CS 6501 Natural Language Processing (Spring 2025)

Yu Meng
University of Virginia
yumeng5@virginia.edu

Jan 15, 2025

(Recap) Course Information & Logistics

- This course is designed to be a **research-oriented graduate-level** course
- Seminar-style: a substantial focus on reading, presenting and discussing important papers and conducting research projects
- A comprehensive overview of cutting-edge developments in NLP
- Prerequisites: CS 4501 NLP or CS 4774 (having deep learning background is important!)
- This course may benefit you if
  - You are working on NLP research (PhD/MS research students)
  - Your research uses NLP models/tools
  - You aim for a job that involves using NLP models/tools
  - You are very interested in the cutting-edge topics of NLP and willing to spend time to learn

(Recap) Course Format & Grading

- Course Website: https://yumeng5.github.io/teaching/2025-spring-cs6501

Schedule (Subject to Changes!)

Date	Topic	Papers	Slides
		Introduction to Large Language Models	
1/13	Course Overview	-	overview
1/15	Language Model Architecture	Distributed Representations of Words and Phrases and their Compositionality (word2vec) Attention Is All You Need (Transformer)	lm_basics
1/20	No Class (MLK Holiday)	-	-
1/22	Language Model Pretraining & Fine-Tuning	Language Models are Unsupervised Multitask Learners (GPT-2) BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding RoBERTa: A Robustly Optimized BERT Pretraining Approach ELECTRA: Pre-training Text Encoders as Discriminators Rather Than Generators BART: Denoising Sequence-to-Sequence Pre-training for Natural Language Generation, Translation, and Comprehension Exploring the Limits of Transfer Learning with a Unified Text-to-Text Transformer (T5)	pretrain

(Recap) Course Format & Grading: Paper Presentation (30%)

- Starting from the 4th lecture (1/27), each lecture will be presented by a group of 1 or 2 students
  - Groups of two are encouraged, but individual presentations are also acceptable
- Every group presents one lecture (3 papers)
- Signup sheet: https://docs.google.com/spreadsheets/d/1h4uuKnL8T71YUtbORgth-y6AAkFZnaZsvZV5ygrzxjw/edit?usp=sharing
- You can sign up for the topic you are interested in – slots are first come, first served!
- The dates listed on the course website are subject to change – please sign up based on the topic rather than the date

(Recap) Course Format & Grading: Paper Presentation (30%)

- **Presentation duration**: strictly limited to 60 minutes, followed by a 10-minute question-and-answer session with the audience & instructor
- **Deadline**: Email your slides to the instructor and TAs at least 48 hours before your presentation (e.g., if presenting on Monday, slides should be emailed by Saturday 2pm)
- You will receive feedback from the instructor to improve your slides (if necessary, the instructor may schedule a meeting with your team to go over the slides)
- Late submissions result in a 50% presentation grade deduction
- Detailed grading rubrics and tips can be found on the course website
- First three student lectures automatically receive **5%, 3%, 1% extra credit of final grade**

(Recap) Course Format & Grading: Participation (20%)

- Starting from the 4th lecture (1/27), everyone is required to complete two mini-assignments
- **Pre-lecture question**: read the 3 papers to be introduced in the lecture, and submit a question you have when you read them
- **Post-lecture feedback**: provide feedback to the presenters after the lecture
- We'll use Google Forms to collect pre-lecture questions and post-lecture feedback and share them with the presenters
- **Deadlines**: pre-lecture questions are due one day before the lecture (e.g., For Monday lectures, you need to submit the question by Sunday 11:59 pm); post-lecture feedback is due each Friday (both Monday & Wednesday feedback is due Friday 11:59 pm)
- Lectures are not recorded, but slides will be posted on the course website

(Recap) Course Format & Grading: Participation (20%)

- Besides student presentations, we'll also invite leading researchers from academia and industry to introduce their cutting-edge research
- Guest lectures do not have pre-lecture questions/post-lecture feedback, and we'll directly take attendance on Zoom
- You can get extra participation credit if you ask questions during guest lectures (details shared later)
- At the end of the semester, you'll get **2% extra credit of final grade** if you complete the teaching evaluation survey about this course (sent from Student Experiences of Teaching)

(Recap) Course Format & Grading: Project (50%)

- Complete a research project, present your results, and submit a project report
- Work in a team of 1 or 2 (a larger team size requires prior approval from the instructor) – may or may not be the same team as your presentation group
- (Type 1) A comprehensive survey report: carefully examine and summarize existing literature on a topic covered in this course; provide detailed and insightful discussions on the unresolved issues, challenges, and potential future opportunities within the chosen topic
- (Type 2) A hands-on project: not constrained to the course topics but must be centered around NLP; doesn't have to involve large language models (e.g., train or analyze smaller-scale language models for specific tasks); eligible for extra credits if publishable
- **Project proposal**: 5% (ddl: 2/5); **Mid-term report**: 10% (ddl: 3/10); **Final presentation** (ddl: 4/15) **and final report**: 35% (ddl: 5/6)

(Recap) Overview of Course Contents

- Introduction to Language Models
  - Language Model Architecture
  - Language Model Pretraining & Fine-Tuning
  - In-Context Learning
  - Scaling and Emergent Ability
- Reasoning with Language Models
  - Chain-of-Thought Generation
  - Inference-Time Scaling
- Knowledge, Factuality and Efficiency
  - Parametric Knowledge in Language Models
  - Retrieval-Augmented Language Generation (RAG)
  - Long-Context Language Models
  - Efficiency
- Language Model Post-Training
  - Instruction Tuning
  - Reinforcement Learning from Human Feedback (RLHF)
- Language Agents
  - Language Agent Basics
  - Language Models for Code
  - Multimodal Language Models
- Ethical Considerations of Language Models
  - Security and Jailbreaking
  - Bias and Calibration
  - Privacy and Legal Issues
- Looking Forward

Agenda: Language Model Architecture

- Introduction to Text Representations
- Word Representations (Word2Vec)
- Transformer Architecture

Motivation: Representing Texts with Vectors

- Word similarity computation is important for understanding semantics

Word similarity (on a scale from 0 to 10) manually annotated by humans

vanish	disappear	9.8
belief	impression	5.95
muscle	bone	3.65
modest	flexible	0.98
hole	agreement	0.3

Word semantics can be multi-faceted

	Valence	Arousal	Dominance
courageous	8.05	5.5	7.38
music	7.67	5.57	6.5
heartbreak	2.45	5.65	3.58
cub	6.71	3.95	4.24

- How to represent words numerically? Using multi-dimensional vectors!

