Language Modeling and Sentence Representation

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Plan of this lecture

- Language modeling
  - Standard *n*-gram language models
  - neural *n*-gram models
  - Recurrent neural networks
- Sentence representation
  - BiLSTM
  - Late and early fusion
  - Transformer network

Slides on *n*-grams are inspired by Dan Jurafsky's class

https://web.stanford.edu/class/cs124/lec/

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:

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

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

- Sequence probability as a product of token probabilities:

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- Indeed we have:

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

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- Recursively applied to a sequence:

$$\begin{aligned} P(w_1, w_2, w_3) &= P(w_1)P(w_2, w_3 \mid w_1) \\ &= P(w_1)P(w_2 \mid w_1)P(w_3 \mid w_2, w_1). \end{aligned}$$

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- Language models estimate probability of upcoming token given past:

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

n-gram language models

Count based language model

Compute probability with counting statistics from a dataset:

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

$$
\begin{aligned}
P(w_t \mid w_{t-1}, \ldots, w_1) &= \frac{P(w_1, \ldots, w_t)}{P(w_1, \ldots, w_{t-1})} \\
&= \frac{c(w_1 \cdots w_t)}{c(w_1 \cdots w_{t-1})}
\end{aligned}
$$

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

Count based language model

- Example:

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

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

Sentence "The moment one learns" appears 75 in dataset

Limitiations of count based language model

- Number of unique sentences increases with dataset size,
- Long sentences are rare: no good statistics for them

$\rightarrow$ **Too many sentences with not enough statistics**

Count based language model

- **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:

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

Count based language model

- **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:

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

Count based language model: unigram

- Probability of a sentence with a unigram model:

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

N = total number of tokens in dataset
$c(w_t)$ = number of occurences of w_t 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 occurences 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"

Count based language model

- 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**

Estimating n-gram probabilites: an example

- 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:

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

- <s>= token for beginning of sentence; $P(<\text{s}>) = 1$.
- Compute sentence probability with them

Estimating n-gram probabilites: an example

- 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

Estimating *n*-gram probabilites: an example

- 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

Estimating *n*-gram probabilites: an example

- Example:

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

<s>= token for beginning of sentence; $P(\text{<s>}) = 1$.

- Result:

$$\begin{aligned} P(\text{<s> i want chinese food}) =& P(\text{<s>})P(\text{i}|\text{<s>})P(\text{want}|\text{i})P(\text{chinese}|\text{want})P(\text{food}|\text{chinese}) \\ =& 1 \times .25 \times 0.33 \times 0.0065 \times 0.52 \\ =& 0.00027885 \end{aligned}$$

Estimating *n*-gram probabilites: an example

	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:

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

- Result:

$$\begin{aligned} P(<\text{s}>\ \text{i bring my lunch to work}) &= P(<\text{s}>) \ldots P(\text{to}|\text{lunch}) \ldots \\ &= 1 \times \cdots \times 0 \times \ldots \\ &= \mathbf{0} \end{aligned}$$

- **Does not generalize well!**

Estimating n-gram probabilites: an example

- 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:

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

where V = vocabulary size

estimating n-gram probabilites

- Add mass to unrealistic bigram ("to to").
- Decrease probability of realistic bigram by factor V.
- Example: $P(\text{want} \mid \text{i})$ decreases from 0.33 to 0.21!

$\rightarrow$ Add-1 is not good in practice

Good-Turing estimation

- **Idea** reallocate probability mass of *n*-grams that occur exactly $c + 1$ times to *n*-grams that occur exactly c times
- reallocate mass of *n*-grams appearing once to unseen *n*-grams

→ **alternative to Add-1**

Good-Turing estimation

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→ **alternative to Add-1**

- the adjusted count:

$$c^* = (c+1)\frac{N_{c+1}}{N_c}$$

where N_c is the number of n-grams that appears exactly c times

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- *n*-gram probability depends on c^* instead of c

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$\rightarrow$ **alternative to Add-1**

- the adjusted count:

$$c^* = (c+1)\frac{N_{c+1}}{N_c}$$

  where N_c is the number of n-grams that appears exactly c times
- n-gram probability depends on c^* instead of c
- **Problem** What if $N_{c+1} = 0$ (but $N_c > 0$)?

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 $c(w_{t-n+1} \cdots w_t) > 0$:

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

- else backoff to $(n-1)$gram:

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

- 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:

$$\begin{aligned} P_L(w_t \mid w_{t-1}, w_{t-2}) &= \lambda_1 P(w_t \mid w_{t-1}, w_{t-2}) + \\ & \lambda_2 P(w_t \mid w_{t-1}) + \\ & \lambda_3 P(w_t) \end{aligned}$$

- Conditioned interpolation:

$$\begin{aligned} P_L(w_t \mid w_{t-1}, w_{t-2}) &= \lambda_1(w_{t-1}, w_{t-2}) P(w_t \mid w_{t-1}, w_{t-2}) + \\ & \lambda_2(w_{t-1}, w_{t-2}) P(w_t \mid w_{t-1}) + \\ & \lambda_3(w_{t-1}, w_{t-2}) P(w_t) \end{aligned}$$

Conditioned Interpolation

- Requires to split training dataset in two
- On one dataset, compute the *n*-gram probabilities
- On the second dataset, learn the λ's that fits the best.
- Learning the λ's is a logistic regression problem:

$$\max_{\lambda} \sum_i \log \left[\sum_j \lambda_j(w_{i-1}, w_{i-2}) P(w_i \mid w_{i-1}, \ldots, w_{i-3+j}) \right]$$

Kneser-Ney Smoothing

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

- You recursively apply this formula to get the explicit probability

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

- You recursively apply this formula to get the explicit probability
- Indeed (with simplified notations):

$$\begin{aligned} P_t &= f_t + \lambda_t P_{t-1} \\ &= f_t + \lambda_t (f_{t-1} + \lambda_{t-1} P_{t-2}) \\ &= f_t + \lambda_t f_{t-1} + \cdots + \prod_{k=0}^{t} \lambda_k P_0 \end{aligned}$$

Kneser-Ney Smoothing

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

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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 is discount factor
  it works as a threshold too: $f_{KN} = 0$ for any n-gram appearing less than d times.

