Neural Sequence Modeling

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Logistics

- HW1 due this Friday at 12pm.
- HW2 will be released this Friday.
- Textbook and readings

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Feature learning

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

Can we learn features from data?

Feature learning

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

Can we learn features from data?

Example:

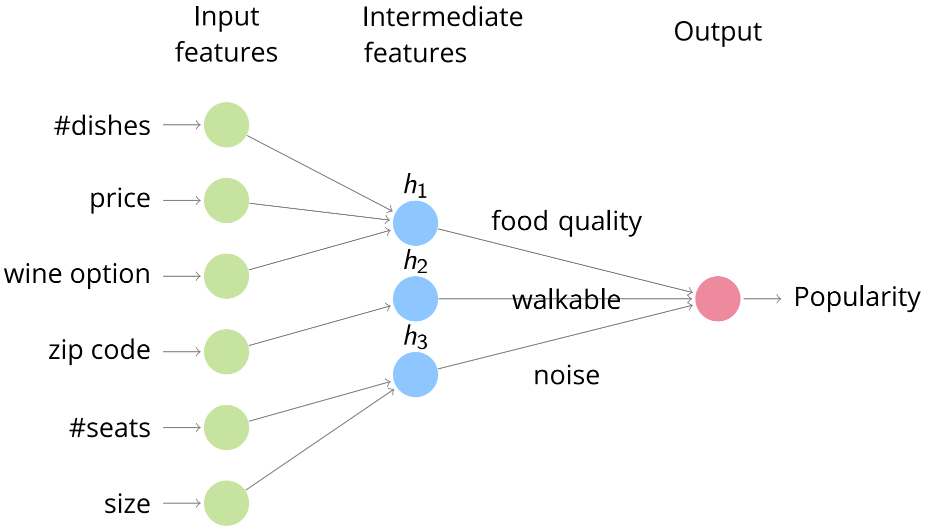
- Predict popularity of restaurants.
- Raw input: #dishes, price, wine option, zip code, #seats, size
- Decompose into subproblems:

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

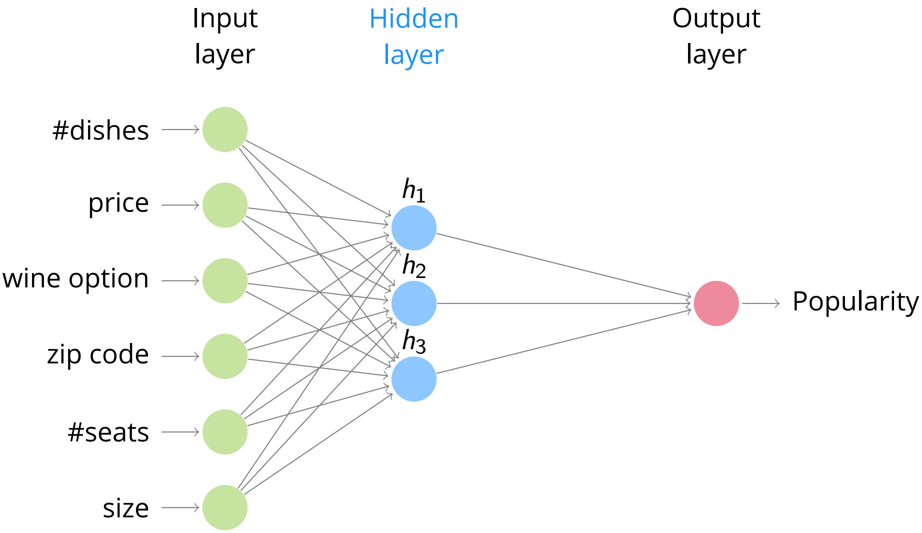
$$h_2([\text{zip code}]) = \text{walkable}$$

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

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

- How should we parametrize h_i's?

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    - E.g., logistic function, hyperbolic tangent function, ReLU

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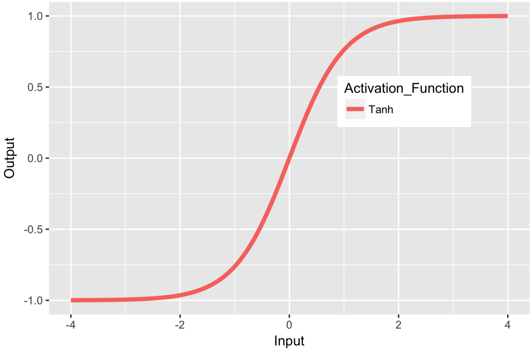
  - *Differentiable* approximations: sigmoid functions.
    - E.g., logistic function, hyperbolic tangent function, ReLU
  - Non-linearity

