

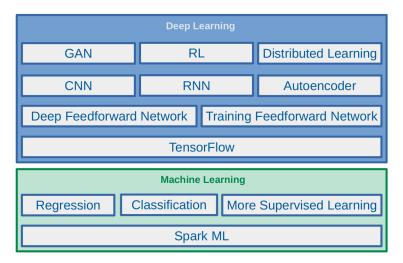
Recurrent Neural Networks

Amir H. Payberah payberah@kth.se 25/11/2019

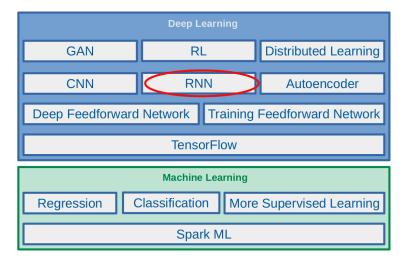


https://id2223kth.github.io







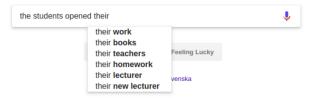




Let's Start With An Example







▶ Language modeling is the task of predicting what word comes next.





Language Modeling (2/2)

▶ More formally: given a sequence of words $x^{(1)}, x^{(2)}, \dots, x^{(t)}$, compute the probability distribution of the next word $x^{(t+1)}$:

$$p(x^{(t+1)} = w_j | x^{(t)}, \cdots x^{(1)})$$





Language Modeling (2/2)

▶ More formally: given a sequence of words $x^{(1)}, x^{(2)}, \dots, x^{(t)}$, compute the probability distribution of the next word $x^{(t+1)}$:

$$p(x^{(t+1)} = w_j | x^{(t)}, \cdots x^{(1)})$$

ightharpoonup w_j is a word in vocabulary $V = \{w_1, \dots, w_v\}$.





▶ the students opened their ___



- ▶ the students opened their ___
- ► How to learn a Language Model?



- ▶ the students opened their ___
- ► How to learn a Language Model?
- ► Learn a n-gram Language Model!



- ▶ the students opened their ___
- ► How to learn a Language Model?
- ► Learn a n-gram Language Model!
- ► A n-gram is a chunk of n consecutive words.



- ▶ the students opened their ___
- ► How to learn a Language Model?
- ► Learn a n-gram Language Model!
- ► A n-gram is a chunk of n consecutive words.
 - Unigrams: "the", "students", "opened", "their"



- ▶ the students opened their ___
- ► How to learn a Language Model?
- ► Learn a n-gram Language Model!
- ► A n-gram is a chunk of n consecutive words.
 - Unigrams: "the", "students", "opened", "their"
 - Bigrams: "the students", "students opened", "opened their"



- ▶ the students opened their ___
- ► How to learn a Language Model?
- ► Learn a n-gram Language Model!
- ► A n-gram is a chunk of n consecutive words.
 - Unigrams: "the", "students", "opened", "their"
 - Bigrams: "the students", "students opened", "opened their"
 - Trigrams: "the students opened", "students opened their"



- ▶ the students opened their ___
- ► How to learn a Language Model?
- ► Learn a n-gram Language Model!
- ► A n-gram is a chunk of n consecutive words.
 - Unigrams: "the", "students", "opened", "their"
 - Bigrams: "the students", "students opened", "opened their"
 - Trigrams: "the students opened", "students opened their"
 - 4-grams: "the students opened their"



- ▶ the students opened their ___
- ► How to learn a Language Model?
- ► Learn a n-gram Language Model!
- ► A n-gram is a chunk of n consecutive words.
 - Unigrams: "the", "students", "opened", "their"
 - Bigrams: "the students", "students opened", "opened their"
 - Trigrams: "the students opened", "students opened their"
 - 4-grams: "the students opened their"
- ► Collect statistics about how frequent different n-grams are, and use these to predict next word.



- ► Suppose we are learning a 4-gram Language Model.
 - $x^{(t+1)}$ depends only on the preceding 3 words $\{x^{(t)}, x^{(t-1)}, x^{(t-2)}\}$.





- ► Suppose we are learning a 4-gram Language Model.
 - $x^{(t+1)}$ depends only on the preceding 3 words $\{x^{(t)}, x^{(t-1)}, x^{(t-2)}\}$.

```
discard condition on this
```

 $p(w_j|students \ opened \ their) = \frac{students \ opened \ their}{students \ opened \ their}$



- ► Suppose we are learning a 4-gram Language Model.
 - $x^{(t+1)}$ depends only on the preceding 3 words $\{x^{(t)}, x^{(t-1)}, x^{(t-2)}\}$.

```
p(w_j|students\ opened\ their) = \frac{\text{students\ opened\ their}}{\text{students\ opened\ their}}
```

- ▶ In the corpus:
 - "students opened their" occurred 1000 times



- ► Suppose we are learning a 4-gram Language Model.
 - $x^{(t+1)}$ depends only on the preceding 3 words $\{x^{(t)}, x^{(t-1)}, x^{(t-2)}\}$.

```
p(w_j|students\ opened\ their) = \frac{\text{students\ opened\ their}}{\text{students\ opened\ their}}
```

- ▶ In the corpus:
 - "students opened their" occurred 1000 times
 - "students opened their books occurred 400 times: p(books|students opened their) = 0.4



- ► Suppose we are learning a 4-gram Language Model.
 - $x^{(t+1)}$ depends only on the preceding 3 words $\{x^{(t)}, x^{(t-1)}, x^{(t-2)}\}$.

```
p(w_j|students\ opened\ their) = \frac{\text{students\ opened\ their}}{\text{students\ opened\ their}}
```

- ▶ In the corpus:
 - "students opened their" occurred 1000 times
 - "students opened their books occurred 400 times: p(books|students opened their) = 0.4
 - "students opened their exams occurred 100 times: p(exams|students opened their) = 0.1



$$p(w_j|students opened their) = \frac{students opened their w_j}{students opened their}$$



$$p(w_j|students opened their) = \frac{students opened their w_j}{students opened their}$$

► What if "students opened their w_j" never occurred in data? Then w_j has probability 0!



$$p(w_j|students opened their) = \frac{students opened their w_j}{students opened their}$$

- ▶ What if "students opened their w_j" never occurred in data? Then w_j has probability 0!
- ► What if "students opened their" never occurred in data? Then we can't calculate probability for any w_j!



$$p(w_j|students \ opened \ their) = \frac{students \ opened \ their \ w_j}{students \ opened \ their}$$

- ▶ What if "students opened their w_j" never occurred in data? Then w_j has probability 0!
- ▶ What if "students opened their" never occurred in data? Then we can't calculate probability for any w_j!
- ▶ Increasing n makes sparsity problems worse.
 - Typically we can't have n bigger than 5.



