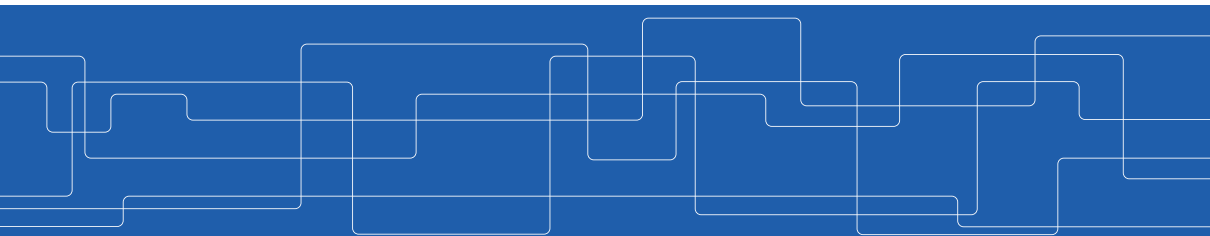




Recurrent Neural Networks

Amir H. Payberah
payberah@kth.se
2020-11-24



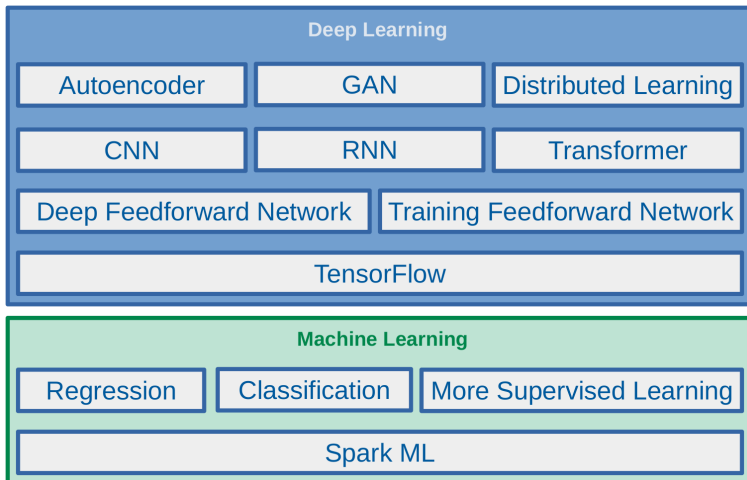


The Course Web Page

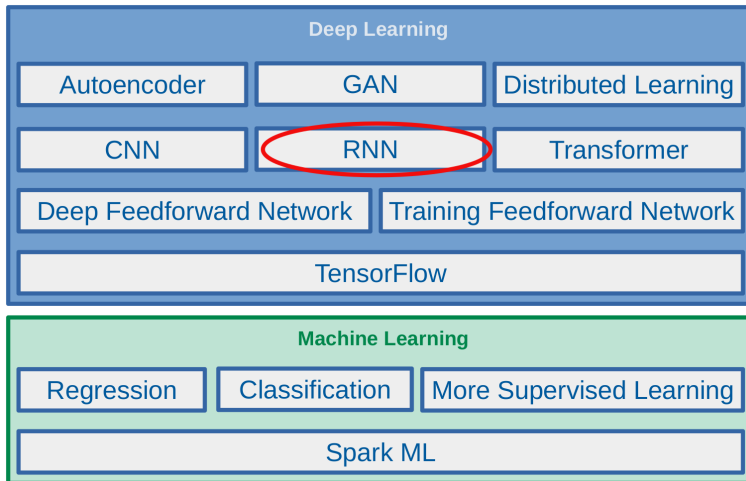
`https://id2223kth.github.io`
`https://tinyurl.com/y6kcpmzy`



Where Are We?



Where Are We?





Let's Start With An Example

Google

the students opened their



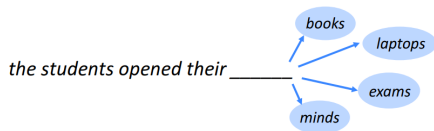
their **work**
their **books**
their **teachers**
their **homework**
their **lecturer**
their **new lecturer**

Feeling Lucky

venska

Language Modeling (1/2)

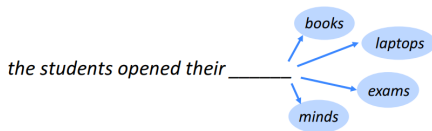
- ▶ **Language modeling** is the task of **predicting** what word comes next.



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** $x^{(t+1)}$:

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

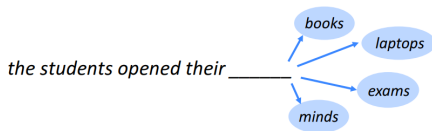


Language Modeling (2/2)

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- ▶ w_j is a word in vocabulary $V = \{w_1, \dots, w_V\}$.





n-gram Language Models

► the students opened their ___



n-gram Language Models

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



n-gram Language Models

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- ▶ Learn a n-gram Language Model!



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 - Unigrams: "the", "students", "opened", "their"



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 - Trigrams: "the students opened", "students opened their"
 - 4-grams: "the students opened their"



n-gram Language Models

- ▶ the students opened their ___
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 - 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.



n-gram Language Models - Example

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

~~as the proctor started the clock, the~~ students opened their _____
discard
condition on this

n-gram Language Models - Example

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

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 $p(\text{books} | \text{students opened their}) = 0.4$

n-gram Language Models - Example

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 - "students opened their" occurred 1000 times
 - "students opened their books" occurred 400 times:
 $p(\text{books} | \text{students opened their}) = 0.4$
 - "students opened their exams" occurred 100 times:
 $p(\text{exams} | \text{students opened their}) = 0.1$



Problems with n-gram Language Models - Sparsity

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



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- ▶ 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

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



Problems with n-gram Language Models - Storage

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

- ▶ 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.