Activation Functions

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

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

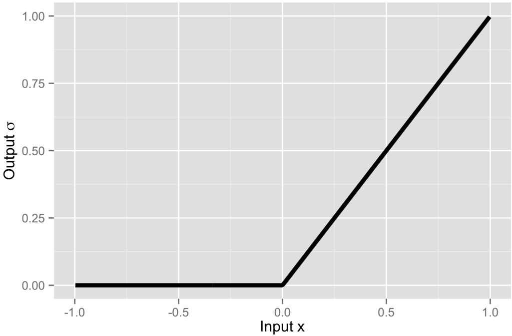


Activation Functions

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

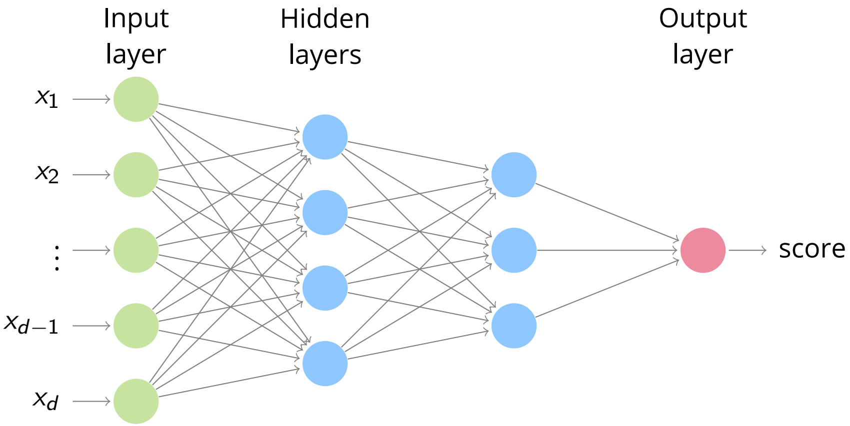
$$\sigma(x) = \max(0, x).$$

- Much faster to calculate the function value and 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

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

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:

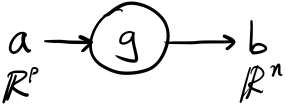
$$f(x) = \left(a \circ h^{(L)} \circ \cdots \circ h^{(1)}\right)(x) \tag{2}$$

Computation graphs

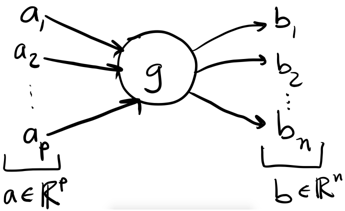
(adpated from David Rosenberg's slides)

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

- Typical computation graph:



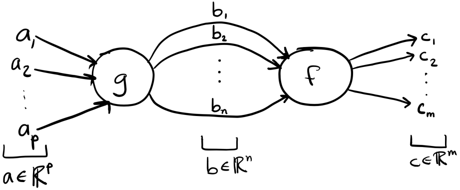
- Broken out into components:



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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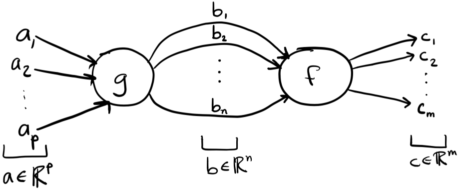

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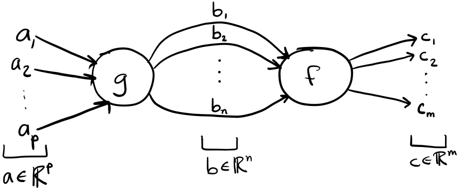

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$$\frac{\partial c_i}{\partial a_j} = \sum_{k=1}^{n} \frac{\partial c_i}{\partial b_k} \frac{\partial b_k}{\partial a_j}.$$

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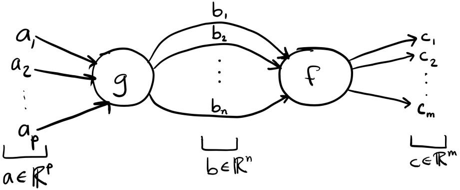

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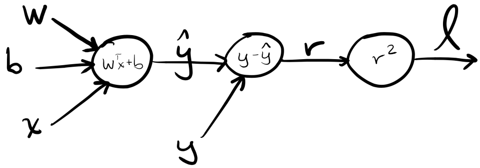
- Visualize the multivariable **chain rule**:
  - Sum changes induced on all paths from a_j to c_i.
  - Changes on one path is the product of changes across each node.

Computation graph example

(adpated from David Rosenberg's slides)



(What is this graph computing?)

Computation graph example

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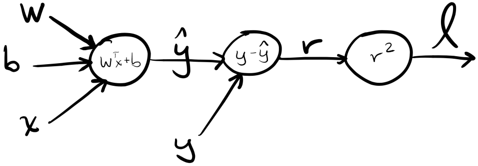

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$$
\begin{aligned}
\frac{\partial \ell}{\partial b} &= \frac{\partial \ell}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial b} = (-2r)\,(1) = -2r \\
\frac{\partial \ell}{\partial w_j} &= \frac{\partial \ell}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial w_j} = (-2r)\,x_j = -2rx_j
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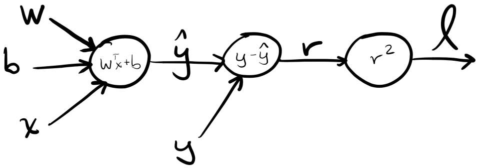

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$$\frac{\partial \ell}{\partial b} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial b} = (-2r)(1) = -2r$$

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

Computation graph example

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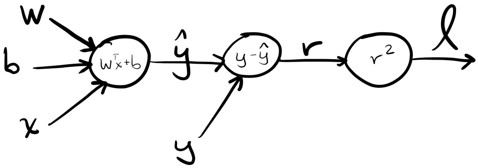

(What is this graph computing?)

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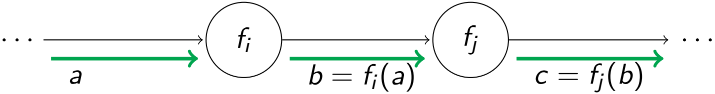
Computing the derivatives in certain order allows us to save compute!

Backpropogation

Backpropogation = chain rule + dynamic programming on a computation graph

Forward pass

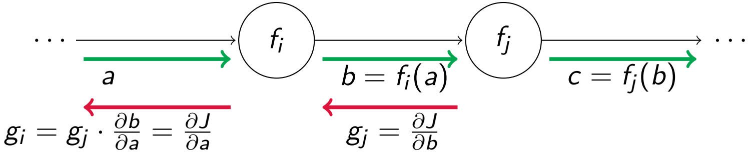
- **Topological order**: every node appears before its children
- For each node, compute the output given the input (from its parents).



