Feature Engineering

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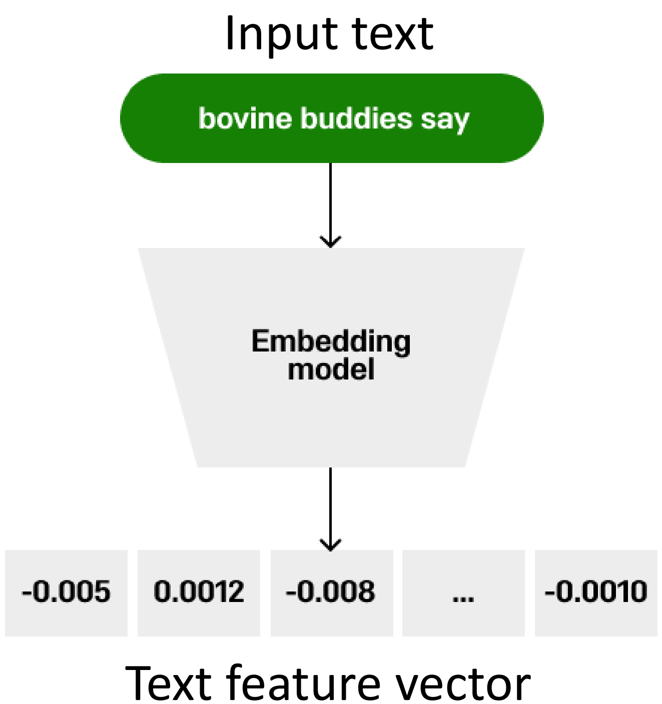
Content outline

- Feature engineering: A definition
- Conventional text encodings
- Modern word embeddings

Feature engineering

- Feature engineering involves selecting, transforming, and creating relevant features from raw data.
- This aims to enhance the performance of ML models.



Input image | Edge features

Feature engineering: Key steps

- Feature selection: Pick the most relevant features from the data to reduce noise and enhance model accuracy.
  - Statistical tests, correlation analysis, or feature importance scores.
- Feature transformation: Modify features to suit the model.
  - Encoding (e.g., one-hot encoding, label encoding), normalization (e.g., min-max, standardization, log/power transforms).
- Feature creation: Generate new features from existing data to capture valuable patterns and insights.
- Dimensionality reduction: Lower the dimensionality of the feature space while retaining the most important information.
  - E.g., Principal Component Analysis (PCA)

Feature engineering: Importance

- Improve model performance: Good features make patterns in the data more apparent, leading to better predictions.
- Reduce overfitting: Deleting irrelevant features help simplify the model.
- Optimize training time: A focused feature set can minimize computational requirements.

- Feature engineering involves creativity, domain expertise, and experimentation to achieve the best results.

Conventional text encodings

Document vectorization

- A vocabulary is built from all words available in the corpus.
- Each word is a column/row in the vector space.

The cat sat on the hat.
The hats are on the table.

Corpus

cat

sat → sit

hats → hat

table

Text processing
- Tokenize
- Remove stop words
- Lemmatize

cat	hat	sit	table
…			
…			

Vector space

One-hot encoding for text

- Each term is encoded by a one-hot vector, in which
  - The vector's length is the number of distinct terms in the corpus.
  - Only the element at the corresponding index is set to one.
- A tensor of multiple one-hot vectors describes a document.

Gain

- Terms are ordered $\rightarrow$ suitable for models like RNN,…

Loss

- The vector is huge due to large real-world vocabulary.
- Binary representation $\rightarrow$ the frequency of words is lost.

One-hot encoding: An example

The quick brown fox jumped over the brown dog

cat	the	quick	brown	fox	jumped	over	dog	bird	flew		kangaroo	house
0	1	0	0	0	0	0	0	0	0	...	0	0
0	0	1	0	0	0	0	0	0	0	...	0	0
0	0	0	1	0	0	0	0	0	0	...	0	0
0	0	0	0	1	0	0	0	0	0	...	0	0
0	0	0	0	0	1	0	0	0	0	...	0	0
0	0	0	0	0	0	1	0	0	0	...	0	0
0	1	0	0	0	0	0	0	0	0	...	0	0
0	0	0	1	0	0	0	0	0	0	...	0	0
0	0	0	0	0	0	0	1	0	0	...	0	0

time

Dictionary Size

Image credit: [Data Science Central]

Binary encoding for text

- Each document is encoded by a binary vector, in which
  - The vector's length is the number of distinct terms in the dataset.
  - If a term is present, the element at the corresponding index is set to one. Otherwise, set it to zero.