Problems with n-gram Language Models - Storage

$$p(w_j|students \ opened \ their) = \frac{students \ opened \ their \ w_j}{students \ opened \ their}$$



Problems with n-gram Language Models - Storage

```
p(w_j|students opened their) = \frac{students opened their w_j}{students opened their}
```

- ▶ For "students opened their w_j ", we need to store count for all possible 4-grams.
- ▶ The model size is in the order of $O(\exp(n))$.
- ▶ Increasing n makes model size huge.



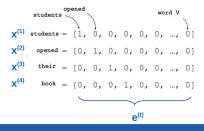
Can We Build a Neural Language Model? (1/3)

- ► Recall the Language Modeling task:
 - Input: sequence of words $x^{(1)}, x^{(2)}, \dots, x^{(t)}$
 - Output: probability dist of the next word $p(x^{(t+1)} = w_i | x^{(t)}, \cdots, x^{(1)})$



Can We Build a Neural Language Model? (1/3)

- ► Recall the Language Modeling task:
 - Input: sequence of words $x^{(1)}, x^{(2)}, \dots, x^{(t)}$
 - Output: probability dist of the next word $p(x^{(t+1)} = w_1 | x^{(t)}, \dots, x^{(1)})$
- ▶ One-Hot encoding
 - Represent a categorical variable as a binary vector.
 - All recodes are zero, except the index of the integer, which is one.
 - Each embedded word $e^{(t)} = E^T x^{(t)}$ is a one-hot vector of size vocabulary size.

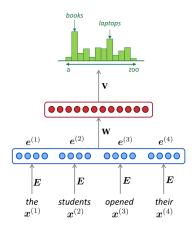




Can We Build a Neural Language Model? (2/3)

► A MLP model

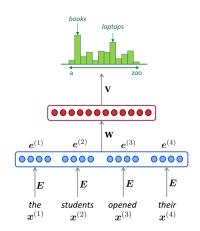
- Input: words $x^{(1)}, x^{(2)}, x^{(3)}, x^{(4)}$
- Input layer: one-hot vectors $\mathbf{e}^{(1)}$, $\mathbf{e}^{(2)}$, $\mathbf{e}^{(3)}$, $\mathbf{e}^{(4)}$
- Hidden layer: $\mathbf{h} = \mathbf{f}(\mathbf{w}^{\mathsf{T}}\mathbf{e})$, \mathbf{f} is an activation function.
- Output: $\hat{\mathbf{y}} = \operatorname{softmax}(\mathbf{v}^{\mathsf{T}}\mathbf{h})$





Can We Build a Neural Language Model? (3/3)

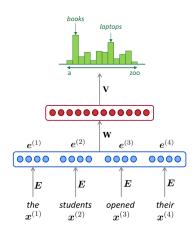
- ► Improvements over n-gram LM:
 - No sparsity problem
 - Model size is O(n) not O(exp(n))





Can We Build a Neural Language Model? (3/3)

- ► Improvements over n-gram LM:
 - No sparsity problem
 - Model size is O(n) not O(exp(n))
- ► Remaining problems:
 - It is fixed 4 in our example, which is small
 - We need a neural architecture that can process any length input





Recurrent Neural Networks (RNN)



Recurrent Neural Networks (1/4)

► The idea behind Recurrent neural networks (RNN) is to make use of sequential data.



- ▶ The idea behind Recurrent neural networks (RNN) is to make use of sequential data.
 - Until here, we assume that all inputs (and outputs) are independent of each other.



- ► The idea behind Recurrent neural networks (RNN) is to make use of sequential data.
 - Until here, we assume that all inputs (and outputs) are independent of each other.
 - Independent input (output) is a bad idea for many tasks, e.g., predicting the next word in a sentence (it's better to know which words came before it).



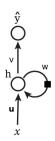
- ► The idea behind Recurrent neural networks (RNN) is to make use of sequential data.
 - Until here, we assume that all inputs (and outputs) are independent of each other.
 - Independent input (output) is a bad idea for many tasks, e.g., predicting the next word in a sentence (it's better to know which words came before it).
- ► They can analyze time series data and predict the future.



- ► The idea behind Recurrent neural networks (RNN) is to make use of sequential data.
 - Until here, we assume that all inputs (and outputs) are independent of each other.
 - Independent input (output) is a bad idea for many tasks, e.g., predicting the next word in a sentence (it's better to know which words came before it).
- ► They can analyze time series data and predict the future.
- ► They can work on sequences of arbitrary lengths, rather than on fixed-sized inputs.

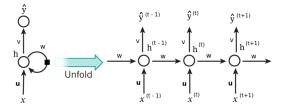


- ▶ Neurons in an RNN have connections pointing backward.
- ► RNNs have memory, which captures information about what has been calculated so far.



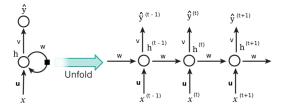


- ▶ Unfolding the network: represent a network against the time axis.
 - We write out the network for the complete sequence.



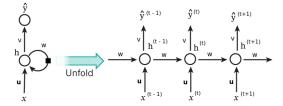


- ▶ Unfolding the network: represent a network against the time axis.
 - We write out the network for the complete sequence.
- ► For example, if the sequence we care about is a sentence of three words, the network would be unfolded into a 3-layer neural network.
 - One layer for each word.



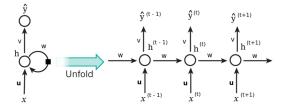


 $h^{(t)} = f(u^T x^{(t)} + wh^{(t-1)})$, where f is an activation function, e.g., tanh or ReLU.



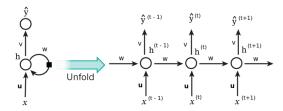


- $h^{(t)} = f(u^T x^{(t)} + wh^{(t-1)})$, where f is an activation function, e.g., tanh or ReLU.
- $\hat{y}^{(t)} = g(vh^{(t)})$, where g can be the softmax function.





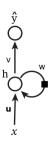
- $h^{(t)} = f(u^T x^{(t)} + wh^{(t-1)})$, where f is an activation function, e.g., tanh or ReLU.
- $\hat{y}^{(t)} = g(vh^{(t)})$, where g can be the softmax function.
- $\blacktriangleright \ \text{cost}(\textbf{y}^{(t)}, \boldsymbol{\hat{y}}^{(t)}) = \text{cross_entropy}(\textbf{y}^{(t)}, \boldsymbol{\hat{y}}^{(t)}) = -\sum \textbf{y}^{(t)} \text{log} \boldsymbol{\hat{y}}^{(t)}$
- $ightharpoonup y^{(t)}$ is the correct word at time step t, and $\hat{y}^{(t)}$ is the prediction.





