Sequence modeling

Armand Joulin

Google DeepMind
ajoulin@google.com

Why?

- Example of temporal sequences:
  - videos
  - robot moving in an environment
  - video games...

...but first an introduction to language modeling

What is language modeling

- **Language modeling** assigning probability to a text
- A text is a sequence of tokens
- tokens can be words, characters or group of characters.
- For example:

$$\{\text{a cat}\} \quad = \quad \{\text{a}, \text{cat}\},$$

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\end{aligned}
$$

- For most of this lecture, we assume that tokens are words

What is language modeling

- Given a sequence $\{w_1, \ldots, w_T\}$ of tokens, a language model estimates its probability:

$$P(w_1, \ldots, w_T)$$

- P depends on a **vocabulary**, i.e., the set of unique tokens.

- P can be conditioned on an external variable, i.e., $P(.) = P(. \mid C)$

Applications of language modeling

Language models are applied in several fields:

- Speech recognition:

$$P(\text{"Vanilla, I scream"}) < P(\text{"Vanilla ice cream"}).$$

- Machine translation:

$$P(\text{"Déçu en bien"} \mid \text{"Pleasantly surprised"}) \quad < \\ P(\text{"Agréablement surpris"} \mid \text{"Pleasantly surprised"})$$

- Optical Character Recognition:

$$P(\text{"m0ve fast"}) < P(\text{"move fast"})$$

Applications of language modeling

- Language models are just models of sequences
- they can apply to any sequence, like video or audio

Probabilistic language model

- Sequence probability as a product of token probabilities:

$$P(w_1, \ldots, w_T) = \prod_{t=1}^{T} P(w_t \mid w_{t-1}, \ldots, w_1)$$

Probabilistic language model

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$$P(a, b) = P(a)P(b \mid a)$$

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- Language models estimate probability of upcoming token given past:

$$P(w_t \mid w_{t-1}, \ldots, w_1).$$

Preliminaries: words as vectors

- We assume a fixed vocabulary of V words
- we represent the i-th word by a V dimensional vector $\mathbf{w}_i$:

$$\mathbf{w}_i[j] = \begin{cases} 1 & \text{if } j = i, \\ 0 & \text{otherwise} \end{cases}$$

- These word vectors are:
    - independent: $\mathbf{w}_i^T \mathbf{w}_j = 0$ if $i \neq j$
    - normalized: $\mathbf{w}_i^T \mathbf{w}_i = 1$
- We call this representation "one-hot vectors"
- For now on, the notation $\mathbf{w}_t$ represents the one-hot vector of the word at the t-th position in the sentence

A linear model for bigrams

- The input is the 1-hot vector of the previous word: $\mathbf{x}_t = \mathbf{w}_{t-1}$
- The output is the 1-hot vector of the upcoming word: $y_t = \mathbf{w}_t$

- **Linear model $\mathbf{z} = \mathbf{A}\mathbf{x}$**
- Build a probability over all possible words:

$$f(\mathbf{y},\ \mathbf{z})[k] = \frac{\exp(\mathbf{z}[k])}{\sum_{i=1}^{V} \exp(\mathbf{z}[i])}$$

- A cross-entropy loss: $\ell(\mathbf{q}, \mathbf{p}) = -\mathbf{q}^T \log(\mathbf{p})$
- Learning a linear bigram model is equivalent to:

$$\min_{\mathbf{A} \in \mathbb{R}^{V \times V}} \ \frac{1}{T} \sum_{t=1}^{T} \ell(\mathbf{y}_t, f(\mathbf{A}\mathbf{x}_t))$$

Limitations of linear models

$$\min_{\mathbf{A}\in\mathbb{R}^{V\times V}} \frac{1}{T}\sum_{t=1}^{T}\ell(\mathbf{y}_t, \mathbf{A}\mathbf{x}_t)$$

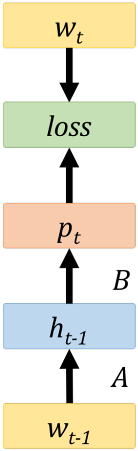
- The matrix **A** is $O(V^2)$
- Example: $V = 10\text{k} \rightarrow 100,000,000$ parameters
- Difficult and slow to scale to longer *n*-grams

