Neural Sequence Modeling

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Logistics

- HW1 due this Friday.
- Lecture (65 min)
- Section on Pytorch and HPC (50 min)

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Feature learning

Linear predictor with handcrafted features: $f(x) = w \cdot \phi(x)$.

Can we learn intermediate features?

Feature learning

Linear predictor with handcrafted features: $f(x) = w \cdot \phi(x)$.

Can we learn intermediate features?

Example:

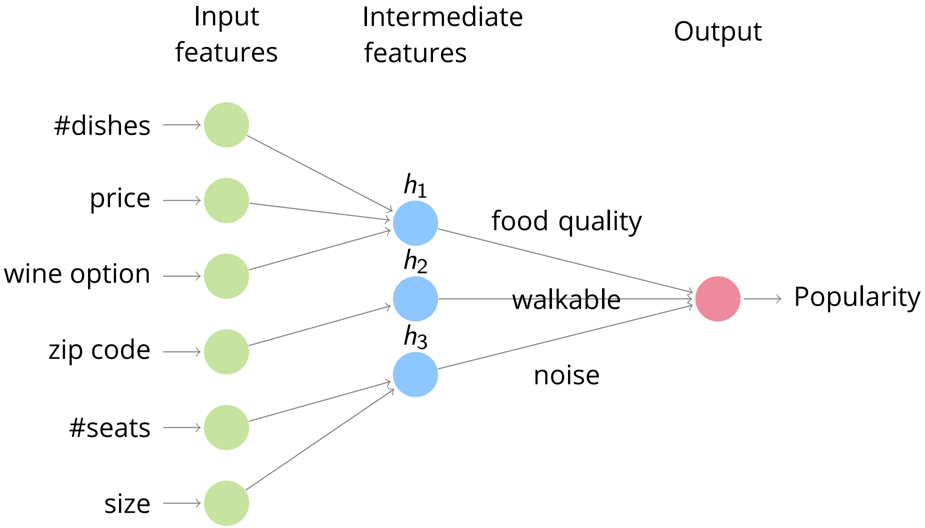
- Predict popularity of restaurants.
- Raw input: #dishes, price, wine option, zip code, #seats, size
- Decompose into subproblems:

$$h_1(\text{[\#dishes, price, wine option]}) = \text{food quality}$$

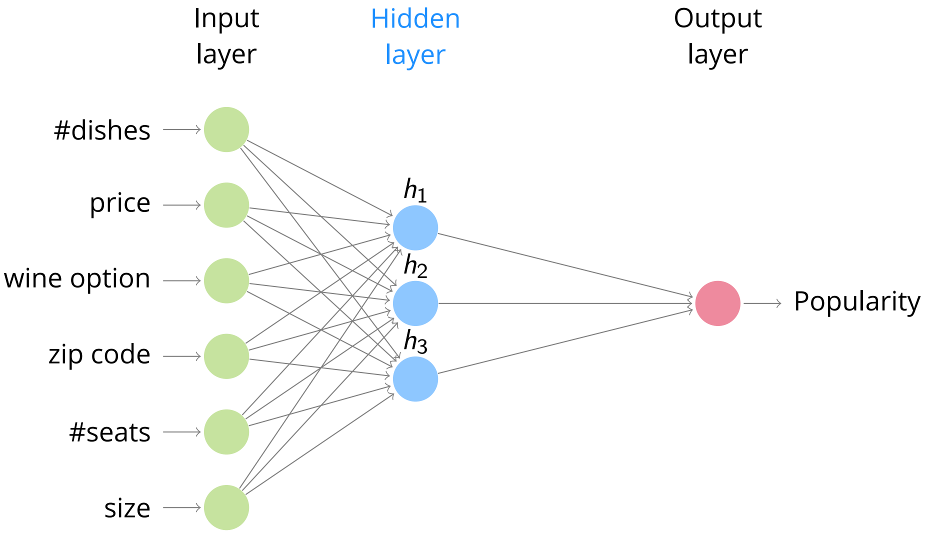
$$h_2(\text{[zip code]}) = \text{walkable}$$

$$h_3(\text{[\#seats, size]}) = \text{nosie}$$

Predefined subproblems



Learning intermediate features



Neural networks

Key idea: automatically learn the intermediate features.

Feature engineering: Manually specify $\phi(x)$ based on domain knowledge and learn the weights:

$$f(x) = w^T \phi(x).$$

Feature learning: Automatically learn both the features (K hidden units) and the weights:

$$h(x) = [h_1(x), \ldots, h_K(x)], \quad f(x) = w^T h(x)$$

Activation function

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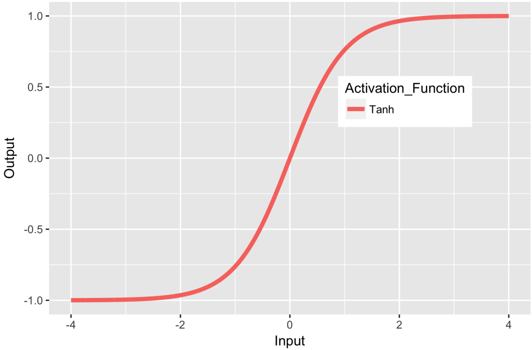
  - *Differentiable* approximations: sigmoid functions.
    - E.g., logistic function, hyperbolic tangent function, ReLU
- Two-layer neural network (one hidden layer and one output layer) with K hidden units:

$$f(x) = \sum_{k=1}^{K} w_k h_k(x) = \sum_{k=1}^{K} w_k \sigma({v_k}^T x) \tag{2}$$

Activation Functions

- The **hyperbolic tangent** is a common activation function:

$$\sigma(x) = \tanh(x) \,.$$

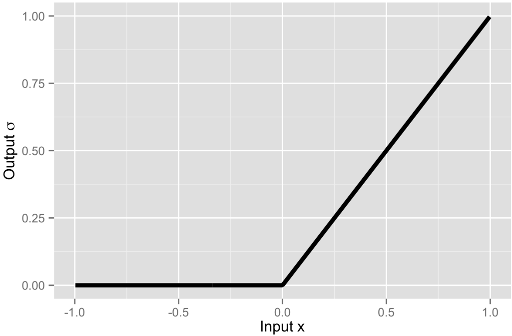


Activation Functions

- More recently, the **rectified linear** (**ReLU**) function has been very popular:

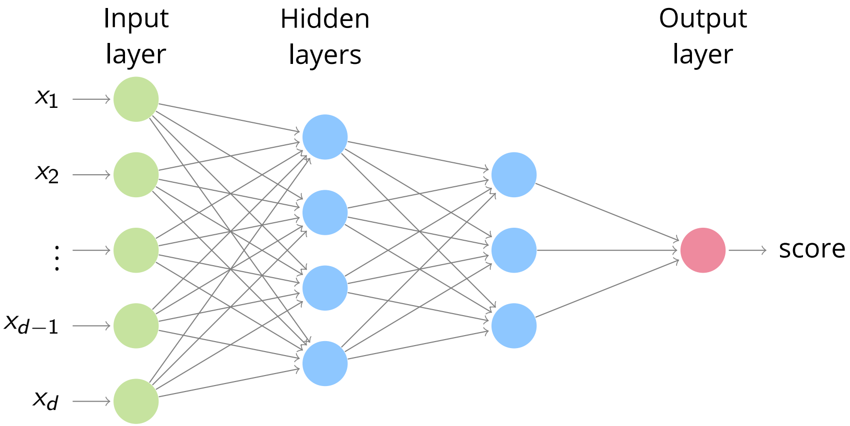
$$\sigma(x) = \max(0, x).$$

- Much faster to calculate, and to calculate its derivatives.
- Work well empirically.



Multilayer perceptron / Feed-forward neural networks

- Wider: more hidden units.
- Deeper: more hidden layers.



Multilayer Perceptron: Standard Recipe

- Each hidden layer takes the output $o \in \mathbb{R}^m$ of previous layer and produces

$$h^{(j)}(o^{(j-1)}) = \sigma\left(W^{(j)} o^{(j-1)} + b^{(j)}\right), \text{ for } j = 2, \ldots, L$$

where $W^{(j)} \in \mathbb{R}^{m \times m}$, $b^{(j)} \in \mathbb{R}^m$.

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- The output layer is an *affine* mapping (no activation function):

$$a(o^{(L)}) = W^{(L+1)}o^{(L)} + b^{(L+1)},$$

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  where $W^{(L+1)} \in \mathbb{R}^{k \times m}$ and $b^{(L+1)} \in \mathbb{R}^k$.
- The full neural network function is given by the *composition* of layers:

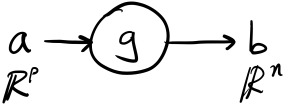
$$f(x) = \left(a \circ h^{(L)} \circ \cdots \circ h^{(1)}\right)(x) \tag{3}$$

Computation graphs

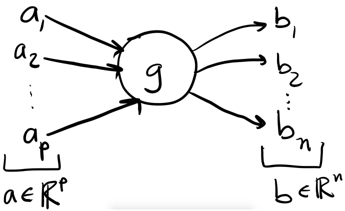
(adpated from David Rosenberg's slides)

Function as a *node* that takes in *inputs* and produces *outputs*.

- Typical computation graph:



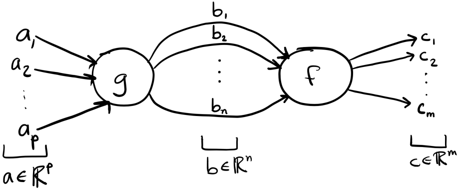
- Broken out into components:



Compose multiple functions

(adpated from David Rosenberg's slides)

Compose two functions $g : \mathbb{R}^p \to \mathbb{R}^n$ and $f : \mathbb{R}^n \to \mathbb{R}^m$: $c = f(g(a))$



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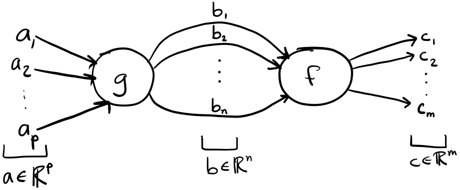

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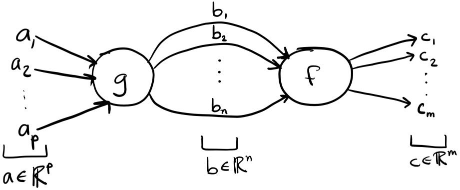

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$$\frac{\partial c_i}{\partial a_j} = \sum_{k=1}^{n} \frac{\partial c_i}{\partial b_k} \frac{\partial b_k}{\partial a_j}.$$

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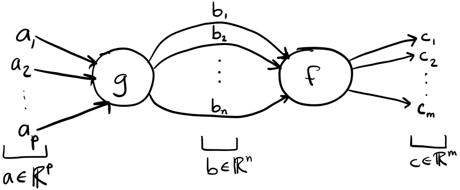

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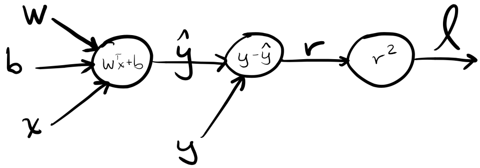
- Visualize the multivariable **chain rule**:
  - Sum changes induced on all paths from a_j to c_i.
  - Changes on one path is the product of changes on each edge.

Computation graph example

(adpated from David Rosenberg's slides)



(What is this graph computing?)

Computation graph example

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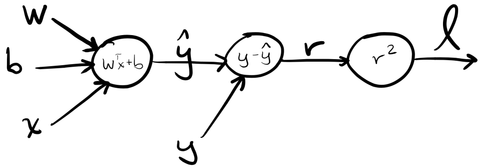

(What is this graph computing?)

$$\frac{\partial \ell}{\partial b} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial b} = (-2r)(1) = -2r$$

$$\frac{\partial \ell}{\partial w_j} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial w_j} = (-2r)\, x_j = -2r x_j$$

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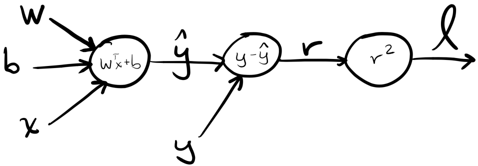

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Computing the derivatives in certain order allows us to save compute!