Figure source: https://web.stanford.edu/~jurafsky/slp3/6.pdf

Vector Semantics

- Represent a word as a point in a multi-dimensional semantic space
- A desirable vector semantic space: words with similar meanings are nearby in space

2D visualization of a desirable high-dimensional vector semantic space

Figure source: https://web.stanford.edu/~jurafsky/slp3/6.pdf

Vector Space Basics

- Vector notation: an N-dimensional vector $\boldsymbol{v} = [v_1, v_2, \ldots, v_N] \in \mathbb{R}^N$
- Vector dot product/inner product:

$$\text{dot product}(\boldsymbol{v}, \boldsymbol{w}) = \boldsymbol{v} \cdot \boldsymbol{w} = v_1 w_1 + v_2 w_2 + \cdots + v_n w_n = \sum_{i=1}^{N} v_i w_i$$

- Vector length/norm:

$$|\boldsymbol{v}| = \sqrt{\boldsymbol{v} \cdot \boldsymbol{v}} = \sqrt{\sum_{i=1}^{N} v_i^2}$$

Other (less commonly-used) vector norms:
Manhattan norm, *p*-norm, infinity norm…

- Cosine similarity between vectors:

$$\cos(\boldsymbol{v}, \boldsymbol{w}) = \frac{\boldsymbol{v} \cdot \boldsymbol{w}}{|\boldsymbol{v}||\boldsymbol{w}|} = \frac{\sum_{i=1}^{N} v_i w_i}{\sqrt{\sum_{i=1}^{N} v_i^2} \sqrt{\sum_{i=1}^{N} w_i^2}}$$

Vector Space Basics: Example

- Consider two 4-dimensional vectors $\boldsymbol{v} = [1, 0, 1, 0] \in \mathbb{R}^4$ $\boldsymbol{w} = [0, 1, 1, 0] \in \mathbb{R}^4$
- Vector dot product/inner product:

$$\boldsymbol{v} \cdot \boldsymbol{w} = \sum_{i=1}^{N} v_i w_i = 1$$

- Vector length/norm:

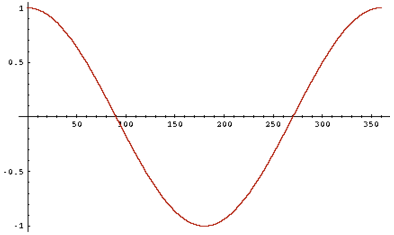
$$|\boldsymbol{v}| = \sqrt{\sum_{i=1}^{N} v_i^2} = \sqrt{2} \quad |\boldsymbol{w}| = \sqrt{\sum_{i=1}^{N} w_i^2} = \sqrt{2}$$

- Cosine similarity between vectors:

$$\cos(\boldsymbol{v}, \boldsymbol{w}) = \frac{\boldsymbol{v} \cdot \boldsymbol{w}}{|\boldsymbol{v}||\boldsymbol{w}|} = \frac{1}{2}$$

Vector Similarity

- Cosine similarity is the most commonly used metric for similarity measurement
  - Symmetric: $\cos(\boldsymbol{v}, \boldsymbol{w}) = \cos(\boldsymbol{w}, \boldsymbol{v})$
  - Not influenced by vector length
  - Has a normalized range: [-1, 1]
  - Intuitive geometric interpretation



Cosine function values under different angles

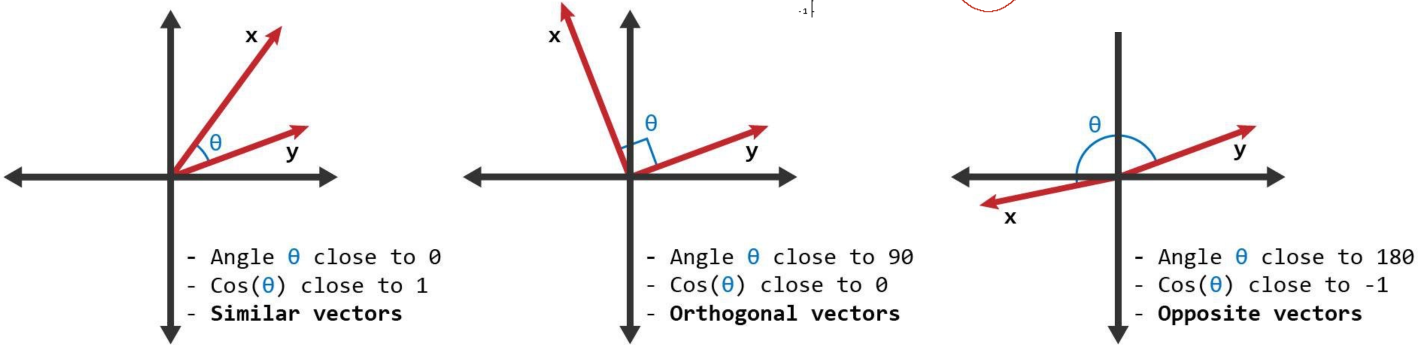


Figure source: https://www.learndatasci.com/glossary/cosine-similarity/

How to Represent Words as Vectors?

- Given a vocabulary $\mathcal{V} = \{\text{good}, \text{feel}, \text{I}, \text{sad}, \text{cats}, \text{have}\}$
- Most straightforward way to represent words as vectors: use their indices
- One-hot vector: only one high value (1) and the remaining values are low (0)
- Each word is identified by a unique dimension

$$
\begin{aligned}
\boldsymbol{v}_{\text{good}} &= [1, 0, 0, 0, 0, 0] \\
\boldsymbol{v}_{\text{feel}} &= [0, 1, 0, 0, 0, 0] \\
\boldsymbol{v}_{\text{I}} &= [0, 0, 1, 0, 0, 0] \\
\boldsymbol{v}_{\text{sad}} &= [0, 0, 0, 1, 0, 0] \\
\boldsymbol{v}_{\text{cats}} &= [0, 0, 0, 0, 1, 0] \\
\boldsymbol{v}_{\text{have}} &= [0, 0, 0, 0, 0, 1]
\end{aligned}
$$

Represent Sequences by Word Occurrences

- Consider the mini-corpus with three documents

$$d_1 = \text{“I feel good”}$$
$$d_2 = \text{“I feel sad”}$$
$$d_3 = \text{“I have cats”}$$

$$\boldsymbol{v}_{\text{good}} = [1, 0, 0, 0, 0, 0]$$
$$\boldsymbol{v}_{\text{feel}} = [0, 1, 0, 0, 0, 0]$$
$$\boldsymbol{v}_{\text{I}} = [0, 0, 1, 0, 0, 0]$$
$$\boldsymbol{v}_{\text{sad}} = [0, 0, 0, 1, 0, 0]$$
$$\boldsymbol{v}_{\text{cats}} = [0, 0, 0, 0, 1, 0]$$
$$\boldsymbol{v}_{\text{have}} = [0, 0, 0, 0, 0, 1]$$

- Straightforward way of representing documents: look at which words are present

$$\boldsymbol{v}_{d_1} = [1, 1, 1, 0, 0, 0]$$
$$\boldsymbol{v}_{d_2} = [0, 1, 1, 1, 0, 0]$$
$$\boldsymbol{v}_{d_3} = [0, 0, 1, 0, 1, 1]$$

Document vector similarity ➡

$$\cos(\boldsymbol{v}_{d_1}, \boldsymbol{v}_{d_2}) = \frac{2}{3}$$
$$\cos(\boldsymbol{v}_{d_1}, \boldsymbol{v}_{d_3}) = \frac{1}{3}$$
$$\cos(\boldsymbol{v}_{d_2}, \boldsymbol{v}_{d_3}) = \frac{1}{3}$$

Agenda: Language Model Architecture

- Introduction to Text Representations
- Word Representations (Word2Vec)
- Transformer Architecture