Neural bigram model

- feedforward network:

$$\begin{aligned}\mathbf{h}_{t-1} &= \sigma(\mathbf{A}\mathbf{w}_{t-1})\\ \mathbf{p}_t &= f(\mathbf{B}\mathbf{h}_{t-1})\end{aligned}$$

$\sigma(x) = 1/(1+\exp(-x))$ pointwise sigmoid function



- $\mathbf{A}$: $V \times H$ matrix; $\mathbf{B}$: $H \times V$ matrix
- $H << V$
- Minimization problem:

$$\min_{\mathbf{A},\,\mathbf{B}} \frac{1}{T}\sum_{t=1}^{T} \ell(\mathbf{w}_t, f(\mathbf{B}\sigma(\mathbf{A}\mathbf{w}_{t-1})))$$

Neural *n*-gram model

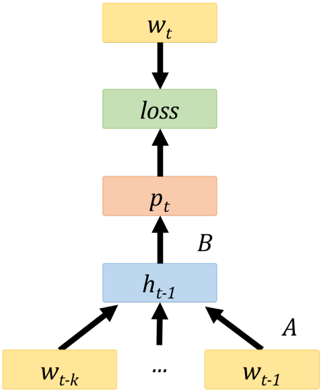
Generalization to any fixed *n*-gram:

- The input is the contactenation of previous words:

$$\mathbf{x}_t = [\mathbf{w}_{t-n+1}, \ldots, \mathbf{w}_{t-1}]$$

- **A**: $nV \times H$ matrix
- Minimization problem:

$$\min_{\mathbf{A},\ \mathbf{B}} \frac{1}{T} \sum_{t=1}^{T} \ell(w_t, f(\mathbf{B}\sigma(\mathbf{A}\mathbf{x}_t)))$$

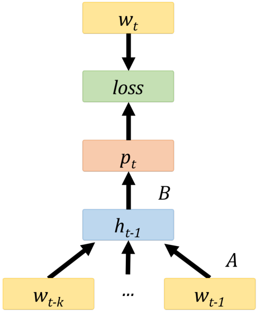


Recurrent Neural Network

- Recurrent network: Keep memory of past in the hidden variables

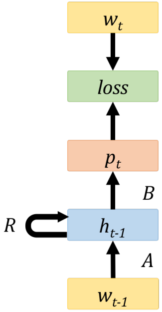
Feedforward

$$\mathbf{h}_{t-1} = \sigma\left(\mathbf{A}[\mathbf{w}_{t-k}, \ldots, \mathbf{w}_{t-1}]\right)$$
$$\mathbf{p}_t = f(\mathbf{B}\mathbf{h}_{t-1})$$

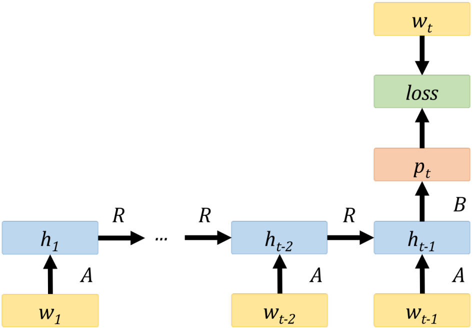


Recurrent Network

$$\mathbf{h}_{t-1} = \sigma\left(\mathbf{A}\mathbf{w}_{t-1} + \mathbf{R}\mathbf{h}_{t-2}\right)$$
$$\mathbf{p}_t = f(\mathbf{B}\mathbf{h}_{t-1})$$