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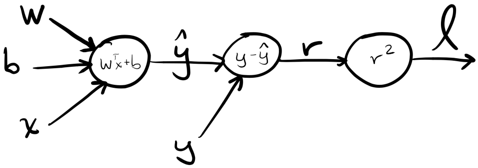

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$$
\begin{aligned}
\frac{\partial \ell}{\partial r} &= 2r \\
\frac{\partial \ell}{\partial \hat{y}} &= \frac{\partial \ell}{\partial r}\frac{\partial r}{\partial \hat{y}} = (2r)(-1) = -2r \\
\frac{\partial \ell}{\partial b} &= \frac{\partial \ell}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial b} = (-2r)(1) = -2r \\
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\end{aligned}
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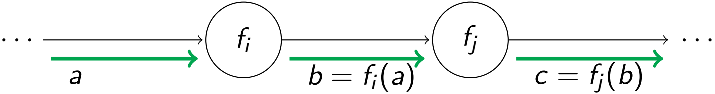
Computing the derivatives in certain order allows us to save compute!

Backpropogation

Backpropogation = chain rule + dynamic programming on a computation graph

Forward pass

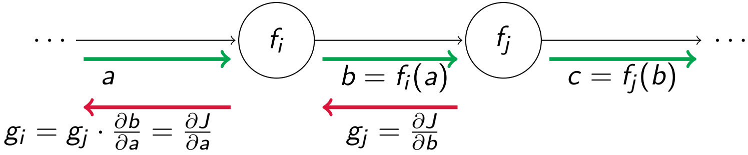
- **Topological order**: every node appears before its children
- For each node, compute the output given the input (from its parents).



Backpropogation

Backward pass

- **Reverse topological order**: every node appear after its children
- For each node, compute the partial derivative of its output w.r.t. its input, multiplied by the partial derivative from its children (chain rule).



Summary

Key idea in neural nets: feature/representation learning

Building blocks:

- Input layer: raw features (no learnable parameters)
- Hidden layer: perceptron + nonlinear activation function
- Output layer: linear (+ transformation, e.g. softmax)

Optimization:

- Optimize by SGD (implemented by back-propogation)
- Objective is non-convex, may not reach a global minimum

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Overview

Problem setup: given an input sequence, come up with a (neural network) model that outputs a representation of the sequence for downstream tasks (e.g., classification)

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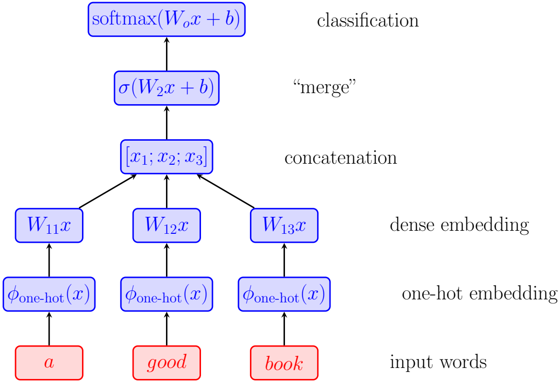
Key challenge: how to model interaction among words?

Approach:

- Aggregation / pooling word embeddings
- Recurrence
- Self-attention

Feed-forward neural network for text classification



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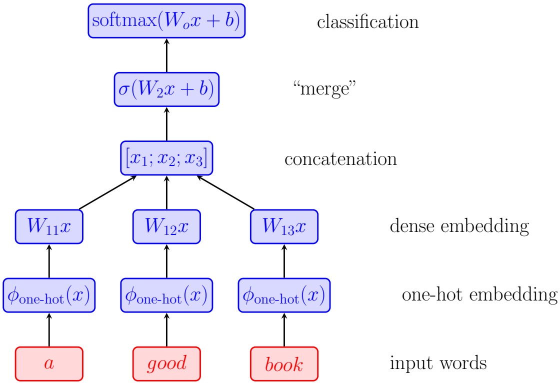

🤔 What kind of features can be learned?
How to adapt the network to handle sequences with arbitrary length?

Recurrent neural networks

- **Goal**: represent a sequence of symbols of varying lengths
- **Idea**: combine new symbols with previous symbols recurrently by modeling the temporal dynamics

$$h_t = f(h_{t-1}, x_t)$$

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  - Compute the **hidden states** h_t recurrently
    - Output from previous time step is the input to the current time step
    - Apply the same transformation f at each time step

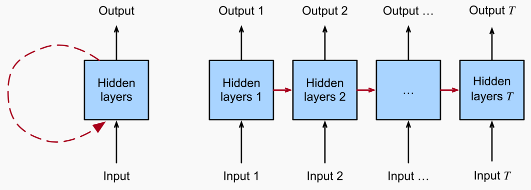
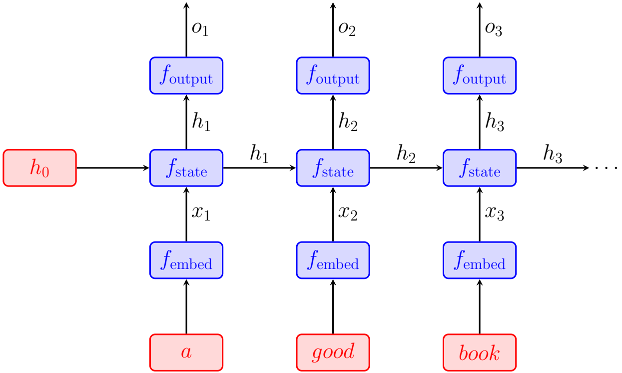


