Sequence Modelling

RNN, biRNN, BPTT, LSTM, RecNN

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Sequence modelling

Recurrent neural network

- Definition
- Training

Gated architectures

RNN generators

The Transformer

Implementation in PyTorch

Take-home message

Bonus: Recursive NN

Sequence modelling

Sequential data

1. Time series
   - Financial data analysis: stock market, commodities, Forex
   - Healthcare: pulse rate, sugar level (from medical equipment and wearables)
2. Text and speech: speech understanding, text generation
3. Spatiotemporal data
   - Self-driving and object tracking
   - Plate tectonic activity
4. Physics: jet identification
5. etc.

Sequence modelling I

Sequence classification

1. $\boldsymbol{x} = x_1, x_2, \ldots, x_n, x_i \in V$ - objects
2. $y \in \{1, \ldots, L\}$ - labels
3. $\{(\boldsymbol{x}^{(1)}, y_1), (\boldsymbol{x}^{(2)}, y_2), \ldots, (\boldsymbol{x}^{(m)}, y_m)\}$ – training data

Classification problem: $\gamma : \boldsymbol{x} \to y$

1. Activity recognition: x – pulse rate, y – activity (walking, running, peace)
2. Opinion mining: x – sentence, y – sentiment (positive, negative)
3. Trading: x – stock market, y – action (sell, buy, do nothing)

Sequence modelling II

Sequence labelling

1. $\boldsymbol{x} = x_1, x_2, \ldots, x_n, x_i \in V$ - objects
2. $\boldsymbol{y} = y_1, y_2, \ldots, y_n, y_i \in \{1, \ldots, L\}$ - labels
3. $\{(\boldsymbol{x}^{(1)}, \boldsymbol{y}^{(1)}), (\boldsymbol{x}^{(2)}, \boldsymbol{y}^{(2)}), \ldots, (\boldsymbol{x}^{(m)}, \boldsymbol{y}^{(m)})\}$ – training data
4. exponential number of possible solutions : if $\texttt{length}(x) = n$, there are L^n possible solutions

Classification problem: $\gamma : \boldsymbol{x} \to \boldsymbol{y}$

1. Part of speech tagging: x – word, y – part of speech (verb, noun, etc.)
2. Genome annotation: x – DNA, y – genes
3. HEP tracking: x - a set of hits with backgrounds, y – hit classification

Sequence modelling III

Sequence transduction / transformation

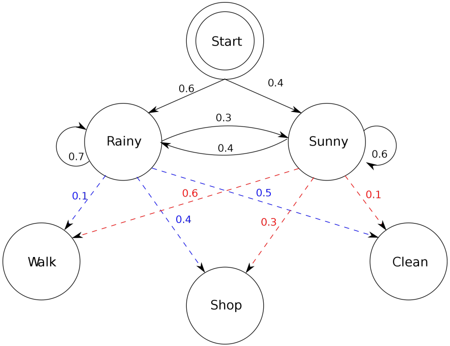
1. $\boldsymbol{x} = x_1, x_2, \ldots, x_n, x_i \in V_{source}$ - objects
2. $\boldsymbol{y} = y_1, y_2, \ldots, y_n, y_i \in V_{target}$ - objects
3. $\{(\boldsymbol{x}^{(1)}, \boldsymbol{y}^{(1)}), (\boldsymbol{x}^{(2)}, \boldsymbol{y}^{(2)}), \ldots, (\boldsymbol{x}^{(m)}, \boldsymbol{y}^{(m)})\}$ – training data
4. $\boldsymbol{x}^{(1)}, \boldsymbol{y}^{(1)}$ are of different length

Transduction problem: $\boldsymbol{x}_{source} \rightarrow \boldsymbol{y}_{target}$

1. Machine translation: x – sentence in German, y – sentence in English
2. Speech recognition: x – spoken language, y – text
3. Chat bots: x – question, y – answer

Traditional ML approaches to sequence modeling

- Hidden Markov Models (HMM)
- Conditional Random Fields (CRF)
- Local classifier: for each x define features, based on x_{-1}, x_{+1}, etc, and perform classification n times