Kneser-Ney Smoothing

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

- λ is the interpolation weight:

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

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

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.

Cache model

- Ngram models compute statstics over the whole dataset
- Locally, this distribution can change!

- Example:
  - Full Dataset = all the news article about football
  - Current prediction is on an article about a specific team
  - The name of the players in this team are more likely to appear than in the full dataset

- **Cache model** keeps an history $\mathcal{H}$ of recent past and adjust prediction to increase the probability of the words in this history:

$$P_C(w_t \mid w_{t-1}, w_{t-2}) = \lambda P(w_t \mid w_{t-1}, w_{t-2}) + (1-\lambda)\frac{|w_t \in \mathcal{H}|}{|\mathcal{H}|}$$

Large scale *n*-gram models

Pruning keep only *n*-grams with counts $>$ threshold

Memory efficiency

- Store *n*-grams in tri trees
- Store indices instead of string
- Quantization: 4-8 bits instead of 8-byte floats

Approximated LM bloom filters instead of indices to retrieve *n*-grams

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 downsstream 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	0.5	**responsability**	0.4	**responsability**	0.8
responsability	0.4	responsabilities	0.3	current	0.1
voltage	0.1	irresponsability	0.3	volt	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 $W = (w_1, \ldots, w_T)$ is:

$$\begin{aligned} PP(W) &= P(w_1, \ldots, w_T)^{-\frac{1}{T}} \\ &= \prod_{t=1}^{T} P(w_t \mid w_{t-1}, \ldots, w_1)^{-\frac{1}{T}} \end{aligned}$$

- 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:

$$\log PP(W) = -\frac{1}{T}\sum_{t=1}^{T} \log P(w_t \mid w_{t-1}, \ldots, w_1)$$

- It is the negative log-likelihood of the sequence

Example of Perplexity

	Unigram	Bigram	Trigram
PP	962	170	109

Lower perplexity means better model

As expected, better model with longer n-grams

On the WJS dataset [Training = 38M tokens, Testing = 1.5M tokens]

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

  $\rightarrow$ Language modeling can cased as a supervised classification

Preliminaries: loss function

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

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:

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

Pros of linear models over n-grams

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

- Can learn the same statistics as those in the n-gram models
- We can put additional features into $\mathbf{x}_t$ (e.g. from WordNet)
- Simple to implement

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

Neural bigram model

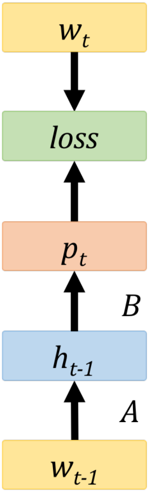
- feedforward network:

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

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

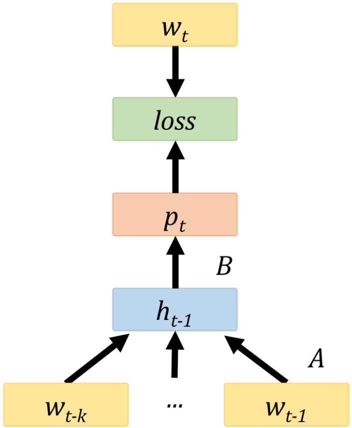
Generalization to any fixed n-gram size:

- The input is the contactenation of previous words:

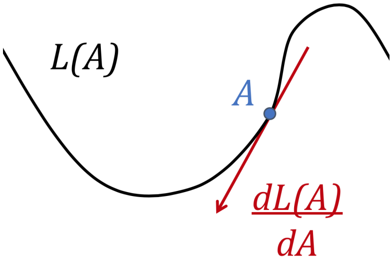
$$\mathbf{x}_t = [\mathbf{w}_{t-n+1}, \ldots, \mathbf{w}_{t-1}]$$

- $\mathbf{A}$: $nV \times H$ matrix
- Minimization problem:

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



Neural n-gram model: training



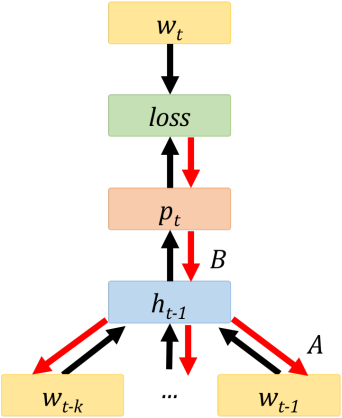
- Loss function: $L(A, B) = \frac{1}{T} \sum_{t=1}^{T} \ell(w_t, f(\mathbf{B}\sigma(\mathbf{A}\mathbf{x}_t)))$
- This loss is differentiable in **A** and **B**
- Minimize the loss by updating parameters in direction of the gradient

Neural n-gram model: training

- Gradient descent:
  - Compute full loss $L(\mathbf{A}, \mathbf{B})$
  - Update parameters:
  $$\mathbf{A} \leftarrow \mathbf{A} - \eta \frac{\partial L}{\partial \mathbf{A}}$$
  - $\eta > 0$ is the learning rate
- Stochastic gradient descent (SGD):
  - Instead of gradient on the full loss $L(\mathbf{A}, \mathbf{B})$
  - Randomly sample an example t
  - Partial loss
  $$L_t(\mathbf{A}, \mathbf{B}) = \ell(y_t, f(\mathbf{B}\sigma(\mathbf{A}\mathbf{x}_t)))$$
  - Update parameters:
  $$\mathbf{A} \leftarrow \mathbf{A} - \eta \frac{\partial L_t}{\partial \mathbf{A}}$$

Computing the gradient with backpropagation

- Compute gradient with **backpropagation**
- Compute the error made by the model when predicting the next word
- Propagate this error back to all of the parameters of the network and the input



Neural n-gram model: backpropagation

- We have $\mathbf{z} = \mathbf{B}\sigma(\mathbf{A}\mathbf{x})$ and $\mathbf{p} = f(\mathbf{z})$
- Loss for one example: $\ell(\mathbf{w}, \mathbf{p}) = \ell(\mathbf{w}, f(\mathbf{B}\sigma(\mathbf{A}\mathbf{x})))$

