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Sparse and dense embeddings as inp

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Input to feedforward neural networks

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- ▶ A bag-of-words model where the input \mathbf{x} is the count of each word (feature) x_i .
 - ▶ The connections from word (feature) x_i to hidden units z_k form a vector \mathbf{w}_k that is used as the emb
 - ▶ With summing within t
- ▶ *Pretrained* word embeddings learn unlabeled data, using techniques such as Word2Vec
- ▶ *Contextualized* word embeddings (e.g., ELMO, BERT) that are computed dynamically for a word sequence. This requires more advanced architectures (Transformers) that we will talk about later in the course.

One-hot encodings for features

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A *one-hot* encoding is one in which each dimension corresponds to a unique feature, and the resulting feature vector of a c instance can be thought of as the sum of indicator vectors in which a single dimension has a value of one and all other dimensions have a value of zero.

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Example:

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When considering a bag-of-words representation of 40000 words. A short document of 20 words will be represented with a very sparse 40000-dimensional vector in which **at most** 20 dimensions have non-zero values

Sparse vectors for text classification

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Sparse vectors for text classification can be viewed as a summation of one-hot features for a text instance:

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$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \end{bmatrix}$$

$$=$$

$$\begin{bmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 \end{bmatrix}$$

Shortcomings for sparse representations

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- ▶ Each feature is a sparse vector in which one dimension is 1 and the rest are 0s (thus “one-hot”)
- ▶ Dimensionality of one-hot vector is same as n features
- ▶ Features can be combined. For example, the feature “word is ‘cat’” as it is to “word is ‘cat’”
- ▶ Features for one classifying instance can be summed.
- ▶ A recent trend is to use dense representations that can capture similarities between features, which lead to better generalizations to new data.

Dense vectors for text classification

- ▶ Extract a set of linguistic features f_1, \dots, f_k that are relevant for predicting the output class.
- ▶ For each feature f_i of interest, retrieve the corresponding vector v_i , which can be pre-trained, pre-co-initialization, or initialized.
- ▶ Each core feature is mapped to a low-dimensional space (typically 50 dimensions).
- ▶ Combine the vectors (either by concatenation, or a combination of both) into an input vector for a classification instance.
 - ▶ Note: concatenation if we care about relative position, but doesn't work for variable-length vectors such as document classification
- ▶ Model training will cause similar features to have similar vectors - information is shared between similar features.

Relationship between one-hot and dense vectors

- ▶ Dense represent pre-trained word embeddings
- ▶ One-hot and dense representations may not be the same one might think
- ▶ In fact, using sparse, one-hot vectors as input to a neural network to learn a task [e.g. word classification feature] based on training data.
- ▶ With task-specific word embedding, the embedding is typically smaller, but the training objective for the embedding and the task objective are one and the same
- ▶ With pre-trained word embeddings, the training data is easy to come by (just unannotated text), but the embedding objective and task objective may diverge.

Two ways of obtaining dense word vectors

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- ▶ Count based methods, known in NLP as Distr
Semantic Models (DSM) or Vector Seman
- ▶ Predictive m rk
community ntations
for words, co
- ▶ Distributed word representations uct of
neural language models and later bec
its own

Distributional semantics

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- ▶ Based on the well-known observation of Z. Harris: Words are similar if they occur in the same context (Harris)
- ▶ Further summarized it as a slogan: "You shall know the company it keeps." (J. R. Firth, 1957)
- ▶ A long history of word meaning representation
represents a context word it can occur with
- ▶ Each word is represented as a sparse vector in a high-dimensional space
- ▶ Then word distances and similarities can be computed with such a matrix

Steps for building a distributional semantic model

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- ▶ Preprocess a (large) corpus (tokenization at a minimum, possibly lemmatization, POS tagging, or syntactic parsing)
- ▶ Define the “context” for a target term (words). The context can be a window centered on the target term, terms that are syntactically related (subject-of, object-of, modifier-of, etc.), or some other set of words.
- ▶ Compute a term-context matrix where each row corresponds to a term and each column corresponds to a context term.
- ▶ Each target term is then represented with a high-dimensional vector of context terms.