Gain

- Tensor is unnecessary, yet the vector is **still** huge.

Loss

- Binary representation $\rightarrow$ lose the frequency of words.
- Terms are unordered $\rightarrow$ lose the context of words.

Binary encoding: An example

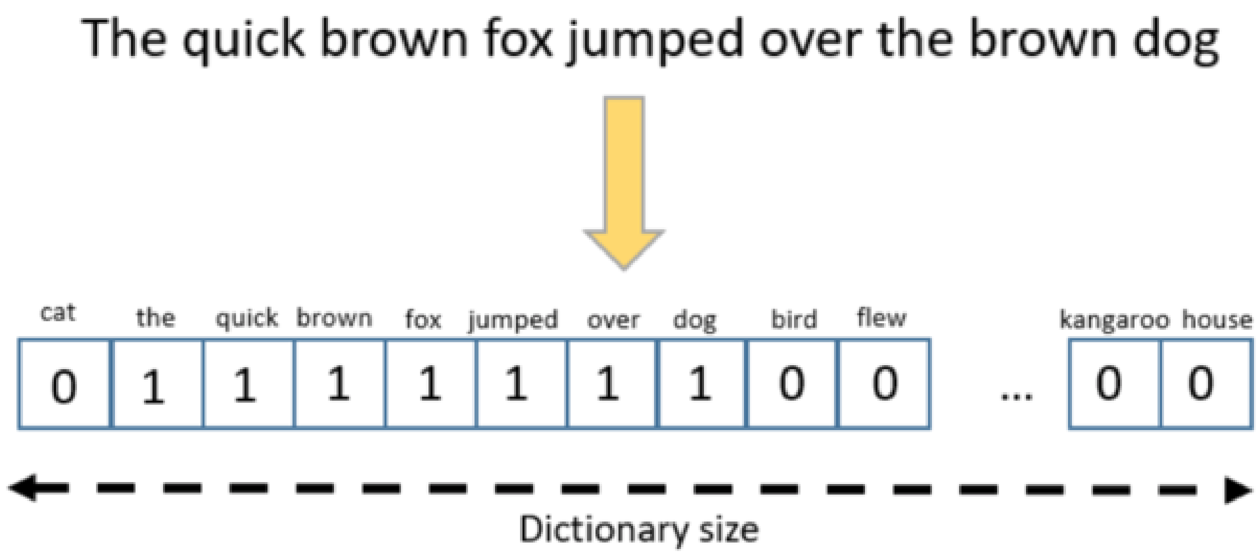


Image credit: [Data Science Central]

Index-based encoding for text

- A dictionary is required to map words to (numeral) indexes.
- We represent each document via a sequence of indices, each encodes one word.

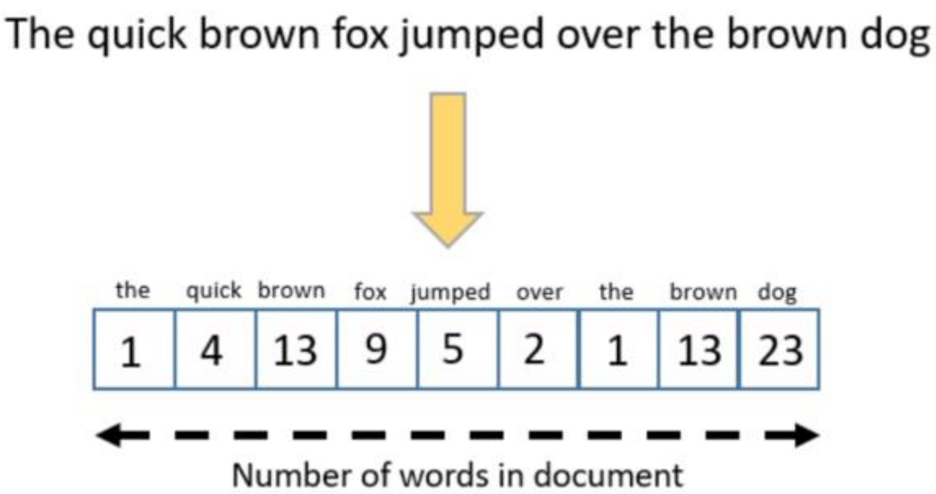


Image credit:
[Data Science Central]

Loss

- It introduces a numerical distance between texts that does not really exist.