Neural n-gram model: backpropagation

- We have $\mathbf{z} = \mathbf{B}\sigma(\mathbf{A}\mathbf{x})$ and $\mathbf{p} = f(\mathbf{z})$
- Loss for one example: $\ell(\mathbf{w}, \mathbf{p}) = \ell(\mathbf{w}, f(\mathbf{B}\sigma(\mathbf{A}\mathbf{x})))$
- The gradient of the loss w.r.t. $\mathbf{B}$ with chain rule:

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

Neural n-gram model: backpropagation

- We have $\mathbf{z} = \mathbf{B}\sigma(\mathbf{A}\mathbf{x})$ and $\mathbf{p} = f(\mathbf{z})$
- Loss for one example: $\ell(\mathbf{w}, \mathbf{p}) = \ell(\mathbf{w}, f(\mathbf{B}\sigma(\mathbf{A}\mathbf{x})))$

- The gradient of the loss w.r.t. $\mathbf{B}$ with chain rule:

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

Neural n-gram model: backpropagation

- We have $\mathbf{z} = \mathbf{B}\sigma(\mathbf{A}\mathbf{x})$ and $\mathbf{p} = f(\mathbf{z})$
- Loss for one example: $\ell(\mathbf{w}, \mathbf{p}) = \ell(\mathbf{w}, f(\mathbf{B}\sigma(\mathbf{A}\mathbf{x})))$

- The gradient of the loss w.r.t. $\mathbf{B}$ with chain rule:

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

Neural n-gram model: backpropagation

- We have $\mathbf{z} = \mathbf{B}\sigma(\mathbf{A}\mathbf{x})$ and $\mathbf{p} = f(\mathbf{z})$
- Loss for one example: $\ell(\mathbf{w}, \mathbf{p}) = \ell(\mathbf{w}, f(\mathbf{B}\sigma(\mathbf{A}\mathbf{x})))$

- The gradient of the loss w.r.t. $\mathbf{B}$ with chain rule:

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

Neural n-gram model: backpropagation

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

- The gradient of the loss w.r.t. $\mathbf{B}$ with chain rule:

$$\begin{aligned}\frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{B}} &= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial \mathbf{p}}{\partial \mathbf{B}} + \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{w}} \frac{\partial \mathbf{w}}{\partial \mathbf{B}} \\ &= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial f(\mathbf{z})}{\partial \mathbf{B}} \qquad \text{where} \quad \mathbf{p} = f(\mathbf{z})\end{aligned}$$

Neural n-gram model: backpropagation

- We have $\mathbf{z} = \mathbf{B}\sigma(\mathbf{A}\mathbf{x})$ and $\mathbf{p} = f(\mathbf{z})$
- Loss for one example: $\ell(\mathbf{w}, \mathbf{p}) = \ell(\mathbf{w}, f(\mathbf{B}\sigma(\mathbf{A}\mathbf{x})))$

- The gradient of the loss w.r.t. $\mathbf{B}$ with chain rule:

$$\begin{aligned}
\frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{B}} &= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial \mathbf{p}}{\partial \mathbf{B}} + \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{w}} \frac{\partial \mathbf{w}}{\partial \mathbf{B}} \\
&= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial f(\mathbf{z})}{\partial \mathbf{B}} \qquad \text{where} \quad \mathbf{p} = f(\mathbf{z})
\end{aligned}$$

Neural *n*-gram model: backpropagation

- We have $\mathbf{z} = \mathbf{B}\sigma(\mathbf{A}\mathbf{x})$ and $\mathbf{p} = f(\mathbf{z})$
- Loss for one example: $\ell(\mathbf{w}, \mathbf{p}) = \ell(\mathbf{w}, f(\mathbf{B}\sigma(\mathbf{A}\mathbf{x})))$

- The gradient of the loss w.r.t. $\mathbf{B}$ with chain rule:

$$
\begin{aligned}
\frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{B}} &= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial \mathbf{p}}{\partial \mathbf{B}} + \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{w}} \frac{\partial \mathbf{w}}{\partial \mathbf{B}} \\
&= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial f(\mathbf{z})}{\partial \mathbf{B}} \qquad \text{where} \quad \mathbf{p} = f(\mathbf{z}) \\
&= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} \frac{\partial \mathbf{z}}{\partial \mathbf{B}}
\end{aligned}
$$

Neural n-gram model: backpropagation

- We have $\mathbf{z} = \mathbf{B}\sigma(\mathbf{A}\mathbf{x})$ and $\mathbf{p} = f(\mathbf{z})$
- Loss for one example: $\ell(\mathbf{w}, \mathbf{p}) = \ell(\mathbf{w}, f(\mathbf{B}\sigma(\mathbf{A}\mathbf{x})))$

- The gradient of the loss w.r.t. $\mathbf{B}$ with chain rule:

$$\begin{aligned}
\frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{B}} &= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial \mathbf{p}}{\partial \mathbf{B}} + \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{w}} \frac{\partial \mathbf{w}}{\partial \mathbf{B}} \\
&= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial f(\mathbf{z})}{\partial \mathbf{B}} \qquad\qquad \text{where} \quad \mathbf{p} = f(\mathbf{z}) \\
&= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} \frac{\partial \mathbf{z}}{\partial \mathbf{B}}
\end{aligned}$$

Neural n-gram model: backpropagation

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

- The gradient of the loss w.r.t. $\mathbf{B}$ with chain rule:

$$\begin{aligned}
\frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{B}} &= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial \mathbf{p}}{\partial \mathbf{B}} + \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{w}} \frac{\partial \mathbf{w}}{\partial \mathbf{B}} \\
&= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial f(\mathbf{z})}{\partial \mathbf{B}} && \text{where} \quad \mathbf{p} = f(\mathbf{z}) \\
&= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} \frac{\partial \mathbf{z}}{\partial \mathbf{B}} \\
&= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} \frac{\partial \left(\mathbf{B}\sigma(\mathbf{Ax})\right)}{\partial \mathbf{B}} && \text{where} \quad \mathbf{z} = \mathbf{B}\sigma(\mathbf{Ax})
\end{aligned}$$

