RNNs and Transformers

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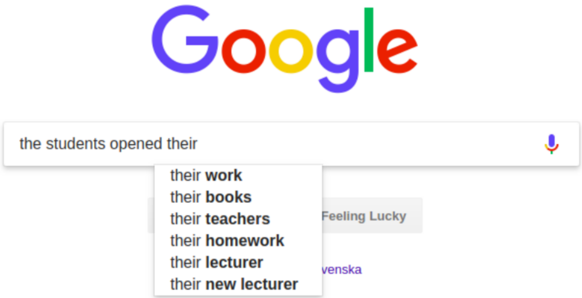
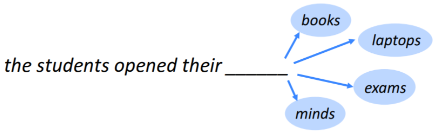
Let's Start With An Example


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.

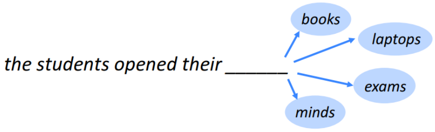


Language Modeling (2/2)

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

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

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



n-gram Language Models

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

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

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

- 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

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

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

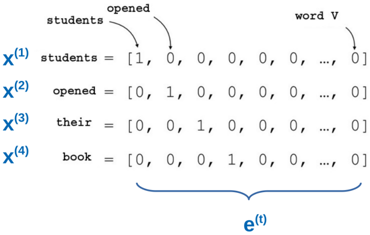
Problems with n-gram Language Models - Storage

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

- 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.

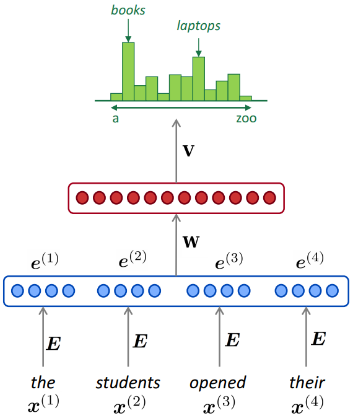
Can We Build a Neural Language Model? (1/3)

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



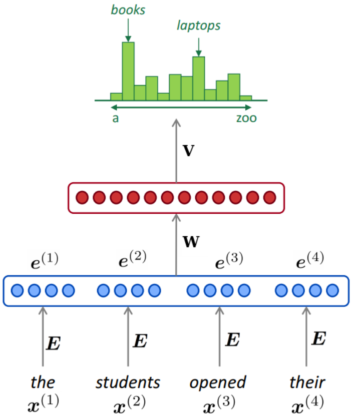
Can We Build a Neural Language Model? (2/3)

- 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))`
- Remaining problems:
  - It is fixed 4 in our example, which is small
  - We need a neural architecture that can process any length input



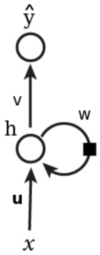
Recurrent Neural Networks (RNN)

Recurrent Neural Networks (1/4)

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

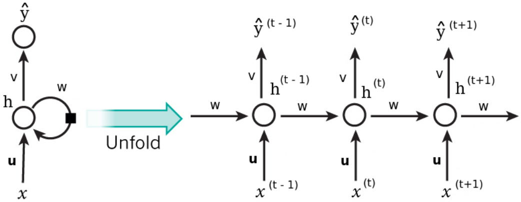
Recurrent Neural Networks (2/4)

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



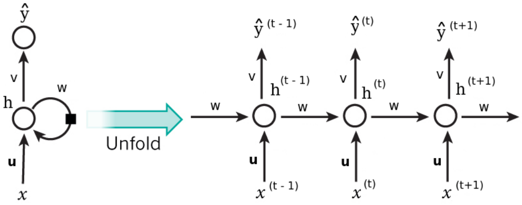
Recurrent Neural Networks (3/4)

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



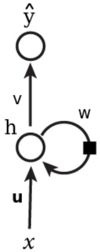
Recurrent Neural Networks (4/4)

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



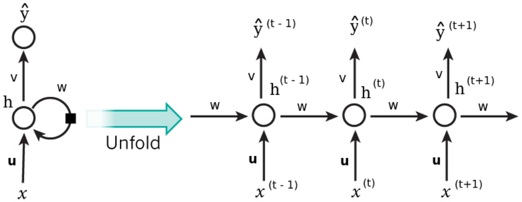
Recurrent Neurons - Weights (1/4)

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



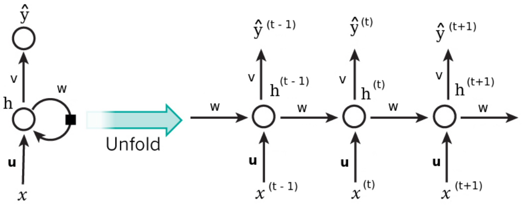
Recurrent Neurons - Weights (2/4)

- $\mathbf{u}$: 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.



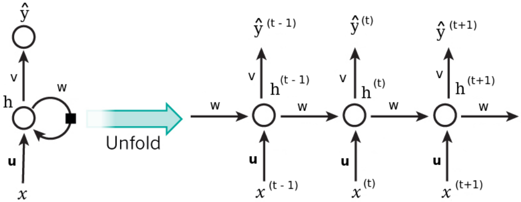
Recurrent Neurons - Weights (3/4)

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



Recurrent Neurons - Weights (4/4)

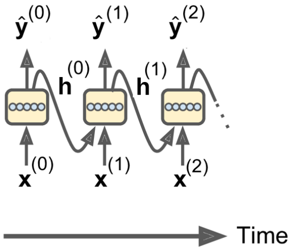
- $\mathtt{v}$: the weights for the hidden state of the current time step $\mathtt{h}^{(\mathtt{t})}$.
- $\hat{\mathbf{y}}^{(\mathtt{t})}$ is the output at step $\mathtt{t}$.
- $\hat{\mathbf{y}}^{(\mathtt{t})} = \mathtt{softmax}(\mathtt{v}\mathtt{h}^{(\mathtt{t})})$
- For example, if we wanted to predict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