UNIVERSITY of VIRGINIA

Word2Vec Paper

Distributed Representations of Words and Phrases and their Compositionality

Tomas Mikolov
Google Inc.
Mountain View
mikolov@google.com

Ilya Sutskever
Google Inc.
Mountain View
ilyasu@google.com

Kai Chen
Google Inc.
Mountain View
kai@google.com

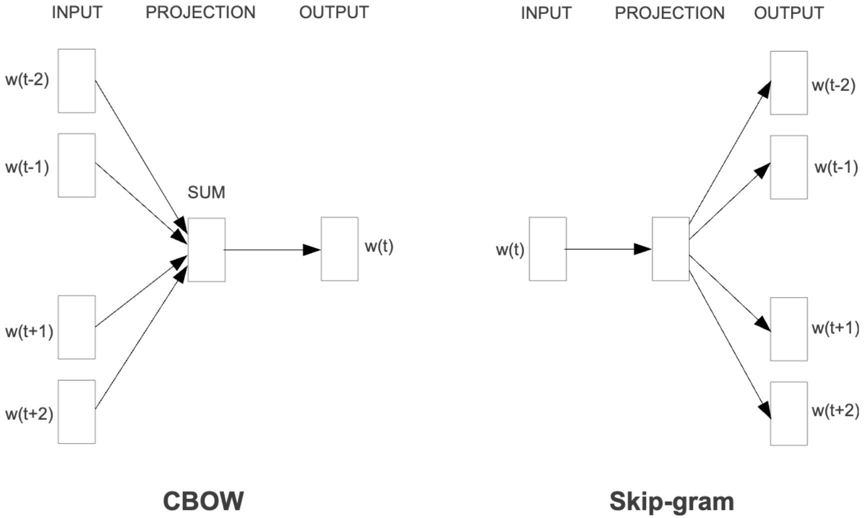
Greg Corrado
Google Inc.
Mountain View
gcorrado@google.com

Jeffrey Dean
Google Inc.
Mountain View
jeff@google.com

Paper: https://arxiv.org/pdf/1310.4546

Overview

- The earliest & most well-known word embedding learning method (published in 2013)
- Two variants: Skip-gram and CBOW (Continuous Bag-of-Words)
- Mainly discuss Skip-gram in this lecture



Distributional Hypothesis

- Words that occur in similar contexts tend to have similar meanings
- A word’s meaning is largely defined by the company it keeps (its context)
- Example: suppose we don’t know the meaning of “Ong choy” but see the following:
  - Ong choy is delicious **sautéed with garlic**
  - Ong choy is superb **over rice**
  - … ong choy **leaves** with **salty** sauces
- And we’ve seen the following contexts:
  - … spinach **sautéed with garlic over rice**
  - … chard stems and **leaves** are **delicious**
  - … collard greens and other **salty** leafy greens
- Ong choy = water spinach!

Example source: https://web.stanford.edu/~jurafsky/slp3/slides/vectorsemantics2024.pdf

Word Embeddings: General Idea

- Learn dense vector representations of words based on distributional hypothesis
- Semantically similar words (based on context similarity) will have similar vector representations
- **Embedding**: a mapping that takes elements from one space and represents them in a different space

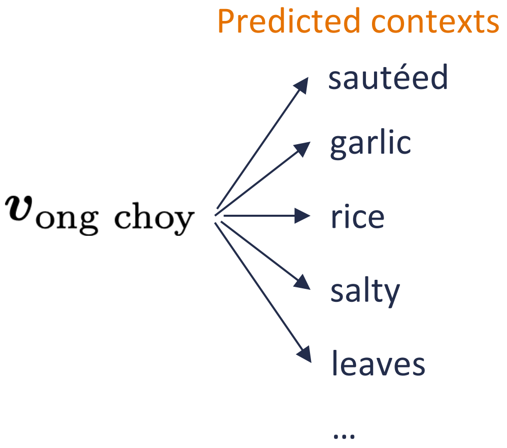
$$\boldsymbol{v}_{\text{to}} = [1, 0, 0, 0, 0, 0, \ldots]$$
$$\boldsymbol{v}_{\text{by}} = [0, 1, 0, 0, 0, 0, \ldots]$$
$$\boldsymbol{v}_{\text{that}} = [0, 0, 1, 0, 0, 0, \ldots]$$
$$\boldsymbol{v}_{\text{good}} = [0, 0, 0, 1, 0, 0, \ldots]$$
$$\boldsymbol{v}_{\text{nice}} = [0, 0, 0, 0, 1, 0, \ldots]$$
$$\boldsymbol{v}_{\text{bad}} = [0, 0, 0, 0, 0, 1, \ldots]$$

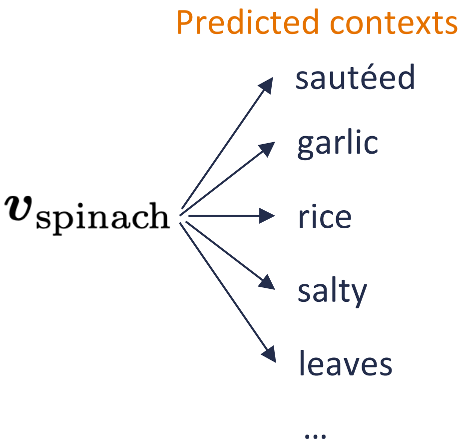
2D visualization of a word embedding space

Figure source: https://web.stanford.edu/~jurafsky/slp3/6.pdf

Learning Word Embeddings

- Assume a large text collection (e.g., Wikipedia)
- Hope to learn similar word embeddings for words occurring in similar contexts
- Construct a prediction task: use a center word's embedding to predict its contexts!
- Intuition: If two words have similar embeddings, they will predict similar contexts, thus being semantically similar!





Word Embedding Is Self-Supervised Learning

- **Self-supervised learning**: a model learns to predict parts of its input from other parts of the same input

Input: *Ong choy is superb over rice*

Prediction task: Ong choy → is, superb, over, rice

- Self-supervised learning vs. supervised learning:
  - Self-supervised learning: **no human-labeled data** – the model learns from unlabeled data by generating supervision through the structure of the data itself
  - Supervised learning: **use human-labeled data** – the model learns from human annotated input-label pairs

Word2Vec Setting

- Input: a corpus D – the larger, the better!
- Training data: word-context pairs (w, c) where w is a center word, and c is a context word
  - Each word in the corpus can act as center word
  - Context words = neighboring words of the center word in a local context window ($\pm l$ words)
- Parameters to learn: $\boldsymbol{\theta} = \{\boldsymbol{v}_{\boldsymbol{w}}, \boldsymbol{v}_{\boldsymbol{c}}\}$ – each word has two vectors (center word representation & context word representation)
- The center word representations $\boldsymbol{v}_{\boldsymbol{w}}$ are usually used as the final word embeddings
- Number of parameters to store: $d \times |V|$
  - d is the embedding dimension; usually 100-300
  - $|V|$ is the vocabulary size; usually > 10K

Word2Vec Training Data Example

- Input sentence: "there is a cat on the mat"
- Suppose context window size = 2
- Word-context pairs as training data:
  - (there, is), (there, a)
  - (is, there), (is, a), (is, cat)
  - (a, there), (a, is), (a, cat), (a, on)
  - (cat, is), (cat, a), (cat, on), (cat, the)
  - (on, a), (on, cat), (on, the), (on, mat)
  - (the, cat), (the, on), (the, mat)
  - (mat, on), (mat, the)

there is a cat on the mat
there is a cat on the mat
there is a cat on the mat
there is a cat on the mat
there is a cat on the mat
there is a cat on the mat
there is a cat on the mat

- "Skip-gram": skipping over some context words to predict the others!
- Training data completely derived from the raw corpus (no human labels!)