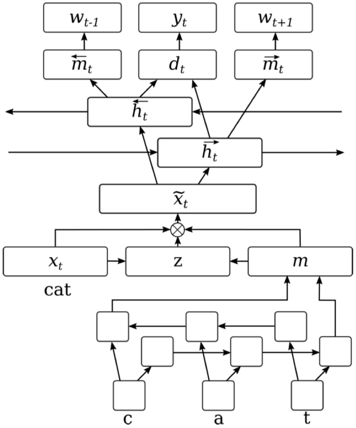


Problems:

1. Markov assumption: fixed length history
2. Computation complexity

DL approaches to sequence modeling

- Recurrent neural network and its modifications: LSTM, GRU, Highway
- Transformer
- 2D Convolutional Neural Network
- Pointer network



Problems:

1. Training time
2. Amount of training data

Recurrent neural network

Definition

Recurrent neural network

- Input: sequence of vectors
- $x_{1:n} = x_1, x_2, \ldots, x_n, x_i \in \mathbb{R}^{d_{in}}$
- Output: a single vector
  $y_n = RNN(x_{1:n}), y_n \in \mathbb{R}^{d_{out}}$
- For each prefix $x_{i:j}$ define an output vector y_i:
  $y_i = RNN(x_{1:i})$
- RNN^* is a function returning this sequence for input sequence $x_{1:n}$:
  $y_{1:n} = RNN^*(x_{1:n}), y_i \in \mathbb{R}^{d_{out}}$

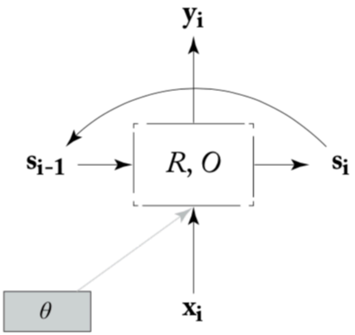


Figure: Goldberg, Yoav. Neural network methods for natural language processing

Sequence modelling with RNN

1. Sequence classification
   Put a dense layer on top of RNN to predict the desired class of the sequence after the whole sequence is processed

$$p(l_j|\boldsymbol{x}_{1:n}) = \texttt{softmax}(RNN(\boldsymbol{x}_{1:n}) \times W + b)_{[j]}$$

2. Sequence labelling
   Produce an output y_i for each input RNN reads in. Put a dense layer on top of each output to predict the desired class of the input

$$p(l_j|\boldsymbol{x}_j) = \texttt{softmax}(RNN(\boldsymbol{x}_{1:j}) \times W + b)_{[j]}$$

More details on RNN

- $RNN^*(x_{1:n}, s_0) = y_{1:n}$
- $y_i = O(s_i)$ – simple activation function
- $s_i = R(s_{i-1,x_i})$, where R is a recursive function, s_i is a state vector
- s_0 is initialized randomly or is a zero vector
- $x_i \in \mathbb{R}^{d_{in}}$, $y_i \in \mathbb{R}^{d_{out}}$, $s_i \in \mathbb{R}^{f(d_{out})}$
- θ – shared weights

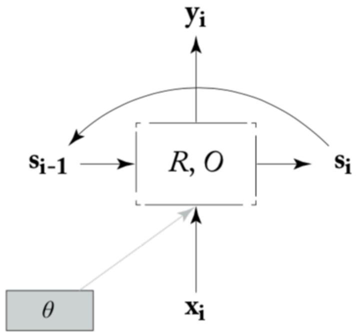


Figure: Goldberg, Yoav. Neural network methods for natural language processing

More details on RNN

- $s_i = R(x_i, s_{i-1}) = g(s_{i-1}W^s + x_iW^x + b)$
- $y_i = O(s_i) = s_i$
- $y_i, s_i, b \in \mathbb{R}^{d_{out}}, x_i \in \mathbb{R}^{d_{in}}$
- $W^x \in \mathbb{R}^{d_{in} \times d_{out}}, W^s \in \mathbb{R}^{d_{out} \times d_{out}}$

