Language Modeling and Sentence Representation

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- Applications of sentence representation
 - question answering
 - fact checking
 - anything where we need to compare sentences

Plan of this lecture

- Language modeling:
 - Pre-deep learning
 - Standard neural Networks
 - Recurrent neural networks
- Sentence representation
 - BiLSTM
 - Transformer network
 - BERT

Slides on $\emph{n}\text{-}$ grams are inspired by Dan Jurafsky's class https://web.stanford.edu/class/cs124/lec/

Introduction to language modeling

• Language modeling: learning a probability distribution of text

• Speech into text:

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P("Vanilla ice cream") or P("Vanilla, I scream")?

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• Image to text:



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$$a cat = \{a, cat\}, \quad (words)$$

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• For example:

$$\label{eq:acat} \begin{array}{ll} \mbox{a cat} &= \{\mbox{a,cat}\}, & \mbox{(words)} \\ &= \{\mbox{a, ,c,a,t}\}, & \mbox{(characters)} \end{array}$$

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

- text = sequence of tokens = $\{w_1, \dots, w_T\}$
- A language model estimates its probability: $P(w_1, ..., w_T)$

Sequence probability as a product of token probabilities:

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Recursively applied to a sequence:

$$P(w_1, w_2, w_3) = P(w_1)P(w_2, w_3 \mid w_1)$$

= $P(w_1)P(w_2 \mid w_1)P(w_3 \mid w_2, w_1).$

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• Language model = learn probability of upcoming token given past:

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

- The probability $P(w_t \mid w_{t-1}, \dots, w_1)$ depends on a vocabulary
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- vocabulary = the set of all unique tokens.
- Naively, the bigger a vocabulary is, the less probable a token is.
- Example: P("car" | I'm driving a") = ?
 - 1 if vocabulary contains "car" but not "moto"
 - 0.5 if vocabulary contains "car" and "moto".

n-gram language models

Idea:

text is discrete \rightarrow count occurences of words to form probabilities

- Advantages:
 - no learning, efficient and simple
 - does not require a lot of computational resources
 - works well in practice

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- Count how many times a sequence of tokens occurs in dataset.
- Compute probability from this count:

$$P(w_{t} \mid w_{t-1}, \dots, w_{1}) = \frac{P(w_{1}, \dots, w_{t})}{P(w_{1}, \dots, w_{t-1})}$$
$$= \frac{c(w_{1} \cdots w_{t})}{c(w_{1} \cdots w_{t-1})}$$

 $c(w_1 \cdots c_T)$ is the number of occurences of the sequence $w_1 \cdots w_T$

Example:

Sentence "The moment one learns English" appears 35 in dataset Sentence "The moment one learns" appears 75 in dataset

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$$P(\text{English} \mid \text{The moment one learns}) = \frac{c(\text{The moment one learns English})}{c(\text{The moment one learns})}$$
$$= \frac{35}{73} = 0.48$$

Limitiations of count based language model

- Number of unique sentences increases with dataset size,
- Long sentences are rare: no good statistics for them
- → Too many sentences with not enough statistics

- Solution: truncate past to a fixed size window
- For example:

$$P(\text{English} \mid \text{The moment one learns}) \approx P(\text{English} \mid \text{one learns})$$

- Implicit assumption: most important information about a word is in its recent history
- **Beware!** In general:

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

- Truncated count based models = n-gram models
- "n" refers to the size of past
- Examples:
 - Unigram:

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

Bigram:

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

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• Bigram:

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Count based language model: unigram

Probability of a sentence with a unigram model:

$$P_U(w_1,...,w_T) = \prod_{t=1}^T P(w_t) = \prod_{t=1}^T \frac{c(w_t)}{N}$$

N = total number of tokens in dataset $c(w_t) = \text{number of occurences of } w_t \text{ in dataset}$

- Unigram only uses word frequency
- Example of text generation with this model:
 the or is ball then car

Count based language model: bigram

Probability of a sentence with a bigram model:

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

 $c(w_{t-1}w_t)$ = number of occurrences of sequence $w_{t-1}w_t$

Predict a word just with the previous word

Count based language model: bigram

• Example of text generation with bigram model:

new car parking lot of the

- "car" is generated from "new", "parking" from "car"...
- But "new" has no influence on "parking"

- Simple to extend to longer dependencies: trigrams, 4-grams...
- n-grams can be "good enough" in some cases
- But n-grams cannot capture long term dependencies required to truely model language

Bigram:

$$P(w_t \mid w_{t-1}) = \frac{c(w_{t-1}w_t)}{c(w_{t-1})}$$

Dataset:

<s>we sat in the house
<s>we sat here we two and we said
<s>how we wish we had something to do

Extract some probabilities:

$$P(sat \mid we) = 0.33, \ P(wish \mid we) = 0.17, \ P(in \mid sat) = 0.5$$

- $\langle s \rangle =$ token for beginning of sentence; $P(\langle s \rangle) = 1$.
- Compute sentence probability with them

- Extract count from Berkeley Restaurant dataset (9222 sentences)
- Unigram counts:

i	want	to	eat	chinese	food	lunch	spend
2533	927	2417	746	158	1093	341	278

• Bigram counts:

	i	want	to	eat	chinese	food	lunch	spend
i	5	827	0	9	0	0	0	2
want	2	0	608	1	6	6	5	1
to	2	0	4	686	2	0	6	211
eat	0	0	2	0	16	2	42	0
chinese	1	0	0	0	0	82	1	0
food	15	0	15	0	1	4	0	0
lunch	2	0	0	0	0	1	0	0
spend	1	0	1	0	0	0	0	0

 The bigram probabilities are obtained by dividing the bigram counts with the unigram counts:

$$P(w_2 \mid w_1) = \frac{c(w_1 w_2)}{c(w_1)}$$

Resulting bigram probabilities:

	i	want	to	eat	chinese	food	lunch	spend
i	0.022	0.33	0	0.036	0	0	0	0.00079
want	0.0022	0	0.66	0.0011	0.0065	0.0065	0.0054	0.0011
to	0.00083	0	0.0017	0.28	0.00083	0	0.0025	0.087
eat	0	0	0.0027	0	0.021	0.0027	0.056	0
chinese	0.0063	0	0	0	0	0.52	0.0063	0
food	0.014	0	0.014	0	0.00092	0.0037	0	0
lunch	0.0059	0	0	0	0	0.0029	0	0
spend	0.0036	0	0.0036	0	0	0	0	0

• Example:

$$P(\langle s \rangle \text{ i want chinese food})$$
?

$$\langle s \rangle =$$
 token for beginning of sentence; $P(\langle s \rangle) = 1$.