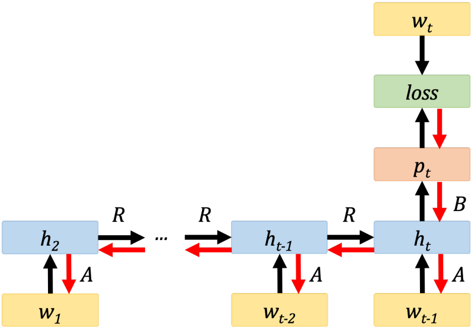


Recurrent Neural Network



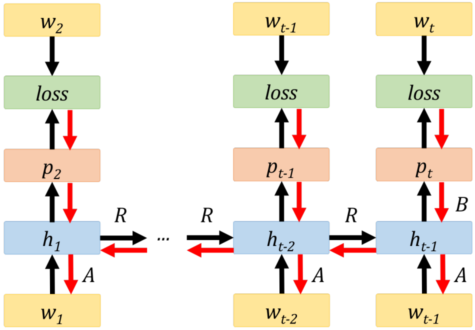
- Recurrent equation: $\mathbf{h}_t = \sigma\left(\mathbf{A}[\mathbf{h}_{t-1}, \mathbf{w}_t]\right)$
- Unfold over time: **very deep feedforward with weight sharing**
- Potentially capture long term dependencies

Recurrent Neural Network: training



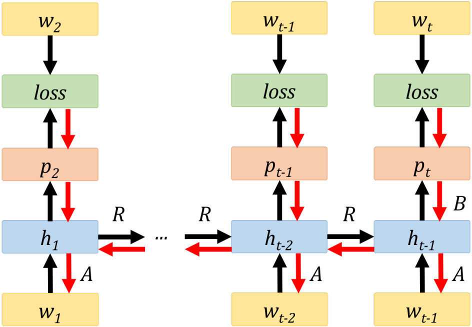
- **Backpropagation through time (BPTT)**: same as backpropagation through a very deepfeedforward network

Recurrent Neural Network: training



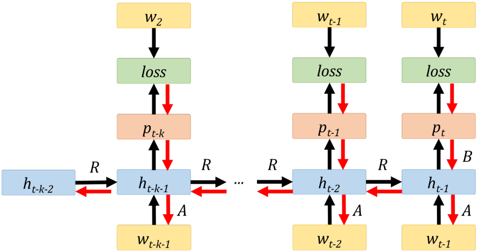
- **batch BPTT**: forward/backward for many words simultaneously

Recurrent Neural Network: training



- **Problem with BPTT**: Computing 1 gradient is $O(T)$. Too slow.

Recurrent Neural Network: training



- **Truncated BPTT**: Go back in time for k step: $O(k)$.

Transformer Networks

Motivation

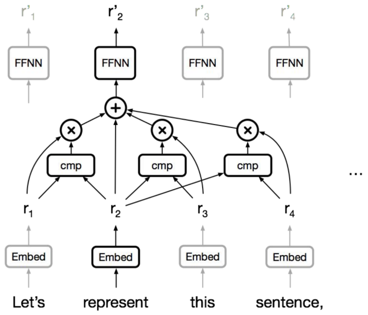
- In recurrent networks, we have

$$\mathbf{h}_t = f(\mathbf{h}_{t-1}, w_t).$$

- RNNs encode the whole history in single vector $\mathbf{h}_{t-1}$
- Instead, can we use all token representations to compute $\mathbf{h}_t$?
- Technical challenge:

  need to combine a variable number of representations!

Convolutional Neural Networks?



- Pros
  - easy to parallelize
  - exploits local context
- Cons
  - span of context increase linearly with number of layers
  - need to be very deep to have large context

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from Vaswani and Huang:
`http://web.stanford.edu/class/cs224n/slides/`

Combining vectors with attention

- Solution: use the (self) attention mechanism
- Given a set of vectors $\mathbf{w}_1$, ..., $\mathbf{w}_T \in \mathbb{R}^d$ representing tokens

$$\mathbf{h}_t = \sum_{i=1}^{T} a_{it} \mathbf{V} \mathbf{w}_i$$

  where $\sum_{i=1}^{T} a_{it} = 1$.
- We could use $a_{it} = \frac{1}{T}$ and get a BoW

Combining vectors with attention

- Introducing matrix $\mathbf{W} \in \mathbb{R}^{d \times T}$ where columns correspond to $\mathbf{w}_i$,

$$\mathbf{h}_t = \mathbf{V}\mathbf{W}\mathbf{a}_t$$

- And finally

$$\mathbf{H} = \mathbf{V}\mathbf{W}\mathbf{A}$$

Combining vectors with attention

- How to compute the matrix $\mathbf{A}$?

$$\mathbf{A} = \text{softmax}(\mathbf{W}^\top \mathbf{K}^\top \mathbf{Q} \mathbf{W})$$

  where the softmax is applied column-wise.