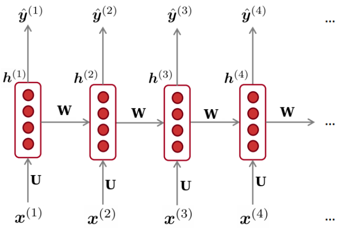


Layers of Recurrent Neurons

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

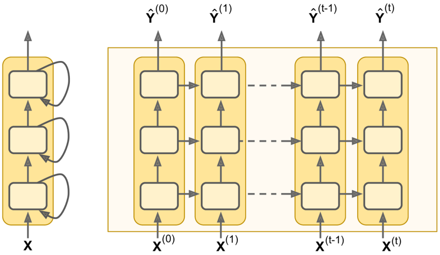
$$\mathbf{h}^{(t)} = \mathtt{tanh}(\mathbf{u}^\intercal \mathbf{x}^{(t)} + \mathbf{w}^\intercal \mathbf{h}^{(t-1)})$$
$$\mathbf{y}^{(t)} = \mathtt{sigmoid}(\mathbf{v}^\intercal \mathbf{h}^{(t)})$$





Deep RNN

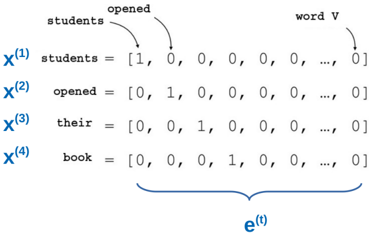
- Stacking multiple layers of cells gives you a deep RNN.

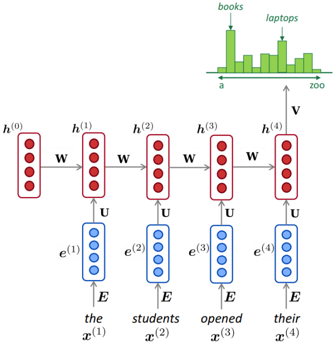


Let's Back to Language Model Example

A RNN Neural Language Model (1/2)

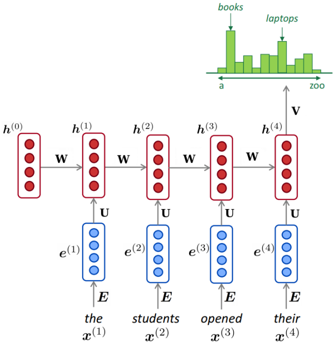
- The input **x** will be a sequence of words (each $\mathtt{x}^{(t)}$ is a single word).
- Each embedded word $\mathbf{e}^{(t)} = \mathbf{E}^{\top}\mathtt{x}^{(t)}$ is a one-hot vector of size vocabulary size.

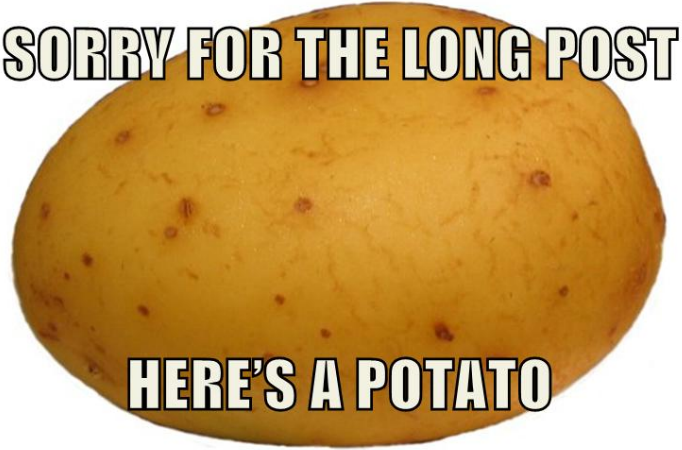




A RNN Neural Language Model (2/2)

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

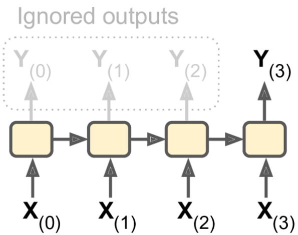



SORRY FOR THE LONG POST
HERE'S A POTATO

RNN Design Patterns

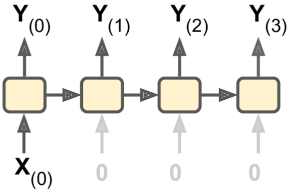
RNN Design Patterns - Sequence-to-Vector

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



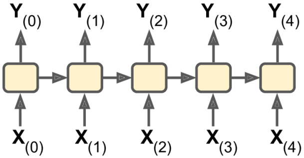
RNN Design Patterns - Vector-to-Sequence

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



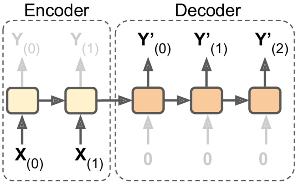
RNN Design Patterns - Sequence-to-Sequence

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

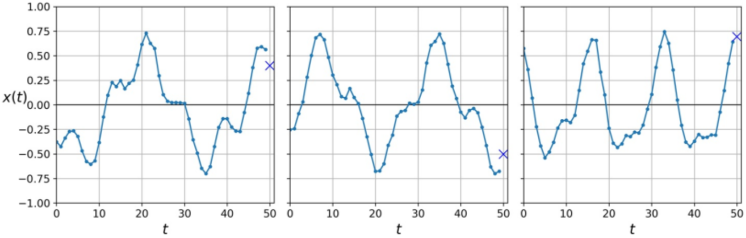
- Encoder-decoder network: a sequence-to-vector network (encoder), followed by a vector-to-sequence network (decoder).
- E.g., translating a sentence from one language to another.
- You would feed the network a sentence in one language, the encoder would convert this sentence into a single vector representation,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

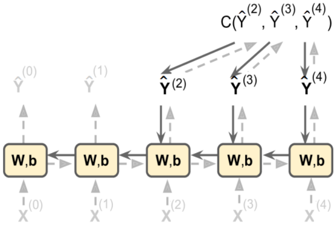
Training RNNs

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

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

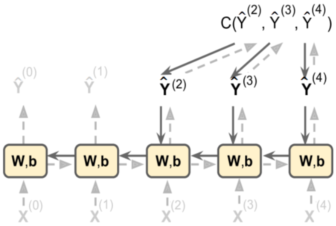
Backpropagation Through Time (1/3)

- 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)

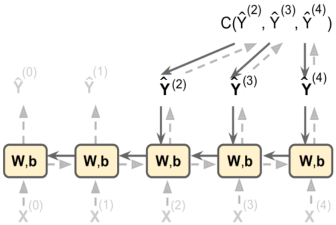
- 3. Propagate backward the gradients of that cost function through the unrolled network (represented by the solid arrows).
- 4. The model parameters are updated using the gradients computed during BPTT.