Result:

$$P(<\text{s}>\text{i want chinese food}) = P(<\text{s}>)P(\text{i}|<\text{s}>)P(\text{want}|\text{i})P(\text{chinese}|\text{want})P(\text{food}|\text{chinese})$$

$$=1\times.25\times0.33\times0.0065\times0.52$$

$$=0.00027885$$

	i	want	to	eat	chinese	food	lunch	spend
i	0.022	0.33	0	0.036	0	0	0	0.00079
food	0.014	0	0.014	0	0.00092	0.0037	0	0
lunch	0.0059	0	0	0	0	0.0029	0	0
spend	0.0036	0	0.0036	0	0	0	0	0

• Example:

$$P(\langle s \rangle \text{ i bring my lunch to work})$$
?

Result:

$$P(~~i bring my lunch to work) = $P(~~) \dots P(to|lunch) \dots~~$
= $1 \times \dots \times 0 \times \dots$
= 0~~$$

Does not generalize well!

Simple fix = Add 1 to each bigram count

	i	want	to	eat	chinese	food	lunch	spend
i	6	828	1	10	1	1	1	3
want	3	1	609	2	7	7	6	2
to	3	1	5	687	3	1	7	212
eat	1	1	3	1	17	3	43	1
chinese	2	1	1	1	1	83	2	1
food	16	1	16	1	2	5	1	1
lunch	3	1	1	1	1	2	1	1
spend	2	1	2	1	1	1	1	1

• Laplace-smoothed bigrams:

$$\frac{c(w_iw_j)+1}{c(w_i)+V},$$

where V = vocabulary size

Estimating *n*-gram probabilites

- Add mass to unrealistic bigram ("to to").
- Decrease probability of realistic bigram by factor V.
- Example: $P(\text{want} \mid i)$ decreases from 0.33 to 0.21!
- ightarrow Add-1 is not good in practice

Backoff and Interpolation

- If no good statistics on long context: use shorter context
- Backoff: use trigram if enough data, else backoff to bigram.
- Interpolation: mix statistics of trigram, bigram and unigram.
- In practice interpolation works better

Backoff model

- Backoff estimates probability with longest reliable available *n*-gram
- It backs off through shorter and shorter *n*-grams until one is reliable
- Examples:
 - Katz's smoothing (Katz, 1987)
 - Stupid backoff model (Brants et al., 2007)

Stupid backoff

- A n-gram is reliable if it appears in the dataset
- If $c(w_{t-n+1}\cdots w_t) > 0$:

$$P_{bo}(w_t \mid w_{t-n+1}, \dots, w_{t-1}) = \frac{c(w_{t-n+1} \cdots w_t)}{c(w_{t-n+1} \cdots w_{t-1})}.$$

• else backoff to (n-1)gram:

$$P_{bo}(w_t \mid w_{t-n+1}, \dots, w_{t-1}) = 0.4 P_{bo}(w_t \mid w_{t-n+2}, \dots, w_{t-1})$$

- Apply recursively until a existing n-gram is found
- **Problem:** probabilities do not sum to 1!
- But works well with a lot of data

Linear Interpolation

Simple linear interpolation:

$$P_{L}(w_{t} \mid w_{t-1}, w_{t-2}) = \lambda_{1} P(w_{t} \mid w_{t-1}, w_{t-2}) + \lambda_{2} P(w_{t} \mid w_{t-1}) + \lambda_{3} P(w_{t})$$

Conditioned interpolation:

$$P_{L}(w_{t} \mid w_{t-1}, w_{t-2}) = \lambda_{1}(w_{t-1}, w_{t-2})P(w_{t} \mid w_{t-1}, w_{t-2}) + \lambda_{2}(w_{t-1}, w_{t-2})P(w_{t} \mid w_{t-1}) + \lambda_{3}(w_{t-1}, w_{t-2})P(w_{t})$$

Kneser-Ney Smoothing (advanced)

- Cover most popular n-gram model: Kneser-Ney Smoothing
- Very efficient, run on CPUs. Best performing *n*-gram model,
- Available in many standard libraries: https://kheafield.com/code/kenlm/estimation/

Kneser-Ney Smoothing (advanced)

- Kneser-Ney is a recursive interpolation model
- The probability of a *n*-gram is:

$$P_{KN}(w_t \mid w_{t-n+1}^{t-1}) = f_{KN}(w_{t-n+1}^t) + \lambda(w_{t-n+1}^{t-1}) P_{KN}(w_t \mid w_{t-n+1}^{t-2})$$
 where $w_{t-n+1}^t = w_{t-n+1} \cdots w_t$.

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 where $w_{t-n+1}^t = w_{t-n+1} \cdots w_t$.

Recursively unroll to get the explicit probability:

$$P_t = f_t + \lambda_t P_{t-1}$$

$$= f_t + \lambda_t (f_{t-1} + \lambda_{t-1} P_{t-2})$$

$$= f_t + \lambda_t f_{t-1} + \dots + \prod_{k=0}^t \lambda_k P_0$$

Kneser-Ney Smoothing: absolute discount

$$P_{KN}(w_t \mid w_{t-n+1}^{t-1}) = f_{KN}(w_{t-n+1}^t) + \lambda(w_{t-n+1}^{t-1}) P_{KN}(w_t \mid w_{t-n+1}^{t-2})$$

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• The contribution of the current *n*-gram is:

$$f_{KN}(w_{t-n+1}^t) = \frac{\max(c(w_{t-n+1}^t) - d, 0)}{c(w_{t-n+1}^{t-1})}$$

where $d \leq 1$ is discount factor

Kneser-Ney Smoothing: absolute discount

$$P_{KN}(w_t \mid w_{t-n+1}^{t-1}) = f_{KN}(w_{t-n+1}^t) + \lambda (w_{t-n+1}^{t-1}) P_{KN}(w_t \mid w_{t-n+1}^{t-2})$$

λ is the interpolation weight:

$$\lambda(w_{t-n+1}^{t-1}) = \frac{d}{c(w_{t-n+1}^{t-1})} \left| \left\{ w \mid c(w_{t-n+1}^{t-1}w) > 0 \right\} \right|$$

It depends on number of words that can appear after w_{t-n+1}^{t-1}

Kneser-Ney Smoothing: lower order distribution

• Let's consider the bigram case:

$$P_{KN}(w_t \mid w_{t-1}) = f_{KN}(w_{t-1} \mid w_t) + \lambda(w_{t-1})P_{KN}(w_t)$$

- How to define $P_{KN}(w_{t-1})$?
- Instead of unigram probability, define probability of unique context:

$$P_{KN}(w_t) = \frac{|\{w \mid c(w \mid w_t) > 0\}|}{|\{w, w' \mid c(w \mid w') > 0\}|}$$

This distribution sum to 1 too.

Open versus closed vocabulary

- Closed vocabulary:
 - The vocabulary of the train set covers the vocabulary of the test set
 - The size of the vocabulary V is fixed
- Open vocabulary:
 - Vocabulary of test set is different from vocabulary of train set
 - We have Out Of Vocabulary (OOV) words
 - Train set is big and test set has same distribution: OOVs are rare words

Training with OOVs

- OOVs do not appear in the training set
- → Need to simulate OOVs in the training set
 - Create a <UNK> token for unknown words
 - Replace the rare words in the training vocabulary to <UNK>
 - Rare words: words that appear less than some times (e.g. 10 times)
 - Your model will learn to predict <UNK> instead of rare words
 - Your vocabulary + < UNK > covers the test set.