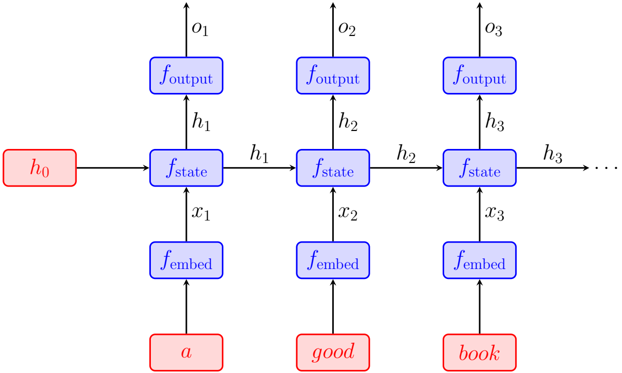
Figure: 9.1 from d2l.ai

Forward pass



A deep neural network with shared weights in each layer

Forward pass



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x_t &= f_{\text{embed}}(s_t) \\
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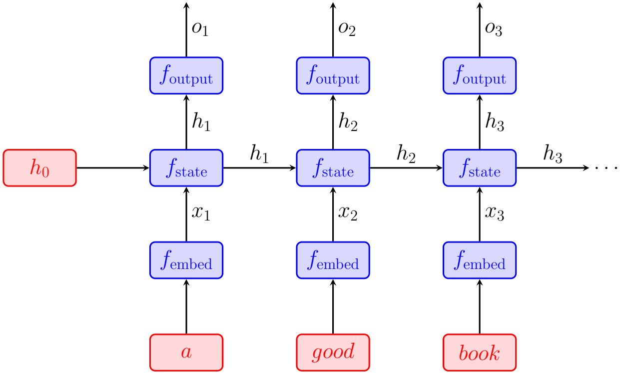

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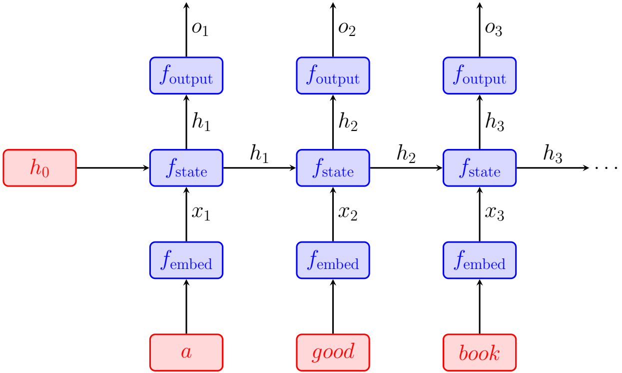

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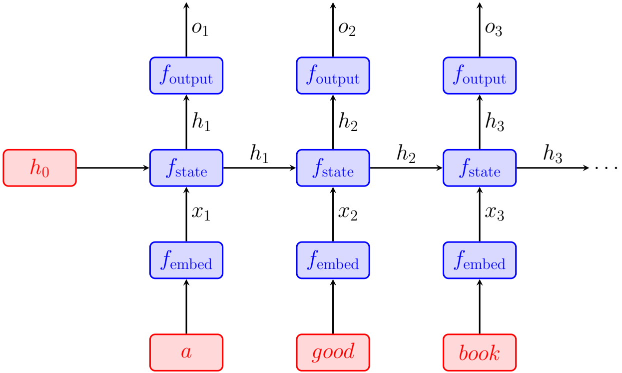
Forward pass

Use o_t's as features



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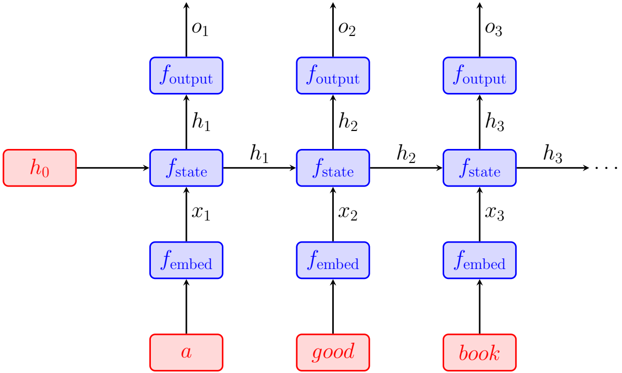

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A deep neural network with shared weights in each layer

Which computation can be parallelized?

Backward pass

Given the loss ℓ, compute the gradient with respect to W_{hh}.

$$\frac{\partial \ell}{\partial W_{hh}} =$$

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Computation graph of h_t:

Backpropagation through time

Problem with standard backpropagation:

- Gradient involves repeated multiplication of W_{hh}
- Gradient will vanish / explode (depending on the eigenvalues of W_{hh})

Quick fixes:

- Reduce the number of repeated multiplication: truncate after k steps (h_{t-k} has no influence on h_t)
- Limit the norm of the gradient in each step: gradient clipping (can only mitigate explosion)

Long-short term memory (LSTM)

Vanilla RNN: always update the hidden state

- Cannot handle long range dependency due to gradient vanishing

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Key idea is to use a **gating mechanism**: multiplicative weights that modulate another variable

- How much should the new input affect the state?
- When to ignore new inputs?
- How much should the state affect the output?

Long-short term memory (LSTM) parametrization

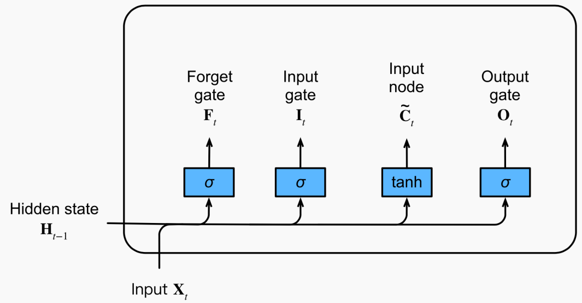

Figure: 10.1.2 from d2l.ai

Update with the new input x_t (same as in vanilla RNN)

$$\tilde{c}_t = \tanh(W_{xc}x_t + W_{hc}h_{t-1} + b_c) \quad \text{new cell content}$$

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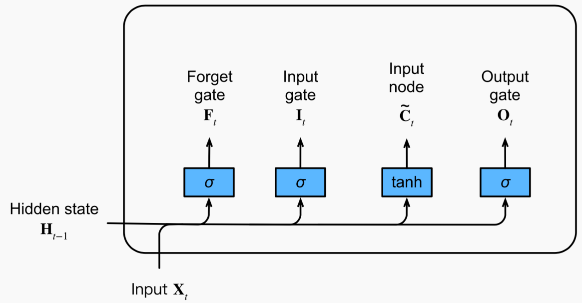

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Can we choose between $\tilde{c}_t$ and another state that doesn't update with x_t?