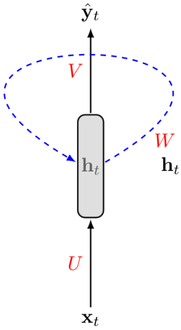
Backpropagation Through Time (3/3)

- 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)



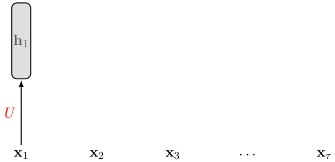
$$\hat{\mathbf{y}}_t = \phi(V\mathbf{h}_t)$$

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

BPTT Step by Step (2/20)

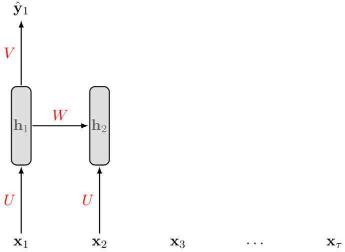
$\mathbf{x}_1 \qquad \mathbf{x}_2 \qquad \mathbf{x}_3 \qquad \cdots \qquad \mathbf{x}_\tau$

BPTT Step by Step (3/20)

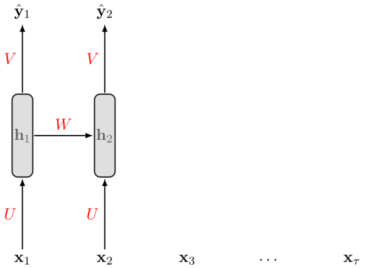


BPTT Step by Step (4/20)

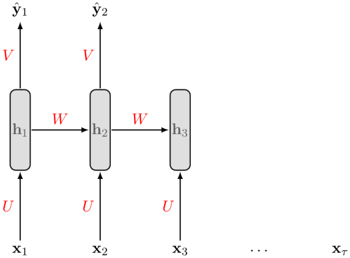
BPTT Step by Step (5/20)



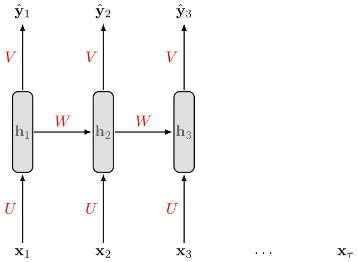
BPTT Step by Step (6/20)



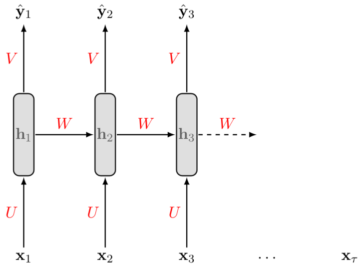
BPTT Step by Step (7/20)



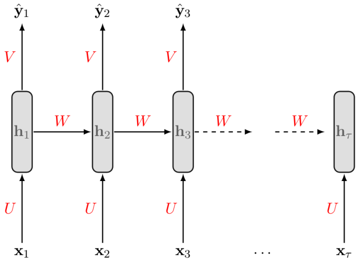
BPTT Step by Step (8/20)



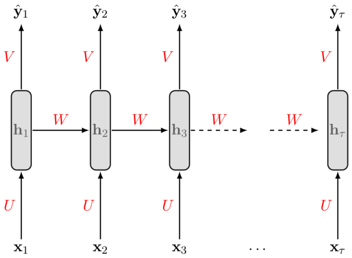
BPTT Step by Step (9/20)



BPTT Step by Step (10/20)



BPTT Step by Step (11/20)



BPTT Step by Step (12/20)

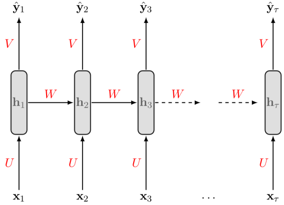
$$\mathbf{s}^{(t)} = \mathbf{u}^T\mathbf{x}^{(t)} + \mathtt{w}\mathtt{h}^{(t-1)}$$

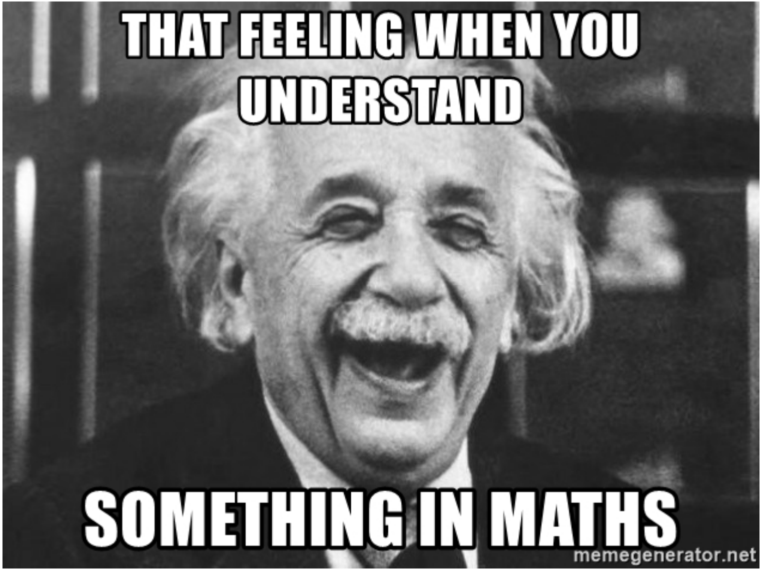
$$\mathtt{h}^{(t)} = \mathtt{tanh}(\mathbf{s}^{(t)})$$