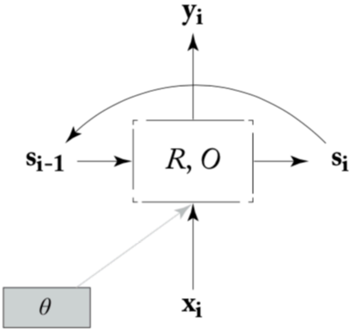
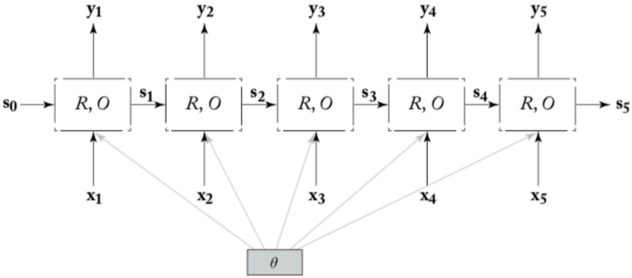


Figure: Goldberg, Yoav. Neural network methods for natural language processing

RNN unrolled

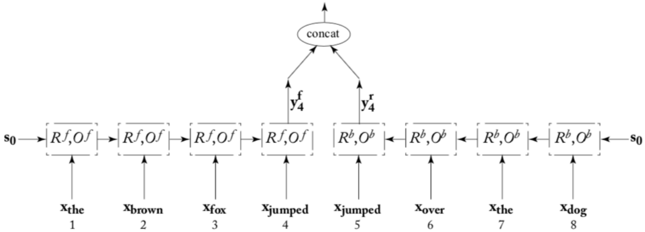


$$s_4 = R(s_3, x_4) = R(R(s_2, x_3), x_4) = R(R(R(s_1, x_2), x_3), x_4) =$$
$$= R(R(R(R(s_0, x1), x_2), x_3), x_4)$$

Figure: Goldberg, Yoav. Neural network methods for natural language processing

Bidirectional RNN (Bi-RNN)

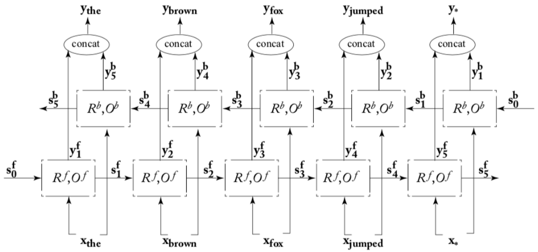
The input sequence can be read from left to right and from right to left. Which direction is better?



$$biRNN(x_{1:n}, i) = y_i = [RNN^f(x_{1:i}); RNN^r(x_{n:i})]$$

Figure: Goldberg, Yoav. Neural network methods for natural language processing

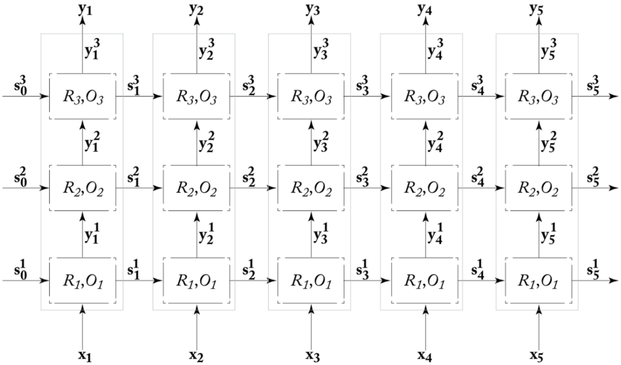
Bi-RNN



$$biRNN^*(x_{1:n}, i) = y_{1:n} = biRNN(x_{1:n}, 1) \dots biRNN(x_{1:n}, n)$$

Figure: Goldberg, Yoav. Neural network methods for natural language processing

Multilayer RNN



Connections between different layers are possible too: $y_1^2 = \texttt{concat}(x_1, y_1^1)$

Figure: Goldberg, Yoav. Neural network methods for natural language processing

Training

Sequence classification

- $\hat{y_n} = O(s_n)$
- `prediction` $= MLP(\hat{y_n})$
- Loss: $L(\hat{y_n}, y_n)$
- L can take any form: cross entropy, hinge, margin, etc.

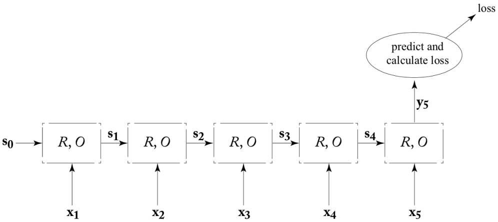


Figure: Goldberg, Yoav. Neural network methods for natural language processing

Sequence labelling

- Output $\hat{t_i}$ for each input $x_{1,i}$
- Local loss: $L_{local}(\hat{t_i}, t_i)$
- Global loss:
  $L(\hat{t_n}, t_n) = \sum_i L_{local}(\hat{t_i}, t_i)$
- L can take any form: cross entropy, hinge, margin, etc.