Mathematical processing for building a DSM

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- Weight the term-context matrix with association strength metrics such as Positive Pointwise Mutual Information (PPMI) to correct frequency bias

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$$PPMI(x, y) = \max(\log \frac{f(x, y)}{f(x)f(y)}, 0)$$

- Its dimensionality reduction techniques such as *singular value decomposition* (SVD)

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$$

$$\mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{U} \in \mathbb{R}^{m \times k}, \mathbf{\Sigma} \in \mathbb{R}^{k \times k}, \mathbf{V} \in \mathbb{R}^{n \times k}, n \gg k$$

- This will result in a matrix that has much lower dimension but retains most of the information of the original matrix.

Getting pre-trained word embeddings using predictive methods

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- ▶ Learns word embeddings from large naturally occurring text, using various language model objectives.
 - ▶ Decide on the context window
 - ▶ Define the objective function that is used to p context et word ba
 - ▶ Train the neur
 - ▶ The resulting weight matrix will serve representation for the target word
- ▶ “Don’t count, predict!” (Baroni et al, 2014) conducted systematic studies and found predict-based word embeddings outperform count-based embeddings.
- ▶ One of popular early word emdeddings are Word2vec embeddings.

Word2vec

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- ▶ Word2vec is a software package that consists of two main models: CBOW (Continuous Bag of Words)
- ▶ It popularized the use of distributed representations to neural networks (inspired by many follow-up models like GloVe and WordNet)
- ▶ It has its roots in language modeling (the use of context to predict the target word), but it's more about getting good language models and focuses instead on getting good word embeddings.

Understanding word2vec: A simple CBOW model with only one context word in

- ▶ Input $\mathbf{x} \in \mathbb{R}^V$ and $x_k = 1$ and $x_{k'} = 0$ for $k' \neq k$. $\Theta \in \mathbb{R}^{N \times V}$ is the weight matrix from the input layer to the hidden layer. Each column of Θ is an N -dimensional vector representation of a word of the input layer.

- ▶ $\Theta' \in \mathbb{R}^{V \times N}$ is the weight matrix from the hidden layer to the output layer and \mathbf{u}_{w_j} is the j -th row of Θ' . The output score o_j for each target word w_j and context word w_i is computed as:

$$o_j = \mathbf{u}_{w_j}^\top \mathbf{v}_{w_i}$$

- ▶ Finally we use softmax to obtain a posterior distribution

$$p(w_j | w_i) = y_j = \frac{\exp(o_j)}{\sum_{j'=1}^V \exp(o_{j'})}$$

where y_j is the output of the j -th unit in the output layer

A simple CBOW model

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Computing the hidden layer is just embedding lookup

Hidden layer computation <https://eduassistpro.github.io/>

$$\mathbf{v}_{w_i} = \mathbf{z} = \Theta \mathbf{x} =$$

$$\begin{bmatrix} 0.1 & 0.3 & 0.5 \\ 0.2 & 0.5 & 0.8 \\ 0.2 & 0.5 & 0.8 \end{bmatrix} \begin{bmatrix} 0.6 \\ 0.1 \\ 0.7 \end{bmatrix} \times \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0.5 \\ 0.8 \\ 0.8 \end{bmatrix}$$

Note there is no activation at the hidden layer (or there is a linear activation function), so this is a “degenerate neural network”.

Computing the output layer

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$\mathbf{o} = \Theta' \mathbf{z}$ <https://eduassistpro.github.io/>

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Each row of Θ' correspond to vector for a target word w_j .

Taking the softmax over the output

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$\begin{bmatrix} 0.11039215 \\ 0.08016116 \end{bmatrix}$

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$\begin{bmatrix} 0.11039215 \\ 0.08016116 \end{bmatrix}$

The output \mathbf{y} is a probabilistic distribution over the entire vocabulary.

