Recurrent Neural Networks

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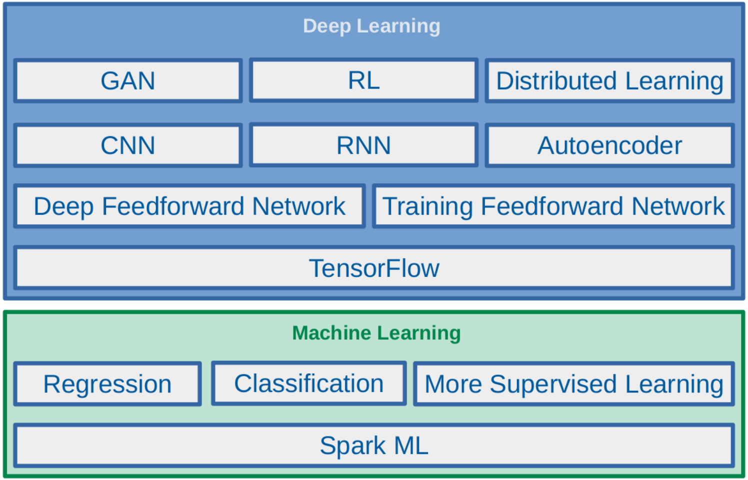
The Course Web Page

https://id2223kth.github.io

Where Are We?



Deep Learning
GAN
RL
Distributed Learning
CNN
RNN
Autoencoder
Deep Feedforward Network
Training Feedforward Network
TensorFlow
Machine Learning
Regression
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More Supervised Learning
Spark ML

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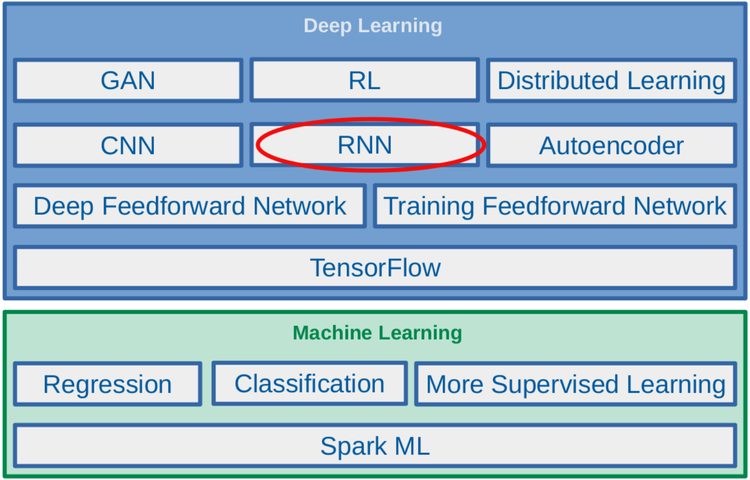
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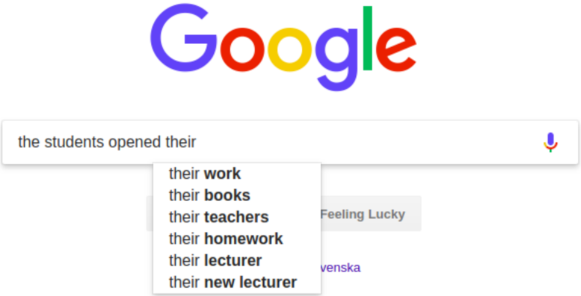
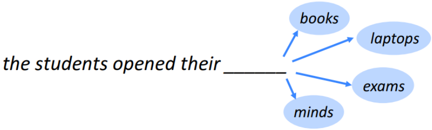
Let's Start With An Example


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)

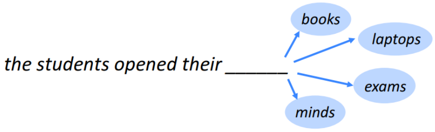
- Language modeling is the task of predicting what word comes next.



Language Modeling (2/2)

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

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



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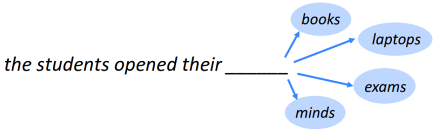
- w_j is a word in vocabulary $V = \{w_1, \cdots, w_v\}$.



n-gram Language Models

- `the students opened their ___`

n-gram Language Models

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

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  - 4-grams: `"the students opened their"`

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  - 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

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  - `"students opened their"` occurred 1000 times

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

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$$p(\mathtt{w}_j|\text{students opened their}) = \frac{\text{students opened their } \mathtt{w}_j}{\text{students opened their}}$$

- In the corpus:
  - `"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

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

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- What if "`students opened their`" never occurred in data? Then we can't calculate probability for any $\mathtt{w_j}$!
- Increasing `n` makes sparsity problems worse.
  - Typically we can't have `n` bigger than 5.

Problems with n-gram Language Models - Storage

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

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

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

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

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

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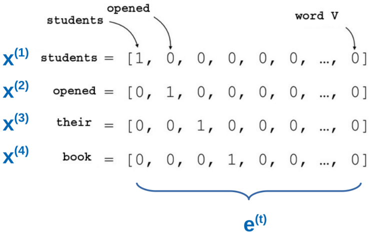
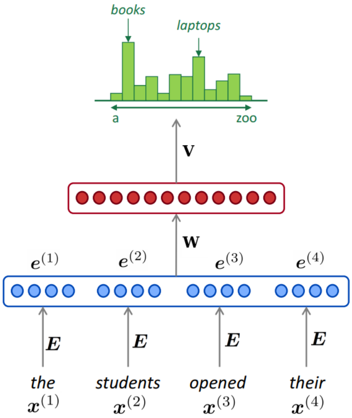
- One-Hot encoding
  - Represent a categorical variable as a binary vector.
  - All recodes are zero, except the index of the integer, which is one.
  - Each embedded word $\mathbf{e}^{(t)} = \mathbf{E}^\intercal x^{(t)}$ is a one-hot vector of size vocabulary size.