- Why softmax? to get positive entries, and columns summing to 1.
- Why $\mathbf{W}^\top \mathbf{K}^\top \mathbf{Q} \mathbf{W}$? Bilinear form over the input

Combining vectors with attention

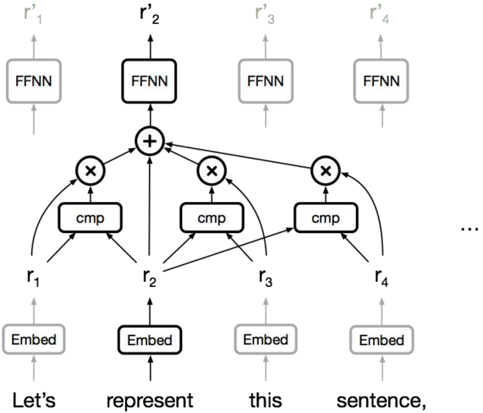
- Putting everything together:

$$\mathbf{H} = \mathbf{V}\mathbf{W}\text{softmax}(\mathbf{W}^\top \mathbf{K}^\top \mathbf{Q}\mathbf{W})$$

  where $\mathbf{H}, \mathbf{W} \in \mathbb{R}^{d \times T}$ and $\mathbf{V}, \mathbf{K}, \mathbf{Q} \in \mathbb{R}^{d \times d}$
- $\mathbf{V}, \mathbf{K}, \mathbf{Q}$ are parameters to be learned.
- This operation is called self-attention

- It can be generalized to multiple heads:
  - Split input vectors into n subvectors of dimension d/n,
  - Apply self attention (with different $\mathbf{V}, \mathbf{K}, \mathbf{Q}$) over these smaller vectors
  - Concatenate the results to get back d dimensional vectors

Combining vectors with attention



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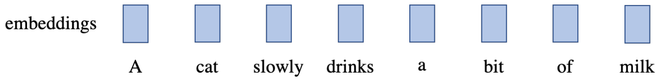
Combining vectors with attention

- Goal: use all the context to update a word
- Idea: look for the most important words in the context
- Solution: self-attention on the sequence of inputs

Combining vectors with attention



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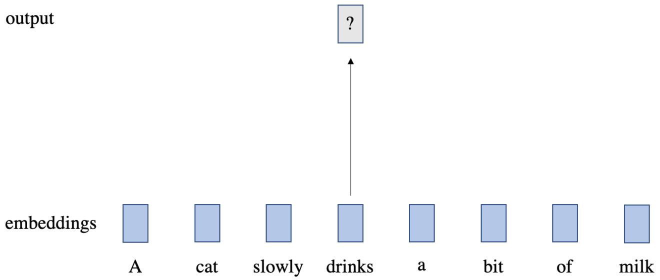

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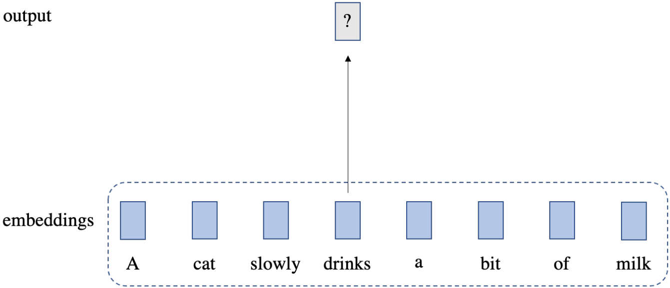

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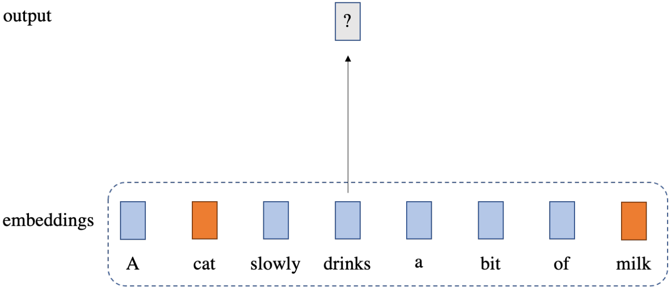