Input vector and output vector

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Since there is no activation function at the hidden layer, the output is really just the dot product of the vector of the in context word and the vector of the output target word

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$$p(w_j|w_i) = y_j = \frac{(\mathbf{u}_{w_j}^\top \mathbf{v}_{w_i})}{\sum_{w_j'} \exp(q_j)}$$

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where \mathbf{v}_{w_i} from Θ is the **input vector** for word w_i and \mathbf{u}_{w_j} from Θ' is the **output vector** for word w_j

Computing the gradient on the hidden-output weights

- Use the familiar cross-entropy loss

$$\ell = - \sum_j \frac{1}{|V|} t_j \log y_j = - \log y_{j^*}$$

where j^* is the index of the target word

- Given y_j is the output on the hidden layer

$$\frac{\partial \ell}{\partial o_j} = y_j - t_j$$

$$\frac{\partial \ell}{\partial \theta'_{ji}} = \frac{\partial \ell}{\partial o_j} \frac{\partial o_j}{\partial \theta'_{ji}} = (y_j - t_j) z_i$$

- Update the hidden→output weights

$$\theta'_{ji} = \theta'_{ji} - \eta (y_j - t_j) z_i$$

Updating input→hidden weights

- Compute the error

$$\frac{\partial \ell}{\partial z_i} = \sum_{j=1}^V \frac{\partial \ell}{\partial o_j} \frac{\partial o_j}{\partial z_i} = \sum_{j=1}^V (y_j - t_j) \theta'_{ji}$$

- Since

$$\frac{\partial \ell}{\partial \theta_{ik}} = \sum_{j=1}^V (y_j - t_j) \theta'_{ji} x_{kj}$$

The derivative of ℓ on the input z_i is:

$$\frac{\partial \ell}{\partial \theta_{ik}} = \frac{\partial \ell}{\partial z_i} \frac{\partial z_i}{\partial \theta_{ik}} = \sum_{j=1}^V (y_j - t_j) \theta'_{ji} x_{kj}$$

- Update the input→hidden weights

$$\theta_{ki} = \theta_{ki} - \eta \sum_{j=1}^V (y_j - t_j) \theta'_{ji} x_{kj}$$

Gradient computation in matrix form

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$$D_o = Y - \begin{bmatrix} 0.11039215 & 9215 \\ 0.10505362 & 6362 \\ 0.11262222 & 37778 \\ & 0.09693485 \\ & 0.13893957 \\ 0.05820895 & 5820895 \\ 0.12922834 & 2322834 \\ 0.063057 & 0 & 0.063057 \\ 0.11039215 & 0 & 0.11039215 \\ 0.08016116 & 0 & 0.08016116 \end{bmatrix}$$

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Computing the errors at the hidden layer

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$$D_z = D_o^T \Theta' =$$

$$\begin{bmatrix} 0.110 & 0.106 & -0.887 & 0.097 & 0.139 & 0.0 & .110 & 0.080 \end{bmatrix}$$

$$\times \begin{bmatrix} 0.3 & 0.4 & 0.6 \\ 0.7 & 0.1 & 0.6 \\ 0.5 & 0.2 & 0.7 \\ 0.2 & 0.6 & 0.3 \\ 0.6 & 0.5 & 0.6 \\ 0.3 & 0.1 & 0.1 \\ 0.2 & 0.4 & 0.8 \\ 0.3 & 0.2 & 0.1 \\ 0.3 & 0.4 & 0.6 \\ 0.3 & 0.5 & 0.1 \end{bmatrix}$$

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Computing the updates to Θ'

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$$\nabla_{\Theta'} = D_o z^T =$$

$$\begin{bmatrix} 0.119 \\ 0.106 \\ -0.887 \\ 0.097 \\ 0.139 \\ 0.058 \\ 0.123 \\ 0.063 \\ 0.110 \\ 0.080 \end{bmatrix} \times \begin{bmatrix} 0.5 & 0.8 & 0.8 \end{bmatrix} = \begin{bmatrix} 0.0595 & 0.0848 & 0.0872 \\ 0.053 & 0.085 & 0.085 \\ -0.4436 & -0.7104 & -0.7104 \\ 0.0485 & 0.0776 & 0.0776 \\ 0.0695 & 0.1112 & 0.1112 \\ 0.029 & 0.0467 & 0.0467 \\ 0.0615 & 0.0992 & 0.0992 \\ 0.032 & 0.050 & 0.050 \\ 0.055 & 0.088 & 0.088 \\ 0.040 & 0.064 & 0.064 \end{bmatrix}$$