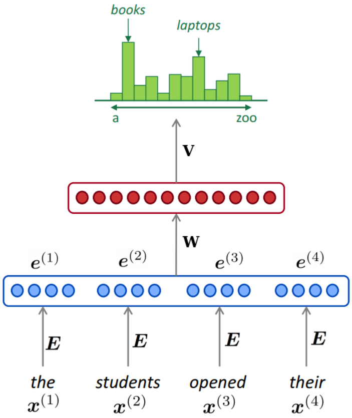
Can We Build a Neural Language Model? (2/3)

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



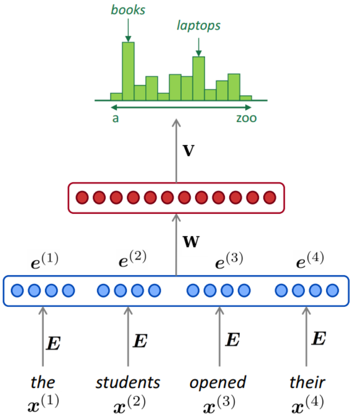
Can We Build a Neural Language Model? (3/3)

- 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)

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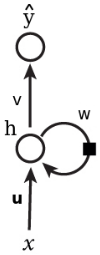
- They can analyze time series data and predict the future.
- They can work on sequences of arbitrary lengths, rather than on fixed-sized inputs.

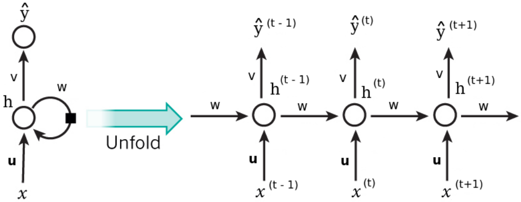
Recurrent Neural Networks (2/4)

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



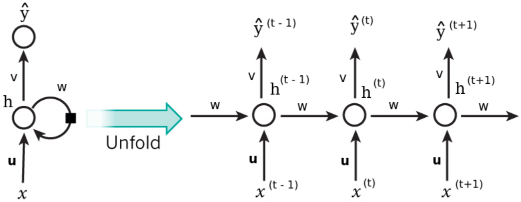
Recurrent Neural Networks (3/4)

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



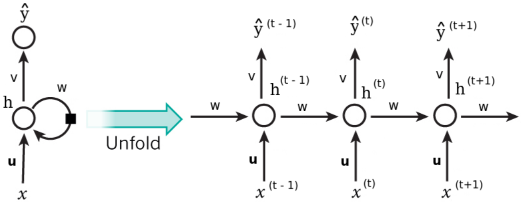
Recurrent Neural Networks (3/4)

- 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)

- $\mathtt{h}^{(t)} = \mathtt{f}(\mathbf{u}^\intercal \mathbf{x}^{(t)} + \mathtt{w}\mathtt{h}^{(t-1)})$, where $\mathtt{f}$ is an activation function, e.g., `tanh` or `ReLU`.



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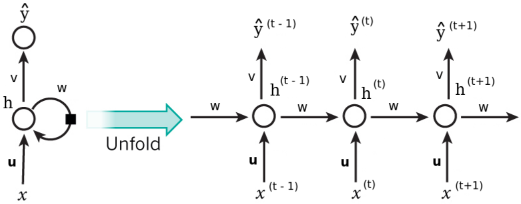
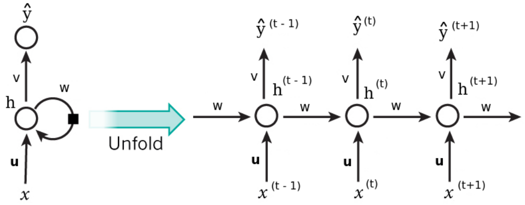
- $\hat{\mathtt{y}}^{(t)} = \mathtt{g}(\mathtt{v}\mathtt{h}^{(t)})$, where $\mathtt{g}$ can be the `softmax` function.



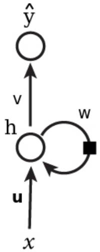
Recurrent Neural Networks (4/4)

- $\mathtt{h}^{(\mathtt{t})} = \mathtt{f}(\mathbf{u}^\intercal \mathbf{x}^{(\mathtt{t})} + \mathtt{w}\mathtt{h}^{(\mathtt{t}-1)})$, where $\mathtt{f}$ is an activation function, e.g., tanh or ReLU.
- $\hat{\mathtt{y}}^{(\mathtt{t})} = \mathtt{g}(\mathtt{v}\mathtt{h}^{(\mathtt{t})})$, where $\mathtt{g}$ can be the softmax function.
- $\mathtt{cost}(\mathtt{y}^{(\mathtt{t})}, \hat{\mathtt{y}}^{(\mathtt{t})}) = \mathtt{cross\_entropy}(\mathtt{y}^{(\mathtt{t})}, \hat{\mathtt{y}}^{(\mathtt{t})}) = -\sum \mathtt{y}^{(\mathtt{t})} \mathtt{log}\hat{\mathtt{y}}^{(\mathtt{t})}$
- $\mathtt{y}^{(\mathtt{t})}$ is the correct word at time step $\mathtt{t}$, and $\hat{\mathtt{y}}^{(\mathtt{t})}$ is the prediction.