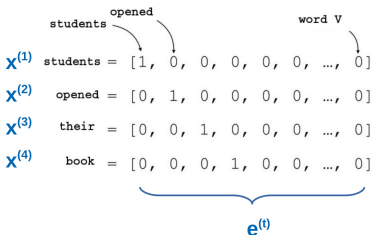
Can We Build a Neural Language Model? (1/3)

► Recall the **Language Modeling** task:

- **Input:** sequence of words $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(t)}$
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Can We Build a Neural Language Model? (1/3)

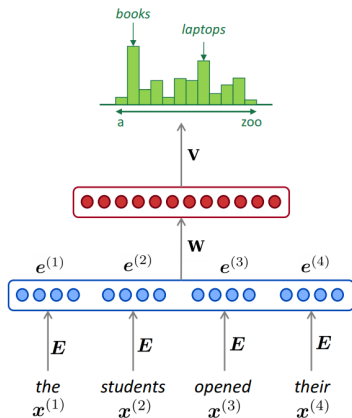
- ▶ Recall the **Language Modeling** task:
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 - **Output:** probability dist of the next word $p(x^{(t+1)} = w_j | x^{(t)}, \dots, x^{(1)})$
- ▶ **One-Hot encoding**
 - Represent a **categorical variable** as a **binary vector**.
 - All recodes are **zero**,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



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

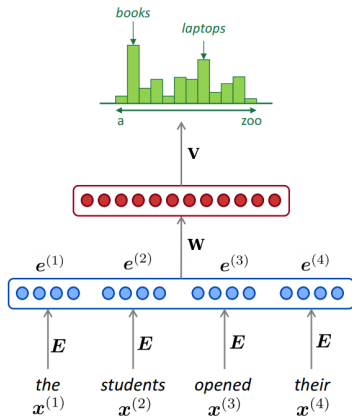
► A MLP model

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



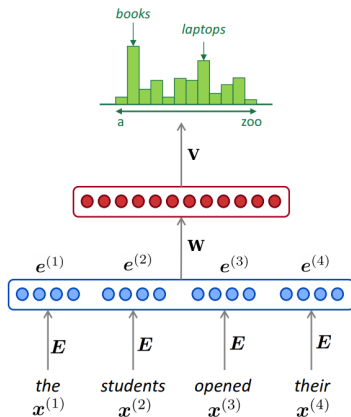
Can We Build a Neural Language Model? (3/3)

- ▶ 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**.



Recurrent Neural Networks (1/4)

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 - Until here, we assume that **all inputs (and outputs)** are **independent** of each other.



Recurrent Neural Networks (1/4)

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



Recurrent Neural Networks (1/4)

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

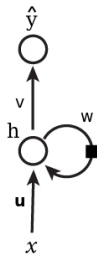


Recurrent Neural Networks (1/4)

- ▶ The idea behind **Recurrent neural networks (RNN)** is to make use of **sequential data**.
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- ▶ They can analyze **time series data** and predict **the future**.
- ▶ They can work on **sequences of arbitrary lengths**, rather than on **fixed-sized inputs**.

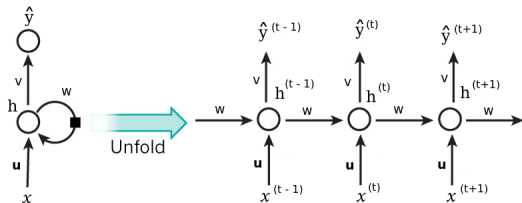
Recurrent Neural Networks (2/4)

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



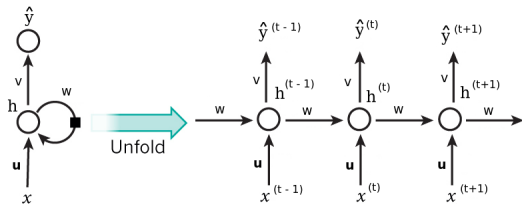
Recurrent Neural Networks (3/4)

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



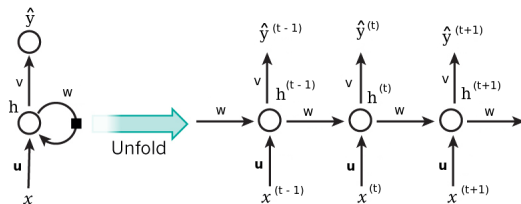
Recurrent Neural Networks (3/4)

- ▶ **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**.



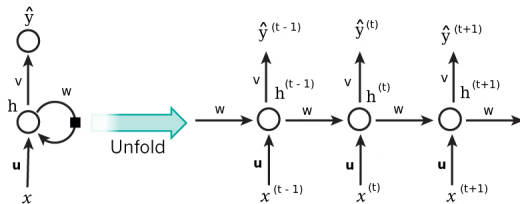
Recurrent Neural Networks (4/4)

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



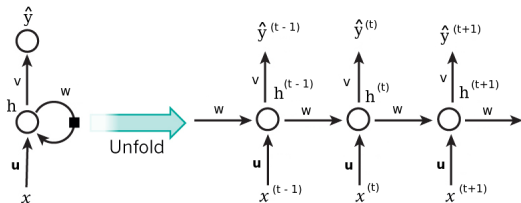
Recurrent Neural Networks (4/4)

- ▶ $\mathbf{h}^{(t)} = \mathbf{f}(\mathbf{u}^\top \mathbf{x}^{(t)} + \mathbf{w} \mathbf{h}^{(t-1)})$, where \mathbf{f} is an activation function, e.g., **tanh** or **ReLU**.
- ▶ $\hat{\mathbf{y}}^{(t)} = \mathbf{g}(\mathbf{v} \mathbf{h}^{(t)})$, where \mathbf{g} can be the **softmax** function.



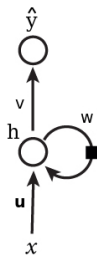
Recurrent Neural Networks (4/4)

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- ▶ $\hat{y}^{(t)} = g(\mathbf{v}h^{(t)})$, where g can be the **softmax** function.
- ▶ $\text{cost}(y^{(t)}, \hat{y}^{(t)}) = \text{cross_entropy}(y^{(t)}, \hat{y}^{(t)}) = -\sum y^{(t)} \log \hat{y}^{(t)}$
- ▶ $y^{(t)}$ is the **correct** word at time step t , and $\hat{y}^{(t)}$ is the **prediction**.



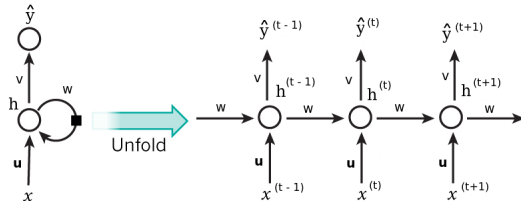
Recurrent Neurons - Weights (1/4)

- ▶ Each recurrent neuron has **three sets of weights**: \mathbf{u} , \mathbf{w} , and \mathbf{v} .