Another alternative: subword segmentation

- Better solution to have a single model that works on open vocabulary:
- need to work at an another level than words
- character level works but is extremelly slow
- How to build bigger units than character with no UNK?
- This units should be at a subword level to cover new words

Subword: goal

- Building subword units by segmenting words into subparts
- wishlist for word segmentation algorithm:
 - open-vocabulary: encode all words through small vocabulary
 - encoding generalizes to unseen words
 - small sequence size (e.g., unlike character level)
 - good translation quality
- Current best solution: segmentation via byte pair encoding (BPE)

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 - 0. Split the vocabulary of a dataset at the character level
 - '[hey, hello, et]' \rightarrow 'h','e','y',' ','h','e','l','l','o',' ','e','t'

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 - 1. Compute frequencies of consecutive symbol pairs
 - $\{'h', 'e'\} = 2; \{'l', 'l'\} = 1;...$

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 - 2. replace most frequent consecutive symbol pair ('A','B') with 'AB'
 - merge 'h', 'e' into 'he'
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 - 3. repeat step 1-2 until desired dictionary size is reached

from Sennrich's class

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 - 3. repeat step 1-2 until desired dictionary size is reached
- Works as a preprocessing of the train set

from Sennrich's class

- For efficiency, we work on the vocabulary + word frequencies instead of the dataset
- Given a dataset, build vocabulary with count:

word	freq.
'low'	5
'lower	2
'newest'	6
'estate'	3

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- Given a dataset, build vocabulary with count:

freq.
5
2
6
3

- Split words into characters
- List of merges *M* = []

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- Given a dataset, build vocabulary with count:

word	freq.
'l o w '	5
'I o w e r $$	2
'n e w e s t $'$	6
'e s t a t e '	3

- Most frequent consecutive symbol pair: 'e s' with freq = 9
- List of merges *M* = []

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word	freq.
'l o w '	5
'I o w e r $$	2
'n e w es t $'$	6
'es t a t e '	3

- Merge 'e s' into 'es'
- List of merges $M = [\text{'e s'} \mapsto \text{'es'}]$

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'n e w est $'$	6
'est a t e $$ '	3

- Merge 'es t' into 'est'
- List of merges $M = [\text{'e s'} \mapsto \text{'es'}, \text{'es t'} \mapsto \text{'est'}]$

from Sennrich's class

Applying BPE preprocessing

Once the BPE codes are computed, we have a list of merges

$$M = [\text{'e s'} \mapsto \text{'es'}, \text{'es t'} \mapsto \text{'est'}, ...]$$

- Steps to preprocess a dataset with BPE codes:
 - 1. split dataset in sequence of characters
 - 2. apply the sequence of merges to the dataset to form BPE codes
- It is a deterministic process with a unique segmentation

BPE: pros and cons

- Pros:
 - Very simple
 - Models trained on BPE segmentations share information between words (e.g., prefix, suffix...)
 - BPE vocabulary is a best trade-off between vocabulary size and average sequence length
- Cons:
 - Characters are not necessarily in the final vocabulary \rightarrow no guarantees open vocabulary (still covers 99.9%)
 - Heuristic, does not work well for all train sets

Language models toolkits

Toolkits for standard *n*-grams based LM models

- SRILM: http://www.speech.sri.com/projects/srilm
- KenLM: https://kheafield.com/code/kenlm

All the *n*-gram models are implemented, simple to use and to deploy!

Evaluation for Language Modeling

- A standardized train/validation/test split
- A metric for model selection
- Build model on train, pick best model based on metric on validation

What is good metric for language modeling?

What is a good model?

- Best option: evaluate the model on a target downstream task
 - machine translation
 - speech recognition
 - ...
- Given two models, keep the one with best result on this task
- This is an **extrinsic** evaluation.

Extrinsic evaluation

Problems:

- Evaluation depends on many other components
- Time consuming
- May require several downstream tasks to assess quality of models

This is why we commonly use an intrinsic evaluation called perplexity

Intuition of Perplexity

With great power comes great _____

Model 1		Model 2		Model 3	
current responsability voltage	0.4	responsability responsabilities irresponsability	0.3	current	0.8 0.1 0.1

What is the best model?

Intuition of Perplexity

With great power comes great _____

Model 1		Model 2		Model 3	
current responsability voltage	0.4	responsability responsabilities irresponsability	0.3	current	0.8 0.1 0.1

What is the best model?

• Accuracy: 2 and 3

• Prec@2: 1, 2 and 3

Highest probability: 3

Best language model assigns highest probability to correct word

Definition of Perplexity

• The perplexity *PP* of a sentence $W = (w_1, ..., w_T)$ is:

$$PP(W) = P(w_1, ..., w_T)^{-\frac{1}{T}}$$

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

In the case of bigram model:

$$PP(W) = \prod_{t=1}^{T} P(w_t \mid w_{t-1})^{-\frac{1}{T}}$$

Perplexity and log likelihood

The logarithm of the perplexity is equal to:

$$\log PP(w) = \log \left(\prod_{t=1}^{T} P(w_t \mid w_{t-1}, \dots, w_1)^{-\frac{1}{T}} \right)$$
$$\log PP(W) = -\frac{1}{T} \sum_{t=1}^{T} \log P(w_t \mid w_{t-1}, \dots, w_1)$$

- It is the negative log-likelihood of the sequence
- In practice: use second expression, then take the exp Avoid numerical underflow

Example of Perplexity

	Unigram	Bigram	Trigram
PP	962	170	109

Lower perplexity means better model As expected, better model with longer *n*-grams

Count based language model

- n-gram based language model works well with "enough data"
- But does not generalize well
- Can we use machine learning instead?

Machine learning and language modeling

Machine learning for language model

- We have an evaluation setting for ML
- Can we cast language modeling as a machine learning problem?

Preliminaries

- Supervised classification:
 - Supervision: Each input X has a fixed given output Y
 - Classification: Y represents a class label among k possibilities
- Language modeling:
 - The input X is the subset of the previous tokens (w_1, \ldots, w_{t-1})
 - The output Y is the current token w_t
 - The token w_t is a class label among V possibilities
- ightarrow Language modeling is a supervised classification problem

Preliminaries: what loss function?

- Intrisic measure for language model: perplexity
- The log of the perplexity is the negative log-likelihood
- Minimizing **negative log-likelihood** optimizes for the right criterion!

