporal information from the previous timestep
- RNNs can be stacked together, or they can be combined to form bidirectional models
- Two specialized RNN architectures designed to address weaknesses associated with long-range context are long short-term memory networks and gated recurrent units
- Both LSTMs and GRUs incorporate gating mechanisms to offer improved control over the flow of information between timesteps