Word2Vec Objective (Skip-gram)

- Intuition: predict the contexts words using the center word (semantically similar center words will predict similar contexts words)
- Objective: using the parameters $\boldsymbol{\theta} = \{\boldsymbol{v_w}, \boldsymbol{v_c}\}$ to maximize the probability of predicting the context word c using the center word w

$$\max_{\boldsymbol{\theta}} \prod_{(w,c)\in\mathcal{D}} \boxed{p_{\boldsymbol{\theta}}(c|w)}$$

Probability expressed as a function of the model parameters

- How to parametrize the probability?

Word2Vec Probability Parametrization

- Word2Vec objective: $\max_{\boldsymbol{\theta}} \prod_{(w,c)\in\mathcal{D}} p_{\boldsymbol{\theta}}(c|w)$
- Assume the log probability (i.e., logit) is proportional to vector dot product

$$\log p_{\boldsymbol{\theta}}(c|w) \propto \boldsymbol{v}_c \cdot \boldsymbol{v}_w$$

- Rationale: a larger vector dot product *can* indicate a higher vector similarity

Word2Vec Parameterized Objective

- Word2Vec objective: $$\max_{\boldsymbol{\theta}} \prod_{(w,c)\in\mathcal{D}} p_{\boldsymbol{\theta}}(c|w)$$
- Assume the log probability (i.e., logit) is proportional to vector dot product
$$\log p_{\boldsymbol{\theta}}(c|w) \propto \boldsymbol{v}_c \cdot \boldsymbol{v}_w$$
- The final probability distribution is given by the softmax function:
$$p_{\boldsymbol{\theta}}(c|w) = \frac{\exp(\boldsymbol{v}_c \cdot \boldsymbol{v}_w)}{\sum_{c'\in|\mathcal{V}|}\exp(\boldsymbol{v}_{c'} \cdot \boldsymbol{v}_w)} \Rightarrow \sum_{c'\in|\mathcal{V}|} p_{\boldsymbol{\theta}}(c'|w) = 1$$
- Word2Vec objective (log-scale):
$$\max_{\boldsymbol{\theta}} \sum_{(w,c)\in\mathcal{D}} \log p_{\boldsymbol{\theta}}(c|w) = \sum_{(w,c)\in\mathcal{D}} \left(\boldsymbol{v}_c \cdot \boldsymbol{v}_w - \log \sum_{c'\in|\mathcal{V}|} \exp(\boldsymbol{v}_{c'} \cdot \boldsymbol{v}_w)\right)$$

UNIVERSITY of VIRGINIA

Word2Vec Negative Sampling

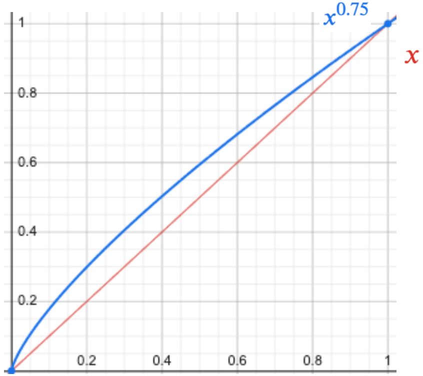
- Challenges with the original objective: Sum over the entire vocabulary – expensive!

$$\max_{\boldsymbol{\theta}} \sum_{(w,c)\in\mathcal{D}} \log p_{\boldsymbol{\theta}}(c|w) = \sum_{(w,c)\in\mathcal{D}} \left(\boldsymbol{v}_c \cdot \boldsymbol{v}_w - \log \boxed{\sum_{c'\in|\mathcal{V}|}} \exp(\boldsymbol{v}_{c'} \cdot \boldsymbol{v}_w) \right)$$

- Randomly sample a few negative terms from the vocabulary to form a negative set N
- How to sample negatives? Based on the (power-smoothed) unigram distribution

$$p_{\text{neg}}(w) \propto \left(\frac{\#(w)}{\sum_{w'\in\mathcal{V}} \#(w')} \right)^{0.75}$$

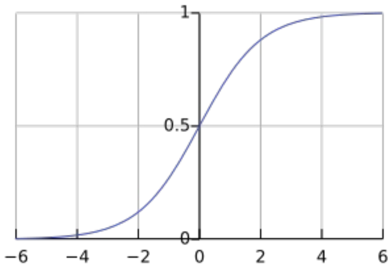
Rare words get a bit boost in sampling probability



Word2Vec Negative Sampling

- Formulate a binary classification task; predict whether (w, c) is a real context pair:

$$p_{\boldsymbol{\theta}}(\text{True}|c, w) = \sigma(\boldsymbol{v}_c \cdot \boldsymbol{v}_w) = \frac{1}{1 + \exp(-\boldsymbol{v}_c \cdot \boldsymbol{v}_w)}$$



$y = \sigma(x)$

- Maximize the binary classification probability for real context pairs, and minimize for negative (random) pairs

$$\max_{\boldsymbol{\theta}} \log \sigma(\boldsymbol{v}_c \cdot \boldsymbol{v}_w) - \sum_{c' \in \mathcal{N}} \log \sigma(\boldsymbol{v}_{c'} \cdot \boldsymbol{v}_w)$$

Real context pair

Negative context pair

Word2Vec Optimization

- How to optimize the following objective?

$$\max_{\boldsymbol{\theta}} \log \sigma(\boldsymbol{v}_c \cdot \boldsymbol{v}_w) - \sum_{c' \in \mathcal{N}} \log \sigma(\boldsymbol{v}_{c'} \cdot \boldsymbol{v}_w)$$

- Stochastic gradient descent (SGD)!
- First, initialize parameters $\boldsymbol{\theta} = \{\boldsymbol{v}_w, \boldsymbol{v}_c\}$ with random d-dimensional vectors
- In each step: update parameters in the direction of the gradient of the objective (weighted by the learning rate)

$$\boldsymbol{\theta}^{(t+1)} \leftarrow \boldsymbol{\theta}^{(t)} - \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}\big|_{\boldsymbol{\theta}=\boldsymbol{\theta}^{(t)}}$$

Learning rate

Loss function

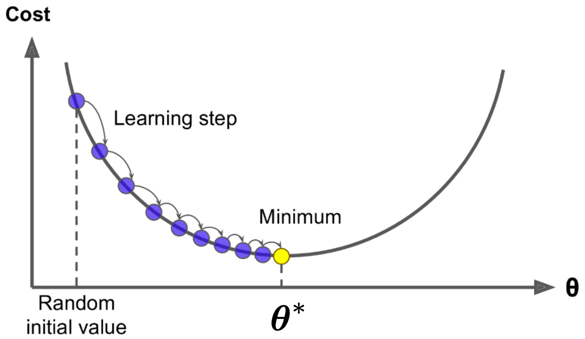


Figure source: https://web.stanford.edu/class/cs224n/slides/cs224n-spr2024-lecture02-wordvecs2.pdf