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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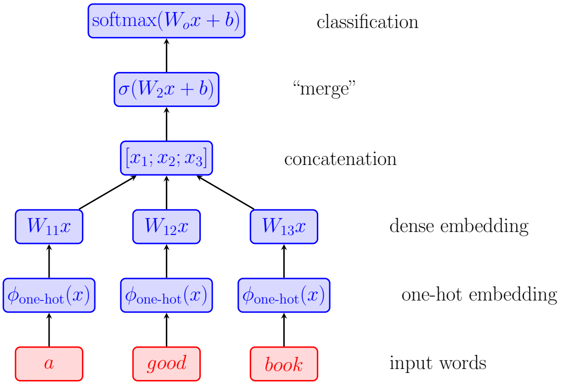
Key challenge: how to model interaction among words?

Approach:

- Aggregation (pooling word embeddings)
- Recurrence
- Self-attention

Feed-forward neural network for text classification



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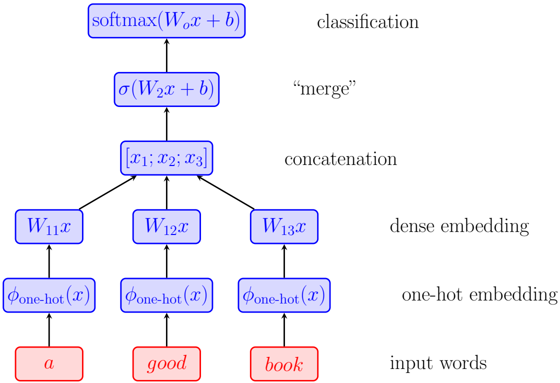


🤔 Where is the interaction between words modeled?
How to adapt the network to handle sequences with arbitrary length?

Recurrent neural networks

- **Goal**: compute representation of sequence $x_{1:T}$ of varying lengths
- **Idea**: combine new symbols with previous symbols recurrently

Recurrent neural networks

- **Goal**: compute representation of sequence $x_{1:T}$ of varying lengths
- **Idea**: combine new symbols with previous symbols recurrently
  - Update the representation, i.e. **hidden states** h_t, recurrently

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

    - Output from previous time step is the input to the current time step
    - Apply the same transformation f at each time step

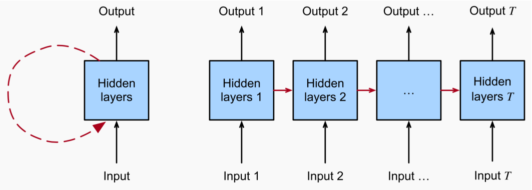
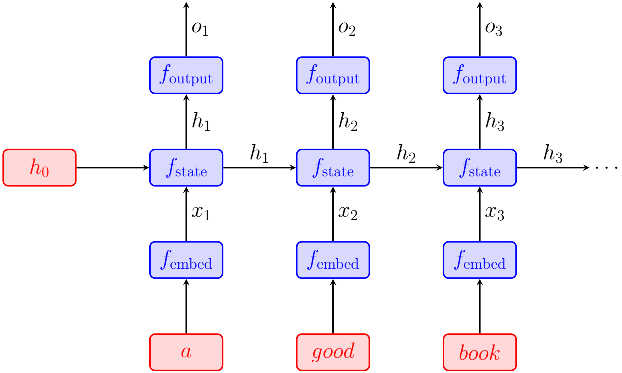


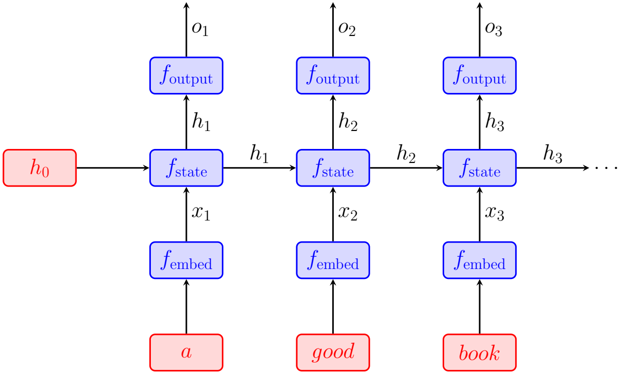
Figure: 9.1 from d2l.ai

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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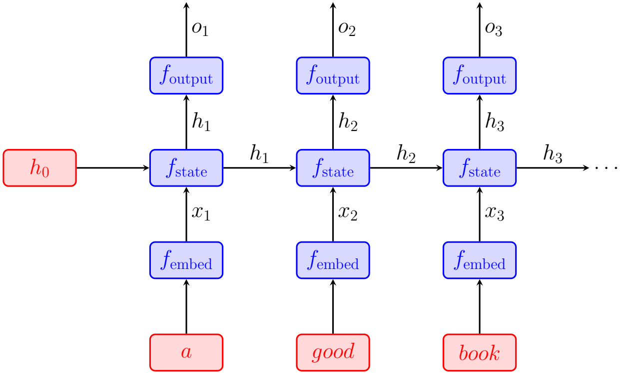

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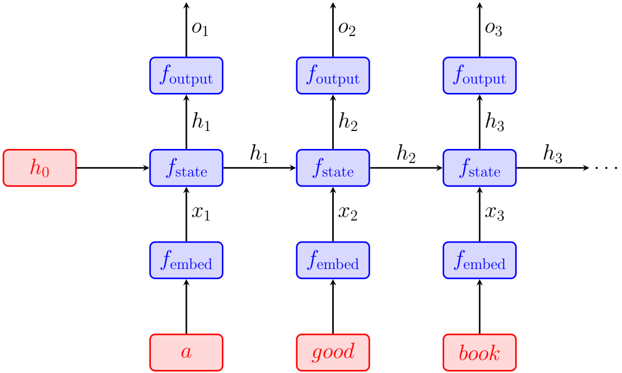