Neural *n*-gram model: backpropagation

- We have $\mathbf{z} = \mathbf{B}\sigma(\mathbf{A}\mathbf{x})$ and $\mathbf{p} = f(\mathbf{z})$
- Loss for one example: $\ell(\mathbf{w}, \mathbf{p}) = \ell(\mathbf{w}, f(\mathbf{B}\sigma(\mathbf{A}\mathbf{x})))$
- The gradient of the loss w.r.t. $\mathbf{B}$ with chain rule:

$$
\begin{aligned}
\frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{B}} &= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial \mathbf{p}}{\partial \mathbf{B}} + \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{w}} \frac{\partial \mathbf{w}}{\partial \mathbf{B}} \\
&= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial f(\mathbf{z})}{\partial \mathbf{B}} && \text{where} \quad \mathbf{p} = f(\mathbf{z}) \\
&= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} \frac{\partial \mathbf{z}}{\partial \mathbf{B}} \\
&= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} \frac{\partial \left(\mathbf{B}\sigma(\mathbf{A}\mathbf{x})\right)}{\partial \mathbf{B}} && \text{where} \quad \mathbf{z} = \mathbf{B}\sigma(\mathbf{A}\mathbf{x})
\end{aligned}
$$

Neural n-gram model: backpropagation

- We have $\mathbf{z} = \mathbf{B}\sigma(\mathbf{A}\mathbf{x})$ and $\mathbf{p} = f(\mathbf{z})$
- Loss for one example: $\ell(\mathbf{w}, \mathbf{p}) = \ell(\mathbf{w}, f(\mathbf{B}\sigma(\mathbf{A}\mathbf{x})))$

- The gradient of the loss w.r.t. $\mathbf{B}$ with chain rule:

$$
\begin{aligned}
\frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{B}} &= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial \mathbf{p}}{\partial \mathbf{B}} + \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{w}} \frac{\partial \mathbf{w}}{\partial \mathbf{B}} \\
&= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial f(\mathbf{z})}{\partial \mathbf{B}} && \text{where} \quad \mathbf{p} = f(\mathbf{z}) \\
&= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} \frac{\partial \mathbf{z}}{\partial \mathbf{B}} \\
&= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} \frac{\partial \left(\mathbf{B}\sigma(\mathbf{A}\mathbf{x})\right)}{\partial \mathbf{B}} && \text{where} \quad \mathbf{z} = \mathbf{B}\sigma(\mathbf{A}\mathbf{x}) \\
&= \frac{\partial \ell(\mathbf{w}, \mathbf{p})}{\partial \mathbf{p}} \frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} \sigma(\mathbf{A}\mathbf{x})
\end{aligned}
$$

Neural *n*-gram model: backpropagation

- Loss function:

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

- The gradients are:

$$\begin{aligned}
\frac{\partial L}{\partial \mathbf{B}} &= \frac{1}{T}\sum_{t=1}^{T}\frac{\partial \ell}{\partial \mathbf{z}_t}\frac{\partial \mathbf{z}_t}{\partial \mathbf{B}} \\
\frac{\partial L}{\partial \mathbf{A}} &= \frac{1}{T}\sum_{t=1}^{T}\frac{\partial \ell}{\partial \mathbf{z}_t}\frac{\partial \mathbf{z}_t}{\partial \mathbf{h}_{t-1}}\frac{\partial \mathbf{h}_{t-1}}{\partial \mathbf{A}}
\end{aligned}$$

with $\mathbf{z}_t = \mathbf{B}\mathbf{h}_t$ and $\mathbf{h}_{t-1} = \sigma(\mathbf{A}\mathbf{x}_t)$

Neural n-gram model: backpropagation

- Loss function:

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

- The gradients are:

$$\begin{aligned}
\frac{\partial L}{\partial \mathbf{B}} &= \frac{1}{T}\sum_{t=1}^{T}\frac{\partial \ell}{\partial \mathbf{z}_t}\frac{\partial \mathbf{z}_t}{\partial \mathbf{B}} \\
\frac{\partial L}{\partial \mathbf{A}} &= \frac{1}{T}\sum_{t=1}^{T}\frac{\partial \ell}{\partial \mathbf{z}_t}\frac{\partial \mathbf{z}_t}{\partial \mathbf{h}_{t-1}}\frac{\partial \mathbf{h}_{t-1}}{\partial \mathbf{A}}
\end{aligned}$$

  with $\mathbf{z}_t = \mathbf{B}\mathbf{h}_t$ and $\mathbf{h}_{t-1} = \sigma(\mathbf{A}\mathbf{x}_t)$

- Note that some intermediate computations are shared to evaluate different gradients

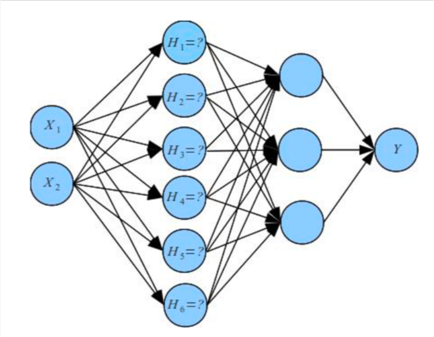
Regularization: dropout

- Specialized units cause overfitting
- **Idea** force model to work even when some units are removed
- Same as activation mask over units
- we replace $\mathbf{h}_t$ by:

  $$\hat{\mathbf{h}}_t = \mathbf{h}_t \odot \mathbf{m}_t$$

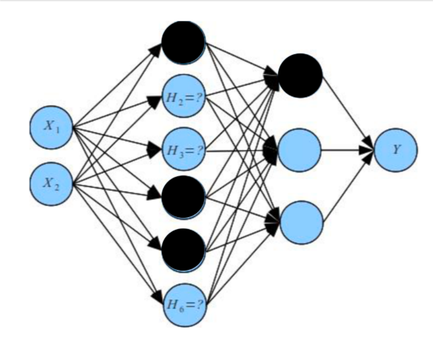
  where $\mathbf{m}_t$ is a binary mask vector.
- This binary mask is randomly drawn for each time step