Recurrent Neurons - Weights (1/4)

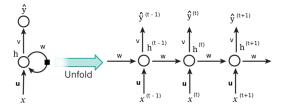
► Each recurrent neuron has three sets of weights: **u**, w, and v.





Recurrent Neurons - Weights (2/4)

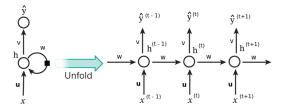
▶ **u**: the weights for the inputs **x**^(t).





Recurrent Neurons - Weights (2/4)

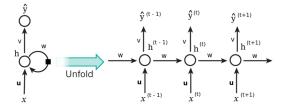
- ▶ **u**: the weights for the inputs **x**^(t).
- ► x^(t): is the input at time step t.
- ► For example, **x**⁽¹⁾ could be a one-hot vector corresponding to the first word of a sentence.





Recurrent Neurons - Weights (3/4)

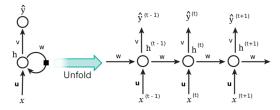
• w: the weights for the hidden state of the previous time step $h^{(t-1)}$.





Recurrent Neurons - Weights (3/4)

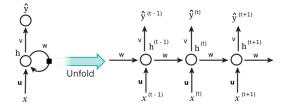
- \triangleright w: the weights for the hidden state of the previous time step $h^{(t-1)}$.
- ▶ h^(t): is the hidden state (memory) at time step t.
 - $h^{(t)} = tanh(\mathbf{u}^\mathsf{T}\mathbf{x}^{(t)} + wh^{(t-1)})$
 - h⁽⁰⁾ is the initial hidden state.





Recurrent Neurons - Weights (4/4)

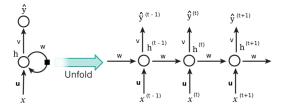
v: the weights for the hidden state of the current time step h^(t).





Recurrent Neurons - Weights (4/4)

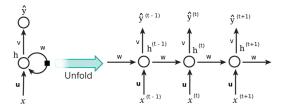
- v: the weights for the hidden state of the current time step h^(t).
- $ightharpoonup \hat{\mathbf{y}}^{(t)}$ is the output at step t.
- $\mathbf{\hat{y}}^{(t)} = softmax(vh^{(t)})$





Recurrent Neurons - Weights (4/4)

- v: the weights for the hidden state of the current time step h^(t).
- $ightharpoonup \hat{\mathbf{y}}^{(t)}$ is the output at step t.
- $\mathbf{\hat{y}}^{(t)} = \text{softmax}(vh^{(t)})$
- ► For example, if we wanted to predict the next word in a sentence, it would be a vector of probabilities across our vocabulary.

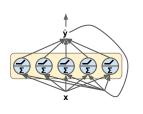




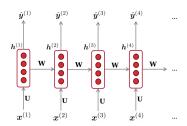
Layers of Recurrent Neurons

At each time step t, every neuron of a layer receives both the input vector $\mathbf{x}^{(t)}$ and the output vector from the previous time step $\mathbf{h}^{(t-1)}$.

$$\begin{aligned} \mathbf{h}^{(t)} &= \text{tanh}(\mathbf{u}^{\mathsf{T}}\mathbf{x}^{(t)} + \mathbf{w}^{\mathsf{T}}\mathbf{h}^{(t-1)}) \\ \mathbf{y}^{(t)} &= \text{sigmoid}(\mathbf{v}^{\mathsf{T}}\mathbf{h}^{(t)}) \end{aligned}$$

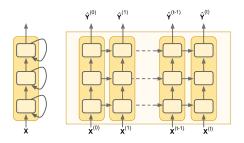








► Stacking multiple layers of cells gives you a deep RNN.



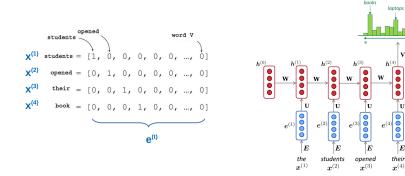


Let's Back to Language Model Example



A RNN Neural Language Model (1/2)

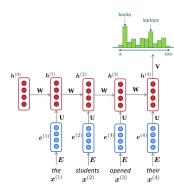
- ▶ The input x will be a sequence of words (each $x^{(t)}$ is a single word).
- ▶ Each embedded word $e^{(t)} = E^T x^{(t)}$ is a one-hot vector of size vocabulary size.





A RNN Neural Language Model (2/2)

- ► Let's recap the equations for the RNN:
 - $\begin{aligned} & \cdot \ \mathbf{h}^{(t)} = \text{tanh}(\mathbf{u}^{\mathsf{T}}\mathbf{e}^{(t)} + \text{wh}^{(t-1)}) \\ & \cdot \ \hat{\mathbf{y}}^{(t)} = \text{softmax}(\text{vh}^{(t)}) \end{aligned}$



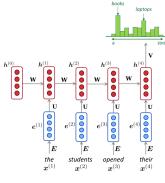


A RNN Neural Language Model (2/2)

Let's recap the equations for the RNN:

```
 \begin{aligned} & \cdot \ \mathbf{h}^{(\texttt{t})} = \mathtt{tanh}(\mathbf{u}^{\intercal} \mathbf{e}^{(\texttt{t})} + \mathtt{wh}^{(\texttt{t}-1)}) \\ & \cdot \ \hat{\mathbf{y}}^{(\texttt{t})} = \mathtt{softmax}(\mathtt{vh}^{(\texttt{t})}) \end{aligned}
```

▶ The output $\hat{\mathbf{y}}^{(t)}$ is a vector of vocabulary size elements.



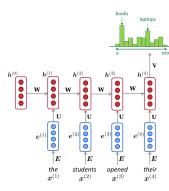


A RNN Neural Language Model (2/2)

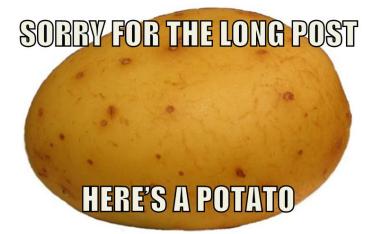
Let's recap the equations for the RNN:

```
 \begin{aligned} & \cdot \ \mathbf{h}^{(\texttt{t})} = \mathtt{tanh}(\mathbf{u}^{\intercal}\mathbf{e}^{(\texttt{t})} + \mathtt{wh}^{(\texttt{t}-1)}) \\ & \cdot \ \hat{\mathbf{y}}^{(\texttt{t})} = \mathtt{softmax}(\mathtt{vh}^{(\texttt{t})}) \end{aligned}
```

- ▶ The output $\hat{\mathbf{y}}^{(t)}$ is a vector of vocabulary size elements.
- ► Each element of ŷ^(t) represents the probability of that word being the next word in the sentence.