Term frequency (TF)

- Let the raw count $f_{t,d}$ of a term t in document d be the number of times that t appears in d.
- The term frequency $\boldsymbol{tf(t,d)}$ of a term t in doc d is given by

$$\boldsymbol{tf(t,d) = \frac{f_{t,d}}{\sum_{t' \in d} f_{t',d}}}$$

  - t' represents every distinct term in the document d.

Term frequency (TF)

Gain

- The frequency of words can be captured.

Loss

- A term that appears in many documents of the corpus may not be discriminative.
- Terms are unordered $\rightarrow$ the context of words are lost.

Term frequency (TF): Example

- Consider a corpus of four documents
  - Doc 1: fast car highway road car
  - Doc 2: car car bike fast fast
  - Doc 3: road road highway fast wheel
  - Doc 4: bike wheel car wheel
- The following table shows the term frequencies.

	bike	car	fast	highway	road	wheel
Doc 1	0	2/5	1/5	1/5	1/5	0
Doc 2	1/5	2/5	2/5	0	0	0
Doc 3	0	0	1/5	1/5	2/5	1/5
Doc 4	1/4	1/4	0	0	0	2/4

Term frequency (TF): Variants

- There are various other ways to define the term frequency.

Weighting scheme	tf weight
Binary	0, 1
Raw count	$f_{t,d}$
Log normalization	$\log\left(1+f_{t,d}\right)$
Double normalization 0.5	$0.5+0.5\frac{f_{t,d}}{\max_{t'\in d} f_{t',d}}$
Double normalization K $K\in[0,1]$	$K+(1-K)\frac{f_{t,d}}{\max_{t'\in d} f_{t',d}}$

Inverse document frequency (IDF)

- The inverse document frequency $\boldsymbol{idf(t, D)}$ of a term t in the document collection D is given by

$$\boldsymbol{idf(t, D) = \log \frac{N}{|\{d \in D: t \in d\}|}}$$

  - N is the number of document in the corpus D
  - The term is not in the corpus $\rightarrow$ division-by-zero $\rightarrow$ adjust the denominator to $1 + |\{\boldsymbol{d} \in \boldsymbol{D}: \boldsymbol{t} \in \boldsymbol{d}\}|$.

- This solves the issue of terms that are too frequent across the documents.

IDF: Example

- Consider a corpus of four documents
  - Doc 1: fast car highway road car
  - Doc 2: car car bike fast fast
  - Doc 3: road road highway fast wheel
  - Doc 4: bike wheel car wheel
- The following table shows the inverse document frequencies.