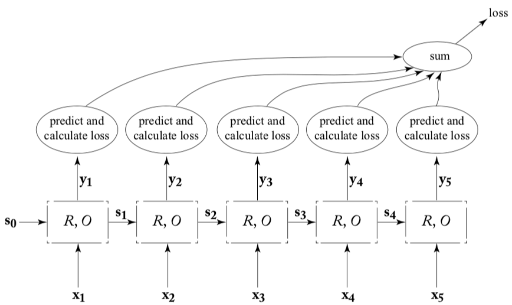


Figure: Goldberg, Yoav. Neural network methods for natural language processing

Backpropogation through time

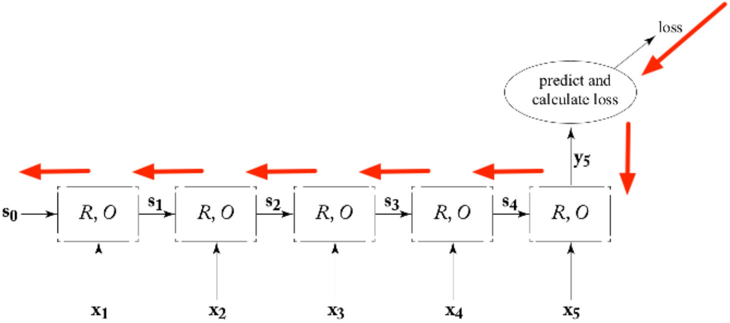


Figure: Goldberg, Yoav. Neural network methods for natural language processing

$s_i = R(x_i, s_{i-1}) = g(s_{i-1}W^s + x_iW^x + b)$

Chain rule: $\frac{\partial L}{\partial w} = \frac{\partial L}{\partial p(\hat{y_5})} \frac{\partial p(\hat{y_5})}{\partial s_4} (\frac{\partial s_4}{\partial w} + \frac{\partial s_4}{\partial s_3} \frac{\partial s_3}{\partial w} + \frac{\partial s_4}{\partial s_3} \frac{\partial s_3}{\partial s_2} \frac{\partial s_2}{\partial s_w} + \ldots)$

Vanishing gradient problem

Chain rule: $\frac{\partial L}{\partial w} = \frac{\partial L}{\partial p(\hat{y_5})} \frac{\partial p(\hat{y_5})}{\partial s_4} (\frac{\partial s_4}{\partial w} + \frac{\partial s_4}{\partial s_3} \frac{\partial s_3}{\partial w} + \frac{\partial s_4}{\partial s_3} \frac{\partial s_3}{\partial s_2} \frac{\partial s_2}{\partial s_w} + \ldots)$
g – sigmoid

1. Many sigmoids near 0 and 1
   - Gradients $\to$ 0
   - Not training for long term dependencies
2. Many sigmoids > 1
   - Gradients $\to + \inf$
   - Not training again

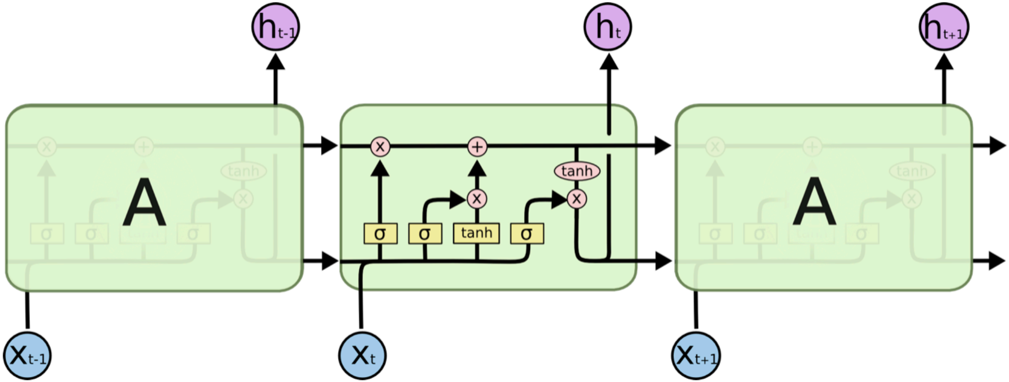
Solution: gated architectures (LSTM and GRU)