CBOW for multiple context words

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$$\begin{aligned} \mathbf{z} &= \frac{1}{M} \Theta(\mathbf{x}_1 + \mathbf{x}_2 + \cdots + \mathbf{x}_M) \\ &= \frac{1}{M} (\mathbf{v}_{w_1} + \mathbf{v}_{w_2} + \cdots + \mathbf{v}_{w_M}) \end{aligned}$$

where M is the number of words in the context, w_1, w_2, \dots, w_M are the words in the context. The loss function is

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$$\begin{aligned} \ell &= -\log p(w_j | w_1, \dots, w_M) \\ &= -o_{j^*} + \log \sum_{j'=1}^V \exp(o_{j'}) \\ &= -\mathbf{u}_{w_j}^\top \mathbf{z} + \log \sum_{j'=1}^V \exp(\mathbf{u}_{w_{j'}}^\top \mathbf{z}) \end{aligned}$$

Computing the hidden layer for multiple context words

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$z = \Theta x =$ Assignment Project Exam Help

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$$\begin{bmatrix} 0.1 & 0.3 & 0.5 & 0.6 \\ 0.2 & 0.5 & 0.8 & 0.7 & 0.9 & 0.4 & 0.8 \\ 0.2 & 0.5 & 0.8 & 0.7 & 0.9 & 0.4 & 0.8 \end{bmatrix} \times \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \\ 0 \\ 1 \\ 1 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1.5 \\ 3.0 \\ 3.0 \end{bmatrix}$$

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During backprop, update vectors for four words instead of just one.

Skip-gram: model

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$p(w_{c,j} = w_{O,c} | w_I) = y_{c,j} = \frac{1}{Z}$
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where $w_{c,j}$ is the output layer, $w_{O,c}$ is the actual output word, w_I is the only input word, $y_{c,j}$ is the output of the c -th panel of the output layer; $o_{c,j}$ is the net input to the j -th unit on the c -th panel of the output layer.

$$o_{c,j} = o_j = \mathbf{u}_{w_j} \cdot \mathbf{z}, \text{ for } c = 1, 2, \dots, C$$

Skip-gram: loss function

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$$\ell = -\log p(w_{O,1}, w_{O,2}, \dots, w_{O,C} | w_I)$$

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$$= -\sum_{c=1}^C \log \frac{\exp(o_{c,j_c^*})}{\sum_{j \in V} \exp(o_{c,j})}$$

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where j_c^* is the index of the actual c -th output context word.

Combine the loss of C context words with multiplication. Note: o_j is the same for all C panels

Skip-gram: updating the weights

- ▶ We take the derivative of ℓ with respect to $o_{c,j}$ for every unit on every p, and obtain

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$$e_{c,j} = \frac{\partial \ell}{\partial o_{c,j}} = y$$

which is the prediction error of the unit.

- ▶ We define a E_j as the sum of the prediction errors for all c: $E_j = \sum_{c=1}^C e_{c,j}$

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$$\frac{\partial \ell}{\partial \theta'_{ji}} = \sum_{c=1}^C \frac{\partial \ell}{\partial o_{c,j}} \cdot \frac{\partial o_{c,j}}{\partial \theta'_{ji}} = E_j \cdot z_i$$

- ▶ Updating the hidden→output weight matrix:

$$\theta'_{ji} = \theta'_{ji} - \eta \cdot E_j \cdot z_i$$

- ▶ No change in how the input→hidden weights are updated.

Additional sources on the skip-gram model

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- Assignment Project Exam Help
- For step-by-step derivation of the Skip-gram model, see the excellent tutorial https://aditya77.github.io/demystifying_neural_network_in_nlp_age_modeling/
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Optimizing computational efficiency