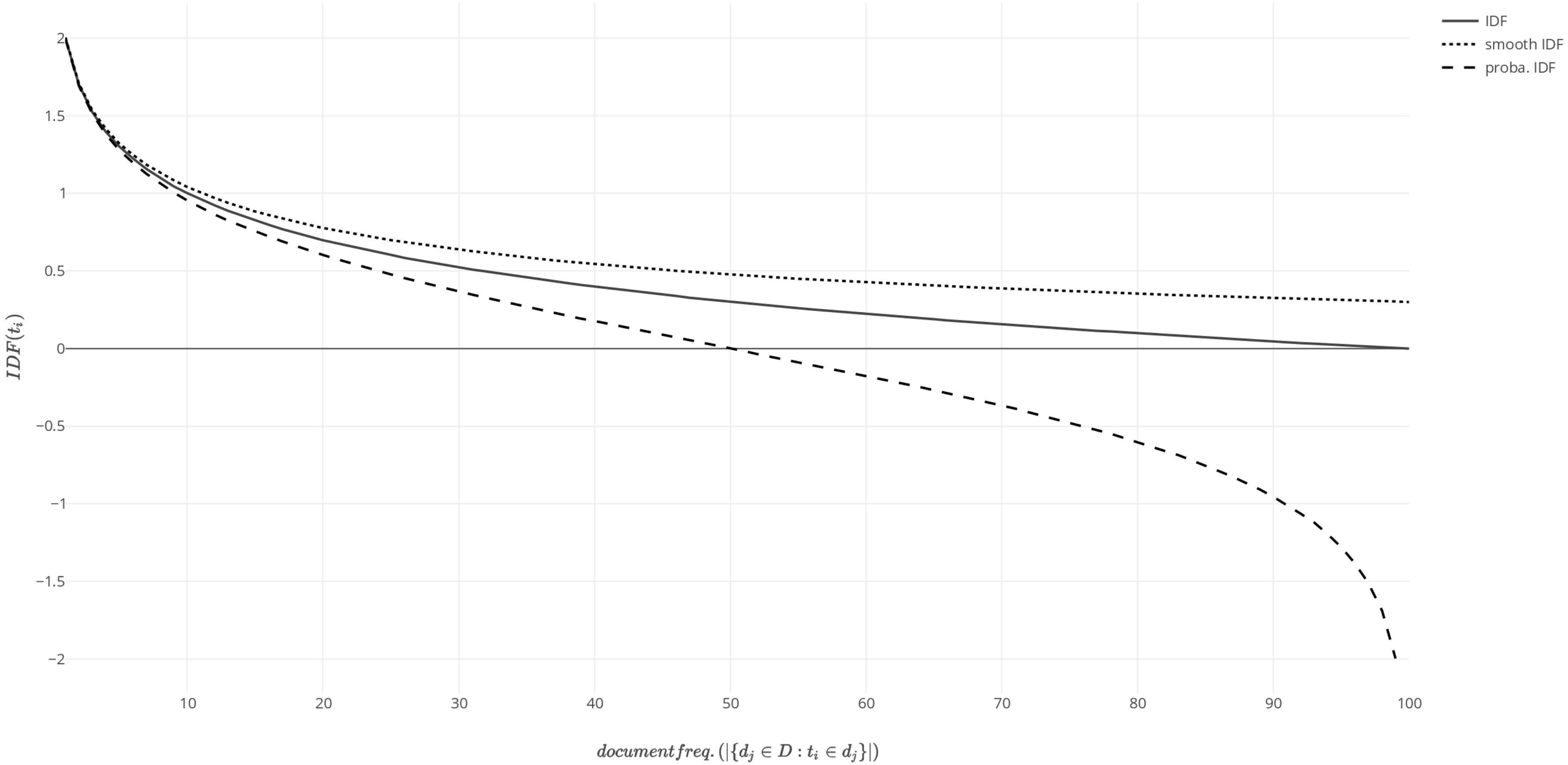
	bike	car	fast	highway	road	wheel
idf(t, D)	log(4/2)	log(4/3)	log(4/3)	log(4/2)	log(4/2)	log(4/2)

IDF: Variants

- There are also many ways to define the inverse document frequency.

Weighting scheme	idf weight ($n_t = \lvert\{d \in D : t \in d\}\rvert$)
Unary	1
Inverse document frequency smooth	$\log\left(\frac{N}{1+n_t}\right)+1$
Inverse document frequency max	$\log\left(\frac{\max_{\{t' \in d\}} n_{t'}}{1+n_t}\right)$
Probabilistic inverse document frequency	$\log\left(\frac{N-n_t}{n_t}\right)$

IDF: Variants



Plot of different inverse document frequency functions: standard, smooth, probabilistic

Image credit: [Wikipedia]