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

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

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

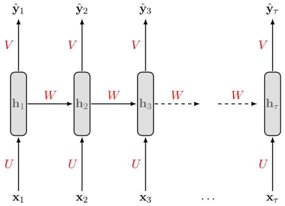



THAT FEELING WHEN YOU UNDERSTAND
SOMETHING IN MATHS
memegenerator.net

BPTT Step by Step (13/20)

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

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



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.
- 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)

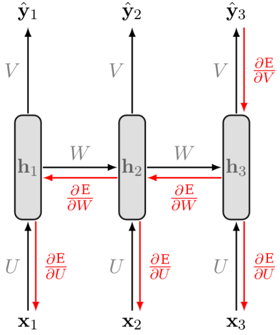
- Let's start with $\frac{\partial E}{\partial v}$.
- A change in v will only impact $J^{(3)}$ at time $t = 3$, because it plays no role in computing the value of anything other than $z^{(3)}$.

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

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

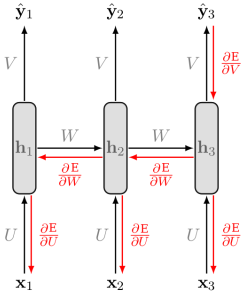
$$\frac{\partial J^{(2)}}{\partial v} = \frac{\partial J^{(2)}}{\partial \hat{y}^{(2)}} \frac{\partial \hat{y}^{(2)}}{\partial z^{(2)}} \frac{\partial z^{(2)}}{\partial v}$$

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



BPTT Step by Step (16/20)

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

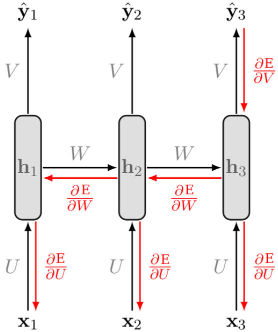


BPTT Step by Step (17/20)

- we compute our individual gradients as:

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

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



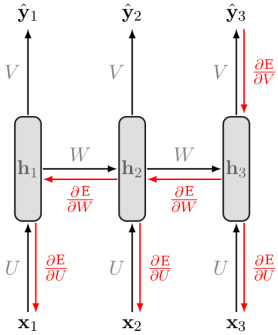
BPTT Step by Step (18/20)

- 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)

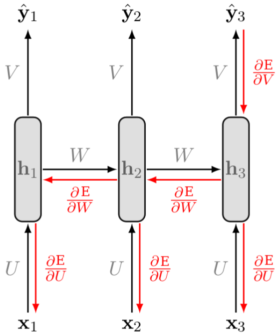
- we compute our individual gradients as:

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

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

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

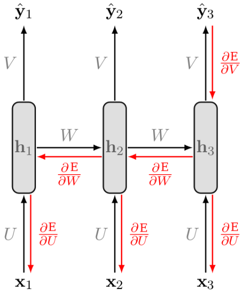
$$\frac{\partial J^{(3)}}{\partial \hat{y}^{(3)}} \frac{\partial \hat{y}^{(3)}}{\partial z^{(3)}} \frac{\partial z^{(3)}}{\partial h^{(3)}} \frac{\partial h^{(3)}}{\partial s^{(3)}} \frac{\partial s^{(3)}}{\partial h^{(2)}} \frac{\partial h^{(2)}}{\partial s^{(2)}} \frac{\partial s^{(2)}}{\partial h^{(1)}}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



BPTT Step by Step (20/20)

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

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



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.

RNN References

- 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`

Word Embeddings

Problem: Word embeddings are context-free

[Peltarion, 2020]

Word Embeddings

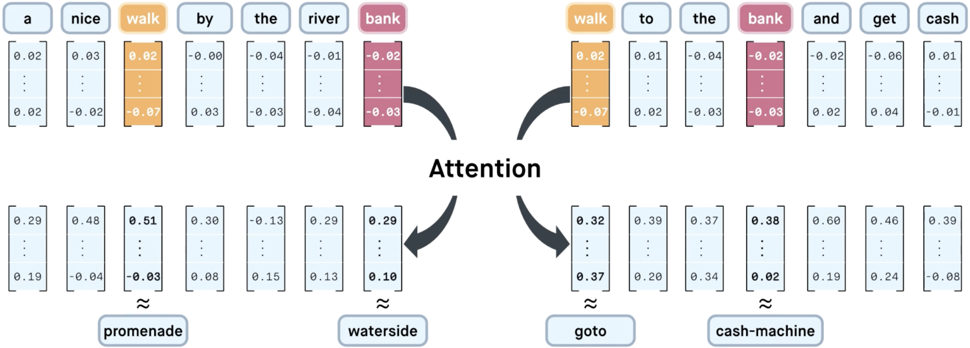
Problem: Word embeddings are context-free

[Peltarion, 2020]

Word Embeddings

Problem: Word embeddings are context-free

Solution: Create contextualized representation



[Peltarion, 2020]

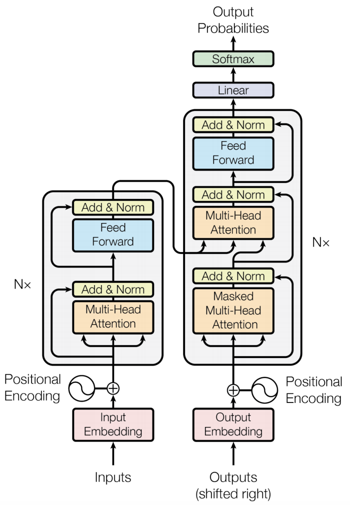
From RNNs to Transformers

Problems with RNNs - Motivation for Transformers

- Sequential computations prevents parallelization
- Despite GRUs and LSTMs, RNNs still need attention mechanisms to deal with long range dependencies
- Attention gives us access to any state...Maybe we don't need the costly recursion?
- Then NLP can have deep models, solves our computer vision envy!