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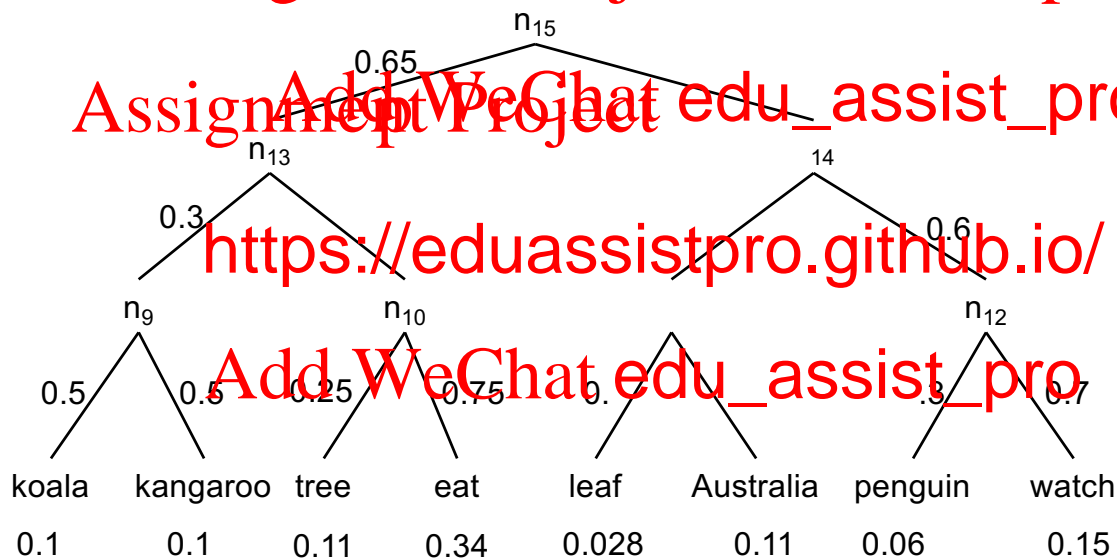
- ▶ Computing softmax at the output layer is expensive. It involves iterative operations over the entire vocabulary.
- ▶ Two methods
 - ▶ **Hierarchical softmax**: Compute the probability from $|V|$ to $\log |V|$.
 - ▶ **Negative sampling**: Instead of computing the probability for all the words in the vocabulary, only sample a small number of words that are not actual context words in the training corpus.

Hierarchical softmax

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Computing the probabilities of the leaf nodes

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$$P(\text{"Kangaroo"}|z) = P_n(\text{Left}|z) \times P_n(\text{Right}|z)$$

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$$P_n(\text{Right}|z) = 1$$

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$$P_n(\text{Left}|z) = \alpha(\gamma)$$

where γ_n is a vector from a set of new parameters that replace Θ

Huffman Tree Building

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A simple algorithm:

- ▶ Prepare a collection of n initial Huffman trees, each is a single leaf node. Put the n trees in a queue organized by weight (frequency).
- ▶ Remove the first two trees from the queue. Create a new tree with these two trees as children, and whose weight is the sum of the two children trees. Put this new tree in the queue.
- ▶ Repeat steps 2-3 until all of the partial Huffman trees have been combined into one.

Negative sampling

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- ▶ Computing softmax over the vocabulary is expensive. Another alternative is to approximate softmax by only sample of (context) words at a time.
- ▶ Given a pair of words (w, c) , let P be the probability of c coming from the corpus, and $P(D = 1|w, c)$ be the probability of c coming from the corpus.
- ▶ This probability can be modeled as a sigmoid function.

$$P(D = 1|w, c) = \sigma(\mathbf{u}_w^\top \mathbf{v}_c) = \frac{1}{1 + e^{-\mathbf{u}_w^\top \mathbf{v}_c}}$$

New learning objective for negative sampling

- ▶ We need a new objective to minimize the following

$$\mathcal{L} = - \sum_{w_j \in D} \log \sigma(o_{w_j}) - \sum_{w_j \in D'} \log \sigma(-o_{w_j})$$

where D is a set of correct context - target word pairs and D' is a set of incorrect context - target word pairs

- ▶ Note that we use multiple positive context words in the original algorithm, there will be only one positive target word.
- ▶ The derivative of the loss function with respect to the output word will be:

$$\frac{\partial \mathcal{L}}{\partial o_{w_j}} = \sigma(o_{w_j}) - t_{w_j}$$

where $t_{w_j} = 1$ if $w_j \in D$ and $t_{w_j} = 0$ if $w_j \in D'$

Updates to the hidden output weights

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- Compute the gradient on the output weights