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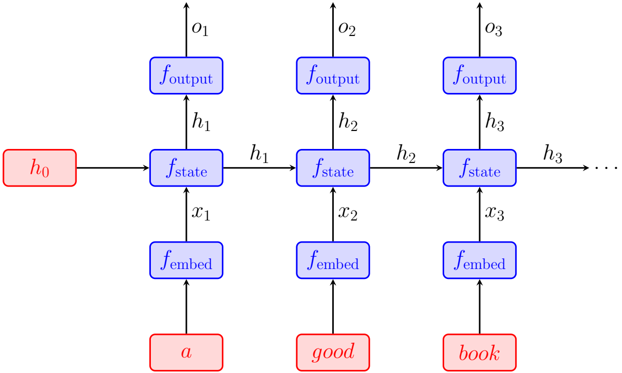
Forward pass

Use o_t's as features



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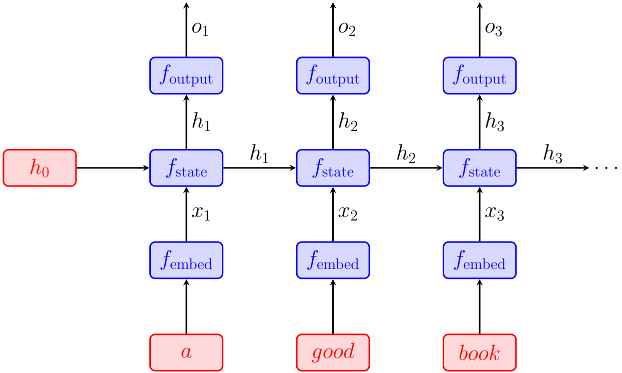

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🤔 Which computation can be parallelized?

A deep neural network with shared weights in each layer

Backward pass

Given the loss $\ell_t(o_t, y_t)$, compute the gradient with respect to W_{hh}.

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Computation graph of h_t: $h_t = \sigma(W_{hh} h_{t-1} + W_{hi} x_t + b)$

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})

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Problem with standard backpropagation:

- Gradient involves repeated multiplication of W_{hh}
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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

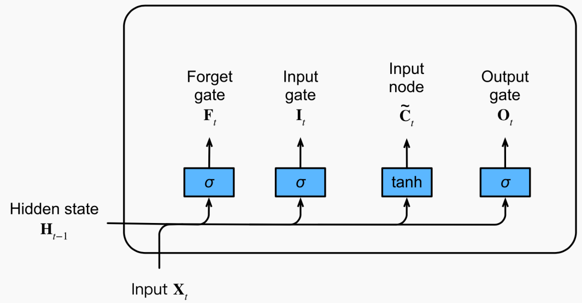

Figure: 10.1.2 from d2l.ai

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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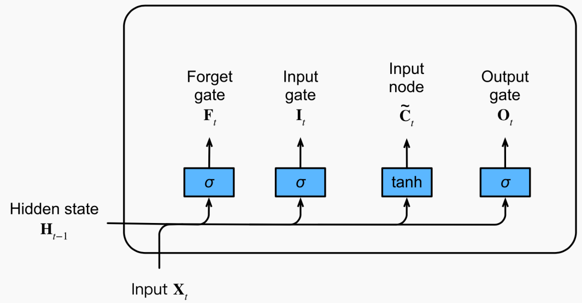

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Should we update with the new input x_t?

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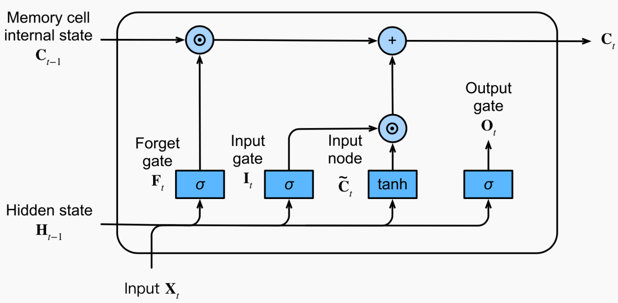


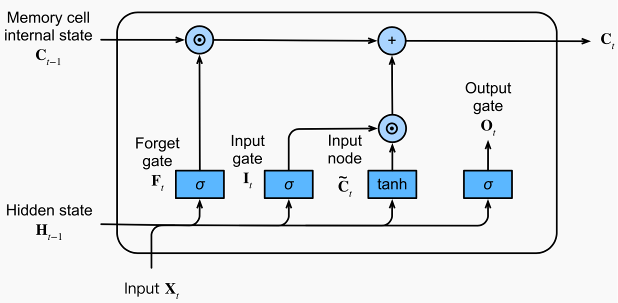
Figure: 10.1.3 from d2l.ai

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

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

- f_t: proportion of the old state (preserve $\uparrow$ or erase $\downarrow$ the old memory)
- i_t: proportion of the new state (write $\uparrow$ or ignore $\downarrow$ 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 depends on data:

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

Each coordinate is between 0 and 1.

Long-short term memory (LSTM) parametrization

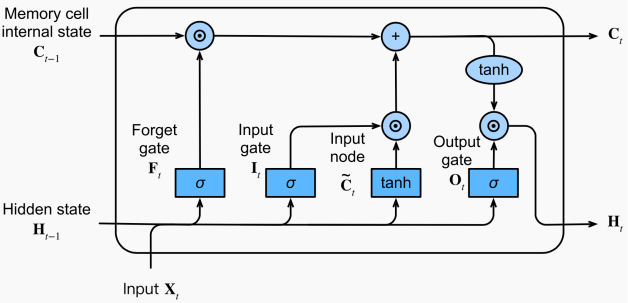


Figure: 10.1.4 from d2l.ai

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

$$h_t = o_t \odot c_t$$

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

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.