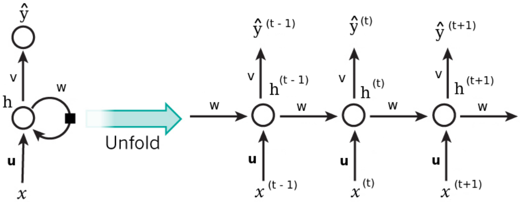
Recurrent Neurons - Weights (1/4)

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



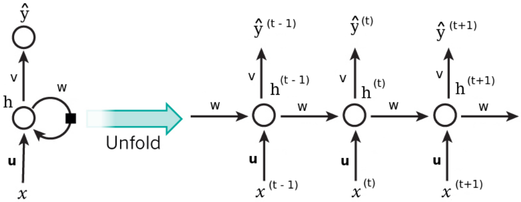
Recurrent Neurons - Weights (2/4)

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



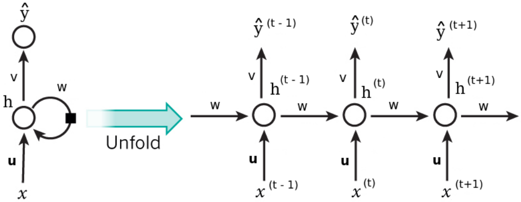
Recurrent Neurons - Weights (2/4)

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



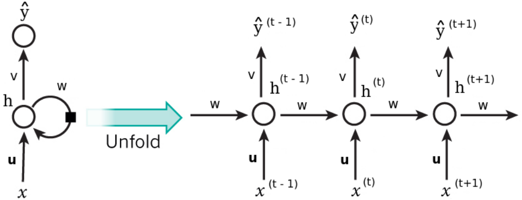
Recurrent Neurons - Weights (3/4)

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



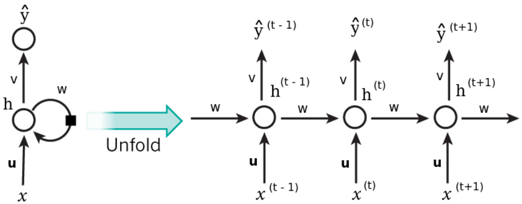
Recurrent Neurons - Weights (3/4)

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



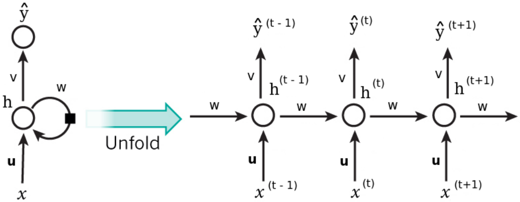
Recurrent Neurons - Weights (4/4)

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



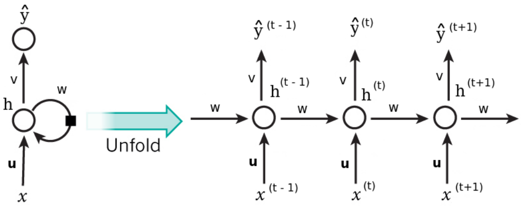
Recurrent Neurons - Weights (4/4)

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



Recurrent Neurons - Weights (4/4)

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

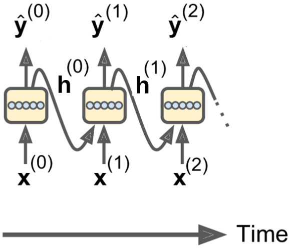


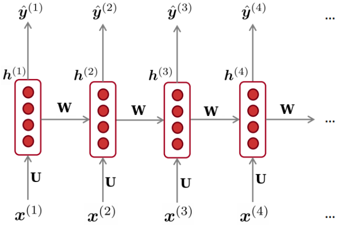
Layers of Recurrent Neurons

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

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

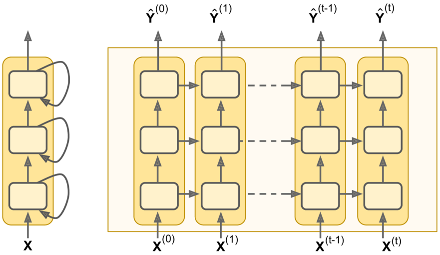
$$\mathbf{y}^{(\mathtt{t})} = \mathtt{sigmoid}(\mathbf{v}^\intercal \mathbf{h}^{(\mathtt{t})})$$





Deep RNN

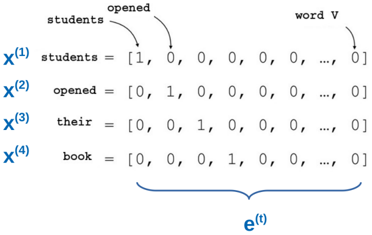
- Stacking multiple layers of cells gives you a deep RNN.

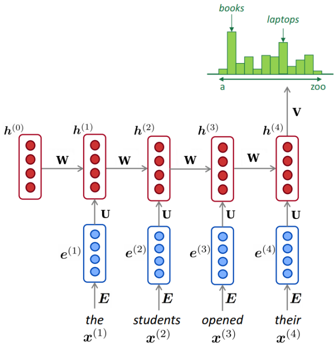


Let's Back to Language Model Example

A RNN Neural Language Model (1/2)

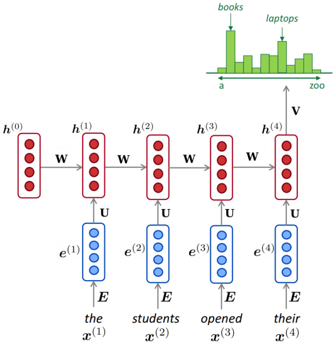
- The input $\mathbf{x}$ will be a sequence of words (each $\mathtt{x}^{(t)}$ is a single word).
- Each embedded word $\mathbf{e}^{(t)} = \mathbf{E}^{\top}\mathtt{x}^{(t)}$ is a one-hot vector of size vocabulary size.