• Assumption: fixed vocabulary of V words

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- Word i maps to a V-dimensional vector w_i:

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 - independent: $\mathbf{w}_i^T \mathbf{w}_j = 0$ if $i \neq j$
 - normalized: $\mathbf{w}_{i}^{T}\mathbf{w}_{i}=1$

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 - normalized: $\mathbf{w}_{i}^{T}\mathbf{w}_{i}=1$
- We call this representation "one-hot vectors"
- w_t = one-hot vector of word at t-th position in sentence

- Input = one-hot vector of previous word: $x_t = w_{t-1}$
- Output = one-hot vector of next word: $y_t = w_t$

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- Linear model z = Ax
- Build a probability over all possible words:

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

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• A cross-entropy loss: $\ell(q, p) = -q^T \log(p)$

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- A cross-entropy loss: $\ell(q, p) = -q^T \log(p)$
- Learning linear bigram model:

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

Pros of linear models over *n*-grams

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

- Can learn the same statistics as those in the *n*-gram models
- We can put additional features into x_t (e.g. from WordNet)
- Simple to implement

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

- The matrix A is $O(V^2)$
- ullet Example: Penn Treebank $V=10{
 m k}
 ightarrow 100,000,000$ parameters
- Difficult and slow to scale to longer n-grams

• What if we replace A by two smaller matrices B and C?

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Limitations of linear models

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with B and C^T of dimension $V \times K$ ($K \ll V$)?

- Bad: Not convex anymore, no guarantee on solution
- Good: fits in memory and faster to run!
- But if not convex: why are we keeping the model linear?

Neural bigram model

Feedforward network:

$$\begin{array}{rcl} {\sf h}_{t-1}&=&\sigma({\sf Aw}_{t-1})\\ &{\sf p}_t&=&f({\sf Bh}_{t-1})\\ \\ \sigma(x)=1/(1+\exp(-x)) \text{ pointwise sigmoid function} \end{array}$$

Neural bigram model

Feedforward network:

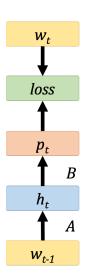
$$h_{t-1} = \sigma(Aw_{t-1})$$

$$p_t = f(Bh_{t-1})$$

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

- A: $V \times H$ matrix; B: $H \times V$ matrix
- H ≪ V
- Minimization problem:

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



Neural *n*-gram model

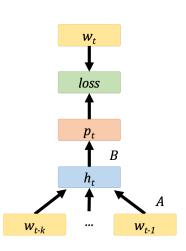
Generalization to any fixed *n*-gram size:

 The input is the contactenation of previous words:

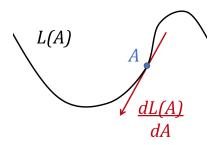
$$\mathbf{x}_t = [\mathbf{w}_{t-n+1}, \dots, \mathbf{w}_{t-1}]$$

- A: nV × H matrix
- Minimization problem:

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



Neural *n*-gram model: training



- Loss function: $L(A, B) = \frac{1}{T} \sum_{t=1}^{T} \ell(w_t, f(B\sigma(Ax_t)))$
- This loss is differentiable in A and B
- Minimize the loss by updating parameters in direction of the gradient

Neural *n*-gram model: training

- Gradient descent:
 - Compute full loss L(A, B)
 - Update parameters:

$$\mathsf{A} \leftarrow \mathsf{A} - \eta \frac{\partial L}{\partial \mathsf{A}}$$

- $\eta > 0$ is the learning rate
- Stochastic gradient descent (SGD):
 - Instead of gradient on the full loss L(A, B)
 - Randomly sample an example t
 - Partial loss

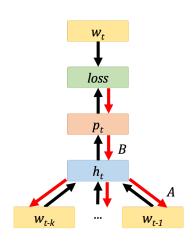
$$L_t(A, B) = \ell(y_t, f(B\sigma(Ax_t)))$$

Update parameters:

$$A \leftarrow A - \eta \frac{\partial L_t}{\partial A}$$

Computing the gradient with backpropagation

- Compute gradient with backpropagation
- Compute error made by network when predicting next word
- Propagate error back to all parameters in network



- We have $z = B\sigma(Ax)$ and p = f(z)
- Loss for one example: $\ell(w, p) = \ell(w, f(B\sigma(Ax)))$

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$$\frac{\partial \ell(w,p)}{\partial B} =$$

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Loss function:

$$\frac{1}{T} \sum_{t=1}^{T} \ell(\mathsf{w}_t, f(\mathsf{B}\sigma(\mathsf{Ax}_t)))$$

• The gradients are:

$$\frac{\partial L}{\partial B} = \frac{1}{T} \sum_{t=1}^{T} \frac{\partial \ell}{\partial z_t} \frac{\partial z_t}{\partial B}$$

$$\frac{\partial L}{\partial A} = \frac{1}{T} \sum_{t=1}^{T} \frac{\partial \ell}{\partial z_t} \frac{\partial z_t}{\partial h_t} \frac{\partial h_t}{\partial A}$$

with $z_t = Bh_t$ and $h_t = \sigma(Ax_t)$

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Intermediate computations shared between different gradients

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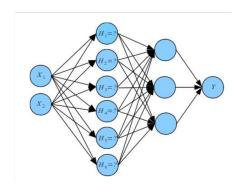
Intermediate computations shared between different gradients
 Backpropagation = chain rule + storing computation

- Specialized units cause overfitting
- Idea force model to work even when some units are removed
- Same as activation mask over units
- we replace h_t by:

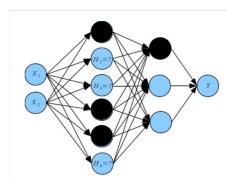
$$\hat{h}_t = h_t \odot m_t$$

where m_t is a binary mask vector.

This binary mask is randomly drawn for each time step

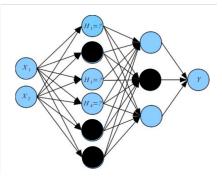


- Units are dropped:
 - with probability p.
 - independently
 - only during training



Iteration 1

- Units are dropped:
 - with probability p.
 - independently
 - only during training
- Dropped unit are in black



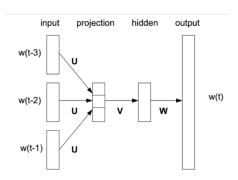
Iteration 2

- Units are dropped:
 - with probability p.
 - independently
 - only during training
 - Dropped unit are in black

Dealing with large vocabulary

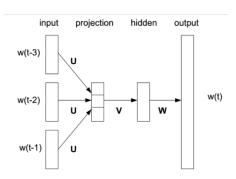
- At each time step, we compute probability over a vocabulary
- If the vocabulary size V is big, computing this probability is very slow
- Similar to text classification with large number of classes
- Solution: use class-based softmax (see prev. lecture)

The neural *n*-gram model from Bengio et al. (2003)



- Their model has one more hidden layer to embed one-hot vectors into low dimensional space
- Resulting vector Uw_t is a distributed word representation
- These representations are passed through a feedforward network

Neural *n*-gram model: example



• The equations are:

$$\begin{aligned} \mathbf{x}_{t-k} &= \sigma(\mathsf{U} \mathbf{w}_{t-k}) \\ \mathbf{h}_{t-1} &= \sigma(\mathsf{V}[\mathbf{x}_{t-3}, \mathbf{x}_{t-2}, \mathbf{x}_{t-1}]) \\ \mathbf{p}_t &= f(\mathsf{W} \mathbf{h}_{t-1}) \end{aligned}$$