Table of Contents

Improve the efficiency of RNN

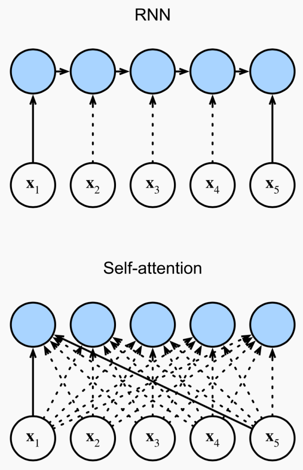


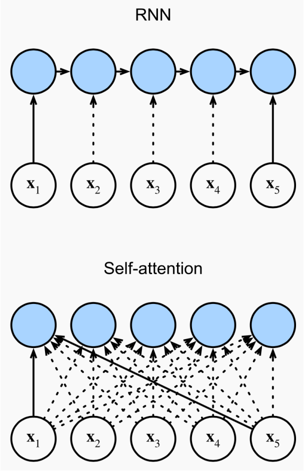
Figure: 11.6.1 from d2l.ai

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 $O(\text{sequence length})$, hard to scale

Improve the efficiency of RNN



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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

Time flies like an arrow: Which word(s) is most related to “time”?

Model interaction between words

Time flies like an arrow: 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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Limitations:

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- A word is related to multiple words in a sentence

  Query should be matched to multiple keys

Model interaction between words using a "soft" database

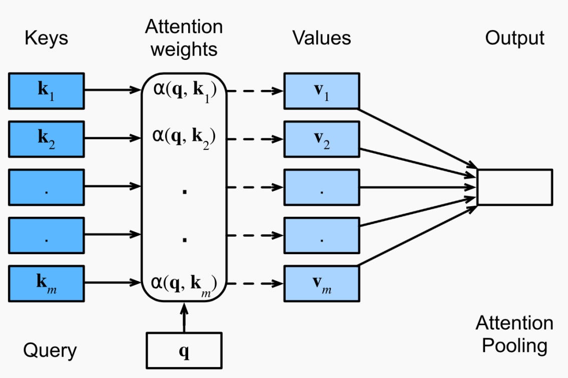

Figure: 11.1.1 from d2l.ai

- **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

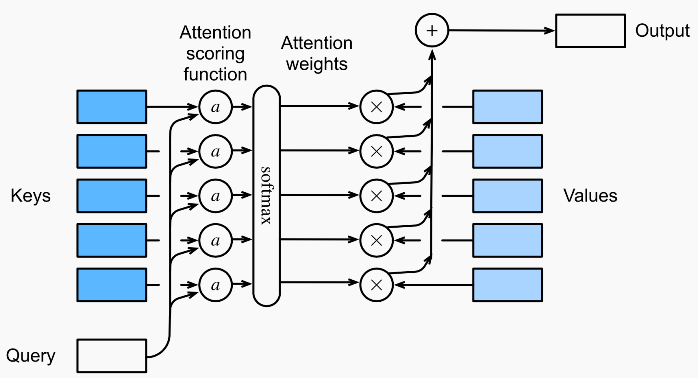

Figure: 11.3.1 from d2l.ai

- 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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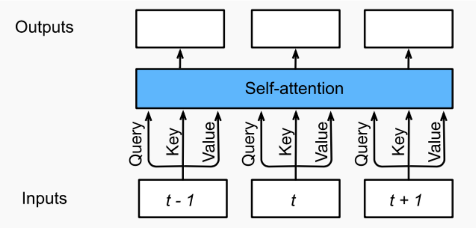

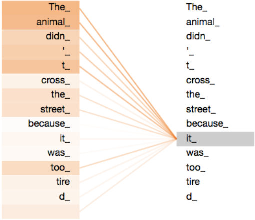

- Input: map each symbol to a query, a key, and a value (embeddings)

Self-attention

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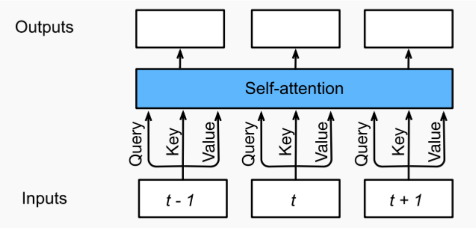

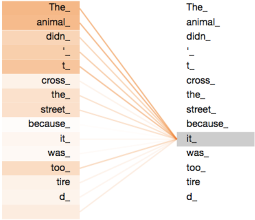

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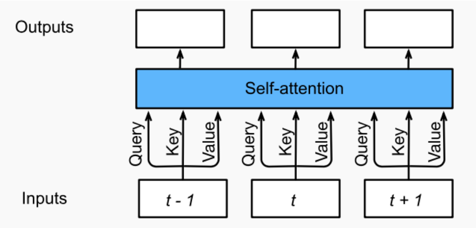

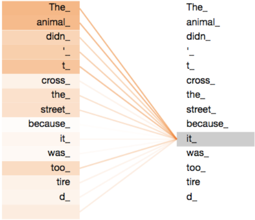

- Input: map each symbol to a query, a key, and a value (embeddings)
- Attend: each word (as a query) interacts with all words (keys)
- Output: *contextualized* representation of each word (weighted sum of values)

Attention scoring functions

Design the function that measures relatedness between queries and keys:

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

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- $\sqrt{d}$: dimension of the key vector
- 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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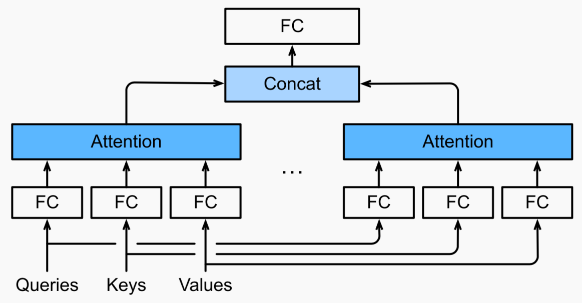
- Which words should “like” attend to?
  - Syntax: “flies”, “arrow” (a preposition)
  - Semantics: “time”, “arrow” (a metaphor)

Multi-head attention: motivation

Time flies like an arrow

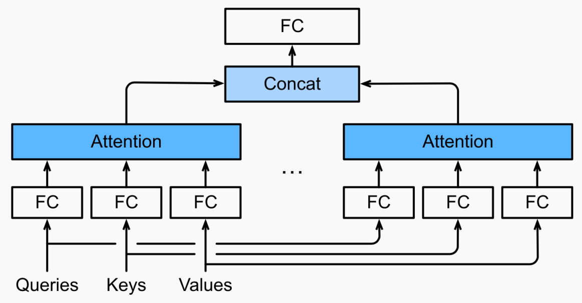
- Each word attends to all other words in the sentence
- Which words should “like” attend to?
  - Syntax: “flies”, “arrow” (a preposition)
  - Semantics: “time”, “arrow” (a metaphor)
- We want to represent different roles of a word in the sentence: need more than a single embedding
- Instantiation: multiple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

Multi-head attention



- Multiple attention modules: same architecture, different parameters

Multi-head attention



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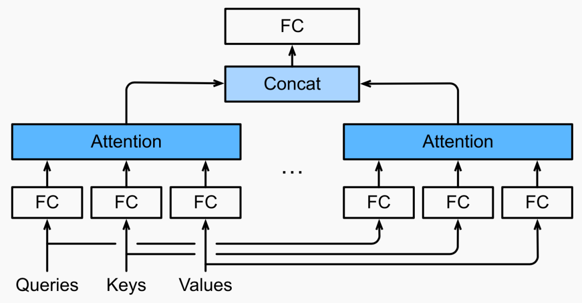
Multi-head attention



- 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

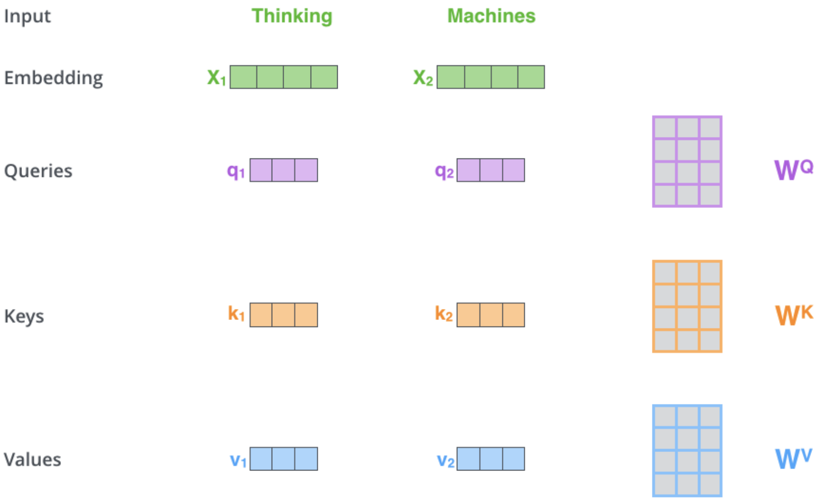
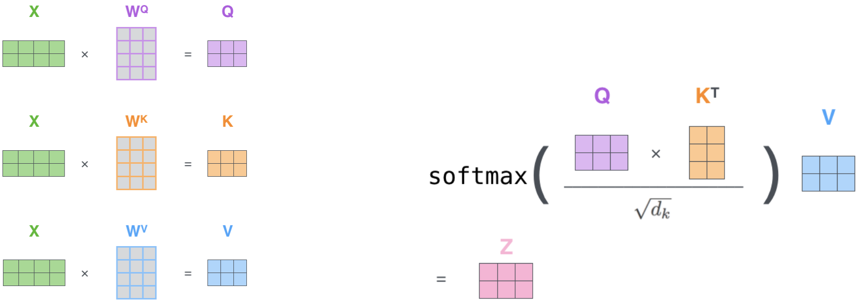


Figure: From The Illustrated Transformer

Matrix representation: attention weights

Scaled dot product attention



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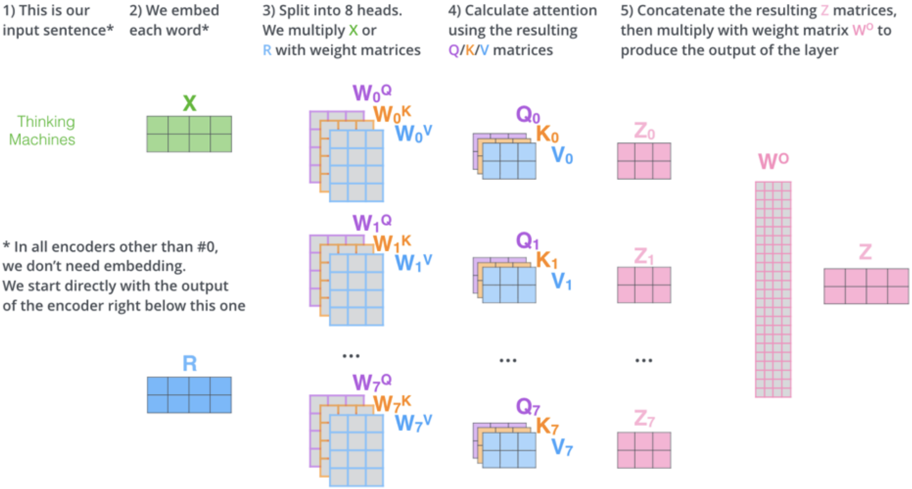
Multi-head attention