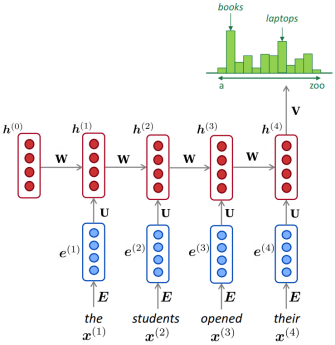
A RNN Neural Language Model (2/2)

- Let's recap the equations for the RNN:
  - $\mathtt{h}^{(\mathtt{t})} = \mathtt{tanh}(\mathbf{u}^\intercal \mathbf{e}^{(\mathtt{t})} + \mathtt{w}\mathtt{h}^{(\mathtt{t}-1)})$
  - $\hat{\mathbf{y}}^{(\mathtt{t})} = \mathtt{softmax}(\mathtt{v}\mathtt{h}^{(\mathtt{t})})$



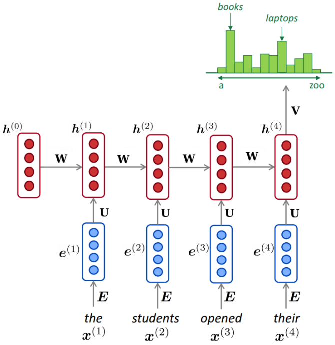
A RNN Neural Language Model (2/2)

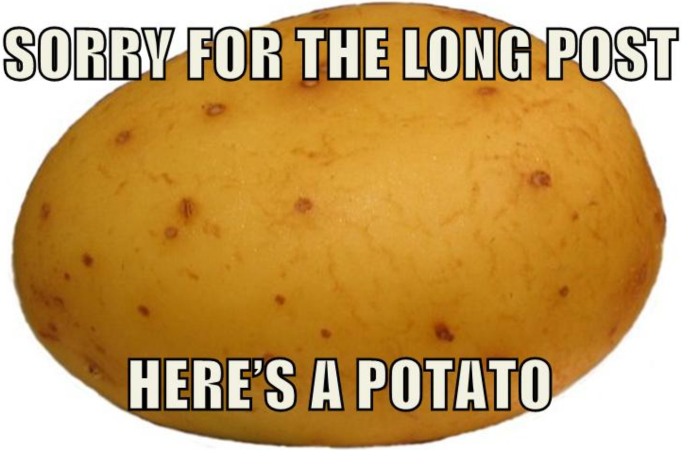
- Let's recap the equations for the RNN:
  - $\mathtt{h}^{(t)} = \mathtt{tanh}(\mathbf{u}^\intercal \mathbf{e}^{(t)} + \mathtt{wh}^{(t-1)})$
  - $\hat{\mathbf{y}}^{(t)} = \mathtt{softmax}(\mathtt{vh}^{(t)})$
- The output $\hat{\mathbf{y}}^{(t)}$ is a vector of vocabulary size elements.



A RNN Neural Language Model (2/2)

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

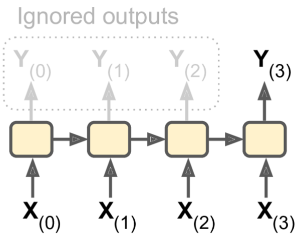



SORRY FOR THE LONG POST
HERE'S A POTATO

RNN Design Patterns

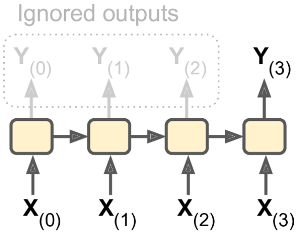
RNN Design Patterns - Sequence-to-Vector

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



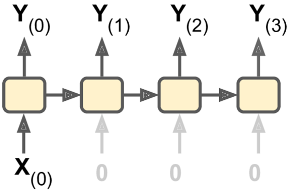
RNN Design Patterns - Sequence-to-Vector

- 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.



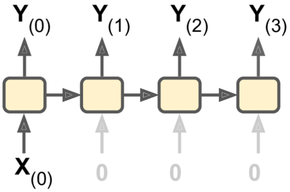
RNN Design Patterns - Vector-to-Sequence

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



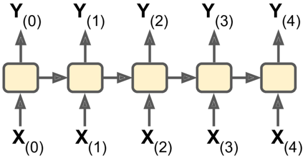
RNN Design Patterns - Vector-to-Sequence

- 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.



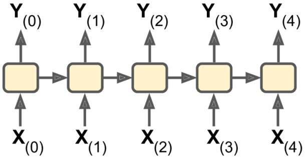
RNN Design Patterns - Sequence-to-Sequence

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



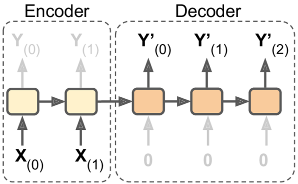
RNN Design Patterns - Sequence-to-Sequence

- 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.



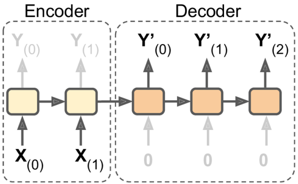
RNN Design Patterns - Encoder-Decoder

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



RNN Design Patterns - Encoder-Decoder

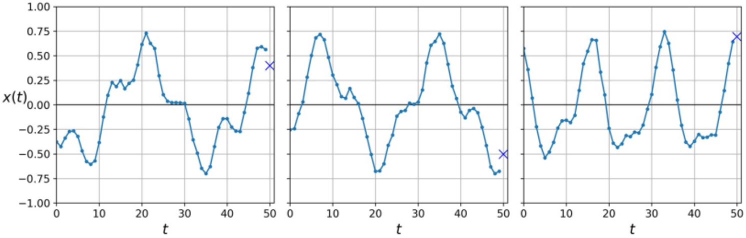
- Encoder-decoder network: a sequence-to-vector network (encoder), followed by a vector-to-sequence network (decoder).
- E.g., translating a sentence from one language to another.
- You would feed the network a sentence in one language, the encoder would convert this sentence into a single vector representation,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

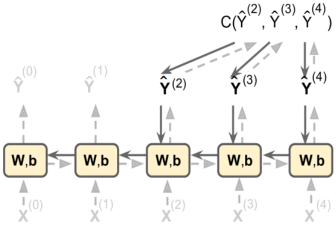
Training RNNs

- To train an RNN, we should unroll it through time and then simply use regular backpropagation.