Word2Vec Hyperparameters

- Word embedding dimension d (usually 100-300)
  - Larger d provides richer vector semantics
  - Extremely large d suffers from inefficiency and curse of dimensionality
- Local context window size l (usually 5-10)
  - Smaller l learns from immediately nearby words – more syntactic information
  - Bigger l learns from longer-ranged contexts – more semantic/topical information
- Number of negative samples k (usually 5-10)
  - Larger k usually makes training more stable but also more costly
- Learning rate η (usually 0.02-0.05)

Summary: Word2Vec

- Distributional hypothesis
  - Words that occur in similar contexts tend to have similar meanings
  - Infer semantic similarity based on context similarity
- Word embeddings
  - Construct a prediction task: use a center word's embedding to predict its contexts
  - Two words with similar embeddings will predict similar contexts => semantically similar
  - Word embedding is a form of self-supervised learningEmploy negative sampling to improve training efficiency
- Use SGD to optimize vector representations
- Word embedding applications & evaluations
  - Word similarity
  - Word analogy
  - Use as input features to downstream tasks

Limitations: Word2Vec

- Limited Context Window:
  - only considers a fixed-size context window when generating embeddings
  - cannot effectively capture long-range dependencies (e.g. words that appear far apart)
- Static Embeddings:
  - the embeddings generated by Word2Vec are static (regardless of the context)
  - polysemy can have different meanings depending on specific context
- Not Capturing Word Order Information:
  - focuses only on co-occurrence within the context window
  - ignores the sequential structure of language

Agenda: Language Model Architecture

- Introduction to Text Representations
- Word Representations (Word2Vec)
- Transformer Architecture

UNIVERSITY of VIRGINIA

Transformer Paper

Attention Is All You Need

Ashish Vaswani[*]
Google Brain
avaswani@google.com

Noam Shazeer[*]
Google Brain
noam@google.com

Niki Parmar[*]
Google Research
nikip@google.com

Jakob Uszkoreit[*]
Google Research
usz@google.com

Llion Jones[*]
Google Research
llion@google.com

Aidan N. Gomez[*, †]
University of Toronto
aidan@cs.toronto.edu

Łukasz Kaiser[*]
Google Brain
lukaszkaiser@google.com

Illia Polosukhin[*, ‡]
illia.polosukhin@gmail.com

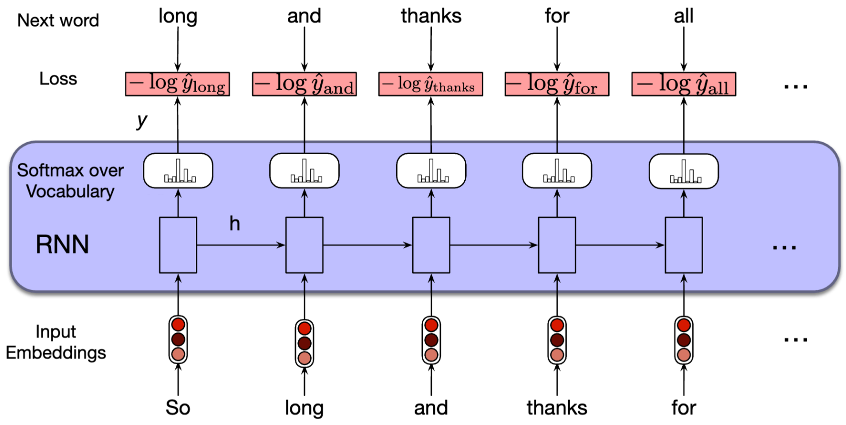
Paper: https://arxiv.org/pdf/1706.03762

Transformer: Overview

- Transformer is a specific kind of sequence modeling architecture (based on DNNs)
- Use attention to replace recurrent operations in RNNs
- The most important architecture for language modeling (almost all LLMs are based on Transformers)!

Transformer vs. RNN

RNN
(recurrent computations)



Transformer
(self-attention computations)

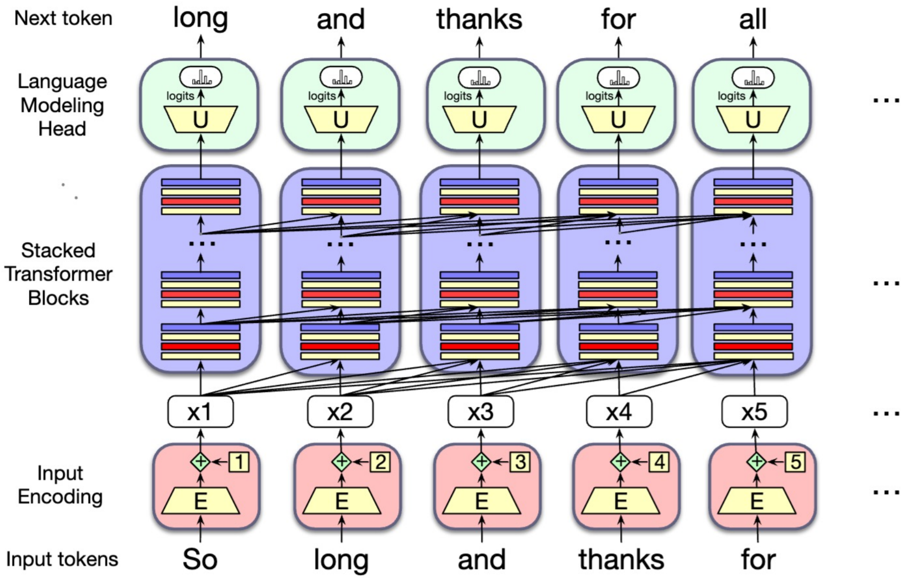


Figure source: https://web.stanford.edu/~jurafsky/slp3/9.pdf

Transformer: Motivation

- Parallel token processing
  - RNN: process one token at a time (computation for each token depends on previous ones)
  - Transformer: process all tokens in a sequence in parallel
- Long-term dependencies
  - RNN: bad at capturing distant relating tokens (vanishing gradients)
  - Transformer: directly access any token in the sequence, regardless of its position
- Bidirectionality
  - RNN: can only model sequences in one direction
  - Transformer: inherently allow bidirectional sequence modeling via attention

Transformer Layer

Each Transformer layer contains the following important components:

- Self-attention
- Feedforward network
- Residual connections + layer norm

Transformer layer

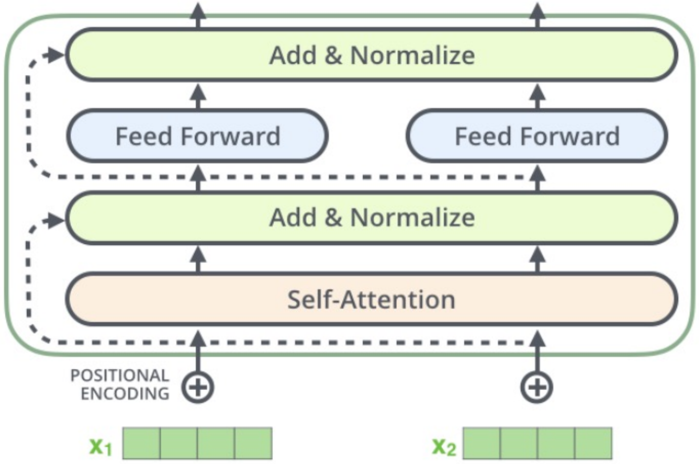


Figure source: https://jalammar.github.io/illustrated-transformer/

Self-Attention: Intuition

- Attention: weigh the importance of different words in a sequence when processing a specific word
  - "When I'm looking at this word, which other words should I pay attention to in order to understand it better?"
- **Self-attention**: each word attends to other words in the **same** sequence
- Example: "The chicken didn't cross the road because it was too tired"
  - Suppose we are learning attention for the word "**it**"
  - With self-attention, "**it**" can decide which other words in the sentence it should focus on to better understand its meaning
  - Might assign high attention to "**chicken**" (the subject) & "**road**" (another noun)
  - Might assign less attention to words like "the" or "didn't"

Self-Attention: Example

Derive the center word representation as a weighted sum of context representations!

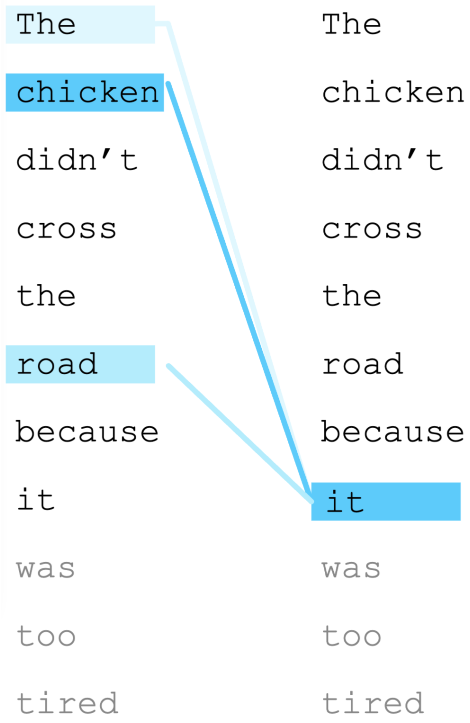
Center word representation

Context word representation

$$\boldsymbol{a}_i = \sum_{x_j \in \boldsymbol{x}} \alpha_{ij} \boldsymbol{x}_j, \quad \sum_{x_j \in \boldsymbol{x}} \alpha_{ij} = 1$$

Attention score $i \rightarrow j$, summed to 1

Context word (key) Center word (query)



Current word = "it"

Figure source: https://web.stanford.edu/~jurafsky/slp3/9.pdf

Self-Attention: Attention Score Computation

- Attention score is given by the softmax function over vector dot product

$$\boldsymbol{a}_i = \sum_{x_j \in \boldsymbol{x}} \alpha_{ij} \boldsymbol{x}_j, \quad \sum_{x_j \in \boldsymbol{x}} \alpha_{ij} = 1$$

$$\alpha_{ij} = \mathrm{Softmax}(\boldsymbol{x}_i \cdot \boldsymbol{x}_j)$$

Center word (query) representation

Context word (key) representation

- Why use two copies of word representations for attention computation?
  - We want to reflect the different roles a word plays (as the target word being compared to others, or as the context word being compared to the target word)
  - If using the same copy of representations for attention calculation, a word will (almost) always attend to itself heavily due to high dot product with itself!

Self-Attention: Query, Key, and Value

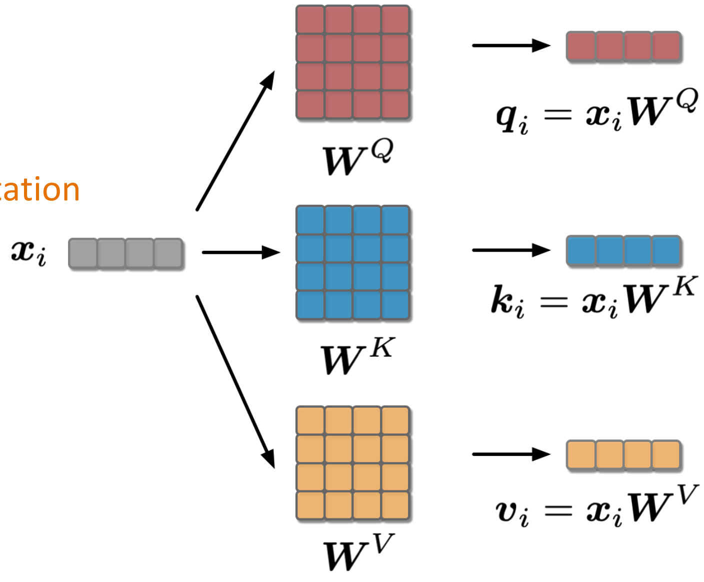
- Each word in self-attention is represented by three different vectors
  - Allow the model to flexibly capture different types of relationships between tokens
- **Query (Q)**:
  - Represent the current word seeking information about
- **Key (K)**:
  - Represent the reference (context) against which the query is compared
- **Value (V)**:
  - Represent the actual content associated with each token to be aggregated as final output

UNIVERSITY of VIRGINIA

Self-Attention: Query, Key, and Value

Each self-attention module has three weight matrices applied to the input word vector to obtain the three copies of representations

Input word representation



query representation

key representation

value representation

Self-Attention: Overall Computation

- Input: single word vector of each word $\boldsymbol{x}_i$
- Compute Q, K, V representations for each word:

$$\boldsymbol{q}_i = \boldsymbol{x}_i \boldsymbol{W}^Q \quad \boldsymbol{k}_i = \boldsymbol{x}_i \boldsymbol{W}^K \quad \boldsymbol{v}_i = \boldsymbol{x}_i \boldsymbol{W}^V$$

- Compute attention scores with Q and K
  - The dot product of two vectors usually has an expected magnitude proportional to $\sqrt{d}$
  - Divide the attention score by $\sqrt{d}$ to avoid extremely large values in softmax function

$$\alpha_{ij} = \text{Softmax}\left(\frac{\boldsymbol{q}_i \cdot \boldsymbol{k}_j}{\sqrt{d}}\right)$$

Dimensionality of q and k

- Sum the value vectors weighted by attention scores

$$\boldsymbol{a}_i = \sum_{x_j \in \boldsymbol{x}} \alpha_{ij} \boldsymbol{v}_j$$

Self-Attention: Illustration

- Example: an input sequence with three words $[x_1, x_2, x_3]$
- Suppose we want to compute the self-attention for x_3