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Summary so far

- Sequence modeling
  - Input: a sequence of words
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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

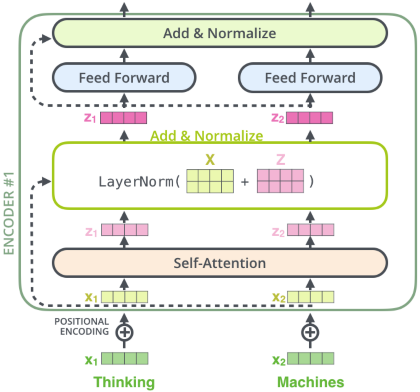

Figure: From The Illustrated Transformer

- Multi-head self-attention

Transformer block

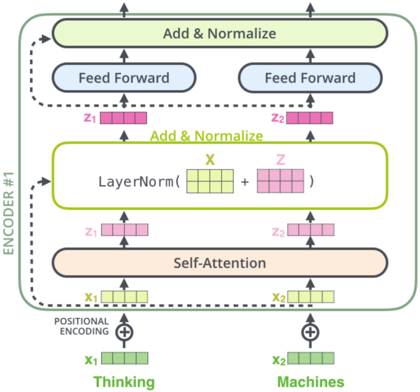

Figure: From The Illustrated Transformer

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

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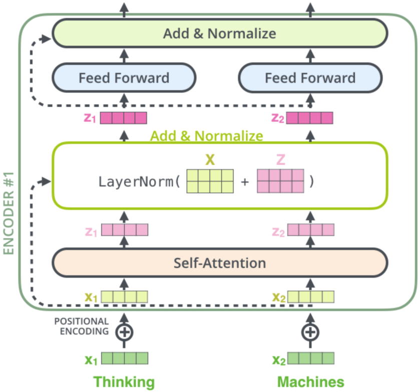
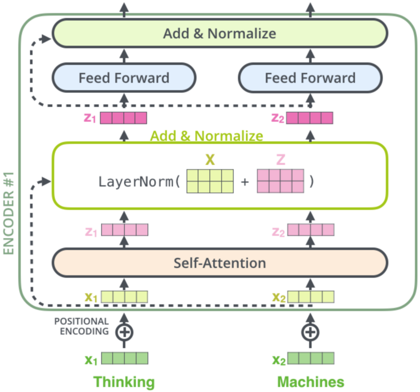


Figure: From The Illustrated Transformer

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

Transformer block



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- Multi-head self-attention
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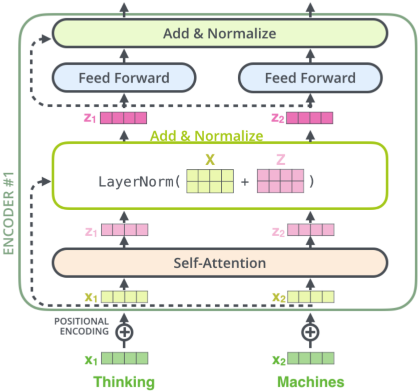

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- Multi-head self-attention
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- Residual connection and layer normalization

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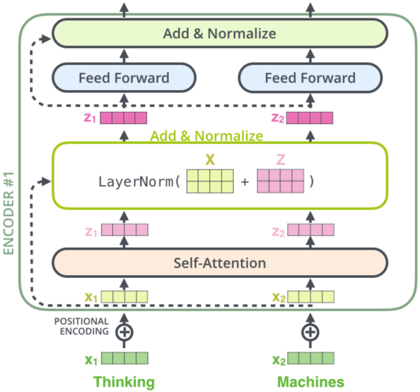
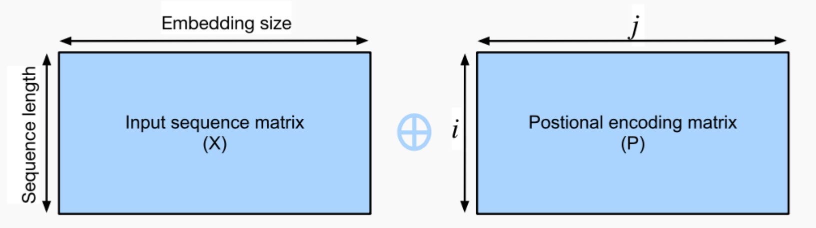


Figure: From The Illustrated Transformer

- 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: continuous approximation of binary encoding of positions (integers)

$0:$	0	0	0	0
$1:$	0	0	0	1
$2:$	0	0	1	0
$3:$	0	0	1	1
$4:$	0	1	0	0
$5:$	0	1	0	1
$6:$	0	1	1	0
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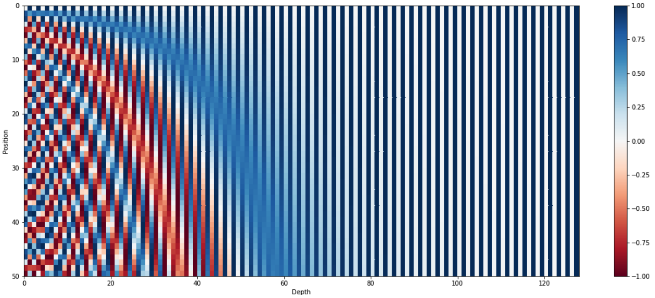