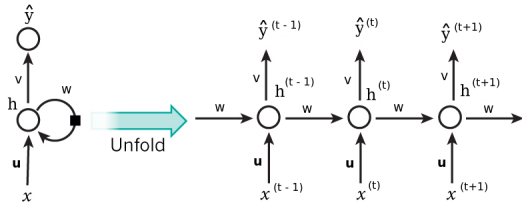
Recurrent Neurons - Weights (2/4)

- u : the weights for the inputs $x^{(t)}$.



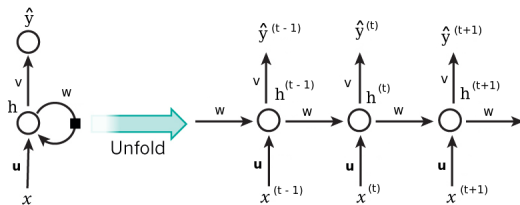
Recurrent Neurons - Weights (2/4)

- ▶ 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.



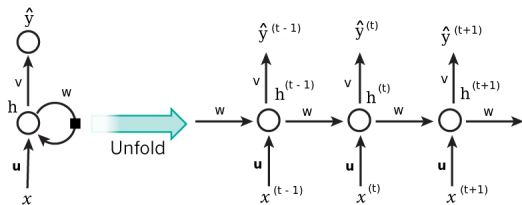
Recurrent Neurons - Weights (3/4)

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



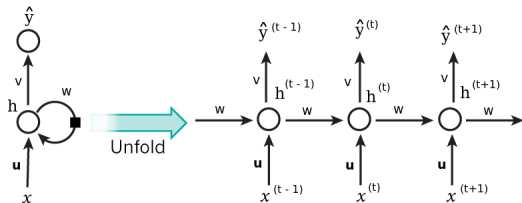
Recurrent Neurons - Weights (3/4)

- ▶ 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 .
 - $h^{(t)} = \tanh(\mathbf{u}^\top \mathbf{x}^{(t)} + w h^{(t-1)})$
 - $h^{(0)}$ is the initial hidden state.



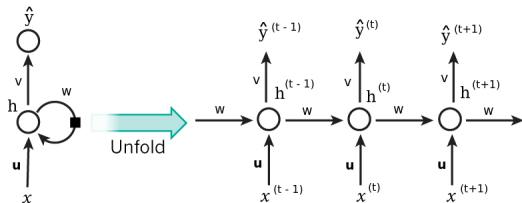
Recurrent Neurons - Weights (4/4)

- ▶ v : the weights for the hidden state of the current time step $h^{(t)}$.



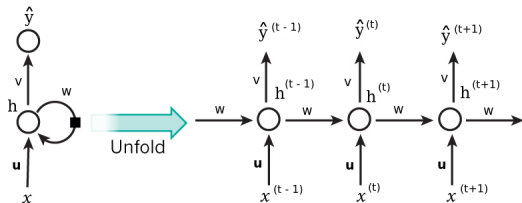
Recurrent Neurons - Weights (4/4)

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



Recurrent Neurons - Weights (4/4)

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

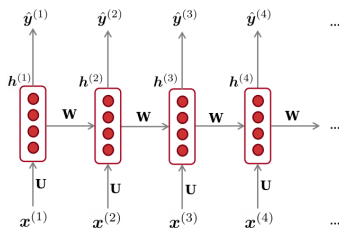
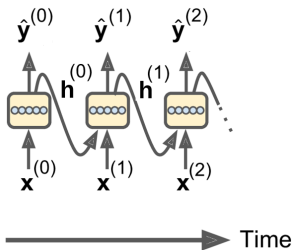


Layers of Recurrent Neurons

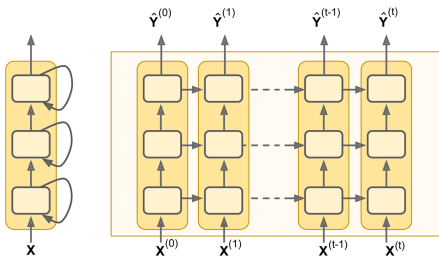
- ▶ At each time step t , every neuron of a **layer** receives both the **input vector** $\mathbf{x}^{(t)}$ and the **output vector** from the previous time step $\mathbf{h}^{(t-1)}$.

$$\mathbf{h}^{(t)} = \tanh(\mathbf{u}^\top \mathbf{x}^{(t)} + \mathbf{w}^\top \mathbf{h}^{(t-1)})$$

$$\mathbf{y}^{(t)} = \text{sigmoid}(\mathbf{v}^\top \mathbf{h}^{(t)})$$



- ▶ Stacking **multiple layers** of cells gives you a **deep RNN**.

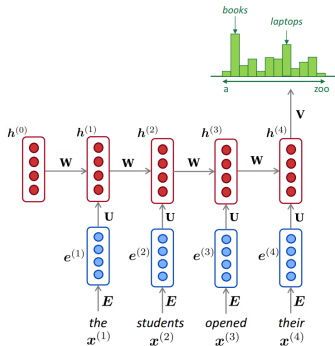
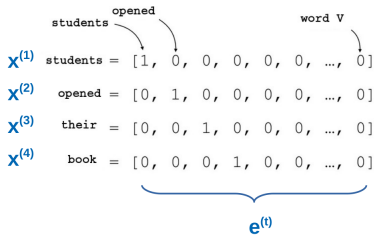




Let's Back to Language Model Example

A RNN Neural Language Model (1/2)

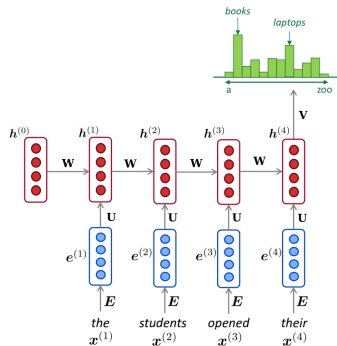
- ▶ The input \mathbf{x} will be a **sequence of words** (each $\mathbf{x}^{(t)}$ is a **single word**).
- ▶ Each embedded word $\mathbf{e}^{(t)} = \mathbf{E}^T \mathbf{x}^{(t)}$ is a **one-hot vector** of size **vocabulary size**.