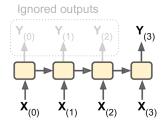


RNN Design Patterns



RNN Design Patterns - Sequence-to-Vector

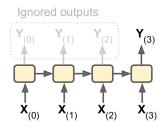
► Sequence-to-vector network: takes a sequence of inputs, and ignore all outputs except for the last one.





RNN Design Patterns - Sequence-to-Vector

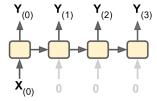
- ► Sequence-to-vector network: takes a sequence of inputs, and ignore all outputs except for the last one.
- ▶ E.g., you could feed the network a sequence of words corresponding to a movie review, and the network would output a sentiment score.





RNN Design Patterns - Vector-to-Sequence

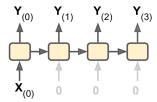
▶ Vector-to-sequence network: takes a single input at the first time step, and let it output a sequence.





RNN Design Patterns - Vector-to-Sequence

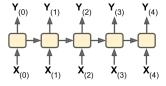
- ▶ Vector-to-sequence network: takes a single input at the first time step, and let it output a sequence.
- ► E.g., the input could be an image, and the output could be a caption for that image.





RNN Design Patterns - Sequence-to-Sequence

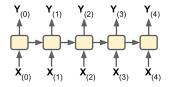
► Sequence-to-sequence network: takes a sequence of inputs and produce a sequence of outputs.





RNN Design Patterns - Sequence-to-Sequence

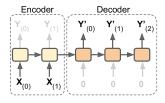
- ► Sequence-to-sequence network: takes a sequence of inputs and produce a sequence of outputs.
- ▶ Useful for predicting time series such as stock prices: you feed it the prices over the last N days, and it must output the prices shifted by one day into the future.
- ▶ Here, both input sequences and output sequences have the same length.





RNN Design Patterns - Encoder-Decoder

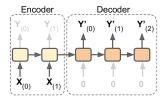
► Encoder-decoder network: a sequence-to-vector network (encoder), followed by a vector-to-sequence network (decoder).





RNN Design Patterns - Encoder-Decoder

- ► Encoder-decoder network: a sequence-to-vector network (encoder), followed by a vector-to-sequence network (decoder).
- ► E.g., translating a sentence from one language to another.
- ▶ You would feed the network a sentence in one language, the encoder would convert this sentence into a single vector representation, and then the decoder would decode this vector into a sentence in another language.



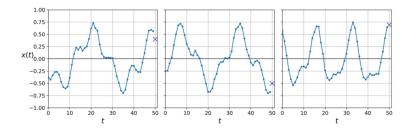


RNN in TensorFlow



RNN in TensorFlow (1/5)

- Forecasting a time series
- ► E.g., a dataset of 10000 time series, each of them 50 time steps long.
- ► The goal here is to forecast the value at the next time step (represented by the X) for each of them.



Use fully connected network

```
model = keras.models.Sequential([
         keras.layers.Flatten(input_shape=[50, 1]),
         keras.layers.Dense(1)
])
model.compile(loss="mse", optimizer="adam")
history = model.fit(X_train, y_train, epochs=20)
model.evaluate(X_test, y_test, verbose=0)
# loss: 0.003993967570985357
```

► Simple RNN

```
model = keras.models.Sequential([
         keras.layers.SimpleRNN(1, input_shape=[None, 1])
])

model.compile(loss="mse", optimizer='adam')
history = model.fit(X_train, y_train, epochs=20)

model.evaluate(X_test, y_test, verbose=0)
# loss: 0.011026302369932333
```



RNN in TensorFlow (4/5)

► Deep RNN

```
model = keras.models.Sequential([
         keras.layers.SimpleRNN(20, return_sequences=True, input_shape=[None, 1]),
         keras.layers.SimpleRNN(20, return_sequences=True),
         keras.layers.SimpleRNN(1)
])

model.compile(loss="mse", optimizer="adam")
history = model.fit(X_train, y_train, epochs=20)

model.evaluate(X_test, y_test, verbose=0)
# loss: 0.003197280486735205
```



RNN in TensorFlow (5/5)

- ► Deep RNN (second implementation)
- ► Make the second layer return only the last output (no return_sequences)

```
model = keras.models.Sequential([
    keras.layers.SimpleRNN(20, return_sequences=True, input_shape=[None, 1]),
    keras.layers.SimpleRNN(20),
    keras.layers.Dense(1)
])

model.compile(loss="mse", optimizer="adam")
history = model.fit(X_train, y_train, epochs=20)

model.evaluate(X_test, y_test, verbose=0)
# loss: 0.002757748544837038
```



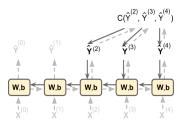
Training RNNs

- ► To train an RNN, we should unroll it through time and then simply use regular backpropagation.
- ► This strategy is called backpropagation through time (BPTT).



Backpropagation Through Time (1/3)

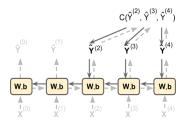
- ▶ To train the model using BPTT, we go through the following steps:
- ▶ 1. Forward pass through the unrolled network (represented by the dashed arrows).
- ▶ 2. The cost function is $C(\hat{y}^{tmin}, \hat{y}^{tmin+1}, \dots, \hat{y}^{tmax})$, where tmin and tmax are the first and last output time steps, not counting the ignored outputs.





Backpropagation Through Time (2/3)

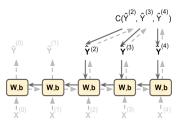
- ▶ 3. Propagate backward the gradients of that cost function through the unrolled network (represented by the solid arrows).
- ▶ 4. The model parameters are updated using the gradients computed during BPTT.



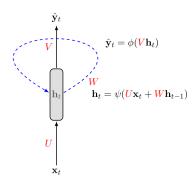


Backpropagation Through Time (3/3)

- ► The gradients flow backward through all the outputs used by the cost function, not just through the final output.
- ► For example, in the following figure:
 - The cost function is computed using the last three outputs, $\hat{\mathbf{y}}^{(2)}$, $\hat{\mathbf{y}}^{(3)}$, and $\hat{\mathbf{y}}^{(4)}$.
 - Gradients flow through these three outputs, but not through $\hat{\mathbf{y}}^{(0)}$ and $\hat{\mathbf{y}}^{(1)}$.