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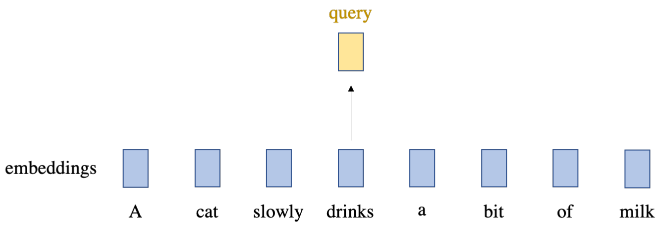

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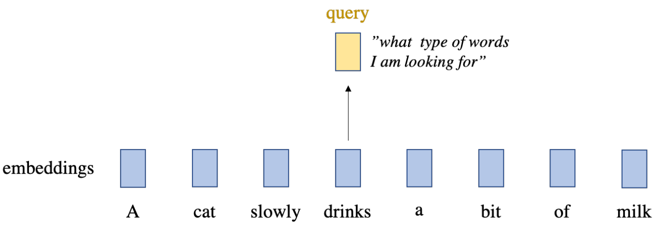

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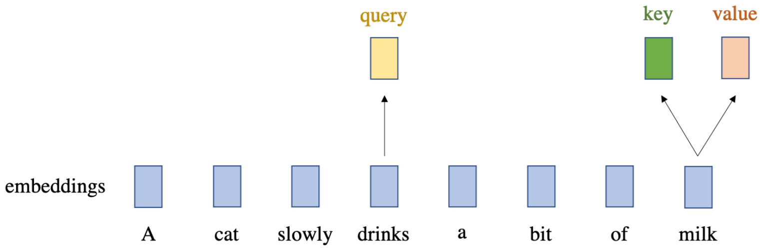

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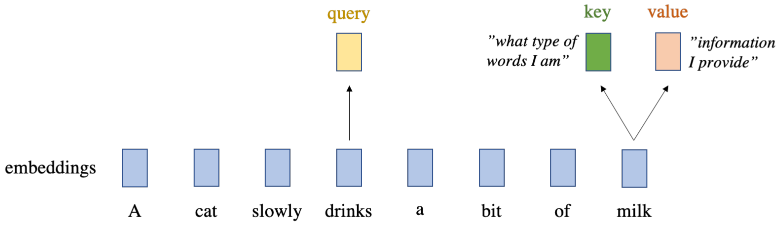

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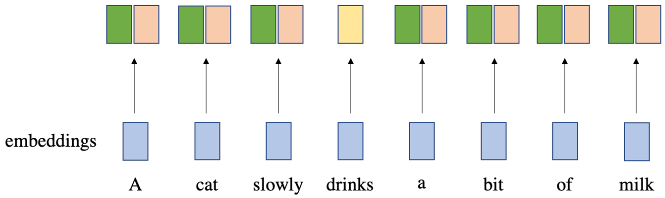

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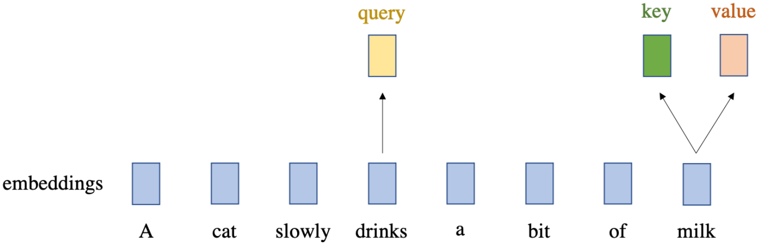

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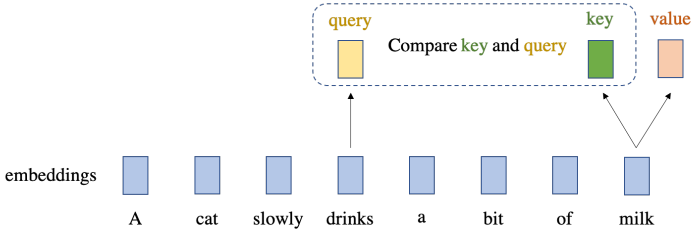