- This strategy is called backpropagation through time (BPTT).

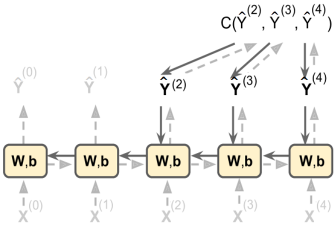
Backpropagation Through Time (1/3)

- 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 $\mathtt{C}(\hat{\mathbf{y}}^{\mathtt{tmin}}, \hat{\mathbf{y}}^{\mathtt{tmin}+1}, \cdots, \hat{\mathbf{y}}^{\mathtt{tmax}})$, where `tmin` and `tmax` are the first and last output time steps, not counting the ignored outputs.



Backpropagation Through Time (2/3)

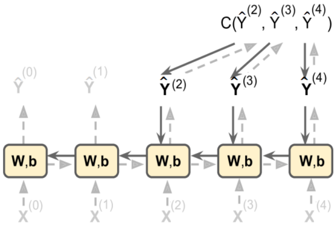
- 3. Propagate backward the gradients of that cost function through the unrolled network (represented by the solid arrows).
- 4. The model parameters are updated using the gradients computed during BPTT.



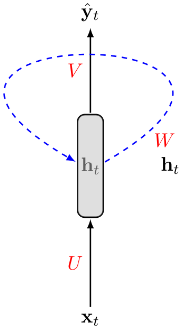
Backpropagation Through Time (3/3)

- 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 $\hat{\mathbf{y}}^{(1)}$.



BPTT Step by Step (1/20)



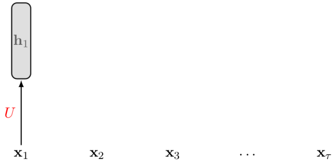
$$\hat{\mathbf{y}}_t = \phi(V\mathbf{h}_t)$$

$$\mathbf{h}_t = \psi(U\mathbf{x}_t + W\mathbf{h}_{t-1})$$

BPTT Step by Step (2/20)

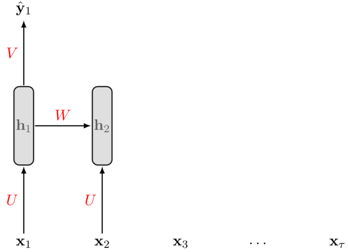
$\mathbf{x}_1 \quad \mathbf{x}_2 \quad \mathbf{x}_3 \quad \cdots \quad \mathbf{x}_\tau$

BPTT Step by Step (3/20)

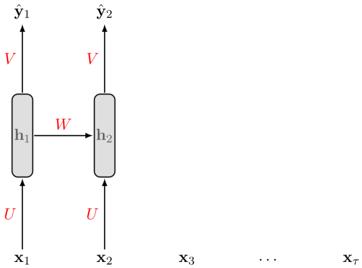


BPTT Step by Step (4/20)

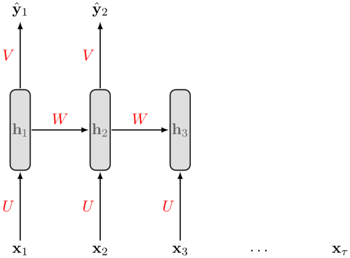
BPTT Step by Step (5/20)



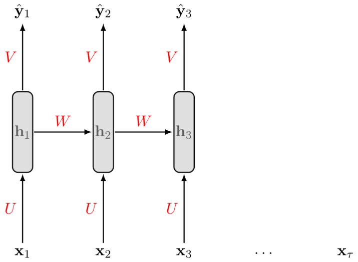
BPTT Step by Step (6/20)



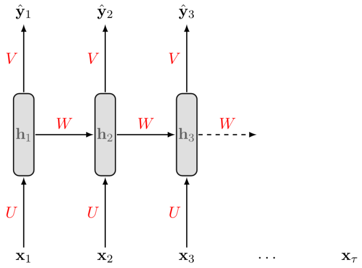
BPTT Step by Step (7/20)



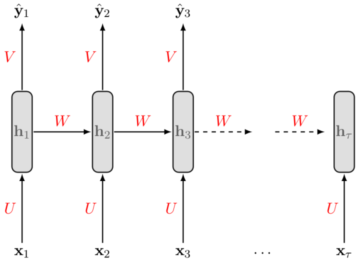
BPTT Step by Step (8/20)



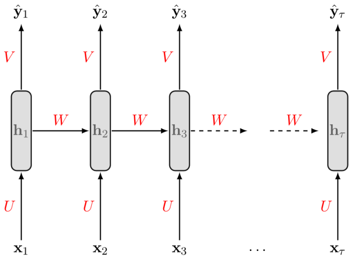
BPTT Step by Step (9/20)



BPTT Step by Step (10/20)



BPTT Step by Step (11/20)



BPTT Step by Step (12/20)

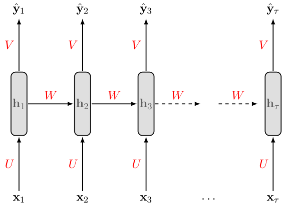
$$\mathbf{s}^{(t)} = \mathbf{u}^{\mathsf{T}}\mathbf{x}^{(t)} + \mathtt{w}\mathtt{h}^{(t-1)}$$