A RNN Neural Language Model (2/2)

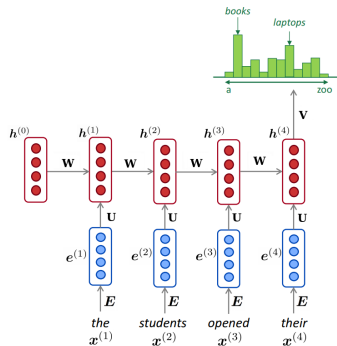
► Let's recap the equations for the RNN:

- $h^{(t)} = \tanh(\mathbf{u}^T \mathbf{e}^{(t)} + \mathbf{w}h^{(t-1)})$
- $\hat{\mathbf{y}}^{(t)} = \text{softmax}(\mathbf{v}h^{(t)})$



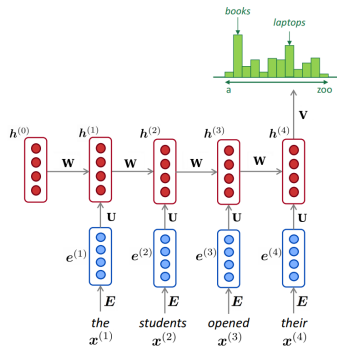
A RNN Neural Language Model (2/2)

- ▶ Let's recap the equations for the RNN:
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- ▶ The output $\hat{\mathbf{y}}^{(t)}$ is a vector of **vocabulary size** elements.

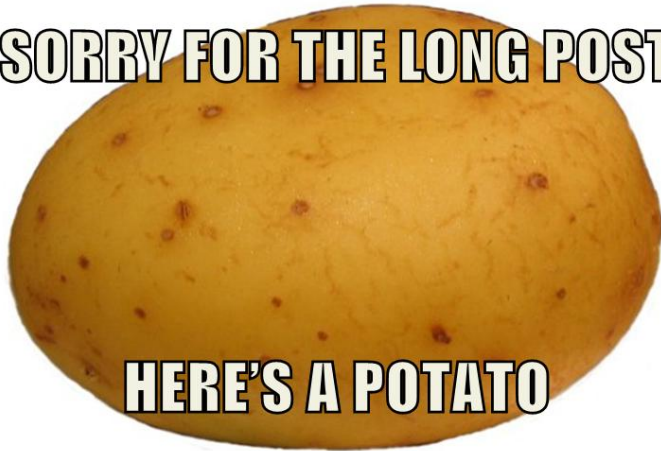


A RNN Neural Language Model (2/2)

- ▶ Let's recap the equations for the RNN:
 - $h^{(t)} = \tanh(\mathbf{u}^T \mathbf{e}^{(t)} + \mathbf{w}h^{(t-1)})$
 - $\hat{\mathbf{y}}^{(t)} = \text{softmax}(\mathbf{v}h^{(t)})$
- ▶ The output $\hat{\mathbf{y}}^{(t)}$ is a vector of **vocabulary size** elements.
- ▶ Each element of $\hat{\mathbf{y}}^{(t)}$ represents the **probability** of that word being the **next word** in the sentence.



SORRY FOR THE LONG POST



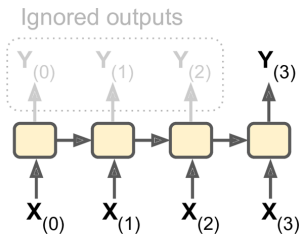
HERE'S A POTATO



RNN Design Patterns

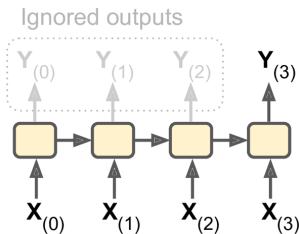
RNN Design Patterns - Sequence-to-Vector

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



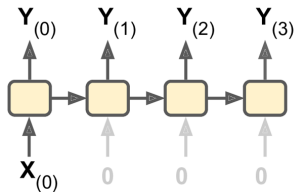
RNN Design Patterns - Sequence-to-Vector

- ▶ **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**.



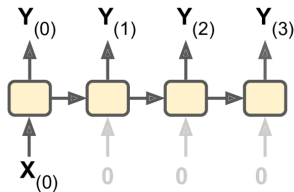
RNN Design Patterns - Vector-to-Sequence

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



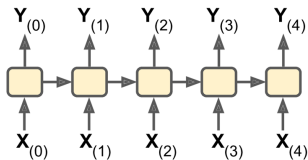
RNN Design Patterns - Vector-to-Sequence

- ▶ **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**.



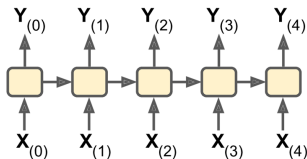
RNN Design Patterns - Sequence-to-Sequence

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



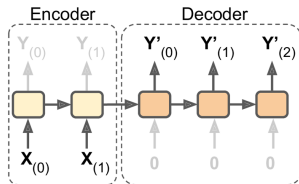
RNN Design Patterns - Sequence-to-Sequence

- ▶ **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**.



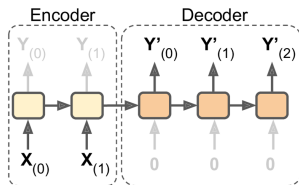
RNN Design Patterns - Encoder-Decoder

- **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.

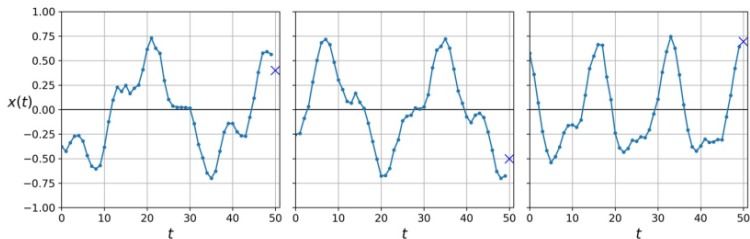




RNN in TensorFlow

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.