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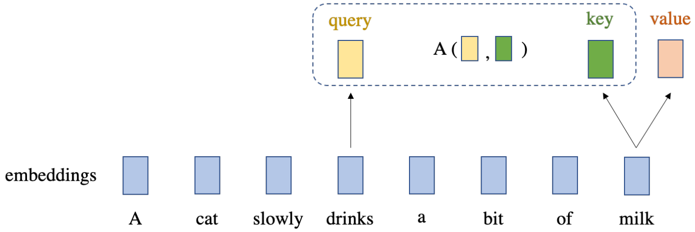

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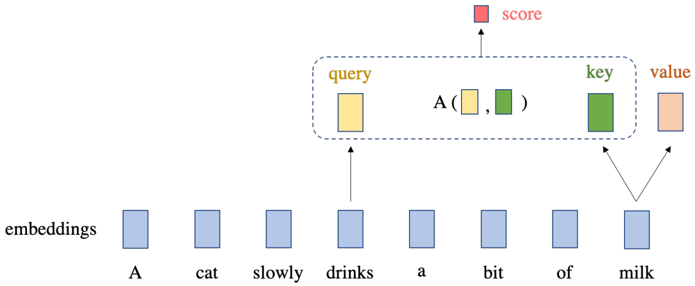

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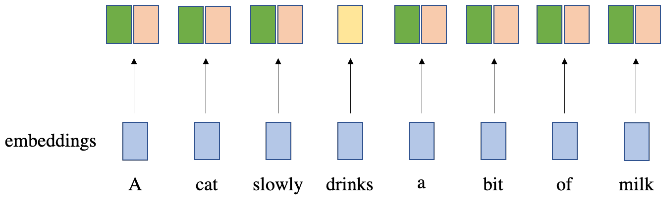

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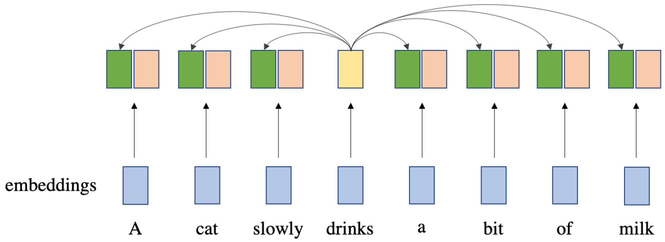

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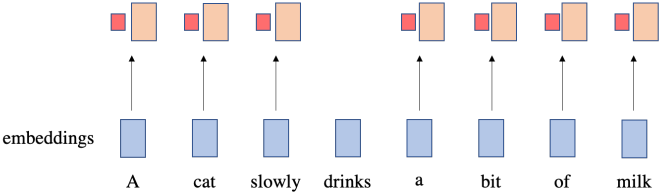

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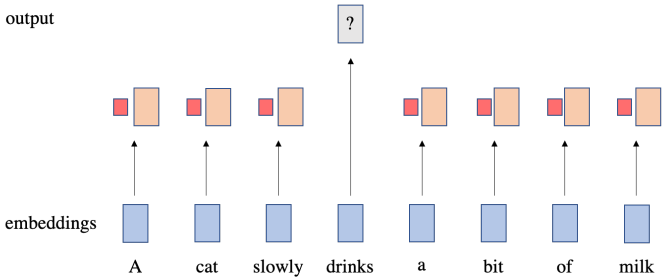

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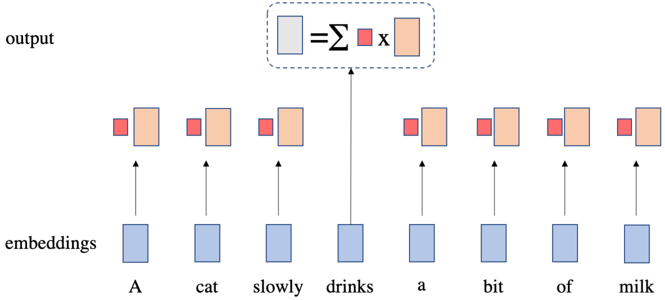