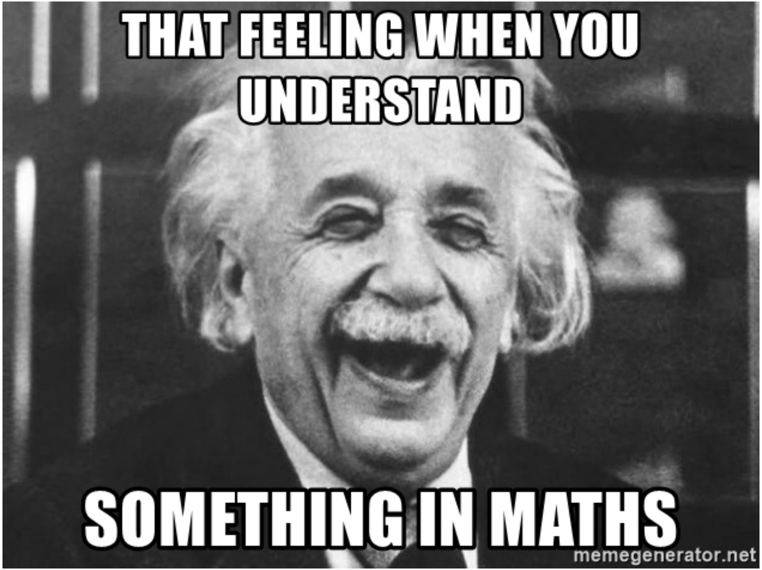
$$\mathtt{h}^{(t)} = \mathtt{tanh}(\mathbf{s}^{(t)})$$

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

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

$$\mathtt{J}^{(t)} = \mathtt{cross\_entropy}(\mathtt{y}^{(t)}, \hat{\mathtt{y}}^{(t)}) = -\sum \mathtt{y}^{(t)} \mathtt{log} \hat{\mathtt{y}}^{(t)}$$

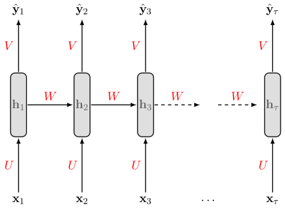



THAT FEELING WHEN YOU UNDERSTAND
SOMETHING IN MATHS
memegenerator.net

BPTT Step by Step (13/20)

$$\mathtt{J}^{(\mathtt{t})} = \mathtt{cross\_entropy}(\mathtt{y}^{(\mathtt{t})}, \hat{\mathtt{y}}^{(\mathtt{t})}) = -\sum \mathtt{y}^{(\mathtt{t})} \mathtt{log} \hat{\mathtt{y}}^{(\mathtt{t})}$$

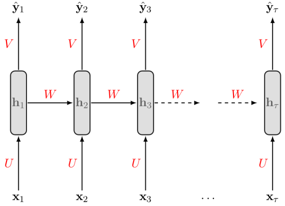
- We treat the full sequence as one training example.



BPTT Step by Step (13/20)

$$\mathtt{J}^{(\mathtt{t})} = \mathtt{cross\_entropy}(\mathtt{y}^{(\mathtt{t})}, \hat{\mathtt{y}}^{(\mathtt{t})}) = -\sum \mathtt{y}^{(\mathtt{t})} \mathtt{log} \hat{\mathtt{y}}^{(\mathtt{t})}$$

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



BPTT Step by Step (14/20)

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

BPTT Step by Step (14/20)

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- The gradient is equal to the sum of the respective gradients at each time step $\mathtt{t}$.

BPTT Step by Step (14/20)

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

BPTT Step by Step (14/20)

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- The gradient is equal to the sum of the respective gradients at each time step t.
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$$\frac{\partial E}{\partial v} = \sum_t \frac{\partial J^{(t)}}{\partial v} = \frac{\partial J^{(3)}}{\partial v} + \frac{\partial J^{(2)}}{\partial v} + \frac{\partial J^{(1)}}{\partial v}$$

BPTT Step by Step (14/20)

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

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

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.
- The gradient is equal to the sum of the respective gradients at each time step t.
- For example if $t = 3$ we have: $E = J^{(1)} + J^{(2)} + J^{(3)}$

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

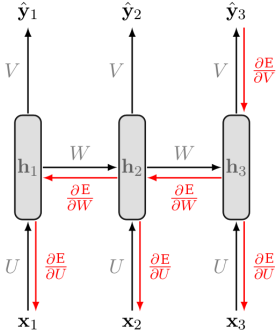
$$\frac{\partial E}{\partial w} = \sum_t \frac{\partial J^{(t)}}{\partial w} = \frac{\partial J^{(3)}}{\partial w} + \frac{\partial J^{(2)}}{\partial w} + \frac{\partial J^{(1)}}{\partial w}$$

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

BPTT Step by Step (15/20)

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

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



BPTT Step by Step (15/20)

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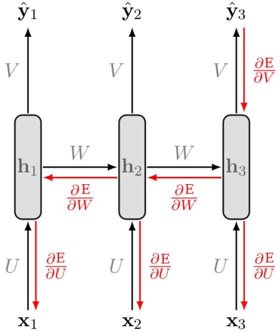
$$\frac{\partial \mathtt{E}}{\partial \mathtt{v}} = \sum_{\mathtt{t}} \frac{\partial \mathtt{J}^{(\mathtt{t})}}{\partial \mathtt{v}} = \frac{\partial \mathtt{J}^{(3)}}{\partial \mathtt{v}} + \frac{\partial \mathtt{J}^{(2)}}{\partial \mathtt{v}} + \frac{\partial \mathtt{J}^{(1)}}{\partial \mathtt{v}}$$

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



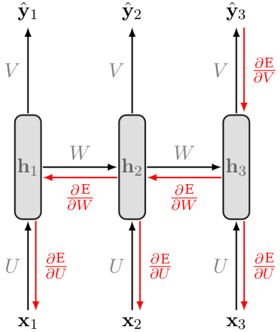
BPTT Step by Step (15/20)

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

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

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

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



BPTT Step by Step (15/20)

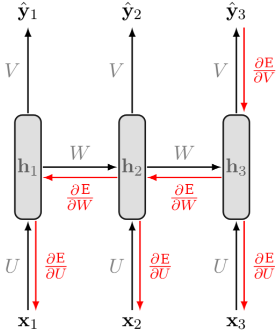
- Let's start with $\frac{\partial E}{\partial v}$.
- A change in v will only impact $J^{(3)}$ at time $t = 3$, because it plays no role in computing the value of anything other than $z^{(3)}$.