Regularization: dropout



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

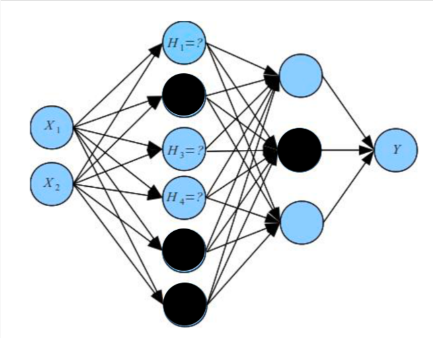
Regularization: dropout



Iteration 1

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

Regularization: dropout



Iteration 2

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

Regularization: tied input-output matrix

- Input matrix $\mathbf{A}$ is a $V \times H$ matrix
- Output matrix $\mathbf{B}$ is a $H \times V$ matrix
- For large vocabulary ($V >> 1$), these matrices holds most of the parameters of the model

$\rightarrow$ This may lead to some overfitting

- **Solution** tie the input and output weights (Press and Wolf, 2016):

$$\mathbf{B} = \mathbf{A}^T$$

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

Dealing with large vocabulary: class-based softmax

- Use a class-based softmax (see lecture on text classification)
- partition vocabulary in L subvocabulary, V_k is k-th subvocabulary

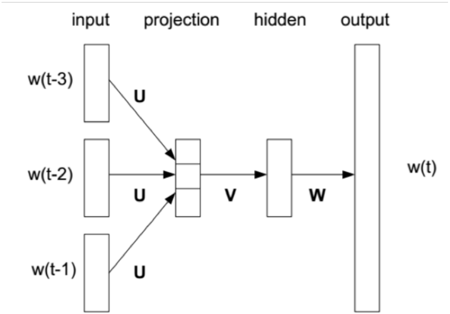
$$P(C = c_k \mid \mathbf{h}_t) P(w_t = k \mid \mathbf{h_t}, C = c_k)$$

- Typically we take $L = \sqrt{V}$

- Subvocabularies are selected to have the same frequency.
- frequency of subvocabulary is the sum of the frequency of its words
- Frequence of words varies greatly ("the" versus "bardiwac")

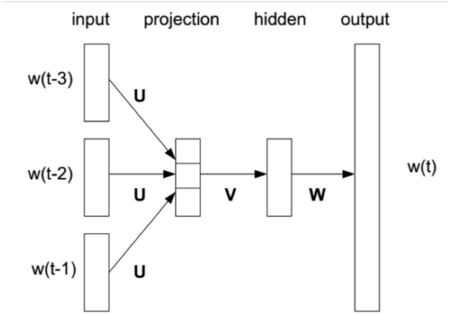
→ size of subvocabularies varies greatly, but large subvocabularies are visited rarely

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 $\mathbf{U}\mathbf{w}_t$ is a distributed word representation
- These representations are passed through a feedforward network

Neural n-gram model: example



- The equations are:

$$\begin{aligned}
\mathbf{x}_{t-k} &= \sigma(\mathbf{U}\mathbf{w}_{t-k}) && \text{(distributed representation)}\\
\mathbf{h}_{t-1} &= \sigma(\mathbf{V}[\mathbf{x}_{t-3}, \mathbf{x}_{t-2}, \mathbf{x}_{t-1}]) && \text{(hidden representation)}\\
\mathbf{p}_{t} &= f(\mathbf{W}\mathbf{h}_{t-1}) && \text{(output probability)}
\end{aligned}$$

Neural n-gram model: example

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

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

Penn Treebank dataset

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

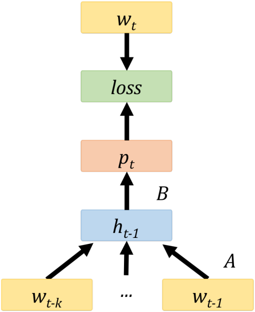
Recurrent Neural Network (RNN)

Recurrent Neural Network

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

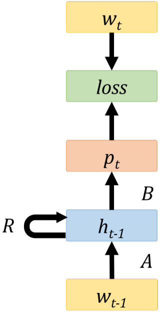
Feedforward

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

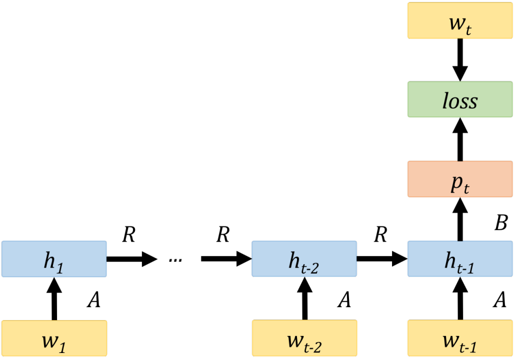


Recurrent Network

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

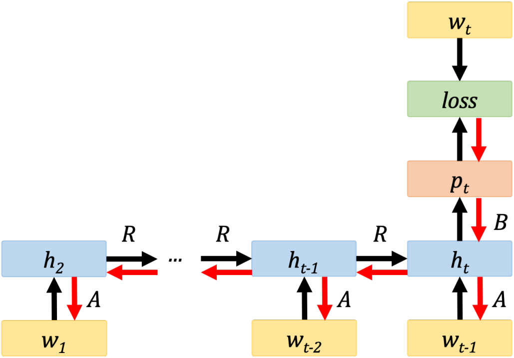


Recurrent Neural Network



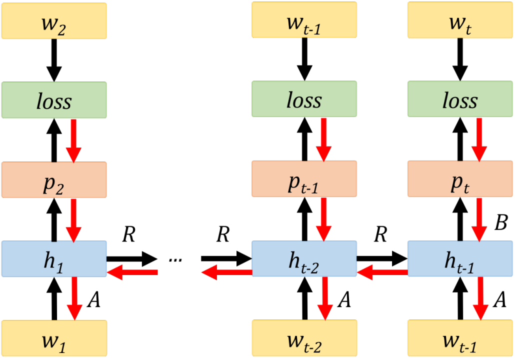
- Recurrent equation: $\mathbf{h}_t = \sigma\left(\mathbf{A}[\mathbf{h}_{t-1}, \mathbf{w}_t]\right)$
- Unfold over time: **very deep feedforward with weight sharing**
- Potentially capture long term dependencies