Attention is all you need! [Vaswani, 2017]

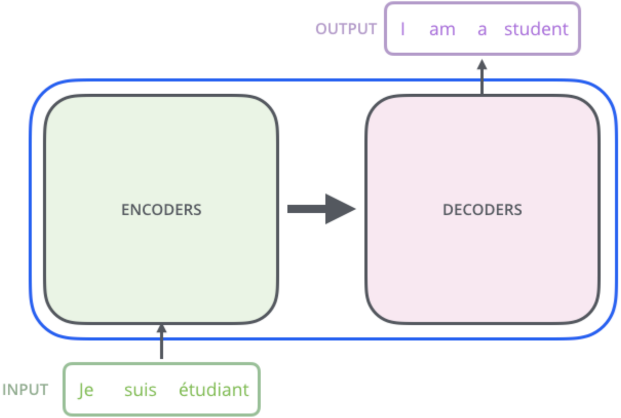
- Sequence-to-sequence model for Machine Translation
- Encoder-decoder architecture
- Multi-headed self-attention
  - Models context and no locality bias



[Vaswani et al., 2017]

Transformers Step-by-Step

Understanding the Transformer: Step-by-Step

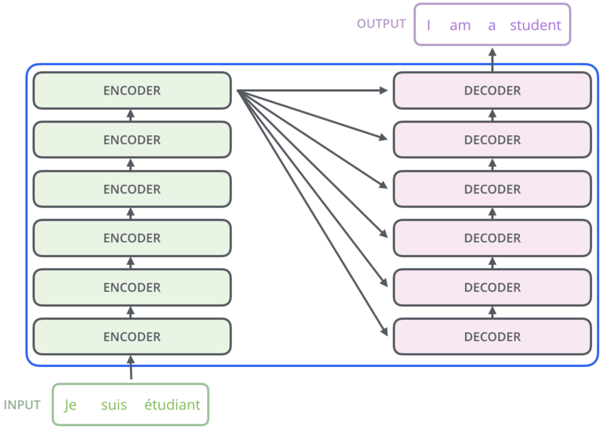


[Alammar, 2018]

Understanding the Transformer: Step-by-Step

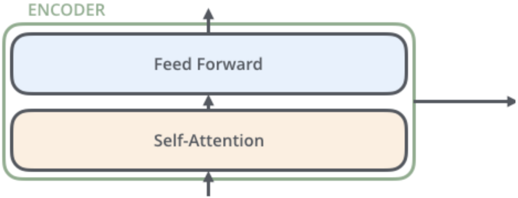
No recursion, instead stacking encoder and decoder blocks

- Originally: 6 layers
- BERT base: 12 layers
- BERT large: 24 layers
- GPT2-XL: 48 layers
- GPT3: 96 layers



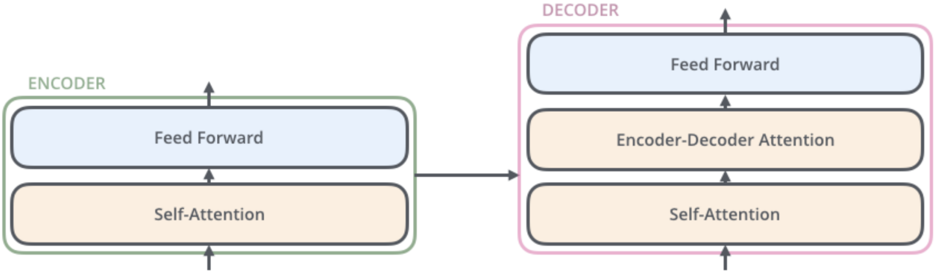
[Alammar, 2018]

The Encoder and Decoder Blocks



[Alammar, 2018]

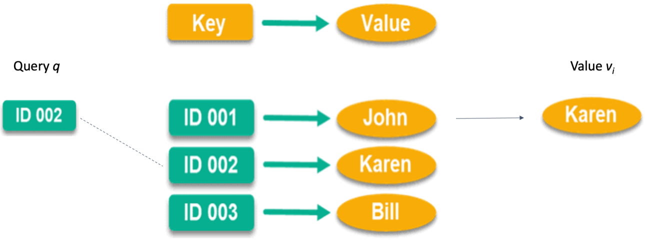
The Encoder Block



[Alammar, 2018]

Attention Preliminaries

Mimics the retrieval of a value v_i for a query q based on a key k_i in a database, but in a probabilistic fashion



Dot-Product Attention

- Queries, keys and values are vectors
- Output is a weighted sum of the values
- Weights are are computed as the scaled dot-product (similarity) between the query and the keys

$$\text{Attention}(q, K, V) = \sum_i \text{Similarity}(q, k_i) \cdot v_i = \sum_i \frac{e^{q \cdot k_i / \sqrt{d_k}}}{\sum_j e^{q \cdot k_j / \sqrt{d_k}}} v_i$$

Output is a row-vector

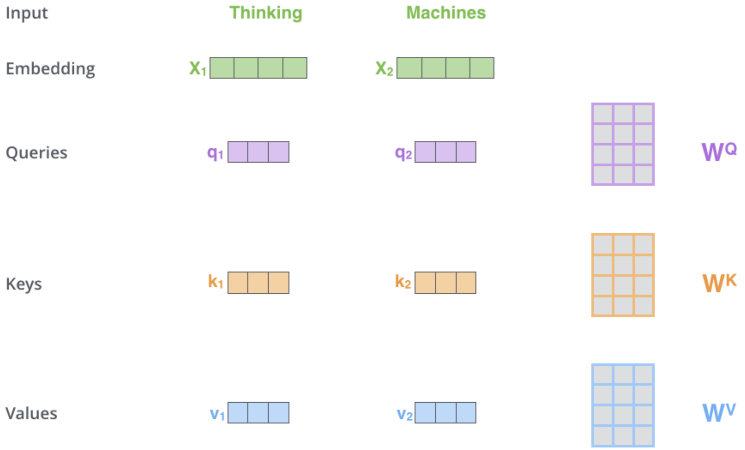
- Can stack multiple queries into a matrix Q