$\frac{\partial \ell}{\partial \mathbf{w}}$

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- When updating the output weights, only
for words in the positive sample and negative
be updated:

Updates to the input hidden weights

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- Computing the derivative of the loss function with respect to the hidden layer

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$$\frac{\partial \mathcal{L}}{\partial \mathbf{u}_{w_j}} = (\sigma(o_w) - t_w) \mathbf{x}_j$$

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- In the CBOW algorithm, the weights for a words will be updated. In the Skip-gram algorithm, the weights for the target word will be updated.

$$\mathbf{v}_{w_i} = \mathbf{v}_{w_i} - \eta(\sigma(o_{w_j}) - t_{w_j}) \mathbf{u}_{w_j} \mathbf{x}_i$$

How to pick the negative samples?

- If we just randomly pick any given word w_i getting picked is:

$$p(w_i) = \frac{\text{freq}(w_i)}{\sum_{j=1}^V \text{freq}(w_j)}$$

More frequent words

may not be ideal

- Adjust the formula to give the less frequent words a higher chance to get picked.

$$p(w_i) = \frac{\text{freq}(w_i)^{\frac{3}{4}}}{\sum_{j=1}^V \text{freq}(w_j)^{\frac{3}{4}}}$$

- Generate a sequence of words using the adjusted probability, and randomly pick $n_{D'}$ words

Use of embeddings: word and short document similarity

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- ▶ Word embeddings can be used to compute word similarity with cosine similarity

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- ▶ How accurate word similarity can also be used
- ▶ They can also be used to compute the similarity of documents

$$sim_{doc}(D_1, D_2) = \sum_{i=1}^m \sum_{j=1}^n \cos(\mathbf{w}_i^1, \mathbf{w}_j^2)$$

Use of embeddings: word analogy

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- What's even more impressive is that they can be used to compute word analogy

$$analogy(m : w \rightarrow k : ?) = \operatorname{argmax}_{k \in V} (\cos(\mathbf{v}, \mathbf{k}) - \cos(\mathbf{v}, \mathbf{w}))$$

$$analogy(m : w \rightarrow k : ?) = \operatorname{argmax}_{k \in V} (\cos(\mathbf{v}, \mathbf{k}) - \cos(\mathbf{v}, \mathbf{w}))$$

$$analogy(m : w \rightarrow k : ?) = \operatorname{argmax}_{k \in V \setminus \{m, w\}} \frac{\cos(\mathbf{v}, \mathbf{k})\cos(\mathbf{v}, \mathbf{w})}{\cos(\mathbf{v}, \mathbf{m}) + \epsilon}$$

Word analogy

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Use of word embeddings

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- ▶ Computing word similarities is not a “real” problem in the eyes of many. [Add WeChat edu_assist_pro](https://eduassistpro.github.io/)
- ▶ The most important use word embeddings is as input to predict the output. <https://eduassistpro.github.io/>
- ▶ Many follow embeddings, e.g., GLOVE
 - ▶ word2vec: <http://vectors.nlp>
 - ▶ fasttext: <https://fasttext.cc/docs/en/english-vectors.html>
 - ▶ GLOVE: <https://nlp.stanford.edu/projects/glove>

Shortcoming of “per-type” word embeddings

- ▶ “Per-type” word embeddings do not account for the context of the word.
 - ▶ “Work out the **solution** in your head.”
 - ▶ “Heat the **solution** to 75° Celsius.”
 - ▶ Having the same embedding for both instances of “solution” doesn’t make sense.
- ▶ The solution is Contextualized word embeddings generated on the fly for each word in each sentence.
 - ▶ ELMO: <https://allenai.org/data/ELMo/>
 - ▶ BERT: <https://github.com/google-research/bert>
 - ▶ Roberta: <https://pytorch.org/hub/pytorch-fairseq-roberta>
- ▶ The contextualized word embeddings can be fine-tuned when used in a new classification task in a process called *transfer learning*.
- ▶ This turns out to be a very powerful idea that leads to many breakthroughs.

Embeddings in Pytorch

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