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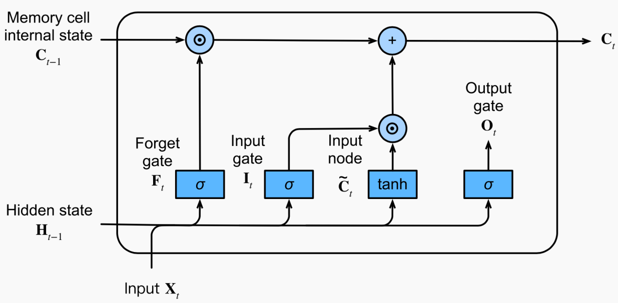


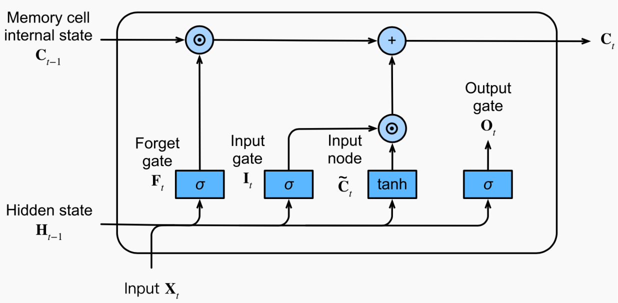
Figure: 10.1.3 from d2l.ai

Choose between $\tilde{c}_t$ (update) and c_{t-1} (no update):

$$\textbf{memory cell} \quad c_t = i_t \odot \tilde{c}_t + f_t \odot c_{t-1}$$

- f_t: proportion of the old state (preserve or erase the old memory)
- i_t: proportion of the new state (write or ignore the new input)
- What is c_t if $f_t = 1$ and $i_t = 0$?

Long-short term memory (LSTM) parametrization



Input gate and forget gate:

$$i_t = \text{sigmoid}(W_{xi}x_t + W_{hi}h_{t-1} + b_i) ,$$
$$f_t = \text{sigmoid}(W_{xf}x_t + W_{hf}h_{t-1} + b_f) .$$

Each coordinate is between 0 and 1.

Long-short term memory (LSTM) parametrization

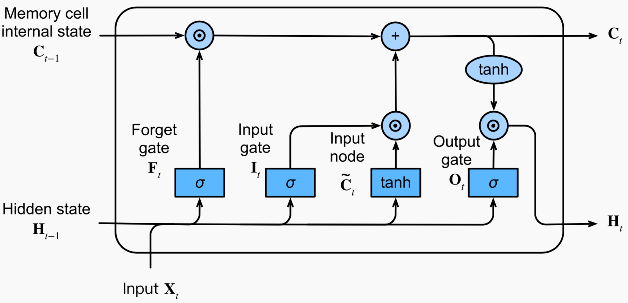


Figure: 10.1.4 from d2l.ai

How much should the memory cell state influence the rest of the network:

$$o_t = \text{sigmoid}(W_{xo}x_t + W_{ho}h_{t-1} + b_o)$$
$$h_t = o_t \odot c_t$$

c_t may accumulate information without impact the network if o_t is close to 0

How does LSTM solve gradient vanishing / explosion?

Intuition: gating allows the network to learn to control how much gradient should vanish.

- Vanilla RNN: gradient depends on repeated multiplication of the same weight matrix
- LSTM: gradient depends on repeated multiplication of some quantity that depends on the data (values of input and forget gates)
- So the network can learn to reset or update the gradient depending on whether there is long-range dependencies in the data.

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Improve the efficiency of RNN

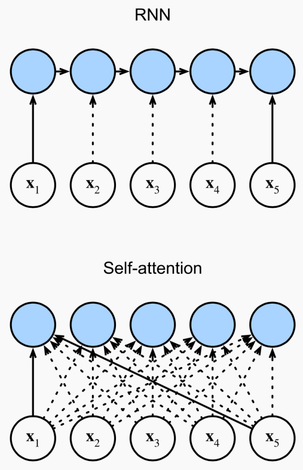

Figure: 11.6.1 from d2l.ai

Recall that our goal is to come up with a good respresentation of a sequence of words.

RNN:

- Past words influence the sentence representation through recurrent update
- Sequential computation O(sequence length), hard to scale

Improve the efficiency of RNN

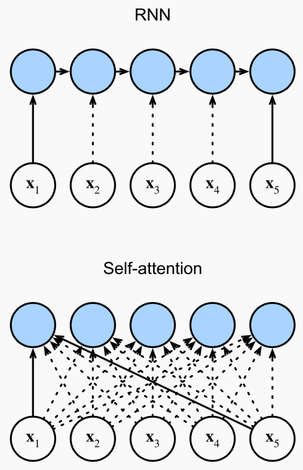

Figure: 11.6.1 from d2l.ai

Recall that our goal is to come up with a good respresentation of a sequence of words.

RNN:

- Past words influence the sentence representation through recurrent update
- Sequential computation O(sequence length), hard to scale

Can we handle dependency more efficiently?

- Direct interaction between any pair of words in the sequence
- Parallelizable computation

Model interaction between words

Which word(s) is most related to “time”?

Model interaction between words

Which word(s) is most related to “time”?