TF-IDF

- The tf-idf is defined as: $\boldsymbol{tfidf(t,d,D) = tf(t,d) \cdot idf(t,D)}$

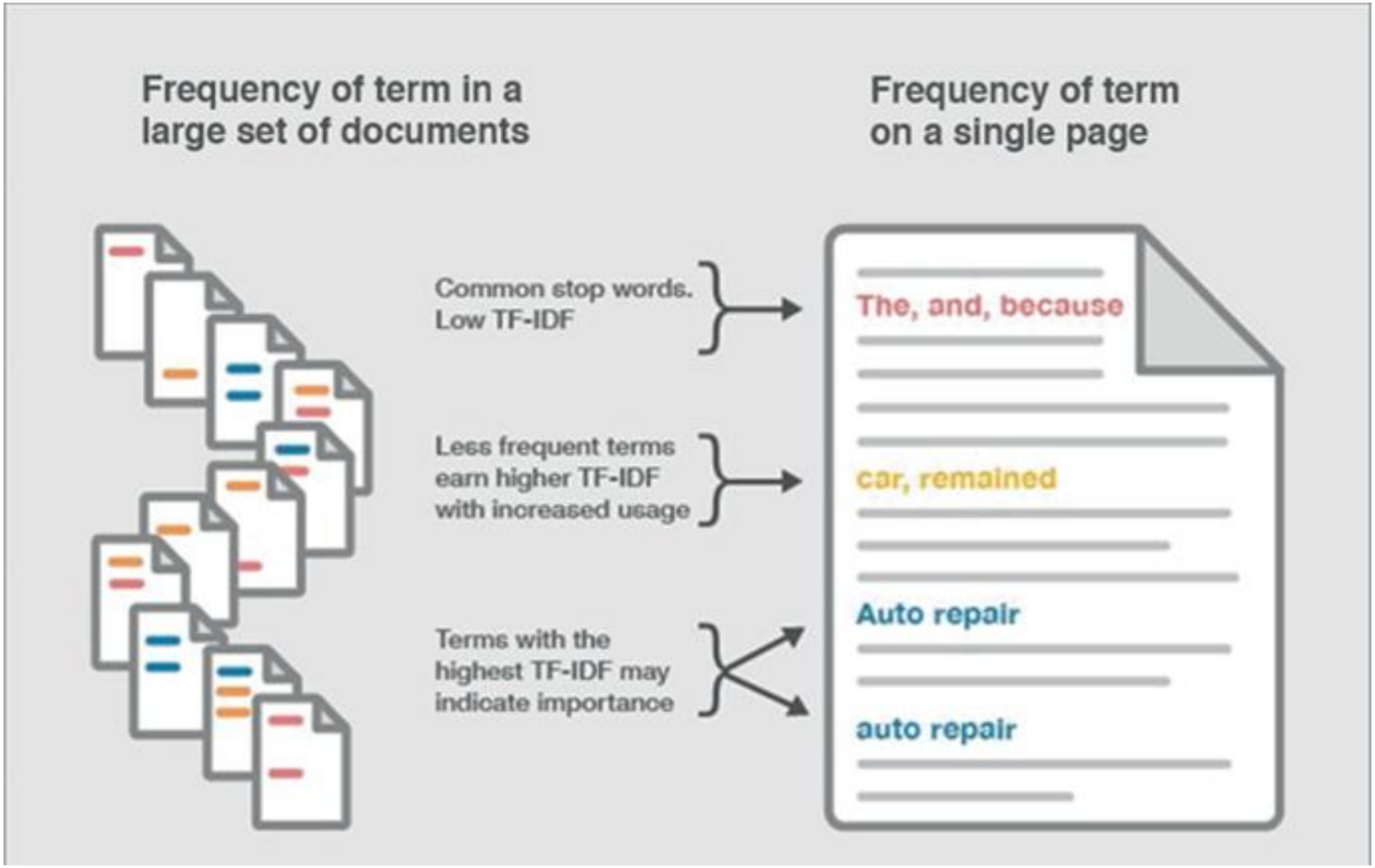


Image credit: [Springer]

TF-IDF: Represent the query

- We describe a query $\boldsymbol{q}$ in the same way as a document d in the corpus, or slightly differently.
- Recommended tf-idf weighting schemes

Document term weight	Query term weight
$f_{t,d} \cdot \log\left(\frac{N}{n_t}\right)$	$\left(0.5 + 0.5 \frac{f_{t,q}}{\max_{t\prime \in q} f_{t\prime,q}} f_{t,d}\right) \cdot \log\left(\frac{N}{n_t}\right)$
$\log\left(1 + f_{t,d}\right)$	$\log\left(1 + \frac{N}{n_t}\right)$
$\left(1 + f_{t,d}\right) \cdot \log\left(\frac{N}{n_t}\right)$	$\left(1 + f_{t,d}\right) \cdot \log\left(\frac{N}{n_t}\right)$