(distributed representation)
(hidden representation)
(output probability)

Neural *n*-gram model: example

Model	Perplexity
Kneser-Ney 5-gram	141
Neural <i>n</i> -gram (Bengio et al., 2003)	140

- Neural *n*-gram perform as as well as Kneser-Ney 5-gram
- Requires much less parameters

Neural *n*-gram model: pros and cons

Pros:

- Performs as well as best count based language models
- Need less parameters
- Naturally generalize to unseen *n*-grams

Cons:

- Number of parameters grows with the window size of n-gram
- Memory of the past limited to n-gram window size

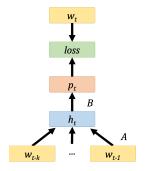
Recurrent Neural Network (RNN)

Recurrent Neural Network

Recurrent network: Keep memory of past in the hidden variables

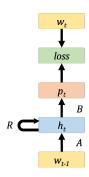
Feedforward

$$h_{t-1} = \sigma(A[w_{t-k}, \dots, w_{t-1}])$$
$$p_t = f(Bh_{t-1})$$

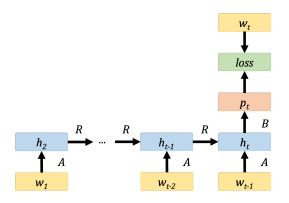


Recurrent Network

$$h_{t-1} = \sigma \left(Aw_{t-1} + Rh_{t-2} \right)$$
$$p_t = f(Bh_{t-1})$$

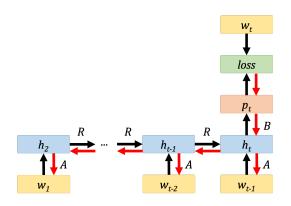


Recurrent Neural Network



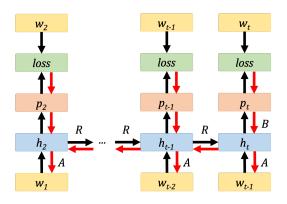
- Recurrent equation: $h_t = \sigma(A[h_{t-1}, w_t])$
- Unfold over time: very deep feedforward with weight sharing
- Potentially capture long term dependencies

Recurrent Neural Network: training



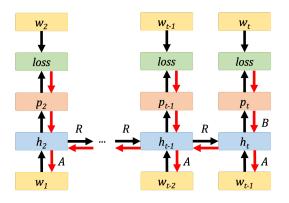
 Backpropagation through time (BPTT): same as backpropagation through a very deepfeedforward network

Recurrent Neural Network: training



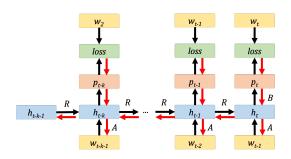
• batch BPTT: forward/backward for many words simultaneously

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).

RNN: results

Model	Perplexity
Kneser-Ney 5-gram	141
Neural <i>n</i> -gram (Bengio et al., 2003)	140 125

- Penn Treebank dataset
- RNN outperforms *n*-gram models
- Faster at test time: does not depend on n-gram length

RNN: Vanishing and exploding gradients

• Consider the partial derivatives of the gradient:

$$\frac{\partial \ell(w_t, p_t)}{\partial h_2} = \frac{\partial \ell(w_t, p_t)}{\partial p_t} \frac{\partial p_t}{\partial h_{t-1}} \underbrace{\frac{\partial h_{t-1}}{\partial h_{t-2}} \cdots \frac{\partial h_3}{\partial h_2}}_{\textit{Ttorms}}$$

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• Each term: $\frac{\partial h_k}{\partial h_{k-1}} = diag(\sigma'(Aw_k + Rh_{k-1}))R$

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- Each term: $\frac{\partial h_k}{\partial h_{k-1}} = diag(\sigma'(Aw_k + Rh_{k-1}))R$
- So the gradient is a serie of multiplication of R and diag(σ'):

$$\frac{\partial \ell(\mathsf{w}_t, \mathsf{p}_t)}{\partial \mathsf{h}_2} = \frac{\partial \ell(\mathsf{w}_t, \mathsf{p}_t)}{\partial \mathsf{p}_t} \frac{\partial \mathsf{p}_t}{\partial \mathsf{h}_{t-1}} \prod_t \left[\mathsf{diag}(\sigma'(\mathsf{z}_t) \mathsf{R} \right]$$

RNN: Exploding gradient

- The matrix R are not directly multiplied in the partial derivatives
- Impossible to lower bound partial derivative norms
- Popular incorrect argument:

$$\prod_{k} \left[\mathsf{diag}(\sigma'(\mathsf{z}_k)) \mathsf{R} \right] \approx \mathsf{R}^k$$

- we cannot lowerbound $diag(\sigma'(z_k))$ nor permute it with R
- Even if we could, R^k is not informative (e.g., nilpotent matrices)
- However the intuition is still correct: if the maximum singluar value of R is such that $\lambda_{\text{max}} \gg 1$: **the gradient might explode**

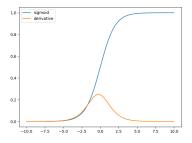
RNN: Exploding gradient

- Consequence: hard to learn a RNN with gradient descent
- Exploding gradient is an optimization problem
- Simple hack to fix this problem: **gradient clipping**:

$$G = \min(\mu, \|G\|) \frac{G}{\|G\|}$$

with $\mu > 0$

ullet it bounds the norm of a gradient ${\it G}$ to be at most μ



• The derivative of σ is mostly close to 0: each multiplication by diag(σ') likely adds 0 to the partial derivative

• Putting R and σ' together, we have:

$$\|\mathsf{diag}(\sigma'(\mathsf{z}_k))\mathsf{R}\| \leq \max_{\mathsf{x}} |\sigma'(\mathsf{x})| |\lambda_{\mathsf{max}}| \leq 0.25 |\lambda_{\mathsf{max}}|$$

• Putting R and σ' together, we have:

$$\|\operatorname{diag}(\sigma'(\mathsf{z}_k))\mathsf{R}\| \leq \max_{\mathsf{x}} |\sigma'(\mathsf{x})| |\lambda_{\mathsf{max}}| \leq 0.25 |\lambda_{\mathsf{max}}|$$

Partial derivative is such that

$$\|\prod_k \mathsf{diag}(\sigma'(\mathsf{z}_k))\mathsf{R}\| \leq 0.25^k \lambda_{\mathsf{max}}^k$$

- If $\lambda_{\text{max}} < 4$: partial derivatives vanish to 0 rapidly.
- The bound depends on the non-linearity

- Consequence of vanishing gradient: long distance information cannot be retained by an RNN
- ullet The flow of information decays exponentially o short memory span
- · Vanishing gradient: model problem, not optimization problem
- Solutions require a change in the structure of the model

• Vanilla RNN:

$$\mathsf{h}_t = \sigma(\mathsf{Aw}_t + \mathsf{Rh}_{t-1})$$

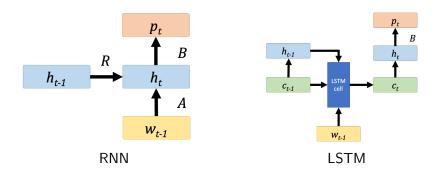
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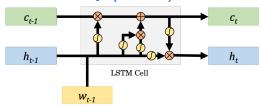
Any function could work:

$$\mathsf{h}_t = \phi(\mathsf{w}_t, \mathsf{h}_{t-1})$$

ullet Preferably ϕ should be mostly differentiable and reduces the vanishing gradient problem



 LSTM introduces an additional hidden variable c_t called the "memory cell"

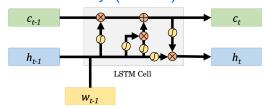


Inspired by "Understanding LSTM Networks", Olah, 2016.