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}}\right) V$$

Output is again a matrix

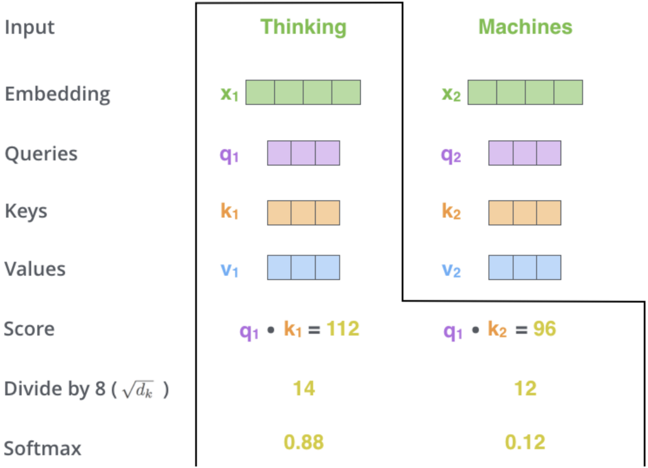
- Self-attention: Let the word embeddings be the queries, keys and values, i.e. let the words select each other

Self-Attention Mechanism



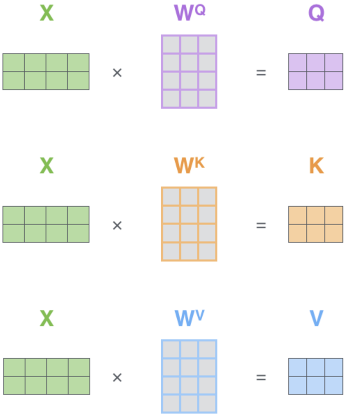
[Alammar, 2018]

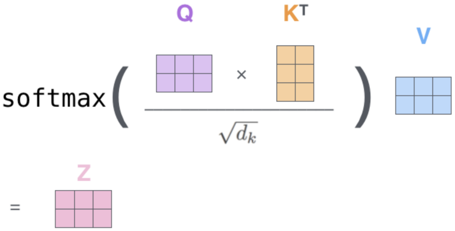
Self-Attention Mechanism



[Alammar, 2018]

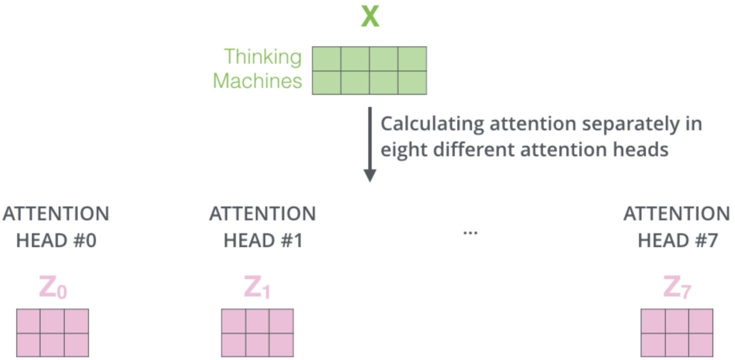
Self-Attention Mechanism in Matrix Notation





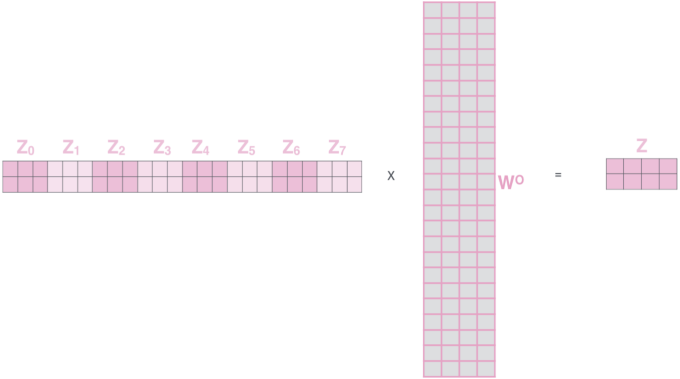
[Alammar, 2018]

Multi-Headed Self-Attention



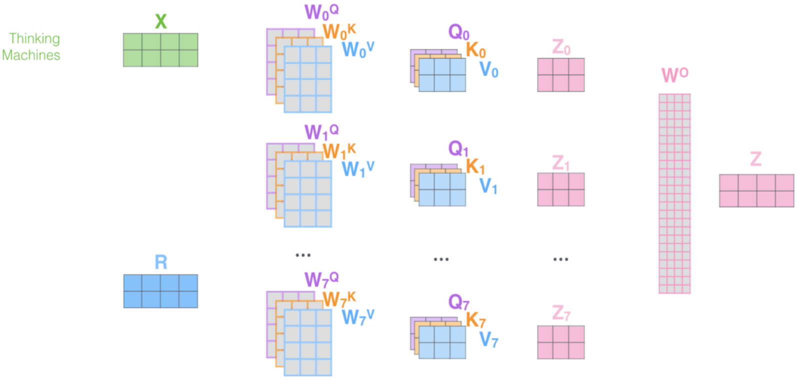
[Alammar, 2018]

Multi-Headed Self-Attention



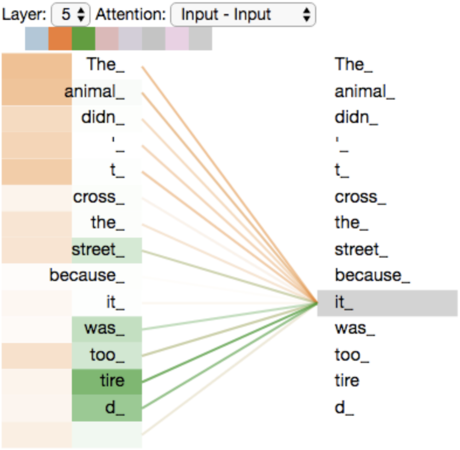
[Alammar, 2018]