Gated architectures

Controlled memory access

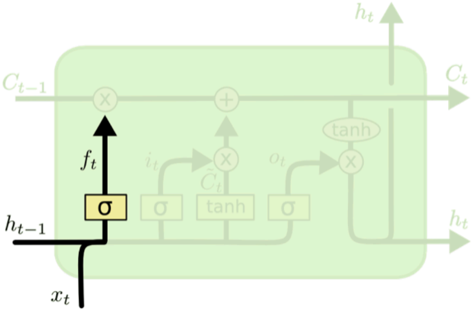
- Entire memory vector is changed: $s_{i+1} = R(x_i, s_i)$
- Controlled memory access: $s_{i+1} = g \odot R(x_i, s_i) + (1 - g)s_i$
  $g \in [0, 1]^d, s, x \in \mathbb{R}^d$
- Differential gates: $\sigma(g), g' \in \mathbb{R}^d$
- This controllable gating mechanism is the basis of the LSTM and the GRU architectures

Long short term memory



http://colah.github.io/posts/2015-08-Understanding-LSTMs/

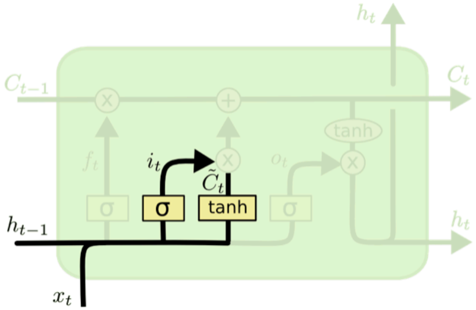
Long short term memory



$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] + b_f\right)$$

http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Long short term memory

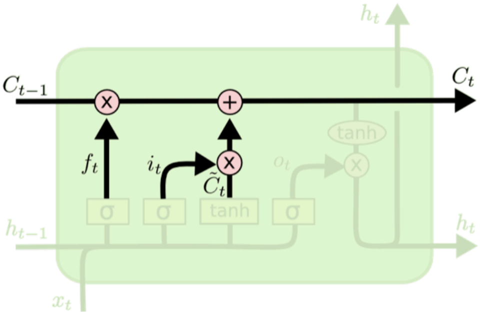


$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] \ + \ b_i\right)$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] \ + \ b_C)$$

`http://colah.github.io/posts/2015-08-Understanding-LSTMs/`

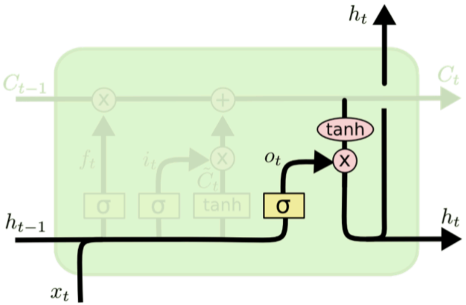
Long short term memory



$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

```
http://colah.github.io/posts/2015-08-Understanding-LSTMs/
```