Recurrent Neural Network: training



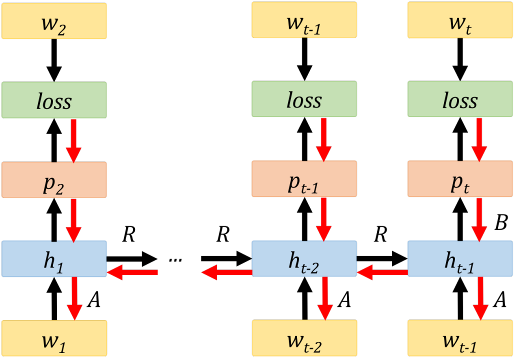
- **Backpropagation through time (BPTT)**: same as backpropagation through a very deepfeedforward network

Recurrent Neural Network: training



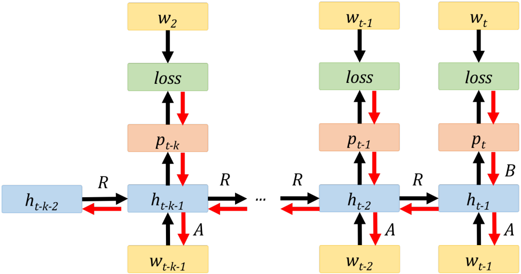
- **batch BPTT**: forward/backward for many words simultaneously

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: $O(k)$.

RNN: results

Model	Perplexity
Kneser-Ney 5-gram	141
Neural *n*-gram (Bengio et al., 2003)	140
RNN	**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:

$$\frac{\partial \ell(\mathbf{w}_t, \mathbf{p}_t)}{\partial \mathbf{h}_2} = \frac{\partial \ell(\mathbf{w}_t, \mathbf{p}_t)}{\partial \mathbf{p}_t} \frac{\partial \mathbf{p}_t}{\partial \mathbf{h}_{t-1}} \underbrace{\frac{\partial \mathbf{h}_{t-1}}{\partial \mathbf{h}_{t-1}} \cdots \frac{\partial \mathbf{h}_3}{\partial \mathbf{h}_2}}_{T \text{ terms}}$$

- Each term: $\frac{\partial \mathbf{h}_k}{\partial \mathbf{h}_{k-1}} = \text{diag}(\sigma'(A\mathbf{w}_k + \mathbf{R}\mathbf{h}_{k-1}))\mathbf{R}$
- So the gradient is a serie of multiplication of $\mathbf{R}$ and $\text{diag}(\sigma')$:

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

RNN: Exploding gradient

- The matrix $\mathbf{R}$ are not direclty multiplied in the partial derivatives
- Impossible to lower bound partial derivative norms
- Popular incorrect argument:

$$\prod_k \left[\mathrm{diag}(\sigma'(\mathbf{z}_k))\mathbf{R}\right] \approx \mathbf{R}^k$$

- we cannot lowerbound $\mathrm{diag}(\sigma'(\mathbf{z}_k))$ nor permute it with $\mathbf{R}$
- Even if we could, $\mathbf{R}^k$ is not informative (e.g., nilpotent matrices)

- However the intuition is still correct: if the maximum singluar value of $\mathbf{R}$ is such that $\lambda_{\mathrm{max}} >> 1$: **the gradient might explode**

RNN: Exploding gradient

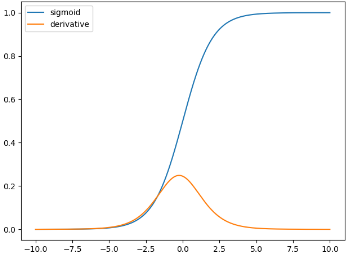
- Consequence: hard to learn a RNN with gradient descent
- **Exploding gradient is an optimization problem**
- Simple hack to fix this problem: **gradient clipping**:

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

  with $\mu > 0$

- it bounds the norm of a gradient G to be at most μ

RNN: Vanishing gradient



- The derivative of σ is mostly close to 0: each multiplication by $\mathrm{diag}(\sigma')$ likely adds 0 to the partial derivative

RNN: Vanishing gradient

- Putting $\mathbf{R}$ and σ' together, we have:

$$\|\text{diag}(\sigma'(\mathbf{z}_k))\mathbf{R}\| \leq \max_x |\sigma'(x)||\lambda_{\text{max}}| \leq 0.25|\lambda_{\text{max}}|$$

- Partial derivative is such that

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

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

RNN: Vanishing gradient

- Consequence of vanishing gradient: long distance information cannot be retained by an RNN
- The flow of information decays exponentially $\rightarrow$ short memory span
- **vanishing gradient is a model problem, not an optimization problem**
- Solutions require a change in the structure of the model

Long Short Term Memory (LSTM)

Long Short Term Memory (LSTM)

- Vanilla RNN:

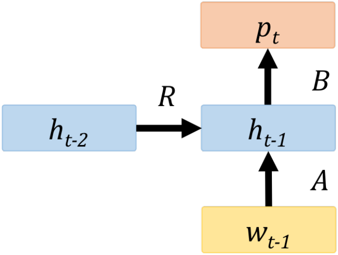
$$\mathbf{h}_t = \sigma(A\mathbf{w}_t + \mathbf{R}\mathbf{h}_{t-1})$$

- Any function could work:

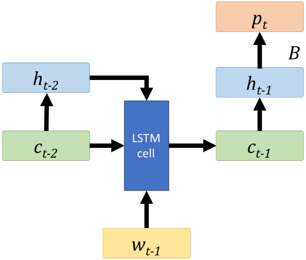
$$\mathbf{h}_t = \phi(\mathbf{w}_t, \mathbf{h}_{t-1})$$

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

Long Short Term Memory (LSTM)



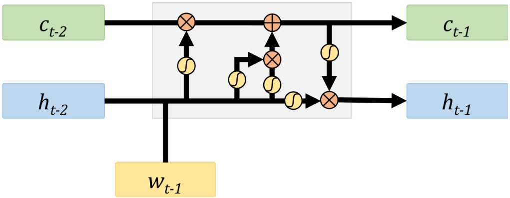
RNN



LSTM

- LSTM introduces an additional hidden variable $\mathbf{c}_t$ called the "memory cell"

Long Short Term Memory (LSTM)



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

- The LSTM equations are:

$$\begin{aligned} \mathbf{c}_t &= f_t \circ \mathbf{c}_{t-1} + i_t \circ \tanh(A\mathbf{w}_t + \mathbf{R}\mathbf{h}_{t-1}) \\ \mathbf{h}_t &= o_t \circ \tanh(W\mathbf{c}_t) \end{aligned}$$

Using $\tanh h(x) = 2\sigma(2x) - 1$ instead of σ is not important.