RNN in TensorFlow (2/5)

- ▶ 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
```



RNN in TensorFlow (3/5)

▶ 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

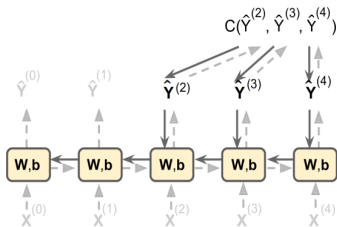


Training RNNs

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

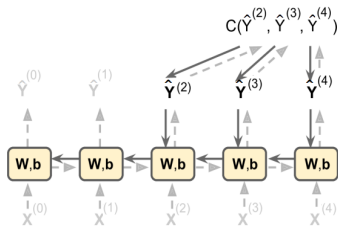
Backpropagation Through Time (1/3)

- ▶ 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 $C(\hat{y}^{t_{\min}}, \hat{y}^{t_{\min}+1}, \dots, \hat{y}^{t_{\max}})$, where t_{\min} and t_{\max} are the first and last output time steps, **not counting the ignored outputs**.



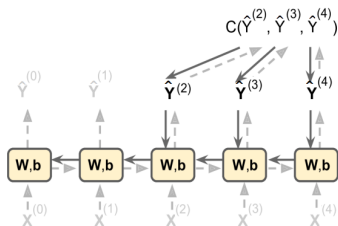
Backpropagation Through Time (2/3)

- ▶ 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.

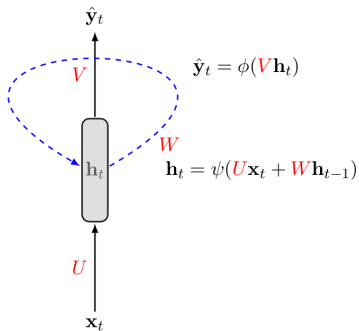


Backpropagation Through Time (3/3)

- ▶ 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**, $\hat{y}^{(2)}$, $\hat{y}^{(3)}$, and $\hat{y}^{(4)}$.
 - Gradients flow through these three outputs, but **not through** $\hat{y}^{(0)}$ and $\hat{y}^{(1)}$.



BPTT Step by Step (1/20)





BPTT Step by Step (2/20)

x_1 x_2 x_3 ... x_r

BPTT Step by Step (3/20)

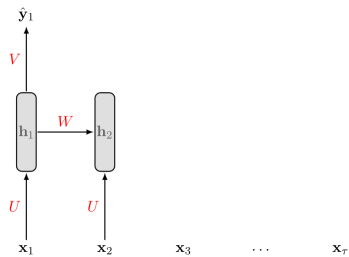




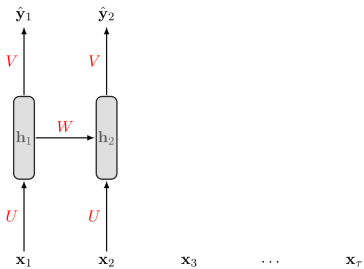
BPTT Step by Step (4/20)



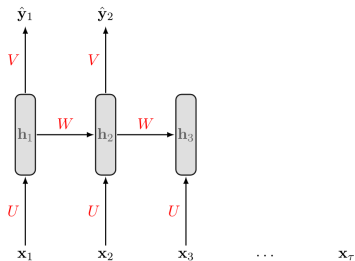
BPTT Step by Step (5/20)



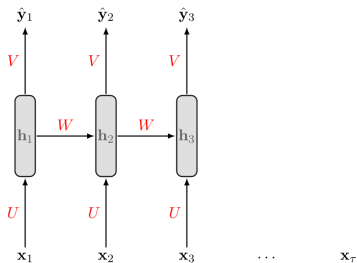
BPTT Step by Step (6/20)



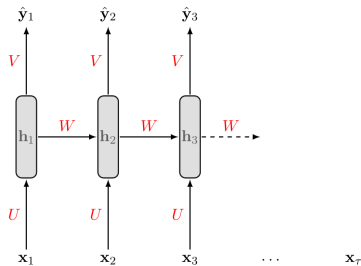
BPTT Step by Step (7/20)



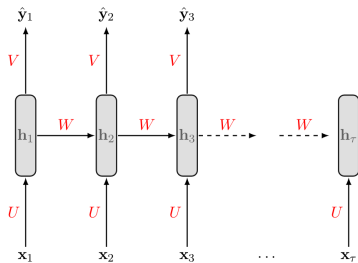
BPTT Step by Step (8/20)



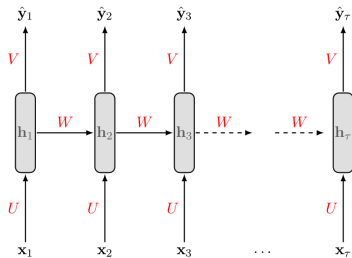
BPTT Step by Step (9/20)



BPTT Step by Step (10/20)



BPTT Step by Step (11/20)



BPTT Step by Step (12/20)

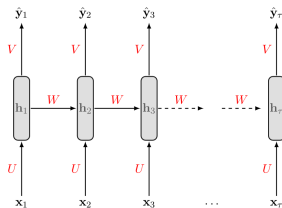
$$\mathbf{s}^{(t)} = \mathbf{u}^T \mathbf{x}^{(t)} + \mathbf{w} \mathbf{h}^{(t-1)}$$

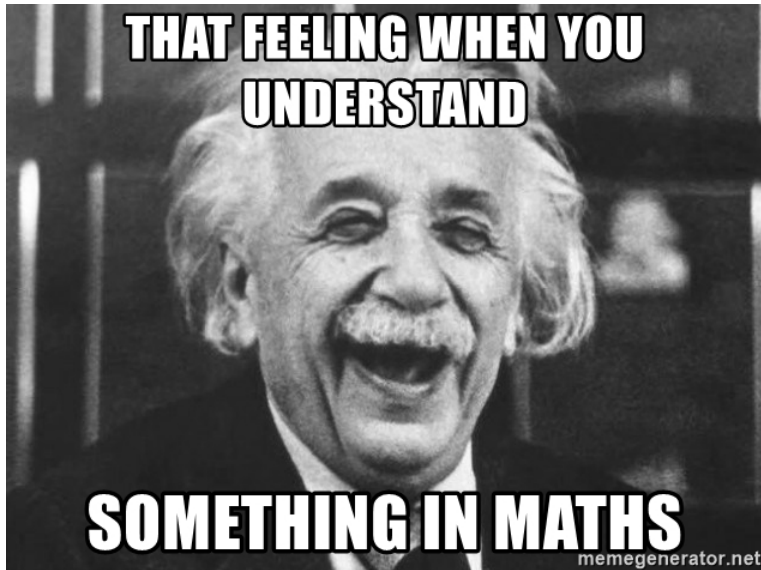
$$\mathbf{h}^{(t)} = \tanh(\mathbf{s}^{(t)})$$

$$\mathbf{z}^{(t)} = \mathbf{v} \mathbf{h}^{(t)}$$

$$\hat{\mathbf{y}}^{(t)} = \text{softmax}(\mathbf{z}^{(t)})$$

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

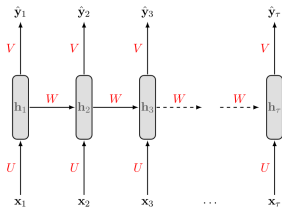




BPTT Step by Step (13/20)

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

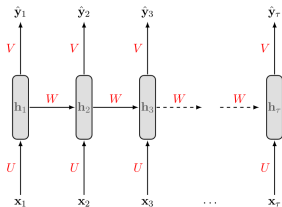
- ▶ We treat the full sequence as **one training example**.



BPTT Step by Step (13/20)

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

- ▶ 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., $E = J^{(1)} + J^{(2)} + \dots + J^{(t)}$





BPTT Step by Step (14/20)

- ▶ $J^{(t)}$ 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.



BPTT Step by Step (14/20)

- ▶ $J^{(t)}$ 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** .



BPTT Step by Step (14/20)

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- ▶ For example if $t = 3$ we have: $E = J^{(1)} + J^{(2)} + J^{(3)}$



BPTT Step by Step (14/20)

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

BPTT Step by Step (14/20)

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

BPTT Step by Step (14/20)

- ▶ $J^{(t)}$ 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.
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- ▶ For example if $t = 3$ we have: $E = J^{(1)} + J^{(2)} + J^{(3)}$

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

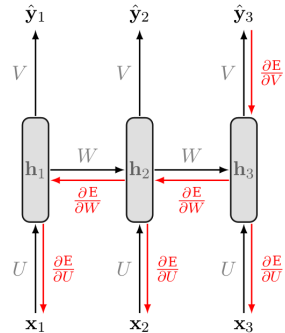
$$\frac{\partial E}{\partial w} = \sum_t \frac{\partial J^{(t)}}{\partial w} = \frac{\partial J^{(3)}}{\partial w} + \frac{\partial J^{(2)}}{\partial w} + \frac{\partial J^{(1)}}{\partial w}$$

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

BPTT Step by Step (15/20)

- ▶ Let's start with $\frac{\partial E}{\partial v}$.
- ▶ 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 $z^{(3)}$.

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

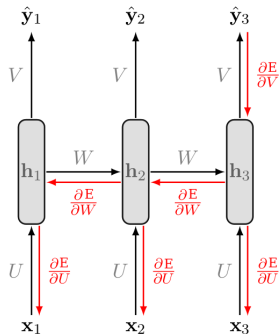


BPTT Step by Step (15/20)

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



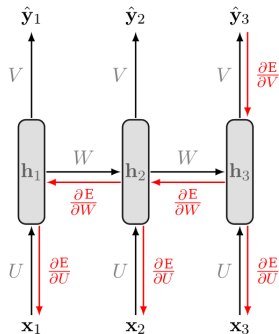
BPTT Step by Step (15/20)

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

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