Long short term memory

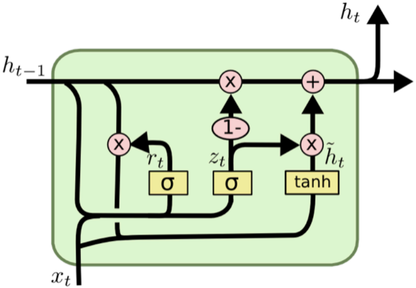


$$o_t = \sigma\left(W_o \left[h_{t-1}, x_t\right] + b_o\right)$$

$$h_t = o_t * \tanh\left(C_t\right)$$

http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Gated recurrent unit



$$z_t = \sigma\left(W_z \cdot [h_{t-1}, x_t]\right)$$

$$r_t = \sigma\left(W_r \cdot [h_{t-1}, x_t]\right)$$

$$\tilde{h}_t = \tanh\left(W \cdot [r_t * h_{t-1}, x_t]\right)$$

$$h_t = (1 - z_t) * h_{t-1} + z_t * \tilde{h}_t$$

`http://colah.github.io/posts/2015-08-Understanding-LSTMs/`

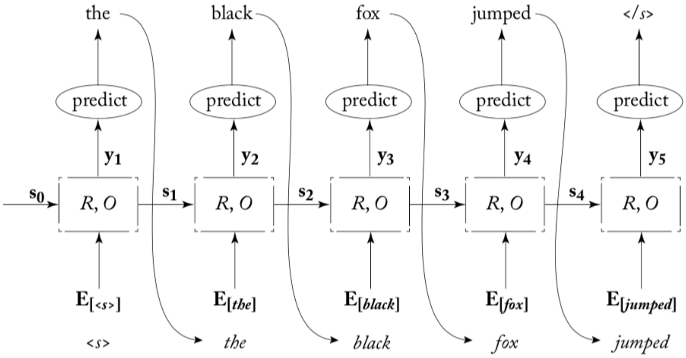
RNN generators

Sequence generation

Teacher forcing: $x :=< s > x, y := x < /s?$

$x :< s > x_1 x_2 \dots x_n$

$y : x_1 x_2 \dots x_n < /s >$



Sequence generation

- Examples of generated texts: `http://karpathy.github.io/2015/05/21/rnn-effectiveness/`
- Examples of generated MIDI music: `https://towardsdatascience.com/how-to-generate-music-using-a-lstm-neural-network-in-keras-6878`

Pros and cons of RNNs

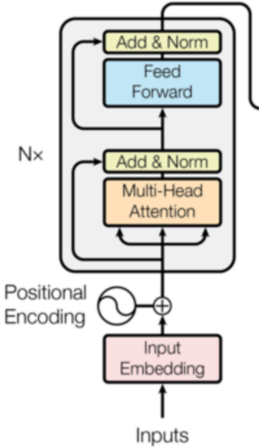
1. Advantages:
   - RNNs are popular and successful for variable-length sequences
   - The gating models such as LSTM are suited for long-range error propagation
2. Problems:
   - The sequentiality prohibits parallelization within instances
   - Long-range dependencies still tricky, despite gating

The Transformer

The Transformer

An alternative architecture to RNN which allows of parallel and faster training

- Several layers of identical modules
- Each module consists of Multi-Head Attention and Feed Forward layers
- Input: embeddings. To get embeddings for numerical input, apply any dense layer
- Positional embeddings to make use of the order of the sequence



Scaled Dot-Product Attention

An attention function can be described as mapping a query and a set of key-value pairs to an output, where the query, keys, values, and output are all vectors:

$$Attention(Q, K, V) = \texttt{softmax}(\frac{QK^T}{\sqrt{d_k}})V,$$

where the input consists of queries Q and keys K of dimension d_k and values V of dimension d_v

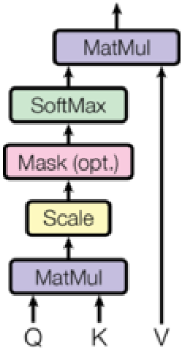
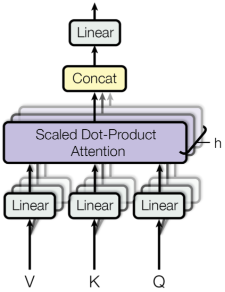


Figure: Vaswani, Ashish, et al. “Attention is all you need.” Advances in neural information processing systems. 2017.

Multi-head Attention

Multi-head attention allows the model to jointly attend to information from different representation subspaces at different positions



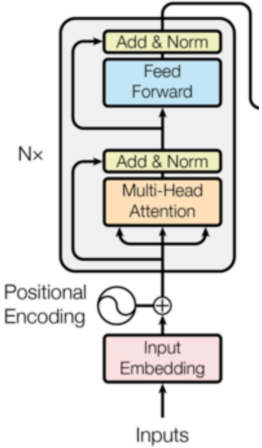
$$MultiHead(Q, K, V) = \texttt{concat}(head_1, ..., head_h)W^O,$$

where $head_i = Attention(QW_i^Q, KW_i^K, VW_i^V)$
and W are projection matrices.

Figure: Vaswani, Ashish, et al. "Attention is all you need." Advances in neural information processing systems. 2017.