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$$
\begin{array}{ll}
0: & 0\ 0\ 0\ 0 \\
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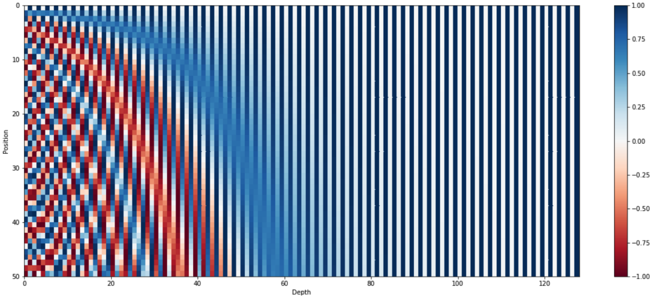
$$



$$
\vec{p_t} = \begin{bmatrix} \sin(\omega_1 . t) \\ \cos(\omega_1 . t) \\ \\ \sin(\omega_2 . t) \\ \cos(\omega_2 . t) \\ \\ \vdots \\ \\ \sin(\omega_{d/2} . t) \\ \cos(\omega_{d/2} . t) \end{bmatrix}_{d \times 1}
$$

Figure: From Amirhossein Kazemnejad's Blog

$$
\omega_{2i} = \omega_{2i+1} = 1/10000^{\frac{2i}{d}}
$$

Learned position embeddings

Sinusoidal position embedding:

- Not learnable
- Can extrapolate to longer sequences but doesn't work well

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Learned absolute position embeddings (most common now):

- Consider each position as a word. Map positions to dense vectors: $W_{d \times n} \phi_{\text{one-hot}}(\text{pos})$
- Column i of W is the embedding of position i

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Learned absolute position embeddings (most common now):

- Consider each position as a word. Map positions to dense vectors: $W_{d \times n} \phi_{\text{one-hot}}(\text{pos})$
- Column i of W is the embedding of position i
- Need to fix maximum position/length beforehand
- Cannot extrapolate to longer sequences

Residual connection

Motivation:

- Gradient explosion/vanishing is not RNN-specific!
- It happens to all very deep networks (which are hard to optimize).

Residual connection

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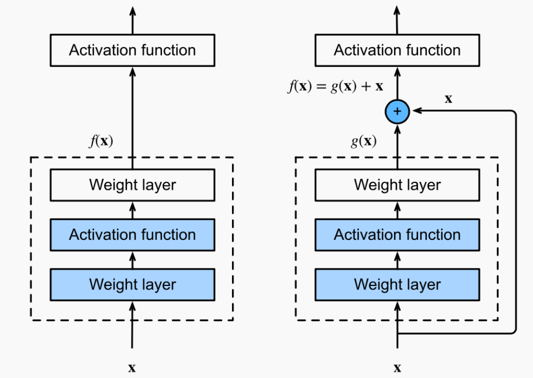
- Gradient explosion/vanishing is not RNN-specific!
- It happens to all very deep networks (which are hard to optimize).
- In principle, a deep network can always represent a shallow network (by setting higher layers to identity functions), thus it should be at least as good as the shallow network.
- How can we make it easier to recover the shallow solution?

Residual connection

Solution: Deep Residual Learning for Image Recognition [He et al., 2015]



Learn the residual layer: $g(x) = f(x) - x$

If the shallow network is better, set $g(x) = 0$ (easier to learn).

Layer normalization

Layer Normalization [Ba et al., 2016]

- Normalize (zero mean, unit variance) across features
- Let $x = (x_1, \ldots, x_d)$ be the input vector (e.g., word embedding, previous layer output)

$$\mathrm{LayerNorm}(x) = \frac{x - \hat{\mu}}{\hat{\sigma}},$$

$$\text{where } \hat{\mu} = \frac{1}{d}\sum_{i=1}^{d} x_i, \quad \hat{\sigma}^2 = \frac{1}{d}\sum_{i=1}^{d}(x_i - \hat{\mu})^2$$

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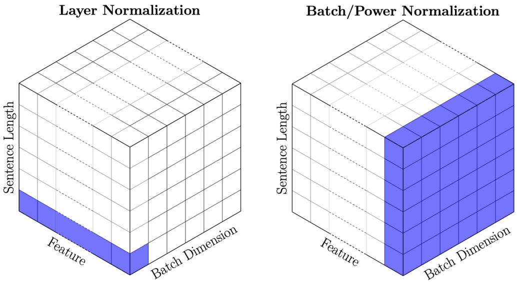
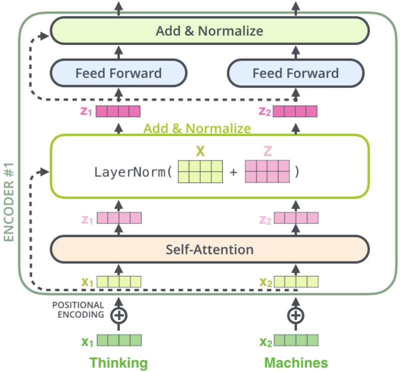


- A deterministic transformation of the input
- Independent of train/inference and batch size

Residual connection and layer normalization in Transformer



- Add (residual connection) & Normalize (layer normalization) after each layer
- Position-wise feed-forward networks: same mapping for all positions

Summary

- We have seen two families of models for sequences modeling: **RNNs** and **Transformers**
- Both take a sequence of (discrete) symbols as input and output a sequence of embeddings
- They are often called **encoders** and are used to represent text
- Transformers are dominating today because of its scalability