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



BPTT Step by Step (15/20)

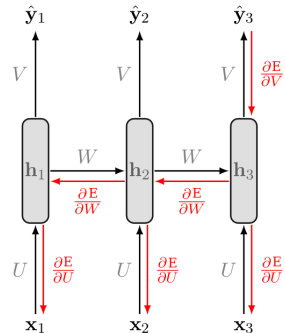
- ▶ Let's start with $\frac{\partial E}{\partial v}$.
- ▶ A change in v will only **impact** $J^{(3)}$ at time $t = 3$, because it plays no role in computing the value of anything other than $z^{(3)}$.

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

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

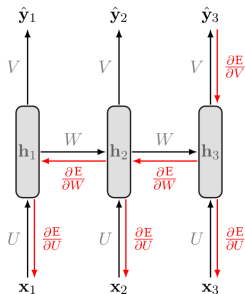
$$\frac{\partial J^{(2)}}{\partial v} = \frac{\partial J^{(2)}}{\partial \hat{y}^{(2)}} \frac{\partial \hat{y}^{(2)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial v}$$

$$\frac{\partial J^{(1)}}{\partial v} = \frac{\partial J^{(1)}}{\partial \hat{y}^{(1)}} \frac{\partial \hat{y}^{(1)}}{\partial z^{(1)}} \frac{\partial z^{(1)}}{\partial v}$$



BPTT Step by Step (16/20)

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

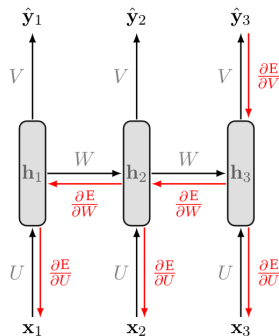


BPTT Step by Step (17/20)

- ▶ we compute our individual gradients as:

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

$$\frac{\partial J(1)}{\partial \mathbf{w}} = \frac{\partial J(1)}{\partial \hat{\mathbf{y}}(1)} \frac{\partial \hat{\mathbf{y}}(1)}{\partial \mathbf{z}(1)} \frac{\partial \mathbf{z}(1)}{\partial \mathbf{h}(1)} \frac{\partial \mathbf{h}(1)}{\partial \mathbf{s}(1)} \frac{\partial \mathbf{s}(1)}{\partial \mathbf{w}}$$



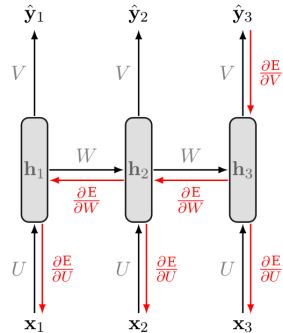
BPTT Step by Step (18/20)

► we compute our individual gradients as:

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

$$\frac{\partial J^{(2)}}{\partial w} = \frac{\partial J^{(2)}}{\partial \hat{y}^{(2)}} \frac{\partial \hat{y}^{(2)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial h^{(2)}} \frac{\partial h^{(2)}}{\partial s^{(2)}} \frac{\partial s^{(2)}}{\partial w} +$$

$$\frac{\partial J^{(2)}}{\partial \hat{y}^{(2)}} \frac{\partial \hat{y}^{(2)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial h^{(2)}} \frac{\partial h^{(2)}}{\partial s^{(2)}} \frac{\partial s^{(2)}}{\partial h^{(1)}} \frac{\partial h^{(1)}}{\partial s^{(1)}} \frac{\partial s^{(1)}}{\partial w}$$



BPTT Step by Step (19/20)

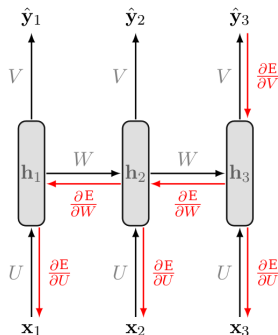
- ▶ we compute our individual gradients as:

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

$$\frac{\partial J^{(3)}}{\partial w} = \frac{\partial J^{(3)}}{\partial \hat{y}^{(3)}} \frac{\partial \hat{y}^{(3)}}{\partial z^{(3)}} \frac{\partial z^{(3)}}{\partial h^{(3)}} \frac{\partial h^{(3)}}{\partial s^{(3)}} \frac{\partial s^{(3)}}{\partial w} +$$

$$\frac{\partial J^{(3)}}{\partial \hat{y}^{(3)}} \frac{\partial \hat{y}^{(3)}}{\partial z^{(3)}} \frac{\partial z^{(3)}}{\partial h^{(3)}} \frac{\partial h^{(3)}}{\partial s^{(3)}} \frac{\partial s^{(3)}}{\partial h^{(2)}} \frac{\partial h^{(2)}}{\partial s^{(2)}} \frac{\partial s^{(2)}}{\partial w} +$$

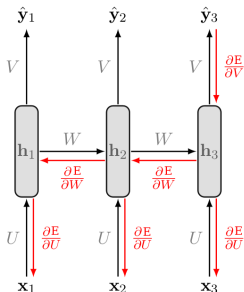
$$\frac{\partial J^{(3)}}{\partial \hat{y}^{(3)}} \frac{\partial \hat{y}^{(3)}}{\partial z^{(3)}} \frac{\partial z^{(3)}}{\partial h^{(3)}} \frac{\partial h^{(3)}}{\partial s^{(3)}} \frac{\partial s^{(3)}}{\partial h^{(2)}} \frac{\partial h^{(2)}}{\partial s^{(2)}} \frac{\partial s^{(2)}}{\partial h^{(1)}} \frac{\partial h^{(1)}}{\partial s^{(1)}} \frac{\partial s^{(1)}}{\partial w}$$



BPTT Step by Step (20/20)

- ▶ More generally, a change in \mathbf{w} will impact our cost $J^{(t)}$ on t separate occasions.

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



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**.



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- ▶ 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**.

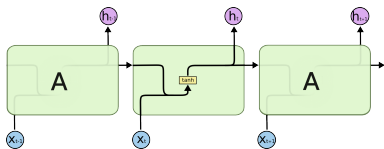


RNN Basic Cell vs. LSTM

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

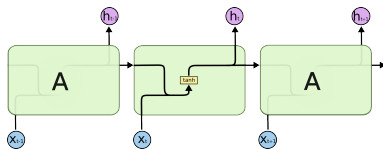
RNN Basic Cell vs. LSTM

- ▶ 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.

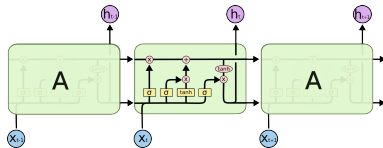


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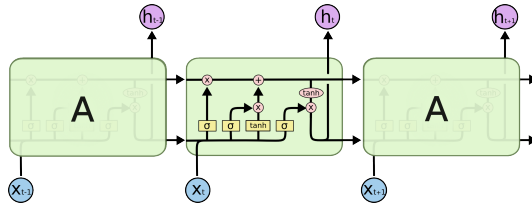


- ▶ An **LSTM** contains **four interacting layers** in each cell.