The Transformer

Bringing it all together:



- LayerNorm: $\frac{x-\mu}{\sigma}$
- Residual connection: LayerNorm(x+Sublayer(x))
- Position-wise Feed-Forward Networks: $FFN(x) = \max(0, xW_1 + b_1)W_2 + b_2$

Positional Encoding

We need to inject some information about the relative or absolute position of x_{pos} in the sequence:

$$PE_{(pos,2i)} = \sin(pos/10000^{2i/d_{model}})$$

$$PE_{(pos,2i+1)} = \cos(pos/10000^{2i/d_{model}})$$

Positional encoding: $x = x + PE(x)$

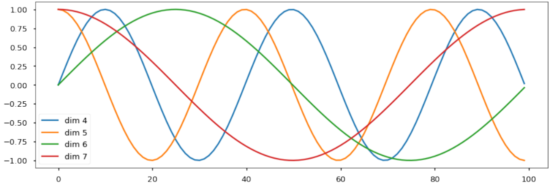


Figure: Vaswani, Ashish, et al. “Attention is all you need.” Advances in neural information processing systems. 2017.

Implementation in PyTorch

Recurrent neural networks

```
torch.nn.RNN(input_size, hidden_size,
    num_layers, nonlinearity, bias,
    batch_first, dropout, bidirectional)

torch.nn.LSTM(input_size, hidden_size,
    num_layers, bias,
    batch_first, dropout, bidirectional)
```

Transformers

```
from fairseq.models import transformer
```

Take-home message

Take-home message

- There is a lot of sequential data around us
- Before DL: HMM, MEMM
- Mid 2010 DL: RNN, LSTM, etc
- Late 2010 DL: the Transformer
- 2020: stack more transformer blocks (Trasformer XL)

Bonus: Recursive NN

Modeling trees with Recursive NN

- Input: $x_1, x_2, \dots, x_n$
- A binary tree T can be represented as a unique set of triplets (i, k, j), s.t. $i < k < j$, $x_{i:j}$ is parent of $x_{i:k}, i_{k+1,j}$
- RecNN takes as an input a binary tree and returns as output a corresponding set of inside state vectors $\boldsymbol{s}^{\boldsymbol{A}}_{\boldsymbol{i:j}} \in \mathbb{R}^d$
- Each state vector $\boldsymbol{s}^{\boldsymbol{A}}_{\boldsymbol{i:j}}$ represents the corresponding tree node $q^A_{i:j}$ and encodes the entire structure rooted at that node

RecNN

- Input: $x_1, x_2, \ldots, x_n$ and a binary tree T
- $RecNN(x_1, x_2, \ldots, x_n, T) = \{\boldsymbol{s^A_{i:j}} \in \mathbb{R}^d | q^A_{i:j} \in T\}$
- $\boldsymbol{s^A_{i:i}} = v(x_i)$
- $\boldsymbol{s^A_{i:j}} = R(A, B, C, \boldsymbol{s^B_{i:k}}, \boldsymbol{s^C_{k+1:j}})\boldsymbol{,}\ q^B_{i:k} \in T, q^C_{k+1:j} \in T$
- $R(A, B, C, \boldsymbol{s^B_{i:k}}, \boldsymbol{s^C_{k+1:j}}) = g([\boldsymbol{s^B_{i:k}}, \boldsymbol{s^C_{k+1:j}}]W)$

RecNN

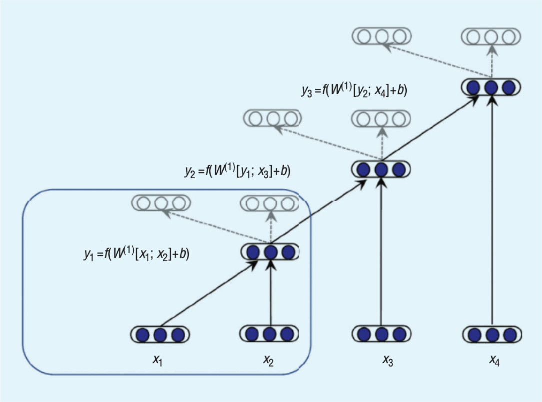


Figure: Zhang, Jiajun & Zong, Chengqing. (2015). Deep Neural Networks in Machine Translation: An Overview