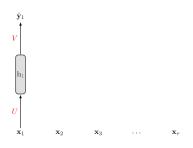


 \mathbf{x}_1 \mathbf{x}_2 \mathbf{x}_3 ... \mathbf{x}_{τ}

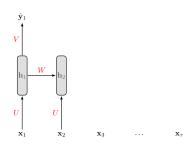




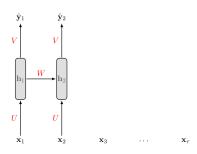




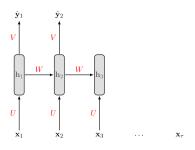




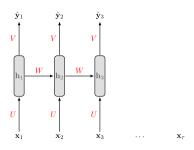




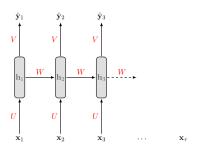




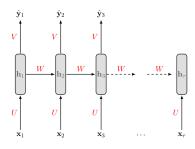




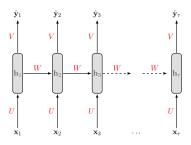




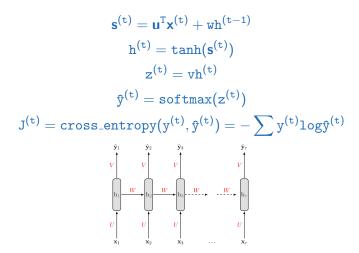




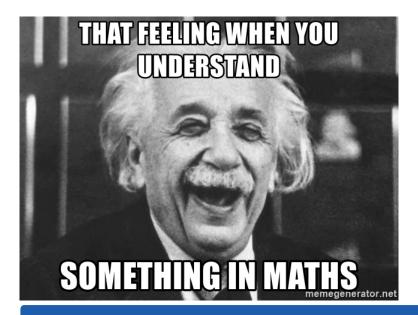








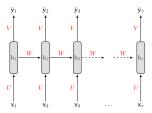






$$\mathbf{J^{(t)}} = \texttt{cross_entropy}(\mathbf{y^{(t)}}, \mathbf{\hat{y}^{(t)}}) = -\sum \mathbf{y^{(t)}log}\mathbf{\hat{y}^{(t)}}$$

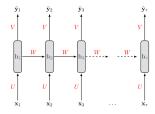
▶ We treat the full sequence as one training example.





$$\textbf{J}^{(t)} = \texttt{cross_entropy}(\textbf{y}^{(t)}, \boldsymbol{\hat{y}}^{(t)}) = -\sum \textbf{y}^{(t)} \texttt{log} \boldsymbol{\hat{y}}^{(t)}$$

- ▶ We treat the full sequence as one training example.
- ► The total error E is just the sum of the errors at each time step.
- E.g., $E = J^{(1)} + J^{(2)} + \cdots + J^{(t)}$





▶ $J^{(t)}$ is the total cost, so we can say that a 1-unit increase in v, w or u will impact each of $J^{(1)}$, $J^{(2)}$, until $J^{(t)}$ individually.



- ▶ $J^{(t)}$ is the total cost, so we can say that a 1-unit increase in v, w or u will impact each of $J^{(1)}$, $J^{(2)}$, until $J^{(t)}$ individually.
- ▶ The gradient is equal to the sum of the respective gradients at each time step t.



- ▶ $J^{(t)}$ is the total cost, so we can say that a 1-unit increase in v, w or u will impact each of $J^{(1)}$, $J^{(2)}$, until $J^{(t)}$ individually.
- ▶ The gradient is equal to the sum of the respective gradients at each time step t.
- ▶ For example if t = 3 we have: $E = J^{(1)} + J^{(2)} + J^{(3)}$



- ▶ $J^{(t)}$ is the total cost, so we can say that a 1-unit increase in v, w or u will impact each of $J^{(1)}$, $J^{(2)}$, until $J^{(t)}$ individually.
- ▶ The gradient is equal to the sum of the respective gradients at each time step t.
- ▶ For example if t = 3 we have: $E = J^{(1)} + J^{(2)} + J^{(3)}$

$$\frac{\partial E}{\partial v} = \sum_{t} \frac{\partial J^{(t)}}{\partial v} = \frac{\partial J^{(3)}}{\partial v} + \frac{\partial J^{(2)}}{\partial v} + \frac{\partial J^{(1)}}{\partial v}$$



- ▶ $J^{(t)}$ is the total cost, so we can say that a 1-unit increase in v, w or u will impact each of $J^{(1)}$, $J^{(2)}$, until $J^{(t)}$ individually.
- ▶ The gradient is equal to the sum of the respective gradients at each time step t.
- ▶ For example if t = 3 we have: $E = J^{(1)} + J^{(2)} + J^{(3)}$

$$\frac{\partial E}{\partial v} = \sum_{t} \frac{\partial J^{(t)}}{\partial v} = \frac{\partial J^{(3)}}{\partial v} + \frac{\partial J^{(2)}}{\partial v} + \frac{\partial J^{(1)}}{\partial v}$$

$$\frac{\partial E}{\partial w} = \sum_{t} \frac{\partial J^{(t)}}{\partial w} = \frac{\partial J^{(3)}}{\partial w} + \frac{\partial J^{(2)}}{\partial w} + \frac{\partial J^{(1)}}{\partial w}$$



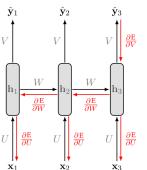
- ▶ $J^{(t)}$ is the total cost, so we can say that a 1-unit increase in v, w or u will impact each of $J^{(1)}$, $J^{(2)}$, until $J^{(t)}$ individually.
- ► The gradient is equal to the sum of the respective gradients at each time step t.
- ▶ For example if t = 3 we have: $E = J^{(1)} + J^{(2)} + J^{(3)}$

$$\begin{split} \frac{\partial E}{\partial v} &= \sum_{t} \frac{\partial J^{(t)}}{\partial v} = \frac{\partial J^{(3)}}{\partial v} + \frac{\partial J^{(2)}}{\partial v} + \frac{\partial J^{(1)}}{\partial v} \\ \frac{\partial E}{\partial w} &= \sum_{t} \frac{\partial J^{(t)}}{\partial w} = \frac{\partial J^{(3)}}{\partial w} + \frac{\partial J^{(2)}}{\partial w} + \frac{\partial J^{(1)}}{\partial w} \\ \frac{\partial E}{\partial u} &= \sum_{t} \frac{\partial J^{(3)}}{\partial u} = \frac{\partial J^{(3)}}{\partial u} + \frac{\partial J^{(2)}}{\partial u} + \frac{\partial J^{(1)}}{\partial u} \end{split}$$



- ► Let's start with $\frac{\partial \mathbf{E}}{\partial \mathbf{v}}$.
- A change in v will only impact $J^{(3)}$ at time t=3, because it plays no role in computing the value of anything other than $z^{(3)}$. \hat{y}_1 \hat{y}_2 \hat{y}_3

$$\frac{\partial E}{\partial v} = \sum_{t} \frac{\partial J^{(t)}}{\partial v} = \frac{\partial J^{(3)}}{\partial v} + \frac{\partial J^{(2)}}{\partial v} + \frac{\partial J^{(1)}}{\partial v}$$