The LSTM equations are:

$$c_t = f_t \circ c_{t-1} + i_t \circ \tanh(Aw_t + Rh_{t-1})$$

$$h_t = o_t \circ \tanh(Wc_t)$$



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$$h_t = o_t \circ \tanh(Wc_t)$$

with:

$$egin{aligned} f_t &= \sigma(A_f \mathbf{w}_{t-1} + R_f \mathbf{h}_{t-1}) & \text{forget gate} \ i_t &= \sigma(A_i \mathbf{w}_{t-1} + R_i \mathbf{h}_{t-1}) & \text{input gate} \ o_t &= \sigma(A_o \mathbf{w}_{t-1} + R_o \mathbf{h}_{t-1}) & \text{output gate} \end{aligned}$$

Attempt at explaining LSTM

- The output gate is not crucial \rightarrow we drop it from this explanation
- The equations are thus the following:

$$c_t = f_t \circ c_{t-1} + i_t \circ \tanh(Aw_t + Rh_{t-1})$$

$$h_t = \tanh(Wc_t)$$

• This way, h_t only depends on c_t

- This is an "hand-wavy" explanation of these equations
- A standard RNN update is:

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• Let us unroll the computation over time:

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- The linear part allows more influence of past on the current update
- Problem: past information is "as important as recent one". After
 T step, a new word contribution is weighted as only 1/T at most.

Possible solution: use a discount factor:

$$\mathsf{c}_t = \eta \mathsf{c}_{t-1} + \mathsf{tanh}(\mathsf{Aw}_t + \mathsf{Rc}_{t-1})$$

 η should be in [0,1]

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 η should be in [0,1]

• We now have:

$$c_t = \sum_{i=0}^t \eta^{t-i} tanh(Aw_i + Rc_{i-1})$$

Problem: This falls back to "vanishing gradient problem"

 Instead, LSTM learns what to store and the importance of the past by learning the weighting:

$$\mathsf{c}_t = f(\mathsf{w}_t, \ \mathsf{c}_{t-1}) \circ \mathsf{c}_{t-1} + i(\mathsf{w}_t, \ \mathsf{c}_{t-1}) \circ \tanh(A\mathsf{w}_t + \mathsf{Rc}_{t-1})$$

- The forget gate weights the contribution of the past
- The input gates weights the contribution of the current word

• So far, we have written the equation in terms of c_t

$$c_t = f(w_t, c_{t-1}) \circ c_{t-1} + i(w_t, c_{t-1}) \circ \tanh(Aw_t + Rc_{t-1})$$

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• But the correct equation is:

$$c_t = f(w_t, \mathbf{h}_{t-1}) \circ c_{t-1} + i(w_t, \mathbf{h}_{t-1}) \circ \tanh(Aw_t + R\mathbf{h}_{t-1})$$

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- Why do we need two different variables?
- $h_t = \tanh(Wc_t) \rightarrow h_t$ is c_t rescaled to [-1, 1]:
- The benefits are:
 - Rescaling h_t avoids gradient explosion
 - Keeping c_t value unbounded allows to learn more patterns, e.g., allows to count

Counting in LSTM

- Counting means that a LSTM can do internally simple arithmetical operation (adding and substracting numbers)
- There are evidences that some memory cells can act as a counter
- This is very interesting for tasks:
 - Learning a latent parser
 - Checking parenthesis in a computer program
 - Storing length of a sentence

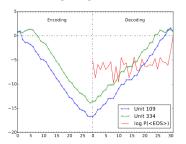


Figure: Evidence from Shi et al. (2016) that some LSTM cells store sentence length in a machine translation system.

LSTM: results

Model	Perplexity
Kneser-Ney 5-gram	141
Neural <i>n</i> -gram	140
RNN	125
LSTM	115

- Penn Treebank dataset
- LSTM outperforms RNN

Sentence Representation

From word to sentence representation

- (Previous lecture) Word vectors: map words to vectors
 Example: word2vec, fasttext, PPMI+SVD...
- **Goal:** Can we build similar representation for sentences?

From word to sentence representation

- (Previous lecture) Word vectors: map words to vectors
 Example: word2vec, fasttext, PPMI+SVD...
- Goal: Can we build similar representation for sentences?
- Several difficulties:
 - Sentences have variable length
 - There is infinite number of sentences, not words
 - Sentences are much richer than words

Simple sentence representation

- A sentence = sequence of words
- Each word has a distributed word vector: w₁,...,w_T
- Average these vectors to form a sentence representation:

$$s = \frac{1}{T} \sum_{t=1}^{T} w_t$$

This is a Bag of Words (BoW) representation

Simple sentence representation

Examples of extensions:

Replace average with taking max value per dimension:

$$\mathsf{s}(i) = \max_{t \in [1,T]} \mathsf{w}_t(i)$$

- Add other features:
 - distributed representation of n-grams or subwords (e.g., fasttext)
 - features from WordNet...
- Make the word vectors depend on context

Simple sentence representation

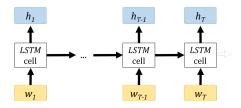
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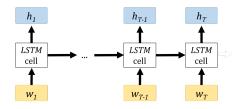
Using an LSTM for sentence representation



- Apply LSTM on sentence \to sequence of word vectors $h_1, \dots, h_{\mathcal{T}}$
- Apply Bag-of-Word sentence representation:

$$s = \frac{1}{T} \sum_{t=1}^{I} h_t$$

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- Apply Bag-of-Word sentence representation:

$$s = \frac{1}{T} \sum_{t=1}^{T} h_t$$

Problem: These word representations depend on past, not future

Simple solution: Bidirectional LSTM (BiLSTM)

- BiLSTM = 2 LSTMs running on opposite direction
- Past: \overrightarrow{LSTM} runs forward on sequence:

$$\overrightarrow{h}_1, \dots, \overrightarrow{h}_T$$

• Future: **ESTM** runs backward on sequence:

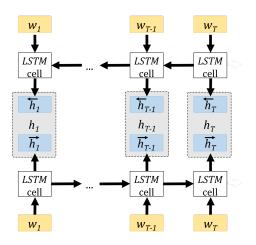
$$\overleftarrow{h}_1, \dots, \overleftarrow{h}_T$$

• Past+Future: biLSTM is the concatenation of both:

$$\mathbf{h}_t = [\overrightarrow{\mathbf{h}_t}, \overleftarrow{\mathbf{h}}_t]$$

• Called "contextualized word vectors" (Peters et al., 2018).