A database approach:

query	**keys**	**values**
	`arrow`	time
	`flies`	flies
	`like`	like
	`an`	an
time	`time`	arrow

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- Relatedness should not be hard-coded

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  Need a function to measure relatedness between keys and values
- A word is related to multiple words in a sentence

  Output should be an aggregation of the values

Model interaction between words using a "soft" database

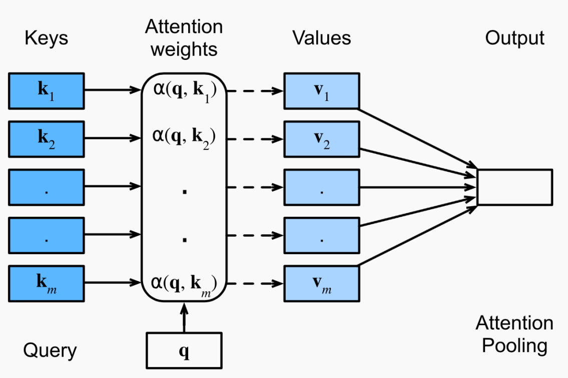

Figure: 11.1.1 from d2l.ai

- **Attention weights** $\alpha(q, k_i)$: how likely is q matched to k_i
- **Attention pooling**: combine v_i's according to their "relatedness" to the query

Model interaction between words using a "soft" database

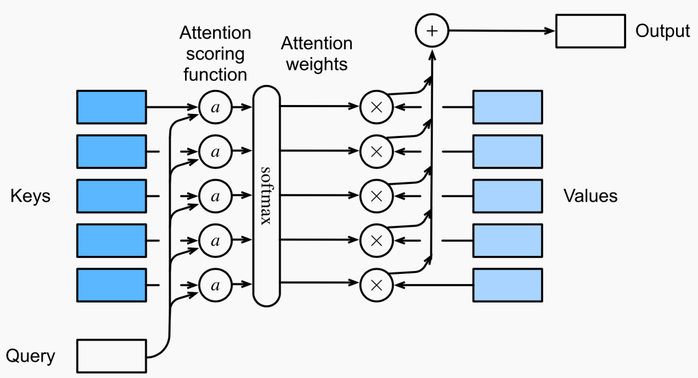

Figure: 11.3.1 from d2l.ai

- Model attention weights as a distribution: $\alpha = \mathrm{softmax}(a(q, k_1), \ldots, a(q, k_m))$
- Output a weighted combination of values: $o_i = \sum_{i=1}^{m} \alpha(q, k_i) v_i$

Self-attention

Goal: an efficient model of the interaction among symbols in a sequence

Idea: model the interaction between each pair of words (in parallel)

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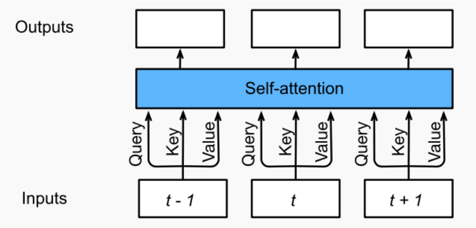

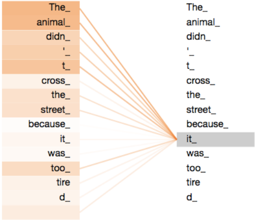

- Input: map each symbol to a query, a key, and a value (embeddings)

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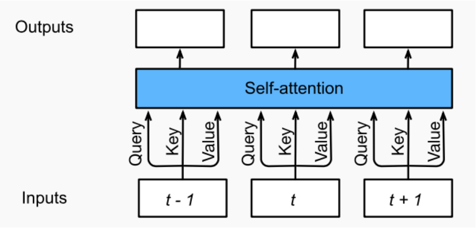

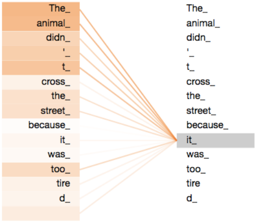

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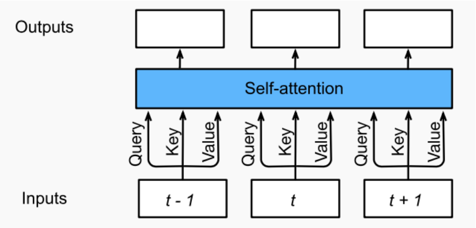

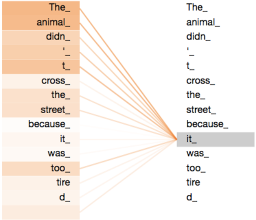

- Input: map each symbol to a query, a key, and a value (embeddings)
- Attend: each word (as a query) interacts with all words (keys)
- Output: *contextualized* representation of each word (weighted sum of values)

Attention scoring functions

Design the function that measures relatedness between queries and keys:

$\alpha = \mathrm{softmax}(a(q, k))$

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Scaled dot-product attention

$$a(q, k) = q \cdot k / \sqrt{d}$$

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- Avoids large attention weights that push the softmax function into regions of small gradients

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MLP attention

$$a(q, k) = u^T \tanh(W[q; k])$$

Multi-head attention: motivation

Time flies like an arrow

- Each word attends to all other words in the sentence
- Which words should “like” attend to?

Multi-head attention: motivation

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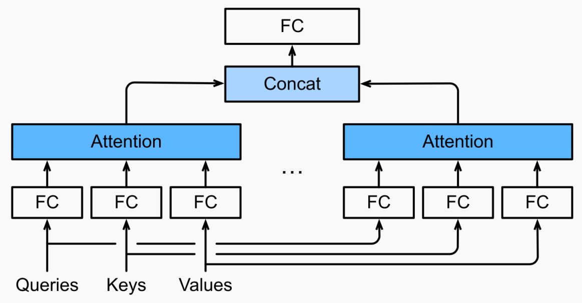
  - Syntax: “flies”, “arrow” (a preposition)
  - Semantics: “time”, “arrow” (a metaphor)

Multi-head attention: motivation

Time flies like an arrow

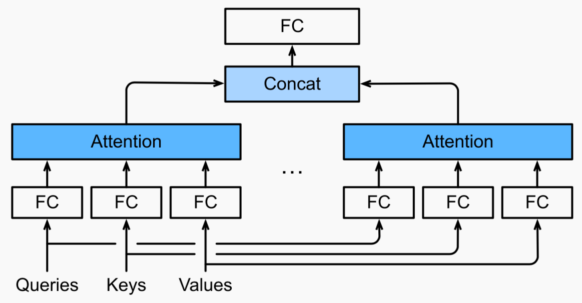
- Each word attends to all other words in the sentence
- Which words should “like” attend to?
  - Syntax: “flies”, “arrow” (a preposition)
  - Semantics: “time”, “arrow” (a metaphor)
- We want to represent different roles of a word in the sentence: need more than a single embedding
- Instantiation: multiple self-attention modules