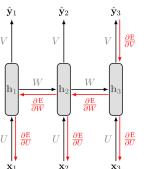




- ► Let's start with $\frac{\partial \mathbf{E}}{\partial \mathbf{v}}$.
- A change in v will only impact $J^{(3)}$ at time t=3, because it plays no role in computing the value of anything other than $z^{(3)}$. \hat{y}_1 \hat{y}_2 \hat{y}_3

$$\frac{\partial E}{\partial v} = \sum_{t} \frac{\partial J^{(t)}}{\partial v} = \frac{\partial J^{(3)}}{\partial v} + \frac{\partial J^{(2)}}{\partial v} + \frac{\partial J^{(1)}}{\partial v}$$

$$\tfrac{\partial J^{(3)}}{\partial v} = \tfrac{\partial J^{(3)}}{\partial \hat{v}^{(3)}} \tfrac{\partial \hat{y}^{(3)}}{\partial z^{(3)}} \tfrac{\partial z^{(3)}}{\partial v}$$



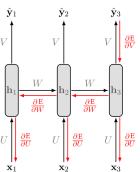


- ► Let's start with $\frac{\partial \mathbf{E}}{\partial \mathbf{v}}$.
- A change in v will only impact $J^{(3)}$ at time t=3, because it plays no role in computing the value of anything other than $z^{(3)}$. \hat{y}_1 \hat{y}_2 \hat{y}_3

$$\frac{\partial E}{\partial v} = \sum_{t} \frac{\partial J^{(t)}}{\partial v} = \frac{\partial J^{(3)}}{\partial v} + \frac{\partial J^{(2)}}{\partial v} + \frac{\partial J^{(1)}}{\partial v}$$

$$\frac{\partial J^{(3)}}{\partial v} = \frac{\partial J^{(3)}}{\partial \hat{y}^{(3)}} \frac{\partial \hat{y}^{(3)}}{\partial z^{(3)}} \frac{\partial z^{(3)}}{\partial v}$$

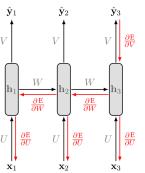
$$\frac{\partial J^{(2)}}{\partial v} = \frac{\partial J^{(2)}}{\partial \hat{y}^{(2)}} \frac{\partial \hat{y}^{(2)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial v}$$





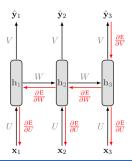
- ► Let's start with $\frac{\partial \mathbf{E}}{\partial \mathbf{v}}$.
- A change in v will only impact $J^{(3)}$ at time t=3, because it plays no role in computing the value of anything other than $z^{(3)}$. \hat{y}_1 \hat{y}_2 \hat{y}_3

$$\begin{split} \frac{\partial E}{\partial v} &= \sum_{\mathbf{t}} \frac{\partial J^{(\mathbf{t})}}{\partial v} = \frac{\partial J^{(3)}}{\partial v} + \frac{\partial J^{(2)}}{\partial v} + \frac{\partial J^{(1)}}{\partial v} \\ \frac{\partial J^{(3)}}{\partial v} &= \frac{\partial J^{(3)}}{\partial \hat{y}^{(3)}} \frac{\partial \hat{y}^{(3)}}{\partial z^{(3)}} \frac{\partial z^{(3)}}{\partial v} \\ \frac{\partial J^{(2)}}{\partial v} &= \frac{\partial J^{(2)}}{\partial \hat{y}^{(2)}} \frac{\partial \hat{y}^{(2)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial v} \\ \frac{\partial J^{(1)}}{\partial v} &= \frac{\partial J^{(1)}}{\partial \hat{y}^{(1)}} \frac{\partial \hat{y}^{(1)}}{\partial z^{(1)}} \frac{\partial z^{(1)}}{\partial v} \end{split}$$





- ▶ Let's compute the derivatives of $\frac{\partial J}{\partial w}$ and $\frac{\partial J}{\partial u}$, which are computed the same.
- A change in w at t = 3 will impact our cost J in 3 separate ways:
 - 1. When computing the value of $h^{(1)}$.
 - 2. When computing the value of $h^{(2)}$, which depends on $h^{(1)}$.
 - 3. When computing the value of $h^{(3)}$, which depends on $h^{(2)}$, which depends on $h^{(1)}$.

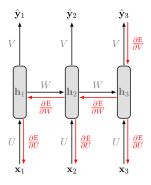




BPTT Step by Step (17/20)

▶ we compute our individual gradients as:

$$\begin{split} &\sum_{\mathbf{t}} \frac{\partial \mathbf{J}^{(\mathbf{t})}}{\partial \mathbf{w}} = \frac{\partial \mathbf{J}^{(3)}}{\partial \mathbf{w}} + \frac{\partial \mathbf{J}^{(2)}}{\partial \mathbf{w}} + \frac{\partial \mathbf{J}^{(1)}}{\partial \mathbf{w}} \\ &\frac{\partial \mathbf{J}^{(1)}}{\partial \mathbf{w}} = \frac{\partial \mathbf{J}^{(1)}}{\partial \hat{\mathbf{y}}^{(1)}} \frac{\partial \hat{\mathbf{y}}^{(1)}}{\partial \mathbf{z}^{(1)}} \frac{\partial \mathbf{z}^{(1)}}{\partial \mathbf{h}^{(1)}} \frac{\partial \mathbf{h}^{(1)}}{\partial \mathbf{z}^{(1)}} \frac{\partial \mathbf{s}^{(1)}}{\partial \mathbf{w}} \end{split}$$

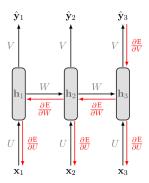




BPTT Step by Step (18/20)

we compute our individual gradients as:

$$\begin{split} \sum_{\mathbf{t}} \frac{\partial J^{(t)}}{\partial w} &= \frac{\partial J^{(3)}}{\partial w} + \frac{\partial J^{(2)}}{\partial w} + \frac{\partial J^{(1)}}{\partial w} \\ \frac{\partial J^{(2)}}{\partial w} &= \frac{\partial J^{(2)}}{\partial \dot{y}^{(2)}} \frac{\partial \dot{y}^{(2)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial h^{(2)}} \frac{\partial h^{(2)}}{\partial s^{(2)}} \frac{\partial s^{(2)}}{\partial w} + \\ &\qquad \qquad \frac{\partial J^{(2)}}{\partial \dot{y}^{(2)}} \frac{\partial \dot{y}^{(2)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial h^{(2)}} \frac{\partial h^{(2)}}{\partial s^{(2)}} \frac{\partial s^{(2)}}{\partial h^{(1)}} \frac{\partial h^{(1)}}{\partial s^{(1)}} \frac{\partial s^{(1)}}{\partial w} \end{split}$$