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

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

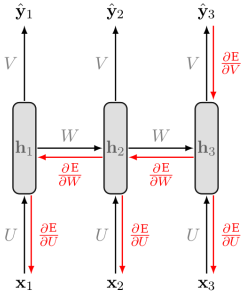
$$\frac{\partial J^{(2)}}{\partial v} = \frac{\partial J^{(2)}}{\partial \hat{y}^{(2)}} \frac{\partial \hat{y}^{(2)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial v}$$

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



BPTT Step by Step (16/20)

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

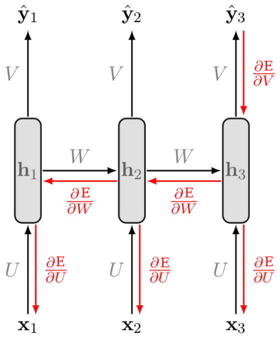


BPTT Step by Step (17/20)

- we compute our individual gradients as:

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

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

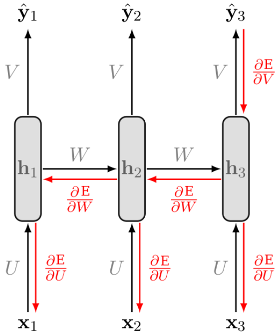


BPTT Step by Step (18/20)

- we compute our individual gradients as:

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

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

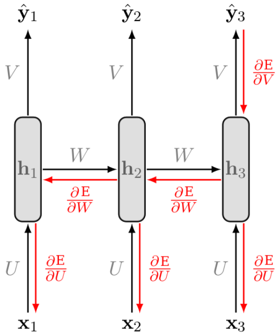


BPTT Step by Step (19/20)

- we compute our individual gradients as:

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

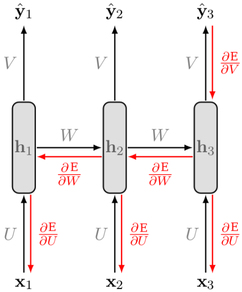
$$\begin{aligned}\frac{\partial J^{(3)}}{\partial w} = &\frac{\partial J^{(3)}}{\partial \hat{y}^{(3)}}\frac{\partial \hat{y}^{(3)}}{\partial z^{(3)}}\frac{\partial z^{(3)}}{\partial h^{(3)}}\frac{\partial h^{(3)}}{\partial s^{(3)}}\frac{\partial s^{(3)}}{\partial w} + \\ &\frac{\partial J^{(3)}}{\partial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



BPTT Step by Step (20/20)

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

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



LSTM

RNN Problems

- Sometimes we only need to look at recent information to perform the present task.
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- 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.

RNN Basic Cell vs. LSTM

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

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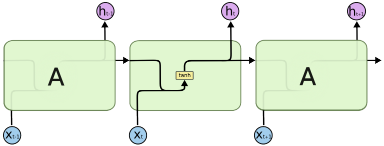

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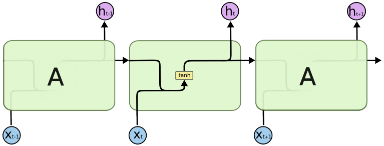
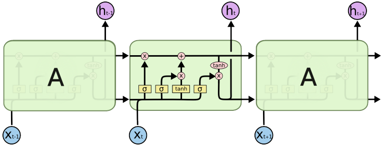
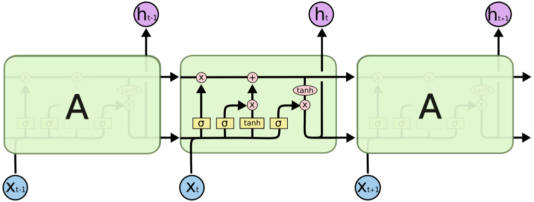


- An LSTM contains four interacting layers in each cell.



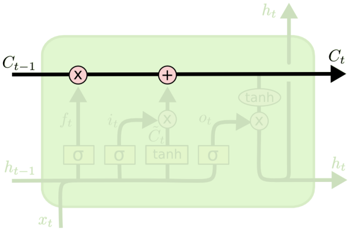
LSTM (1/2)

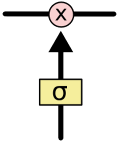
- In LSTM state is split in two vectors:
    1. $\mathtt{h}^{(t)}$ ($\mathtt{h}$ stands for hidden): the short-term state
    2. $\mathtt{c}^{(t)}$ ($\mathtt{c}$ stands for cell): the long-term state



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

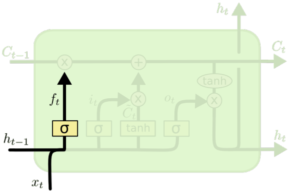




Step-by-Step LSTM Walk Through (1/4)

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

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



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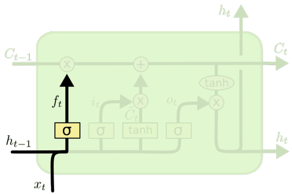
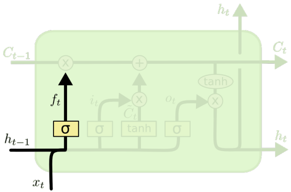


Step-by-Step LSTM Walk Through (1/4)

- 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.
- It looks at $\mathtt{h}^{(t-1)}$ and $\mathbf{x}^{(t)}$, and outputs a number between 0 and 1 for each number in the cell state $\mathtt{c}^{(t-1)}$.
  - 1 represents completely keep this, and 0 represents completely get rid of this.