- with:

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

Attempt at explaining LSTM

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

$$\begin{aligned} \mathbf{c}_t &= f_t \circ \mathbf{c}_{t-1} + i_t \circ \tanh(A\mathbf{w}_t + \mathbf{R}\mathbf{h}_{t-1}) \\ \mathbf{h}_t &= \tanh(W\mathbf{c}_t) \end{aligned}$$

- This way, $\mathbf{h}_t$ only depends on $\mathbf{c}_t$

Attempt at explaining the memory cell update

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

$$\mathbf{c}_t = \tanh(A\mathbf{w}_t + \mathbf{R}\mathbf{c}_{t-1})$$

- A simple way to keep longer memory of past is to add a linear part:

$$\mathbf{c}_t = \mathbf{c}_{t-1} + \underbrace{\tanh(A\mathbf{w}_t + \mathbf{R}\mathbf{c}_{t-1})}_{\text{Same as RNN}}$$

- Let us unroll the computation over time:

$$\mathbf{c}_t = \sum_{i=0}^{t} \tanh(A\mathbf{w}_i + \mathbf{R}\mathbf{c}_{i-1})$$

- 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.

LSTM: memory cell update

- Possible solution: use a discount factor:

$$\mathbf{c}_t = \eta \mathbf{c}_{t-1} + \tanh(A\mathbf{w}_t + \mathbf{R}\mathbf{c}_{t-1})$$

η should be in $[0, 1]$

- We now have:

$$\mathbf{c}_t = \sum_{i=0}^{t} \eta^{t-i} \tanh(A\mathbf{w}_i + \mathbf{R}\mathbf{c}_{i-1})$$

- **Problem**: This falls back to "vanishing gradient problem"

LSTM: memory cell update

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

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

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

LSTM: memory cell update

- So far, we have written the equation in terms of $\mathbf{c}_t$

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

- but the correct equation is:

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

- Why do we need two different variables?
- $\mathbf{h}_t = \tanh(W\mathbf{c}_t) \rightarrow \mathbf{h}_t$ is $\mathbf{c}_t$ rescaled to $[-1, 1]$:
- The benefits are:
  - Rescaling $\mathbf{h}_t$ avoids gradient explosion
  - Keeping $\mathbf{c}_t$ 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

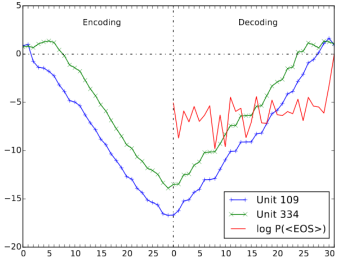


Figure: Evidence from Shi et al. (2016) that some LSTM cells store sentence length in a machine translation system.

LSTM: results

Model	Perplexity
Kneser-Ney 5-gram	141
Neural *n*-gram	140
RNN	125
LSTM	**115**

- Penn Treebank dataset
- LSTM outperforms RNN

Sentence Representation

From word to sentence representation

- **Distributed word vectors** Assign a fixed size vector to a word
- Example: word2vec, fasttext, PPMI+SVD...

- **Goal** Build a similar representation for sentences

- Several difficulties:
  - Sentences have variable length
  - Sentences are much richer than words

Simple sentence representation

- A sentence is a sequence of words $w_1, \ldots, w_T$
- each word has a distributed word vector: $\mathbf{w}_1, \ldots, \mathbf{w}_T$
- Average these vectors to form a sentence representation:

$$\mathbf{s} = \frac{1}{T} \sum_{t=1}^{T} \mathbf{w}_t$$

- This is a Bag of Words (BoW) representation

Extensions of simple sentence representation

- Replace average with another operation, e.g., take the max value per dimension:

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

- Add additional features:
  - distributed representation of *n*-grams or subwords
  - features from WordNet...

- Use a representation of words that depends on context

Extensions of simple sentence representation

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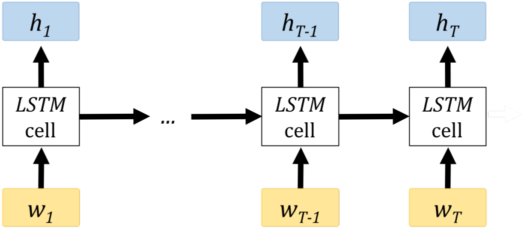
Using an LSTM for sentence representation



- Apply LSTM on a sentence to produce sequence of vectors

$$\mathbf{h}_1, \ldots, \mathbf{h}_T$$

- Use these representations in the BoW sentence representation:

$$\mathbf{s} = \frac{1}{T} \sum_{t=1}^{T} \mathbf{h}_t$$

- LSTM computes representations with history, not future

Bidirectional LSTM (BiLSTM)

- **BiLSTM = 2 LSTMs running on opposite direction**
- $\overrightarrow{LSTM}$ runs forward on sequence to produce its representations:

$$\overrightarrow{\mathbf{h}}_1, \ldots, \overrightarrow{\mathbf{h}}_T$$

- $\overleftarrow{LSTM}$ runs backward on sequence to produce its representations:

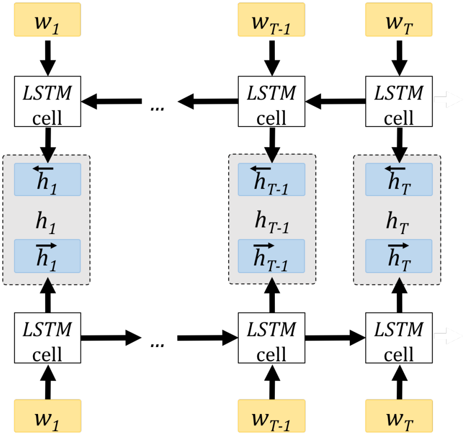
$$\overleftarrow{\mathbf{h}}_1, \ldots, \overleftarrow{\mathbf{h}}_T$$

- The output of biLSTM is the concatenation of both representations:

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

- These vectors are called "contextualized word vectors" (Peters et al., 2018).