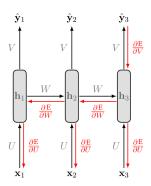




BPTT Step by Step (19/20)

▶ we compute our individual gradients as:

$$\begin{split} \sum_{\mathbf{t}} \frac{\partial J^{(\mathbf{t})}}{\partial w} &= \frac{\partial J^{(3)}}{\partial w} + \frac{\partial J^{(2)}}{\partial w} + \frac{\partial J^{(1)}}{\partial w} \\ \frac{\partial J^{(3)}}{\partial w} &= \frac{\partial J^{(3)}}{\partial \hat{\mathbf{y}}^{(3)}} \frac{\partial \hat{\mathbf{y}}^{(3)}}{\partial \mathbf{z}^{(3)}} \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{h}^{(3)}} \frac{\partial \mathbf{h}^{(3)}}{\partial \mathbf{s}^{(3)}} \frac{\partial \mathbf{s}^{(3)}}{\partial w} + \\ & \frac{\partial J^{(3)}}{\partial \hat{\mathbf{y}}^{(3)}} \frac{\partial \hat{\mathbf{y}}^{(3)}}{\partial \mathbf{z}^{(3)}} \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{h}^{(3)}} \frac{\partial \mathbf{h}^{(3)}}{\partial \mathbf{s}^{(3)}} \frac{\partial \mathbf{s}^{(3)}}{\partial \mathbf{h}^{(2)}} \frac{\partial \mathbf{h}^{(2)}}{\partial \mathbf{s}^{(2)}} \frac{\partial \mathbf{s}^{(2)}}{\partial w} + \\ & \frac{\partial J^{(3)}}{\partial \hat{\mathbf{y}}^{(3)}} \frac{\partial \hat{\mathbf{y}}^{(3)}}{\partial \mathbf{z}^{(3)}} \frac{\partial \mathbf{z}^{(3)}}{\partial \mathbf{h}^{(3)}} \frac{\partial \mathbf{h}^{(3)}}{\partial \mathbf{s}^{(3)}} \frac{\partial \mathbf{s}^{(3)}}{\partial \mathbf{h}^{(2)}} \frac{\partial \mathbf{h}^{(2)}}{\partial \mathbf{s}^{(2)}} \frac{\partial \mathbf{s}^{(2)}}{\partial \mathbf{h}^{(1)}} \frac{\partial \mathbf{h}^{(1)}}{\partial \mathbf{s}^{(1)}} \frac{\partial \mathbf{s}^{(1)}}{\partial \mathbf{w}} \end{split}$$

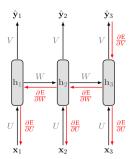




BPTT Step by Step (20/20)

▶ More generally, a change in w will impact our cost J^(t) on t separate occasions.

$$\frac{\partial \mathbf{J^{(t)}}}{\partial \mathbf{W}} = \sum_{k=1}^t \frac{\partial \mathbf{J^{(t)}}}{\partial \hat{\mathbf{y}^{(t)}}} \frac{\partial \hat{\mathbf{y}^{(t)}}}{\partial \mathbf{z^{(t)}}} \frac{\partial \hat{\mathbf{z}^{(t)}}}{\partial \mathbf{h^{(t)}}} \left(\prod_{\mathbf{j}=k+1}^t \frac{\partial \mathbf{h^{(j)}}}{\partial \mathbf{s^{(j)}}} \frac{\partial \mathbf{s^{(j)}}}{\partial \mathbf{h^{(j-1)}}}\right) \frac{\partial \mathbf{h^{(k)}}}{\partial \mathbf{s^{(k)}}} \frac{\partial \mathbf{s^{(k)}}}{\partial \mathbf{W}}$$





LSTM

RNN Problems

- ▶ Sometimes we only need to look at recent information to perform the present task.
 - E.g., predicting the next word based on the previous ones.

RNN Problems

- Sometimes we only need to look at recent information to perform the present task.
 - E.g., predicting the next word based on the previous ones.
- ▶ In such cases, where the gap between the relevant information and the place that it's needed is small, RNNs can learn to use the past information.

RNN Problems

- Sometimes we only need to look at recent information to perform the present task.
 - E.g., predicting the next word based on the previous ones.
- ▶ In such cases, where the gap between the relevant information and the place that it's needed is small, RNNs can learn to use the past information.
- ▶ But, as that gap grows, RNNs become unable to learn to connect the information.
- ► RNNs may suffer from the vanishing/exploding gradients problem.

- Sometimes we only need to look at recent information to perform the present task.
 - E.g., predicting the next word based on the previous ones.
- ▶ In such cases, where the gap between the relevant information and the place that it's needed is small, RNNs can learn to use the past information.
- ▶ But, as that gap grows, RNNs become unable to learn to connect the information.
- ► RNNs may suffer from the vanishing/exploding gradients problem.
- ► To solve these problem, long short-term memory (LSTM) have been introduced.

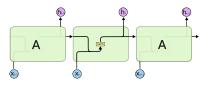
- Sometimes we only need to look at recent information to perform the present task.
 - E.g., predicting the next word based on the previous ones.
- ▶ In such cases, where the gap between the relevant information and the place that it's needed is small, RNNs can learn to use the past information.
- ▶ But, as that gap grows, RNNs become unable to learn to connect the information.
- ► RNNs may suffer from the vanishing/exploding gradients problem.
- ► To solve these problem, long short-term memory (LSTM) have been introduced.
- ▶ In LSTM, the network can learn what to store and what to throw away.

▶ Without looking inside the box, the LSTM cell looks exactly like a basic RNN cell.



RNN Basic Cell vs. LSTM

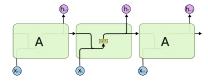
- ▶ Without looking inside the box, the LSTM cell looks exactly like a basic RNN cell.
- ► A basic RNN contains a single layer in each cell.



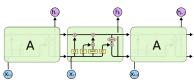


RNN Basic Cell vs. LSTM

- ▶ Without looking inside the box, the LSTM cell looks exactly like a basic RNN cell.
- ► A basic RNN contains a single layer in each cell.

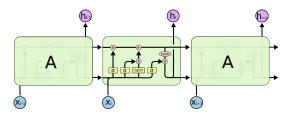


► An LSTM contains four interacting layers in each cell.



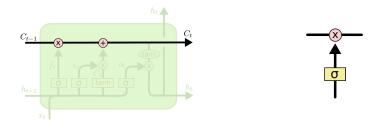
LSTM (1/2)

- ► In LSTM state is split in two vectors:
 - 1. h^(t) (h stands for hidden): the short-term state
 - 2. c^(t) (c stands for cell): the long-term state



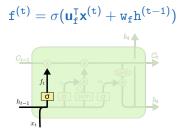
LSTM (2/2)

- ▶ The cell state (long-term state), the horizontal line on the top of the diagram.
- ▶ The LSTM can remove/add information to the cell state, regulated by three gates.
 - Forget gate, input gate and output gate



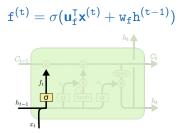


► Step one: decides what information we are going to throw away from the cell state.