Self-Attention: Putting It All Together



[Alammar, 2018]

Attention Visualized

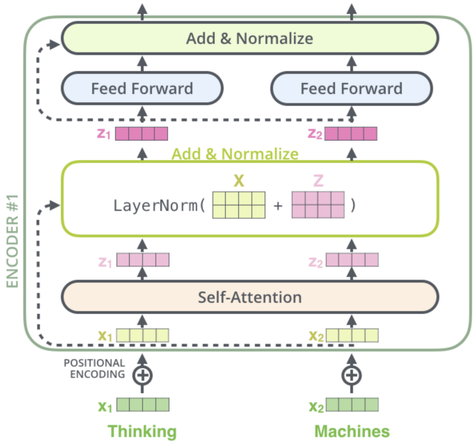


[Alammar, 2018]

The Full Encoder Block

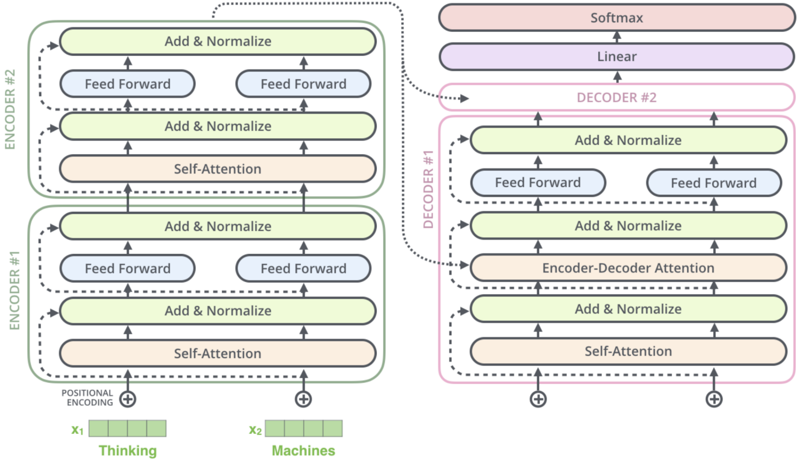
Encoder block consisting of:

- Multi-headed self-attention
- Feedforward NN (FC 2 layers)
- Skip connections
- Layer normalization - Similar to batch normalization but computed over features (words/tokens) for a single sample



[Alammar, 2018]

Encoder-Decoder Architecture - Small Example



[Alammar, 2018]

Complexity Comparison

Layer Type	Complexity per Layer	Sequential Operations	Maximum Path Length
Self-Attention	$O(n^2 \cdot d)$	$O(1)$	$O(1)$
Recurrent	$O(n \cdot d^2)$	$O(n)$	$O(n)$
Convolutional	$O(k \cdot n \cdot d^2)$	$O(1)$	$O(log_k(n))$

[Vaswani et al., 2017]

Results

Model	BLEU		Training Cost (FLOPs)	
	EN-DE	EN-FR	EN-DE	EN-FR
ByteNet [15]	23.75			
Deep-Att + PosUnk [32]		39.2		$1.0 \cdot 10^{20}$
GNMT + RL [31]	24.6	39.92	$2.3 \cdot 10^{19}$	$1.4 \cdot 10^{20}$
ConvS2S [8]	25.16	40.46	$9.6 \cdot 10^{18}$	$1.5 \cdot 10^{20}$
MoE [26]	26.03	40.56	$2.0 \cdot 10^{19}$	$1.2 \cdot 10^{20}$
Deep-Att + PosUnk Ensemble [32]		40.4		$8.0 \cdot 10^{20}$
GNMT + RL Ensemble [31]	26.30	41.16	$1.8 \cdot 10^{20}$	$1.1 \cdot 10^{21}$
ConvS2S Ensemble [8]	26.36	**41.29**	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$
Transformer (base model)	27.3	38.1	$\mathbf{3.3 \cdot 10^{18}}$	
Transformer (big)	**28.4**	**41.0**	$2.3 \cdot 10^{19}$	

[Vaswani et al., 2017]

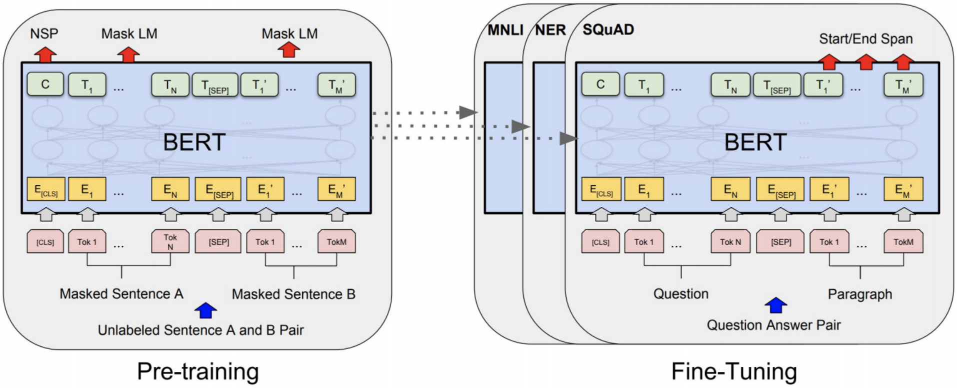
BERT

BERT

Bidirectional **E**ncoder **R**epresentations from **T**ransformers

- Self-supervised pre-training of Transformers encoder for language understanding
- Fine-tuning for specific downstream task

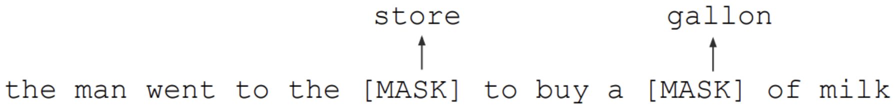
BERT Training Procedure



[Devlin et al., 2018]

BERT Training Objectives

Masked Language Modelling



Next Sentence prediction

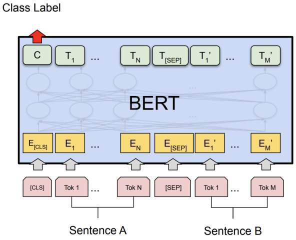
Sentence A = The man went to the store.
Sentence B = He bought a gallon of milk.
Label = IsNextSentence

Sentence A = The man went to the store.
Sentence B = Penguins are flightless.
Label = NotNextSentence

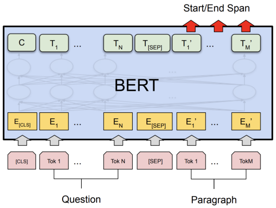
[Devlin et al., 2018]

BERT Fine-Tuning Examples

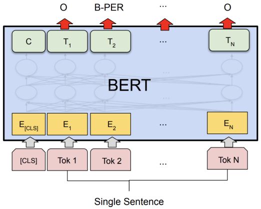
Sentence Classification



Question Answering



Named Entity Recognition



[Devlin et al., 2018]

How good are transformers?