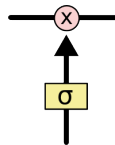
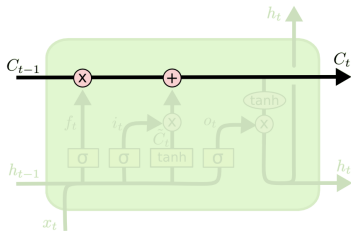
LSTM (1/2)

- ▶ 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)

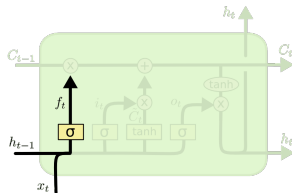
- ▶ The **cell state** (long-term state), the **horizontal line** on the top of the diagram.
- ▶ The LSTM can **remove/add information** to the **cell state**, regulated by **three gates**.
 - Forget gate, input gate and output gate



Step-by-Step LSTM Walk Through (1/4)

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

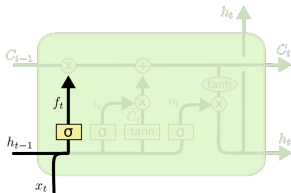
$$f(t) = \sigma(\mathbf{u}_f^T \mathbf{x}^{(t)} + \mathbf{w}_f \mathbf{h}^{(t-1)})$$



Step-by-Step LSTM Walk Through (1/4)

- ▶ **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.

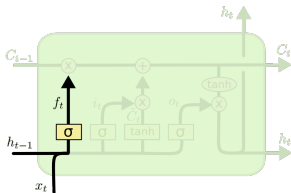
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- ▶ **Step one:** decides **what information** we are going to **throw away** from the **cell state**.
- ▶ This decision is made by a **sigmoid layer**, called the **forget gate** layer.
- ▶ It looks at $\mathbf{h}^{(t-1)}$ and $\mathbf{x}^{(t)}$,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

$$\mathbf{f}^{(t)} = \sigma(\mathbf{u}_f^T \mathbf{x}^{(t)} + \mathbf{w}_f \mathbf{h}^{(t-1)})$$

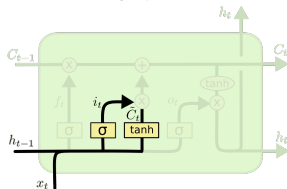


Step-by-Step LSTM Walk Through (2/4)

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

$$i^{(t)} = \sigma(\mathbf{u}_i^T \mathbf{x}^{(t)} + \mathbf{w}_i \mathbf{h}^{(t-1)})$$

$$\tilde{c}^{(t)} = \tanh(\mathbf{u}_{\tilde{c}}^T \mathbf{x}^{(t)} + \mathbf{w}_{\tilde{c}} \mathbf{h}^{(t-1)})$$

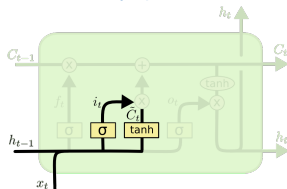


Step-by-Step LSTM Walk Through (2/4)

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 - ▶ 1. A **sigmoid layer**, called the **input gate** layer, decides **which values** we will update.

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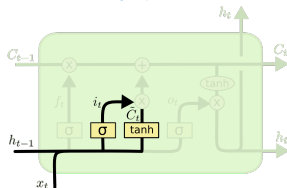


Step-by-Step LSTM Walk Through (2/4)

- ▶ **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.

$$i^{(t)} = \sigma(\mathbf{u}_i^T \mathbf{x}^{(t)} + \mathbf{w}_i \mathbf{h}^{(t-1)})$$

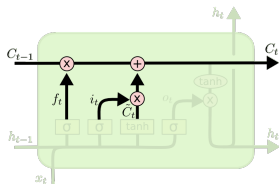
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Step-by-Step LSTM Walk Through (3/4)

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

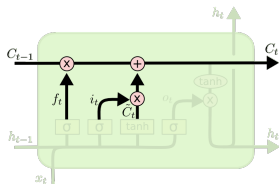
$$c^{(t)} = f^{(t)} \otimes c^{(t-1)} + i^{(t)} \otimes \tilde{c}^{(t)}$$



Step-by-Step LSTM Walk Through (3/4)

- ▶ **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.

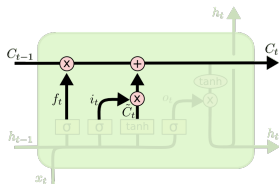
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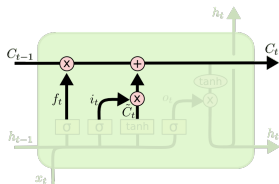
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- ▶ We multiply the old state by $f^{(t)}$, forgetting the things we decided to forget earlier.
- ▶ Then we add it $i^{(t)} \otimes \tilde{c}^{(t)}$.
- ▶ This is the new candidate values, scaled by how much we decided to update each state value.

$$c^{(t)} = f^{(t)} \otimes c^{(t-1)} + i^{(t)} \otimes \tilde{c}^{(t)}$$

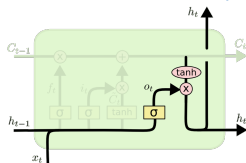


Step-by-Step LSTM Walk Through (4/4)

- **Fourth step:** decides about the **output**.

$$o^{(t)} = \sigma(\mathbf{u}_o^T \mathbf{x}^{(t)} + \mathbf{w}_o \mathbf{h}^{(t-1)})$$

$$\mathbf{h}^{(t)} = o^{(t)} \otimes \tanh(\mathbf{c}^{(t)})$$

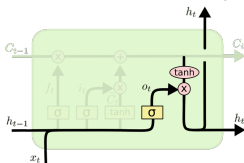


Step-by-Step LSTM Walk Through (4/4)

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

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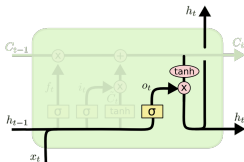


Step-by-Step LSTM Walk Through (4/4)

- ▶ **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**.

$$o^{(t)} = \sigma(\mathbf{u}_o^T \mathbf{x}^{(t)} + \mathbf{w}_o \mathbf{h}^{(t-1)})$$

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LSTM in TensorFlow

► Use LSTM

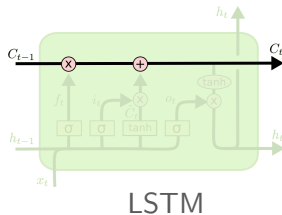
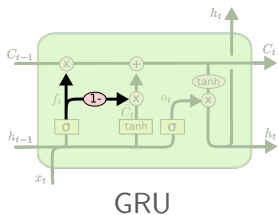
```
model = keras.models.Sequential([
    keras.layers.LSTM(20, return_sequences=True, input_shape=[None, 1]),
    keras.layers.LSTM(20),
    keras.layers.Dense(1)
])