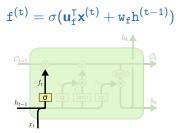


- ► Step one: decides what information we are going to throw away from the cell state.
- ► This decision is made by a sigmoid layer, called the forget gate layer.



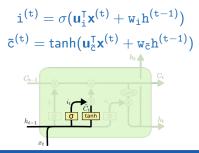


- ▶ Step one: decides what information we are going to throw away from the cell state.
- ► This decision is made by a sigmoid layer, called the forget gate layer.
- It looks at h^(t-1) and x^(t), and outputs a number between 0 and 1 for each number in the cell state c^(t-1).
 - 1 represents completely keep this, and 0 represents completely get rid of this.



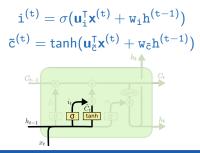


► Second step: decides what new information we are going to store in the cell state. This has two parts:



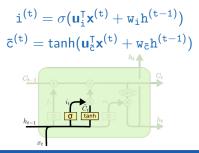


- ► Second step: decides what new information we are going to store in the cell state. This has two parts:
- ▶ 1. A sigmoid layer, called the input gate layer, decides which values we will update.



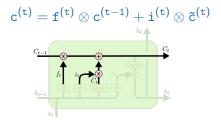


- ► Second step: decides what new information we are going to store in the cell state. This has two parts:
- ▶ 1. A sigmoid layer, called the input gate layer, decides which values we will update.
- ▶ 2. A tanh layer creates a vector of new candidate values that could be added to the state.



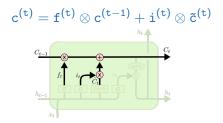


▶ Third step: updates the old cell state $c^{(t-1)}$, into the new cell state $c^{(t)}$.



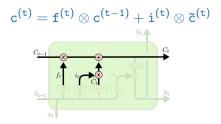


- ▶ Third step: updates the old cell state $c^{(t-1)}$, into the new cell state $c^{(t)}$.
- ▶ We multiply the old state by f^(t), forgetting the things we decided to forget earlier.



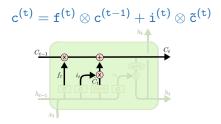


- ▶ Third step: updates the old cell state $c^{(t-1)}$, into the new cell state $c^{(t)}$.
- ▶ We multiply the old state by f^(t), forgetting the things we decided to forget earlier.
- ▶ Then we add it $i^{(t)} \otimes \tilde{c}^{(t)}$.



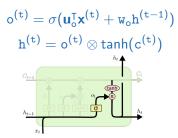


- ▶ Third step: updates the old cell state $c^{(t-1)}$, into the new cell state $c^{(t)}$.
- ▶ We multiply the old state by f^(t), forgetting the things we decided to forget earlier.
- ▶ Then we add it $i^{(t)} \otimes \tilde{c}^{(t)}$.
- ► This is the new candidate values, scaled by how much we decided to update each state value.



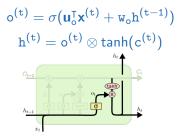


► Fourth step: decides about the output.



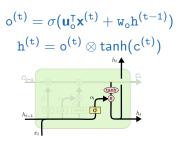


- ► Fourth step: decides about the output.
- ► First, runs a sigmoid layer that decides what parts of the cell state we are going to output.





- ► Fourth step: decides about the output.
- ► First, runs a sigmoid layer that decides what parts of the cell state we are going to output.
- ► Then, puts the cell state through tanh and multiplies it by the output of the sigmoid gate (output gate), so that it only outputs the parts it decided to.



► Use LSTM

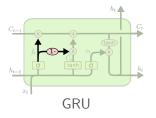
```
model = keras.models.Sequential([
    keras.layers.LSTM(20, return_sequences=True, input_shape=[None, 1]),
    keras.layers.LSTM(20),
    keras.layers.Dense(1)
])

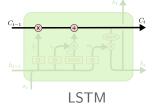
model.compile(loss="mse", optimizer="adam", metrics=[last_time_step_mse])
history = model.fit(X_train, y_train, epochs=20)

model.evaluate(X_test, y_test, verbose=0)
```



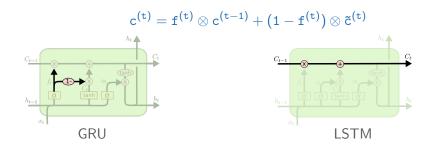
▶ The GRU cell is a simplified version of the LSTM cell.





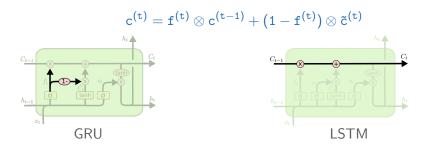


- ▶ The GRU cell is a simplified version of the LSTM cell.
- ► Instead of separately deciding what to forget and what to add to the new information to, it makes those decisions together.



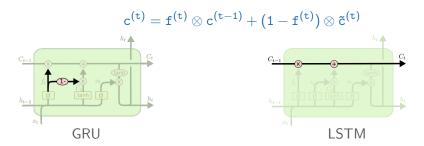


- ▶ The GRU cell is a simplified version of the LSTM cell.
- ► Instead of separately deciding what to forget and what to add to the new information to, it makes those decisions together.
 - It only forgets when it is going to input something in its place.





- ▶ The GRU cell is a simplified version of the LSTM cell.
- ► Instead of separately deciding what to forget and what to add to the new information to, it makes those decisions together.
 - It only forgets when it is going to input something in its place.
 - It only inputs new values to the state when it forgets something older.



▶ Use GRU

```
model = keras.models.Sequential([
    keras.layers.GRU(20, return_sequences=True, input_shape=[None, 1]),
    keras.layers.GRU(20),
    keras.layers.Dense(1)
])

model.compile(loss="mse", optimizer="adam", metrics=[last_time_step_mse])
history = model.fit(X_train, y_train, epochs=20)

model.evaluate(X_test, y_test, verbose=0)
```



Summary

Summary

- ► RNN
- ► Unfolding the network
- ► Three weights
- ► RNN design patterns
- ► Backpropagation through time
- ► LSTM and GRU

Reference

- ▶ Ian Goodfellow et al., Deep Learning (Ch. 10)
- ► Aurélien Géron, Hands-On Machine Learning (Ch. 15)
- Understanding LSTM Networks http://colah.github.io/posts/2015-08-Understanding-LSTMs
- ► CS224d: Deep Learning for Natural Language Processing http://cs224d.stanford.edu



Questions?