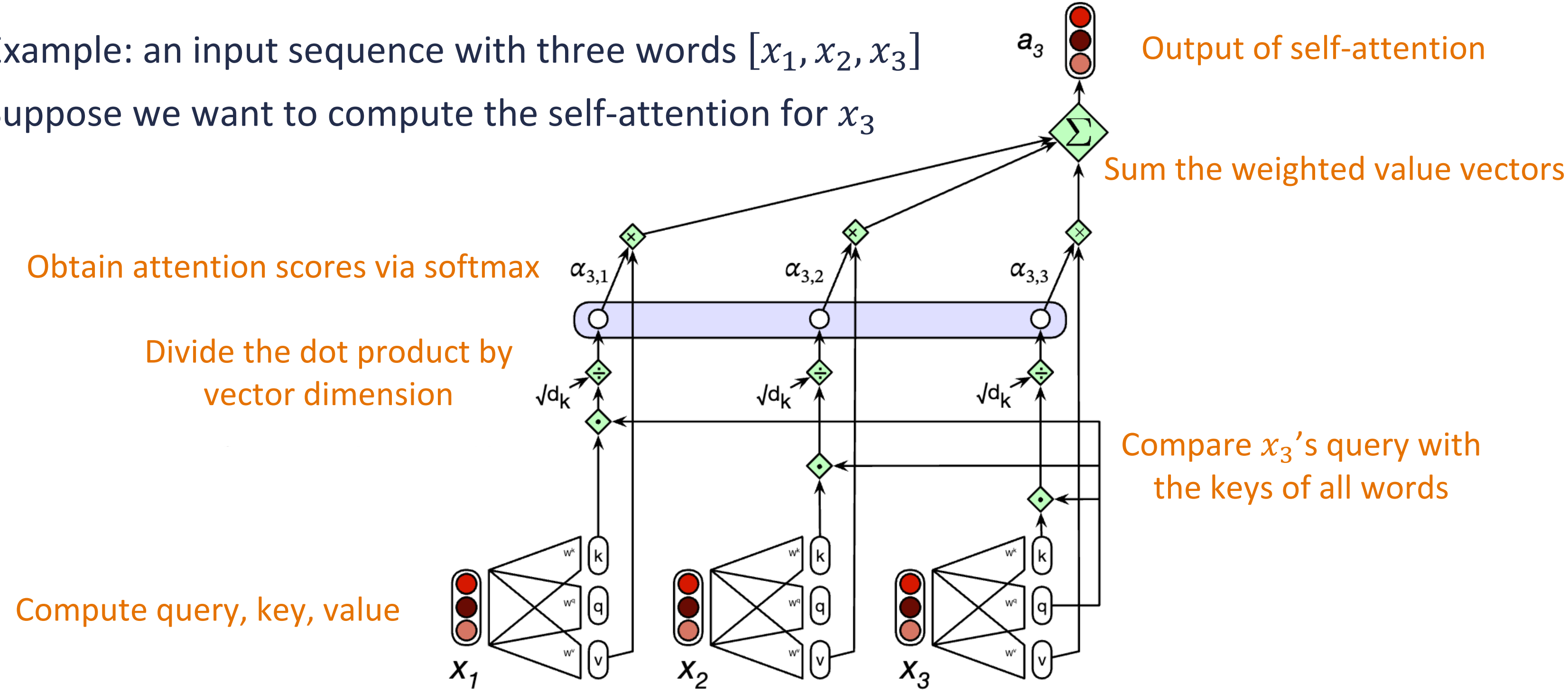
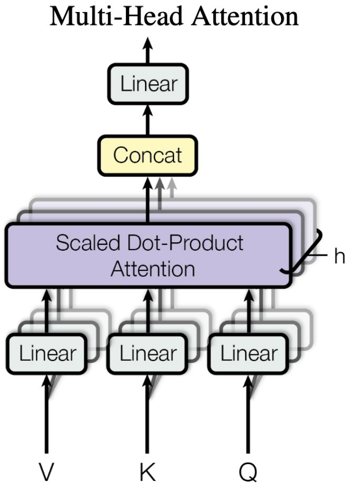


Figure source: https://web.stanford.edu/~jurafsky/slp3/9.pdf

Multi-Head Self-Attention

- Transformers use multiple attention heads for each self-attention module
- Intuition:
  - Each head might attend to the context for different purposes (e.g., particular kinds of patterns in the context)
  - Heads might be specialized to represent different linguistic relationships



Concatenate the outputs of all heads

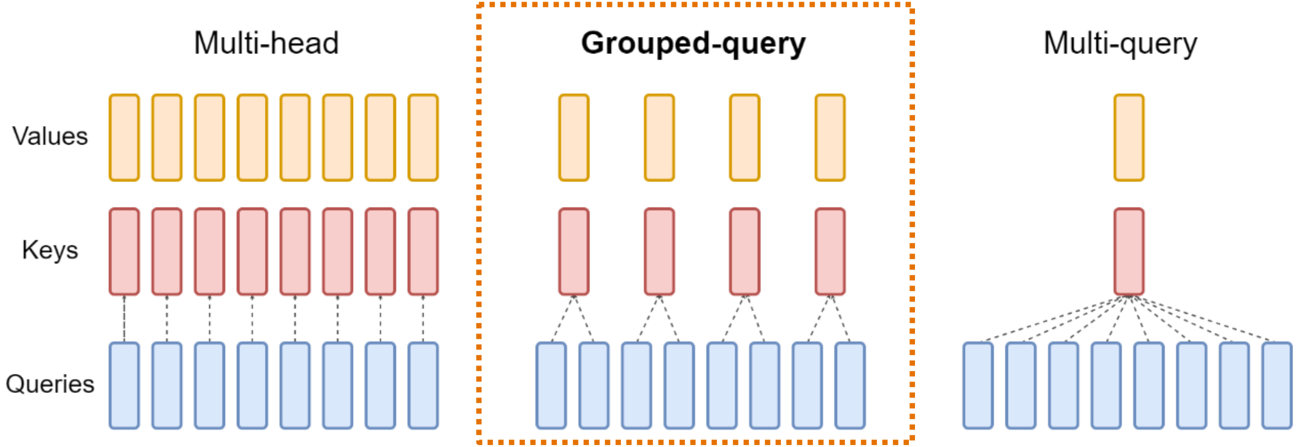
h attention heads are computed separately

Figure source: https://arxiv.org/pdf/1706.03762

UNIVERSITY of VIRGINIA

Multi-Head Self-Attention Variants

- Multi-query attention ([Fast Transformer Decoding: One Write-Head is All You Need](#)): share keys and values across all attention heads
- Grouped-query attention ([GQA: Training Generalized Multi-Query Transformer Models from Multi-Head Checkpoints](#)): share keys and values within groups of heads



Used in latest LLMs (e.g., Llama3)

Figure source: https://arxiv.org/pdf/2305.13245

UNIVERSITY of VIRGINIA

Parallel Computation of QKV

- Self-attention computation performed for each token is independent of other tokens
- Easily parallelize the entire computation, taking advantage of the efficient matrix multiplication capability of GPUs
- Process an input sequence with N words in parallel

Compute QKV for one word: $\boldsymbol{q}_i = \boldsymbol{x}_i \boldsymbol{W}^Q \quad \boldsymbol{k}_i = \boldsymbol{x}_i \boldsymbol{W}^K \quad \boldsymbol{v}_i = \boldsymbol{x}_i \boldsymbol{W}^V \in \mathbb{R}^d$