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)
```

Gated Recurrent Unit (GRU)

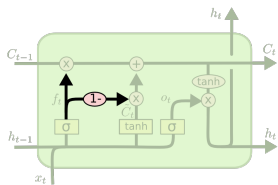
- ▶ The **GRU** cell is a **simplified version** of the **LSTM** cell.



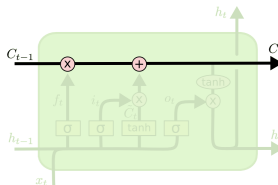
Gated Recurrent Unit (GRU)

- ▶ 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**.

$$c^{(t)} = f^{(t)} \otimes c^{(t-1)} + (1 - f^{(t)}) \otimes \tilde{c}^{(t)}$$



GRU

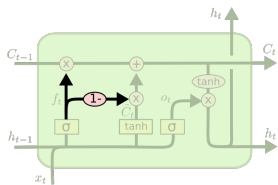


LSTM

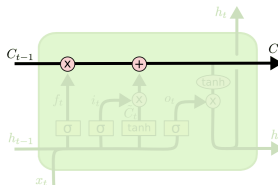
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- ▶ The **GRU** cell is a **simplified version** of the LSTM cell.
- ▶ Instead of separately deciding **what to forget** and **what to add** to the new information to, it **makes those decisions together**.
 - It only **forgets** when it is going to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

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GRU

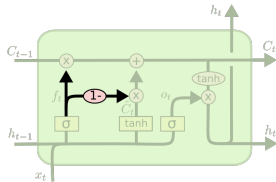


LSTM

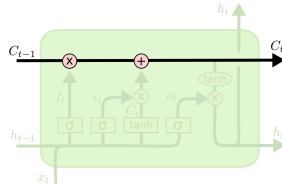
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- ▶ Instead of separately deciding **what to forget** and **what to add** to the new information to, it **makes those decisions together**.
 - It only **forgets** when it is going to input something in its place.
 - It only **inputs new values** to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

$$c^{(t)} = f^{(t)} \otimes c^{(t-1)} + (1 - f^{(t)}) \otimes \tilde{c}^{(t)}$$



GRU



LSTM



GRU in TensorFlow

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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?