Bidirectional LSTM (BiLSTM)



- A BoW sentence representation from an biLSTM is:

$$\mathbf{s} = \frac{1}{T}\sum_{t=1}^{T}\mathbf{h}_t = \frac{1}{T}\sum_{t=1}^{T}[\overrightarrow{\mathbf{h}}_t, \overleftarrow{\mathbf{h}}_t]$$

Training of a biLSTM as a Language model

- Train both LSTMs independently

- The forward $\overrightarrow{LSTM}$ is train to predict the upcoming word:

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

- The backward $\overleftarrow{LSTM}$ is train to predict the previous word:

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

- Equivalently the biLSTM can be trained with joint objective:

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

- Both solutions merge the LSTMs at the last layer $\rightarrow$ **late fusion**

Deep biLSTM architecture with early fusion

- Deep biLSTM: more than one layer
- We merge forward and backward representations at each layer k:

$$
\begin{aligned}
\overrightarrow{\mathbf{h}}_t^k &= \overrightarrow{LSTM}(\mathbf{h}_t^{k-1}), \\
\overleftarrow{\mathbf{h}}_t^k &= \overleftarrow{LSTM}(\mathbf{h}_t^{k-1}). \\
\mathbf{h}_t^k &= [\overrightarrow{\mathbf{h}}_t^k, \overleftarrow{\mathbf{h}}_t^k],
\end{aligned}
$$

- the hidden states $\mathbf{h}_t^k$ depends on the past and the future
- impossible to train this model with language modeling!
- This is often refered to as **early fusion**

Deep biLSTM with early fusion

- 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

Cloze procedure in practice (Devlin et al., 2018)

Sentence The cat is drinking milk in the kitchen

Cloze procedure in practice (Devlin et al., 2018)

Sentence	The cat is drinking milk in the kitchen
input	The cat <MASK> drinking <MASK> in the kitchen

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

Cloze procedure in practice (Devlin et al., 2018)

Sentence	The cat is drinking milk in the kitchen
input	The cat <MASK> drinking <MASK> 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

Cloze procedure in practice (Devlin et al., 2018)

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>

Transformer Networks

Self attention: 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 word representations to compute $\mathbf{h}_t$?
- Technical challenge:

  need to combine a variable number of representations!

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 words

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

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

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:

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

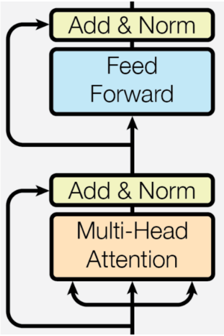
  where $\mathbf{H}, \mathbf{W} \in \mathbb{R}^{d \times T}$ and $\mathbf{V}, \mathbf{K}, \mathbf{Q} \in \mathbb{R}^{d \times d}$
- $\mathbf{V}, \mathbf{K}, \mathbf{Q}$ are parameters to be learned.
- This operation is called self-attention

- 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

Transformer network

Transformer block:

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



Vaswani et al. (2017)

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

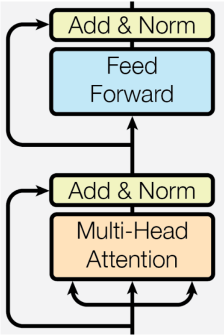
Transformer network

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 $\mathbf{E} \in \mathbb{R}^{d \times T}$

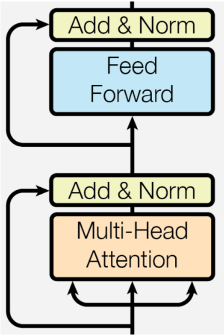
- $\mathbf{E}$ can be learned, or defined using sin and cos:

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

Transformer network

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)

Masking for Transformer Language Models

- In transformer, $\mathbf{h}_t$ depends on all inputs
- Could not be used as is for language modeling
- Solution: use mask in attention, to only use past

- Reminder:

$$\begin{aligned}\mathbf{H} &= \mathbf{V}\mathbf{W}\mathrm{softmax}(\mathbf{W}^\top\mathbf{K}^\top\mathbf{Q}\mathbf{W}) \\ &= \mathbf{V}\mathbf{W}\mathbf{A}\end{aligned}$$

  Hence, $\mathbf{a}_{it}$ 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 $\mathbf{a}_{it} = 0$ for $i \geq t$

Masked softmax

- We introduce the masked softmax operator
- Given an input $\mathbf{x}$ and a binary mask $\mathbf{m}$,

$$[\text{masked\_softmax}(\mathbf{x}, \mathbf{m})]_i = \frac{m_i \exp(x_i)}{\sum_{i=1}^{d} m_i \exp(x_i)}$$

- Still sums to one, $m_i = 0$ implies $[\text{masked\_softmax}(\mathbf{x}, \mathbf{m})]_i = 0$
- Sometimes implemented as:

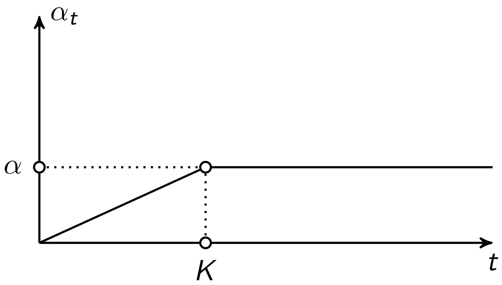
$$\text{softmax}(\mathbf{x} + \log(\mathbf{m}))$$

- **Beware:** do not learn the mask (e.g. PyTorch: `register_buffer`)

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 $(\alpha_t)_t$

- Set a target learning rate α

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

where K is the "warm-up" parameter

Evaluation of sentence representations

- Apply representation on downstream tasks like text classification
- Compare representation of similar sentences (e.g. obtained from paraphrasing)
- Identify relations between sentences: is one the negation of the other? Does one imply the other?
- Question answering: are the embeddings of a question and its answer similar?

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.

Leaderboard available at `https://gluebenchmark.com/`

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	**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

Conclusion

- Neural networks have been very successful in language modeling
- They are also dominant in applications (machine translation sentence representation...)
- Big progress in architectures until recently with early fusion and transformers

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