Stacking N input vectors: $\boldsymbol{Q} = \boldsymbol{X}\boldsymbol{W}^Q \quad \boldsymbol{K} = \boldsymbol{X}\boldsymbol{W}^K \quad \boldsymbol{V} = \boldsymbol{X}\boldsymbol{W}^V \in \mathbb{R}^{N \times d}$

$$\boldsymbol{X} = \begin{bmatrix} \text{——} & \boldsymbol{x}_1 & \text{——} \\ \text{——} & \boldsymbol{x}_2 & \text{——} \\ \cdots & \cdots & \cdots \\ \text{——} & \boldsymbol{x}_N & \text{——} \end{bmatrix}$$

UNIVERSITY of VIRGINIA

Parallel Computation of Attention

Attention computation can also be written in matrix form

Compute attention for one word: $\boldsymbol{a}_i = \mathrm{Softmax}\left(\frac{\boldsymbol{q}_i \cdot \boldsymbol{k}_j}{\sqrt{d}}\right) \cdot \boldsymbol{v}_j$

Compute attention for one N words: $\boldsymbol{A} = \mathrm{Softmax}\left(\frac{\boldsymbol{Q}\boldsymbol{K}^\top}{\sqrt{d}}\right) \boldsymbol{V}$

Attention matrix

N

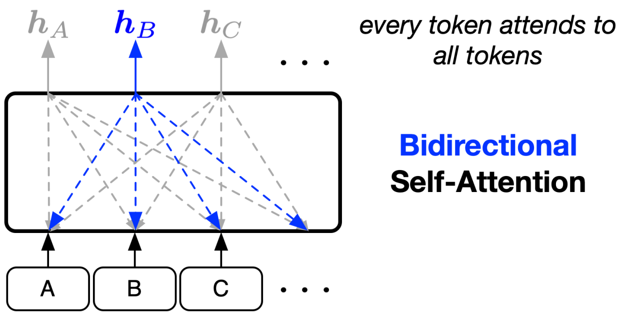
q1•k1	q1•k2	q1•k3	q1•k4
q2•k1	q2•k2	q2•k3	q2•k4
q3•k1	q3•k2	q3•k3	q3•k4
q4•k1	q4•k2	q4•k3	q4•k4

N

Figure source: https://web.stanford.edu/~jurafsky/slp3/9.pdf

Bidirectional vs. Unidirectional Self-Attention

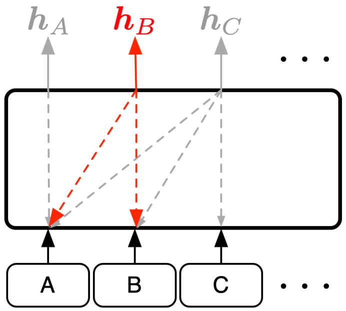
- Self-attention can capture different context dependencies
- **Bidirectional** self-attention:
  - Each position to attend to all other positions in the input sequence
  - Transformers with bidirectional self-attention are called Transformer **encoders** (e.g., BERT)
  - Use case: natural language understanding (NLU) where the entire input is available at once, such as text classification & named entity recognition



Bidirectional vs. Unidirectional Self-Attention

- Self-attention can capture different context dependencies
- **Unidirectional** (or **causal**) self-attention:
  - Each position can only attend to earlier positions in the sequence (including itself).
  - Transformers with unidirectional self-attention are called Transformer **decoders** (e.g., GPT)
  - Use case: natural language generation (NLG) where the model generates output sequentially

upper-triangle portion set to -inf



every token attends to its previous tokens

Unidirectional Self-Attention

N

q1·k1	$-\infty$	$-\infty$	$-\infty$
q2·k1	q2·k2	$-\infty$	$-\infty$
q3·k1	q3·k2	q3·k3	$-\infty$
q4·k1	q4·k2	q4·k3	q4·k4

N

Position Encoding

- Motivation: inject positional information to input vectors

$$\boldsymbol{q}_i = \boldsymbol{x}_i \boldsymbol{W}^Q \quad \boldsymbol{k}_i = \boldsymbol{x}_i \boldsymbol{W}^K \quad \boldsymbol{v}_i = \boldsymbol{x}_i \boldsymbol{W}^V \in \mathbb{R}^d$$

$$\boldsymbol{a}_i = \mathrm{Softmax}\left(\frac{\boldsymbol{q}_i \cdot \boldsymbol{k}_j}{\sqrt{d}}\right) \cdot \boldsymbol{v}_j$$

When $\boldsymbol{x}$ is word embedding, $\boldsymbol{q}$ and $\boldsymbol{k}$ do not have positional information!

- How to know the word positions in the sequence? Use position encoding!

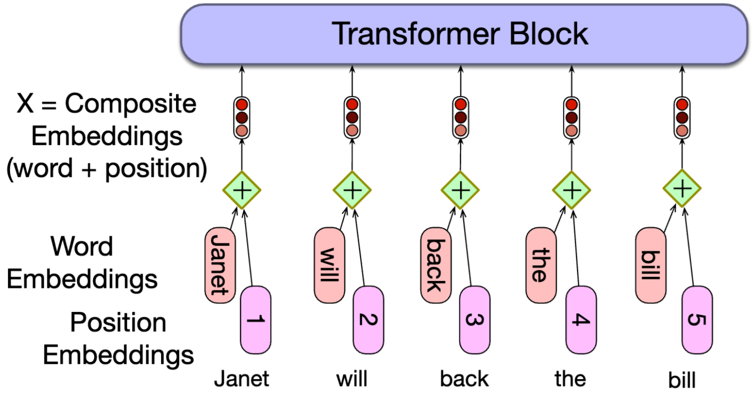


Figure source: https://web.stanford.edu/~jurafsky/slp3/9.pdf

Position Encoding Methods

- Absolute position encoding (the original Transformer paper)
  - Learn position embeddings for each position
  - Not generalize well to sequences longer than those seen in training
- Relative position encoding (Self-Attention with Relative Position Representations)
  - Encode the relative distance between words rather than their absolute positions
  - Generalize better to sequences of different lengths
- Rotary position embedding (RoFormer: Enhanced Transformer with Rotary Position Embedding)
  - Apply a rotation matrix to the word embeddings based on their positions
  - Incorporate both absolute and relative positions
  - Generalize effectively to longer sequences
  - Widely-used in latest LLMs

Summary: Transformer

- Motivation: weigh the importance of different words in a sequence when processing a specific word
- Implementation: represent each word with three vectors:
  - Query: the current word that seeks information
  - Key: context word to be retrieved information from
  - Value: semantic content to be aggregated as the new word representation
- Allow parallel computation of all input words
- Usually deployed with multiple heads to capture various linguistic relationships
- Can be either unidirectional (only attend to previous words) or bidirectional (attend to all words)
- Need to use position encodings to inject positional information

Limitations: Transformer

- Quadratic Complexity wrt Sequence Length:
  - self-attention has a quadratically complexity with the sequence length
  - processing long sequences is extremely compute & memory expensive
- Interpretability & Explainability:
  - complex architecture with many layers and attention heads (totaling billions of parameters)
  - difficult to understand how they arrive at their predictions & debug
- Positional Encoding:
  - the original Transformer paper adopts manually-defined position encodings – likely suboptimal
  - follow-up works propose advance position encoding methods to enhance expressiveness

Thank You!

Yu Meng
University of Virginia
yumeng5@virginia.edu