- Scaling up models size and amount of training data helps a lot
- Best model is 10B (!!) parameters
- Two models have already surpassed human performance!!!
- Exact pre-training objective (MLM, NSP, corruption) doesn't matter too much
- SuperGLUE benchmark:

	Rank	Name	Model	URL	Score	BoolQ	CB	COPA	MultiRC	ReCoRD	RTE	WiC	WSC	AX-g	AX-b
	1	ERNIE Team - Baidu	ERNIE 3.0		90.6	91.0	98.6/99.2	97.4	88.6/63.2	94.7/94.2	92.6	77.4	97.3	92.7/94.7	68.6
+	2	Zirui Wang	T5 + UDG, Single Model (Google Brain)		90.4	91.4	95.8/97.6	98.0	88.3/63.0	94.2/93.5	93.0	77.9	96.6	92.7/91.9	69.1
+	3	DeBERTa Team - Microsoft	DeBERTa / TuringNLRv4		90.3	90.4	95.7/97.6	98.4	88.2/63.7	94.5/94.1	93.2	77.5	95.9	93.3/93.8	66.7
	4	SuperGLUE Human Baselines	SuperGLUE Human Baselines		89.8	89.0	95.8/98.9	100.0	81.8/51.9	91.7/91.3	93.6	80.0	100.0	99.3/99.7	76.6
+	5	T5 Team - Google	T5		89.3	91.2	93.9/96.8	94.8	88.1/63.3	94.1/93.4	92.5	76.9	93.8	92.7/91.9	65.6
+	6	Huawei Noah's Ark Lab	NEZHA-Plus		86.7	87.8	94.4/96.0	93.6	84.6/55.1	90.1/89.6	89.1	74.6	93.2	87.1/74.4	58.0

[Raffel et al., 2019]

Practical Examples

BERT in low-latency production settings

GOOGLE \ TECH \ ARTIFICIAL INTELLIGENCE

Google is improving 10 percent of searches by understanding language context

Say hello to BERT

By Dieter Bohn | @backlon | Oct 25, 2019, 3:01am EDT

Bing says it has been applying BERT since April

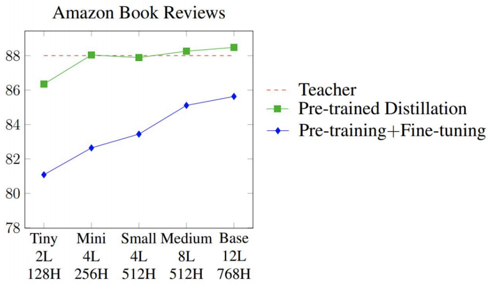
The natural language processing capabilities are now applied to all Bing queries globally.

George Nguyen on November 19, 2019 at 1:38 pm

[Devlin, 2020]

Distillation

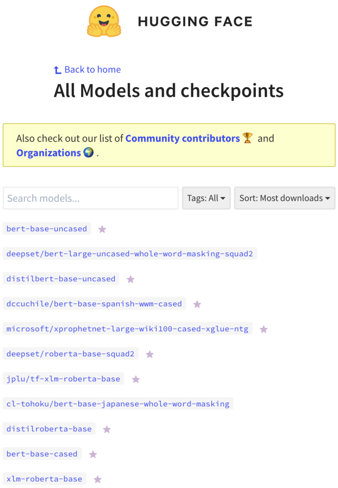
- Modern pre-trained language models are huge and very computationally expensive
- How are these companies applying them to low-latency applications?
- Distillation!
  - Train SOTA teacher model (pre-training + fine-tuning)
  - Train smaller student model that mimics the teacher's output on a large dataset on unlabeled data
- Distillation works *much* better than pre-training + fine-tuning with smaller model



[Devlin, 2020] [Turc, 2020]

Transformers in TensorFlow using HuggingFace 🤗

- The HuggingFace Library contains a majority of the recent pre-trained State-of-the-art NLP models, as well as over 4 000 community uploaded models
- Works with both TensorFlow and PyTorch



Transformers in TensorFlow using HuggingFace 🤗

```
from transformers import BertTokenizerFast, TFBertForSequenceClassification
from datasets import load_dataset
import tensorflow as tf

dataset = load_dataset("imdb").shuffle()
tokenizer = BertTokenizerFast.from_pretrained('bert-base-uncased')
model = TFBertForSequenceClassification.from_pretrained('bert-base-uncased', num_labels=2)

train_encodings = tokenizer(dataset['train']['text'], truncation=True, padding=True)
train_dataset = tf.data.Dataset.from_tensor_slices((dict(train_encodings), dataset['train']['label']))
val_dataset = ... // Analogously

optimizer = tf.keras.optimizers.Adam(learning_rate=5e-5)
model.compile(optimizer=optimizer, loss=model.compute_loss)
model.fit(train_dataset.batch(16), epochs=3, batch_size=16)

model.evaluate(val_dataset.batch(16), verbose=0)
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Wrap Up

Summary

- Transformers have blown other architectures out of the water for NLP
- Get rid of recurrence and rely on self-attention
- NLP pre-training using Masked Language Modelling
- Most recent improvements using larger models and more data
- Distillation can make model serving and inference more tractable