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

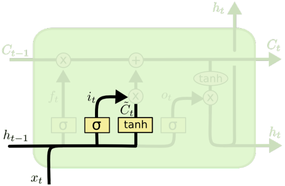


Step-by-Step LSTM Walk Through (2/4)

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

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

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



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

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

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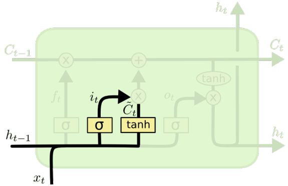
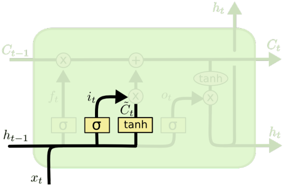


Step-by-Step LSTM Walk Through (2/4)

- 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.

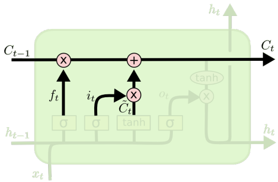
$$\mathtt{i}^{(\mathtt{t})} = \sigma(\mathbf{u}_{\mathtt{i}}^{\mathsf{T}}\mathbf{x}^{(\mathtt{t})} + \mathtt{w}_{\mathtt{i}}\mathtt{h}^{(\mathtt{t}-1)})$$
$$\tilde{\mathtt{c}}^{(\mathtt{t})} = \tanh(\mathbf{u}_{\tilde{\mathtt{c}}}^{\mathsf{T}}\mathbf{x}^{(\mathtt{t})} + \mathtt{w}_{\tilde{\mathtt{c}}}\mathtt{h}^{(\mathtt{t}-1)})$$



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

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

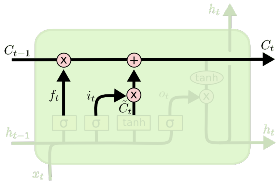
$$\mathbf{c}^{(t)} = \mathbf{f}^{(t)} \otimes \mathbf{c}^{(t-1)} + \mathbf{i}^{(t)} \otimes \tilde{\mathbf{c}}^{(t)}$$



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

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

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



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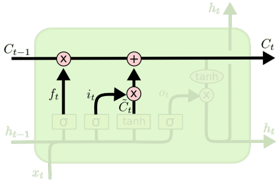
- Then we add it $\mathtt{i}^{(t)} \otimes \tilde{\mathtt{c}}^{(t)}$.

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



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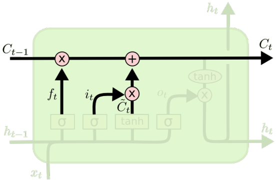
- We multiply the old state by $\mathtt{f}^{(t)}$, forgetting the things we decided to forget earlier.
- Then we add it $\mathtt{i}^{(t)} \otimes \tilde{\mathtt{c}}^{(t)}$.
- This is the new candidate values, scaled by how much we decided to update each state value.

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

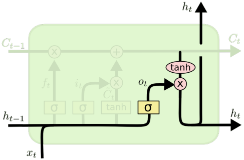


Step-by-Step LSTM Walk Through (4/4)

- Fourth step: decides about the output.

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

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

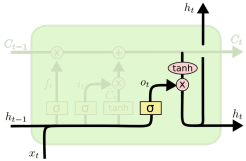


Step-by-Step LSTM Walk Through (4/4)

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

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

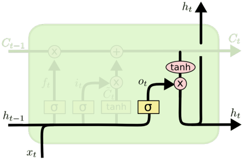
$$\mathbf{h}^{(t)} = \mathbf{o}^{(t)} \otimes \tanh(\mathbf{c}^{(t)})$$



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.
- 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.

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



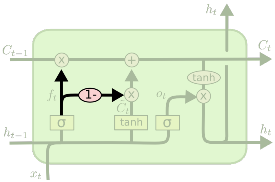
LSTM in TensorFlow

- Use LSTM

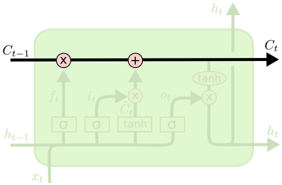
```
model = keras.models.Sequential([
    keras.layers.LSTM(20, return_sequences=True, input_shape=[None, 1]),
    keras.layers.LSTM(20),
    keras.layers.Dense(1)
])

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.



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.

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

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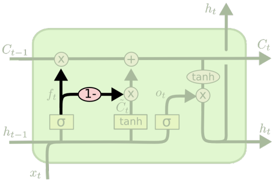
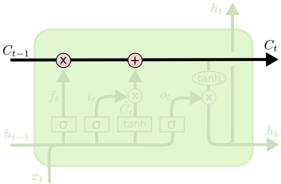


GRU

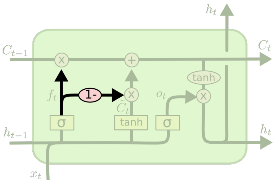


LSTM

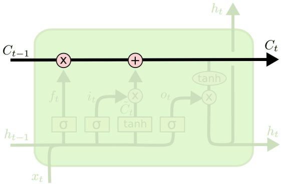
Gated Recurrent Unit (GRU)

- 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.
  - 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.

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



GRU



LSTM

GRU in TensorFlow

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model.evaluate(X_test, y_test, verbose=0)
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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)
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Questions?