Multi-head attention



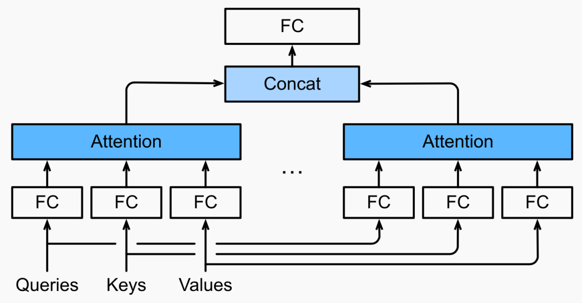
- Multiple attention modules: same architecture, different parameters

Multi-head attention



- Multiple attention modules: same architecture, different parameters
- A **head**: one set of attention outputs

Multi-head attention



- Multiple attention modules: same architecture, different parameters
- A **head**: one set of attention outputs
- Concatenate all heads (increased output dimension)
- Linear projection to produce the final output

Matrix representation: input mapping

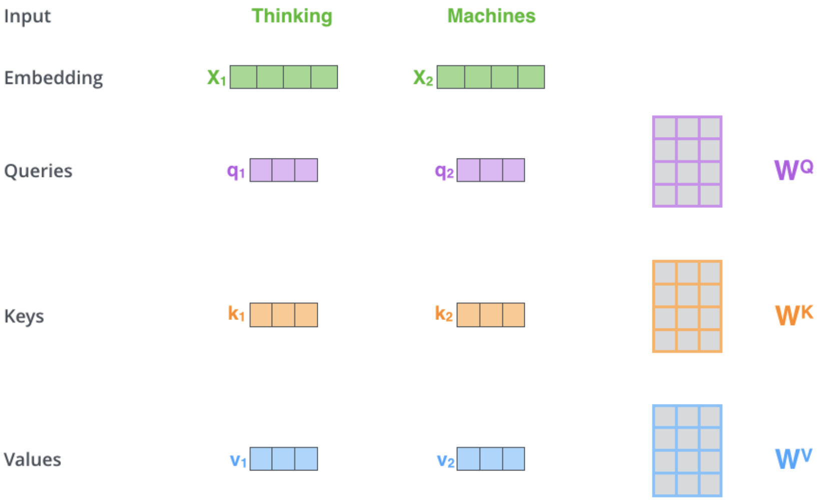


Figure: From The Illustrated Transformer

Matrix representation: attention weights

Scaled dot product attention

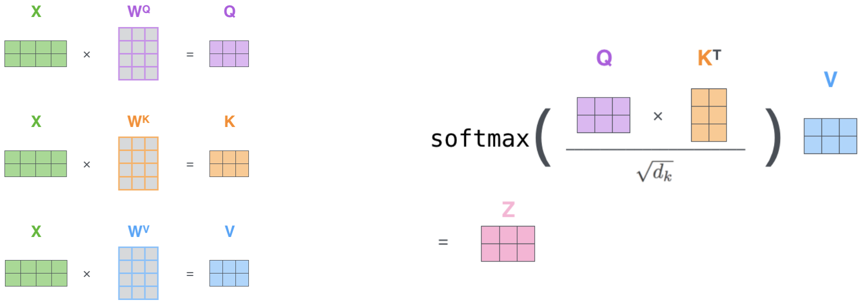
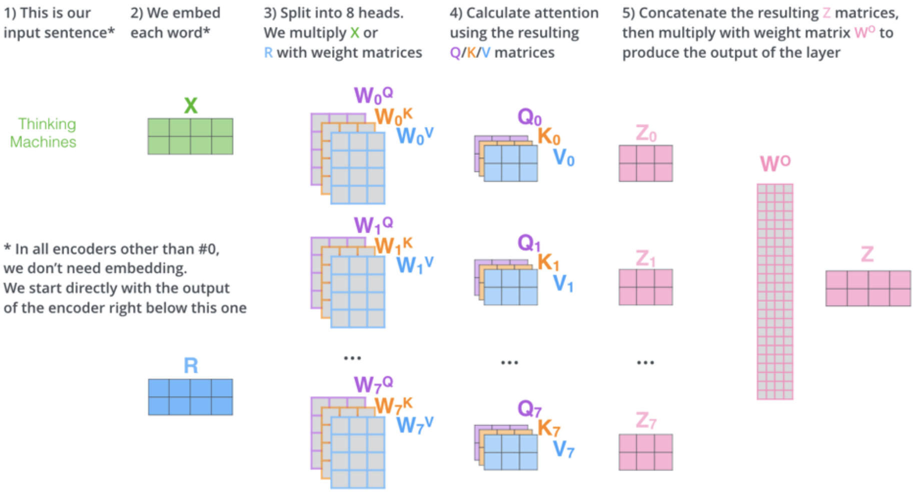


Figure: From The Illustrated Transformer

Multi-head attention



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Summary so far

- Sequence modeling
  - Input: a sequence of words
  - Output: a sequence of contextualized embeddings for each word
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🤔 Which of these can handle sequences of arbitrary length?

Table of Contents

Overview

- Use self-attention as the core building block
- Vastly increased scalability (model and data size) compared to recurrence-based models
- Initially designed for machine translation (next week)
    - *Attention is all you need*. Vaswani et al., 2017.
- The backbone of today's large-scale models
- Extended to non-sequential data (e.g., images and molecules)