Bidirectional LSTM (BiLSTM)



BoW from biLSTM:
$$\mathbf{s} = \tfrac{1}{T} \textstyle \sum_{t=1}^T \mathbf{h}_t = \tfrac{1}{T} \textstyle \sum_{t=1}^T [\overrightarrow{\mathbf{h}}_t, \overleftarrow{\mathbf{h}}_t]$$

Training biLSTM with Language modeling

- Train both LSTMs independently:
 - The forward \overrightarrow{LSTM} predicts upcoming word:

$$P_{\text{forward}}(w_t \mid w_{t-1}, \dots, w_1)$$

- The backward \overline{LSTM} predicts previous word:

$$P_{\mathsf{backward}}(w_t \mid w_{t+1}, \dots, w_T)$$

Equivalent to train biLSTM with joint objective:

$$P_{\mathsf{forward}}(w_t \mid w_{t-1}, \dots, w_1) + P_{\mathsf{backward}}(w_t \mid w_{t+1}, \dots, w_T)$$

LSTMs are merged at the last layer → late fusion

Transformer Networks

Motivations

- BiLSTM = concatenation of two sequence models
- Not designed to learn word representation from whole context
- Can we build a model that directly look at the whole context?
- Insipration: c-bow for word representations

Self attention: motivation

• LSTM: $y_t = f(h_{t-1}, w_t) \rightarrow \text{whole past in 1 vector, } h_{t-1}$

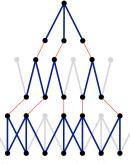
Self attention: motivation

- LSTM: $y_t = f(h_{t-1}, w_t) \rightarrow \text{whole past in 1 vector, } h_{t-1}$
- biLSTM: $y_t = f(h_{t-1}, h_{t+1}, w_t) \rightarrow \text{whole past+future in 2 vectors.}$

Self attention: motivation

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- biLSTM: $y_t = f(h_{t-1}, h_{t+1}, w_t) \rightarrow \text{whole past+future in 2 vectors.}$
- Can we use all past+future vectors?

Convolutional Neural Networks?

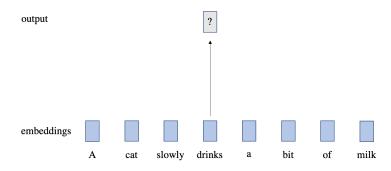


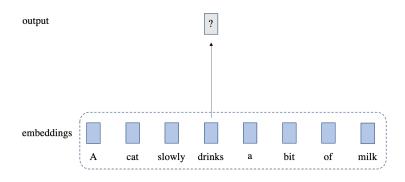
The cat sat on the red mat

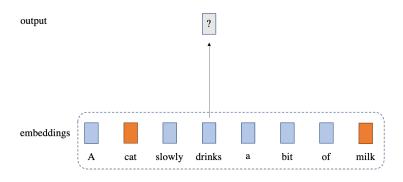
- Pros
 - easy to parallelize
 - exploits local context
- Cons
 - limited context
 - hard to capture long term dependency

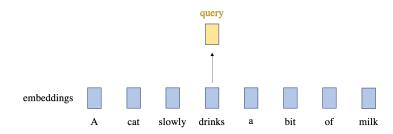
- Goal: use all the context to update a word
- Idea: look for the most important words in the context
- Solution: self-attention on the sequence of inputs

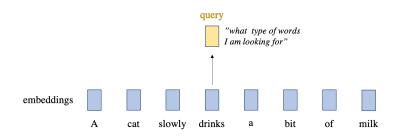


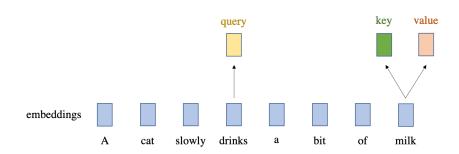


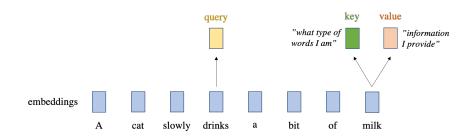


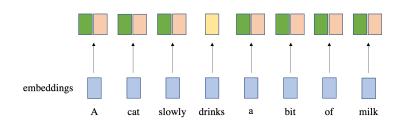


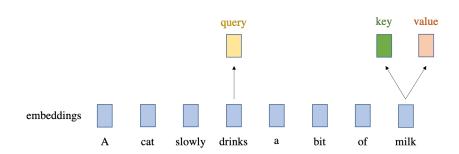


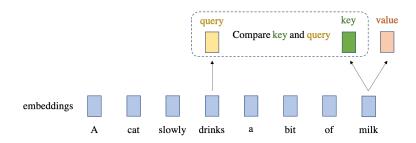


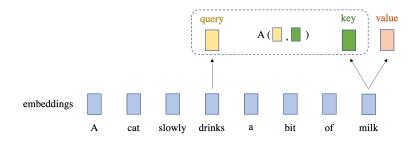


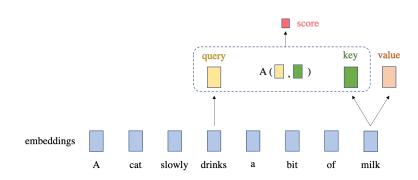


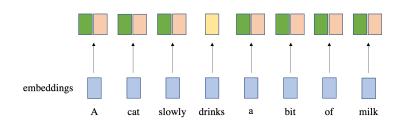


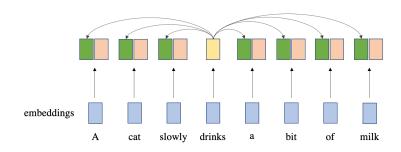


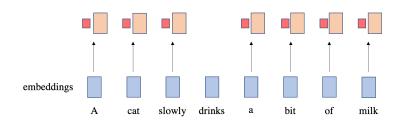


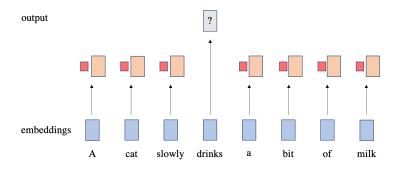


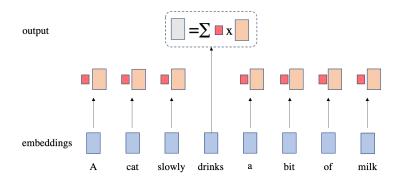










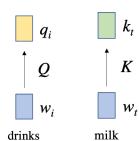


• "query vector" for word *i* ("drinks"):

$$q_i = Qw_i$$

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

$$k_t = Kw_t$$

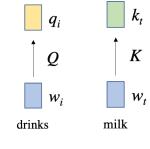


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Their similarity score is then:

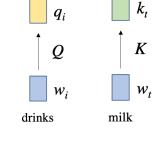
$$s_{it} = \mathsf{q}_i^{\top} \mathsf{k}_t$$