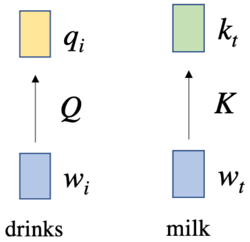
Combining vectors with attention

- "query vector" for word i ("drinks"):

$$\mathbf{q}_i = \mathbf{Q}\mathbf{w}_i$$

- "key vector" for word t ("milk"):

$$\mathbf{k}_t = \mathbf{K}\mathbf{w}_t$$



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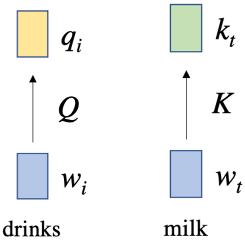
- Their similarity score is then:

$$s_{it} = \mathbf{q}_i^\top \mathbf{k}_t$$



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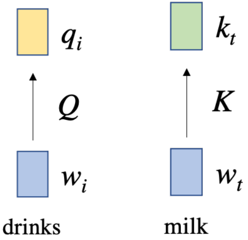
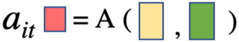
- Normalize over sequence with softmax:

$$a_{it} = \frac{\exp(s_{it})}{\sum_k \exp(s_{ik})}$$

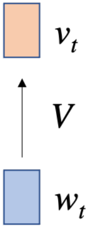




Combining vectors with attention

- "value vector" for word t ("milk"):

$$\mathbf{v}_t = \mathbf{V}\mathbf{w}_t$$



Combining vectors with attention

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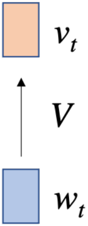
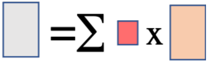


- Finally, compute output for "drinks":

$$\mathbf{y}_i = \sum_t a_{it}\mathbf{v}_t$$



Transformer network

Transformer block:

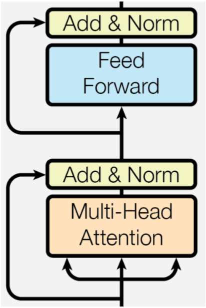
- Multi-head attention layer with skip connection and normalization
- Followed by feed forward with skip connection and normalization

Skip connection+normalization:

- Given a network block **nn** and input **x**
- The output **y** is computed as

$$\mathbf{y} = \mathbf{norm}(\mathbf{x} + \mathbf{nn}(\mathbf{x}))$$

where **norm** normalize the input



Vaswani et al. (2017)

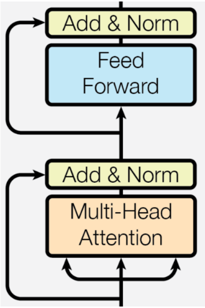
Transformer network

Feed forward block

- Two layer network, with ReLU activation

$$\mathbf{y} = \mathbf{W}_2 \texttt{ReLU}(\mathbf{W}_1 \mathbf{x})$$

- Usually, $\mathbf{W}_1 \in \mathbb{R}^{4d \times d}$ and $\mathbf{W}_2 \in \mathbb{R}^{d \times 4d}$
- i.e. hidden layer of dimension $4d$.



Vaswani et al. (2017)

Position embeddings

- **Limitation:** self attention does not take position into account!
- Indeed, shuffling the input gives the same results

- **Solution:** add position encodings.
- Replace the matrix $\mathbf{W}$ by $\mathbf{W} + \mathbf{E}$, where $\mathbf{E} \in \mathbb{R}^{d \times T}$

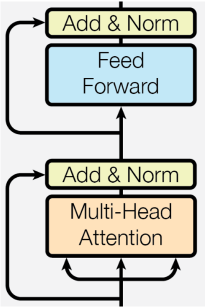
- $\mathbf{E}$ can be learned, or defined using sin and cos:

$$e_{2i,j} = \sin\left(\frac{j}{10000^{2i/d}}\right)$$
$$e_{2i+1,j} = \cos\left(\frac{j}{10000^{2i/d}}\right)$$

Transformer network: take away

Transformer network:

- Token embeddings + Position embeddings
- Then N transformer blocks (e.g. $N = 12$)
- Softmax classifier



Vaswani et al. (2017)

References I

Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., Kaiser, L., and Polosukhin, I. (2017). Attention is all you need. In *Advances in Neural Information Processing Systems*, pages 5998–6008.