Transformer block

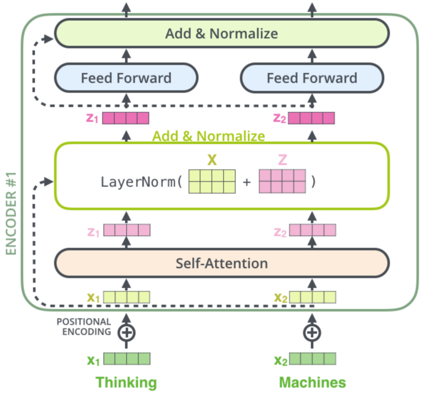

Figure: From The Illustrated Transformer

- Multi-head self-attention

Transformer block

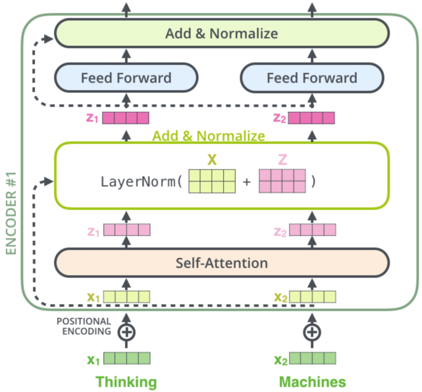

Figure: From The Illustrated Transformer

- Multi-head self-attention
  - Capture dependence among input symbols

Transformer block

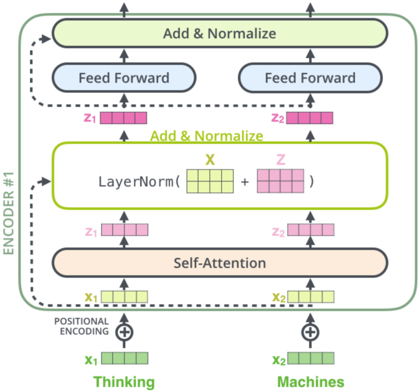

Figure: From The Illustrated Transformer

- Multi-head self-attention
  - Capture dependence among input symbols
- Positional encoding

Transformer block

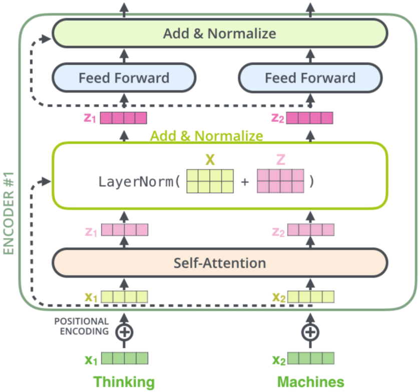

Figure: From The Illustrated Transformer

- Multi-head self-attention
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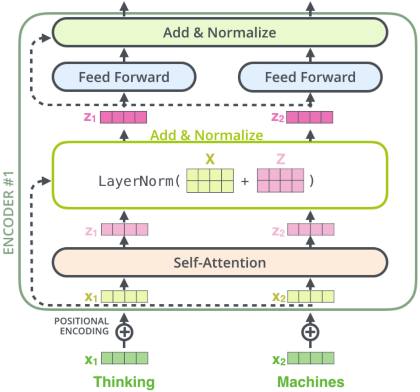

Figure: From The Illustrated Transformer

- Multi-head self-attention
  - Capture dependence among input symbols
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  - Capture the order of symbols
- Residual connection and layer normalization

Transformer block

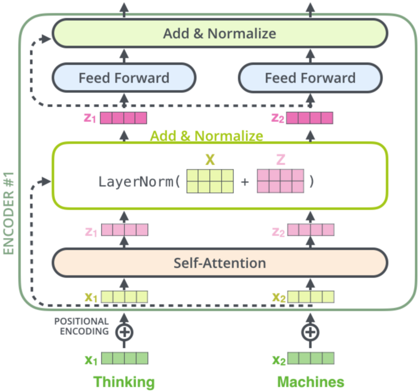


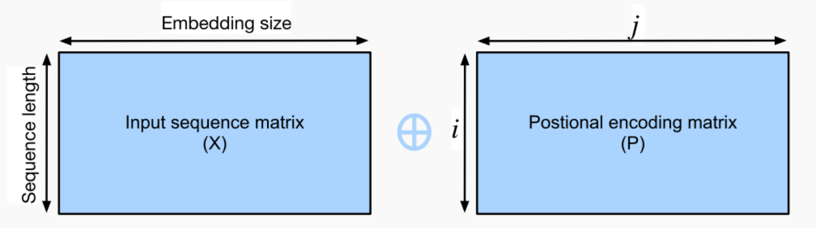
Figure: From The Illustrated Transformer

- Multi-head self-attention
  - Capture dependence among input symbols
- Positional encoding
  - Capture the order of symbols
- Residual connection and layer normalization
  - More efficient and better optimization

Position embedding

Motivation: model word order in the input sequence

Solution: add a position embedding to each word



Position embedding:

- Encode absolute and relative positions of a word
- (Same dimension as word embeddings)
- Learned or deterministic

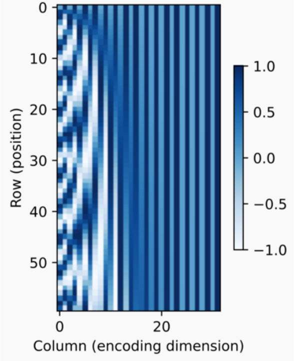
Sinusoidal position embedding

Intuition: binary encoding

- The frequency of bit flips increases from left to right

$0 \rightarrow 000$
$1 \rightarrow 001$
$2 \rightarrow 010$
$3 \rightarrow 011$
$4 \rightarrow 100$
$5 \rightarrow 101$
$6 \rightarrow 110$
$7 \rightarrow 111$

Continuous version $\longrightarrow$

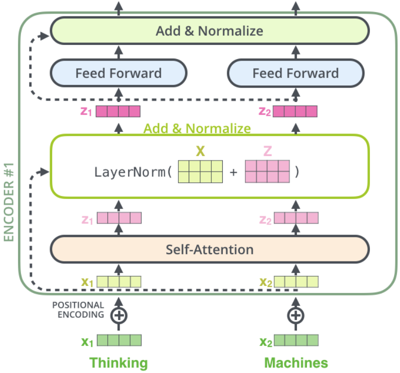


[https://www.d2l.ai]

Col 1: $\sin(w_1 t)$
Col 2: $\cos(w_1 t)$
Col 3: $\sin(w_2 t)$
Col 4: $\cos(w_2 t)$
...

w_i: frequency
t: position

Residual connection and layer normalization



- Residual connection: add input to the output of each layer
- Layer normalization: normalize (zero mean, unit variance) over all features for each sample in the batch
- Position-wise feed-forward networks: same mapping for all positions