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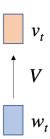
Normalize over sequence with softmax:

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

$$a_{it} \blacksquare = A \left(\boxed{}, \boxed{} \right)$$

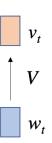
• "value vector" for word t ("milk"):

$$v_t = Vw_t$$



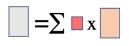
• "value vector" for word t ("milk"):

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



• Finally, compute output for "drinks":

$$y_i = \sum_t a_{it} v_t$$



Efficient self-attention with matrix operations

• Compute query, key and value matrix:

QW, KW, VW

Efficient self-attention with matrix operations

Compute query, key and value matrix:

Compute attention weights

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

where softmax is applied column-wise

Efficient self-attention with matrix operations

Compute query, key and value matrix:

Compute attention weights

$$A = softmax(W^{T}K^{T}QW)$$

where softmax is applied column-wise

• Then, output is obtained with

$$\mathsf{Y} = \mathsf{VWsoftmax}(\mathsf{W}^{\top}\mathsf{K}^{\top}\mathsf{QW})$$

Transformer block:

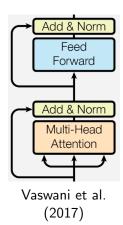
- Multi-head attention layer with skip connection and normalization
- Followed by feed forward with skip connection and normalization

Skip connection+normalization:

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

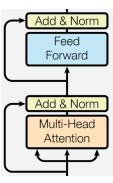
$$y = norm(x + nn(x))$$

where norm normalize the input



Multi-head self-attention block

- Split each input vector into k non overlapping sub-vectors
- \rightarrow the *T* input vectors of dimension *d* are split into *k* sets of *T* vectors of dimension d/k
 - k self-attention layer run in parallel
- The d/k dimension output vector are concatenated back into a d dimensional vector



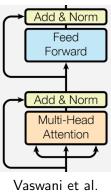
Vaswani et al. (2017)

Feed forward block

• Two layer network, with ReLU activation

$$y = W_2 ReLU(W_1 x)$$

- Usually, $W_1 \in \mathbb{R}^{4d \times d}$ and $W_2 \in \mathbb{R}^{d \times 4d}$
- 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

Position embeddings

- Limitation: self attention does not take position into account!
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- Solution: add position encodings.
- Replace the matrix W by W + E, where $E \in \mathbb{R}^{d \times T}$

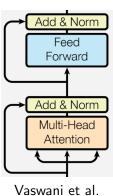
Position embeddings

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- Indeed, shuffling the input gives the same results
- Solution: add position encodings.
- Replace the matrix W by W + E, where $E \in \mathbb{R}^{d \times T}$
- E can be learned, or defined using sin and cos:

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

Transformer network:

- Word embeddings + Position embeddings
- Then N transformer blocks (e.g. N = 12)
- Softmax classifier (e.g. for language modeling)

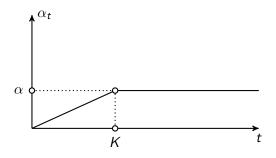


Vaswani et al (2017)

Training of a Transformer

- In practice, transformers are very unstable during training
- If the learning rate is too large, it diverges
- However if the learning rate is too small, it does not learn well

Training of a Transformer



Learning rate scheduler $(\alpha_t)_t$

ullet Set a target learning rate lpha

$$\alpha_t = \min(1, \ \frac{t}{K})\alpha$$

where K is the "warm-up" parameter

BERT: Transformers with early fusion

Introduction

- We consider a deep Transformer, i.e. with more than one layer.
- Embeddings sees the past and the future: impossible to train with language modeling!
- These models fuse information from past and future early in layers \rightarrow early fusion

- A task to train models with early fusion: Cloze procedure (Taylor, 1953)
- Key idea remove words from the input and predict them with the remaining input
- Share similarities with the training of the cbow model for distributed word vectors
- Transformer + Cloze Procedure + Wikipedia Corpus = BERT

Sentence The cat is drinking milk in the kitchen

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Input The cat <MASK> drinking <MASK> in the kitchen

randomly replace 15% of words in sentence with a <MASK> token

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Input The cat <MASK> drinking <MASK> in the kitchen

Targets { "is", "milk" }

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- Take the masked words as targets for the model to predict

Sentence The cat is drinking milk in the kitchen

Input The cat mushroom drinking shoes in the kitchen

Targets { "is", "milk" }

- randomly replace 15% of words in sentence with a <MASK> token
- Take the masked words as targets for the model to predict
- Extension: use random words from vocabulary instead of <MASK>

Sentence The cat is drinking milk in the kitchen

Input The cat <MASK> drinking <MASK> in the kitchen

Targets { "is", "milk" }

- ullet randomly replace 15% of words in sentence with a <MASK> token
- Take the masked words as targets for the model to predict
- Extension: use random words from vocabulary instead of <MASK>
- Related to noisy autoencoders

Evaluation of sentence representations

- Apply representation on downstream tasks (e.g., text classification)
- Compare representations of similar sentences (e.g. paraphrases)
- Identify relations between sentences:
 - is one the negation of the other?
 - Does one imply the other?
- Question answering: match question representation to possible answer representations

GLUE: a benchmark for sentence representations

GLUE (Wang et al., 2018) contains 11 tasks covering:

- Single-Sentence Tasks (e.g., text classification)
- Similarity and Paraphrase Tasks
- Inference tasks, i.e., predicting relations between sentences (e.g., coreference, NLI,...)

Caveat of GLUE finetuning of models on each task is allowed.

GLUE: a benchmark for sentence representations

Model	Avg. Acc.
CBoW	58.9
BiLSTM with late fusion	64.2
Transformer with late fusion	72.8
Transformer with early fusion (BERT)	80.5

- CBoW is a Bag-of-Word representation on top of word GloVe vectors
- Beware! Numbers are not directly comparable because models are trained on different datasets

Transformers for Language Modeling

Masking for Transformer Language Models

- In transformer, h_t depends on all inputs
- Could not be used as is for language modeling
- Solution: use mask in attention, to only use past

Masking for Transformer Language Models

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Reminder:

$$H = VWsoftmax(W^{\top}K^{\top}QW)$$
$$= VWA$$

Hence, a_{it} is weight of input i in representation of position t

- We want representation at time t to only depends on $i \leq t$
- We could enforce $a_{it} = 0$ for $i \ge t$

Masked softmax

- We introduce the masked softmax operator
- Given an input x and a binary mask m,

$$[\mathsf{masked_softmax}(\mathsf{x},\mathsf{m})]_i = \frac{m_i \exp(x_i)}{\sum_{i=1}^d m_i \exp(x_i)}$$

• Still sums to one, $m_i = 0$ implies [masked_softmax(x, m)]_i = 0

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- Sometimes implemented as:

$$softmax(x + log(m))$$

• Beware: do not learn the mask (e.g. PyTorch: register_buffer)

Transformer network for Language Modeling: Results

Model	bpc
LSTM	1.25
Transformer	1.07

- Text8
- Character level language modeling
- bpc = bit per character.

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