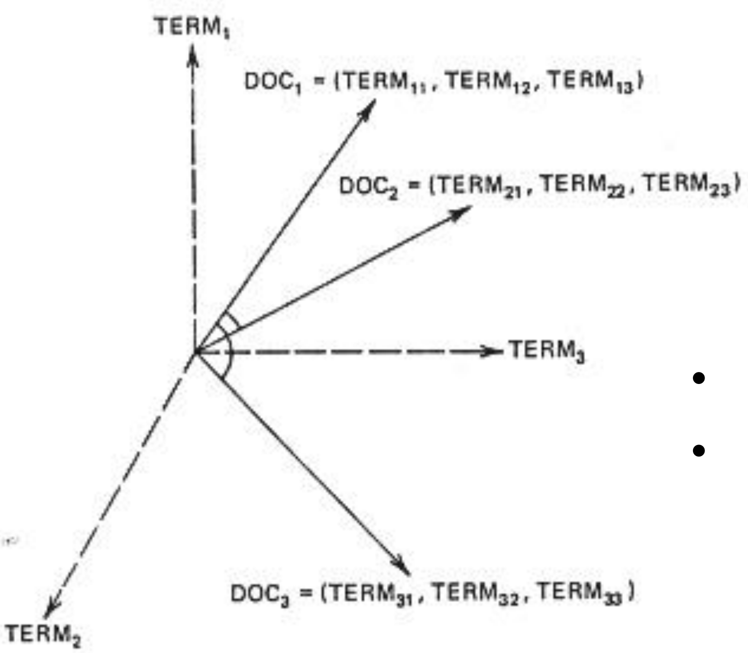
TF-IDF: Calculate the similarity

- The similarity between tf-idf vectors can be estimated by using common metrics.

- Cosine similarity:

$$cosine(\mathbf{d}, \mathbf{q}) = \frac{\langle \overset{\text{document}}{\mathbf{d}} \cdot \overset{\text{query}}{\mathbf{q}} \rangle}{\|\mathbf{d}\| \times \|\mathbf{q}\|}$$

$$= \frac{\sum_{i=1}^{|V|} w_{id} \times w_{iq}}{\sqrt{\sum_{i=1}^{|V|} w_{id}^2} \times \sqrt{\sum_{i=1}^{|V|} w_{iq}^2}}$$



- $|V|$ is the number of terms being considered.
- w_{id} and w_{iq} are the weights of term i in document d and query q, respectively.

TF-IDF: Cosine similarity example

- The following table shows the tfidf weights for the four documents.

	bike	car	fast	highway	road	wheel
Doc 1	0	$2/5 \cdot \log(4/3)$	$1/5 \cdot \log(4/3)$	$1/5 \cdot \log(4/2)$	$1/5 \cdot \log(4/2)$	0
Doc 2	$1/5 \cdot \log(4/2)$	$2/5 \cdot \log(4/3)$	$2/5 \cdot \log(4/3)$	0	0	0
Doc 3	0	0	$1/5 \cdot \log(4/3)$	$1/5 \cdot \log(4/2)$	$2/5 \cdot \log(4/2)$	$1/5 \cdot \log(4/2)$
Doc 4	$1/5 \cdot \log(4/2)$	$1/5 \cdot \log(4/3)$	0	0	0	$2/4 \cdot \log(4/2)$

- Consider the query Q: “fast fast car bike”. For simplicity, we apply the same tfidf scheme for the query.

Query	$1/4 \cdot \log(4/2)$	$1/4 \cdot \log(4/3)$	$2/4 \cdot \log(4/3)$	0	0	0

- Calculate the similarity between the query and the documents

$$\text{sim(Doc 2, Q)} = 0.967 > \text{sim(Doc 4, Q)} = 0.315$$
$$> \text{sim(Doc 1, Q)} = 0.299 > \text{sim(Doc 3, Q)} = 0.102$$

Quiz 01: Construct TF-IDF vectors

- Consider a collection of three documents. No preprocessing required.
- The vocabulary is V = { arrived, gold, shipment, silver, truck }.

  d1: shipment of gold damaged in a fire

  d2: shipment of gold arrived in a truck

  d3: delivery of silver arrived in a silver truck

- Define the TF-IDF vectors for the above documents on the given vocabulary
- Consider the queries q: **gold silver truck.** Compute the Cosine similarity between q and each of the above documents.

Modern word embeddings

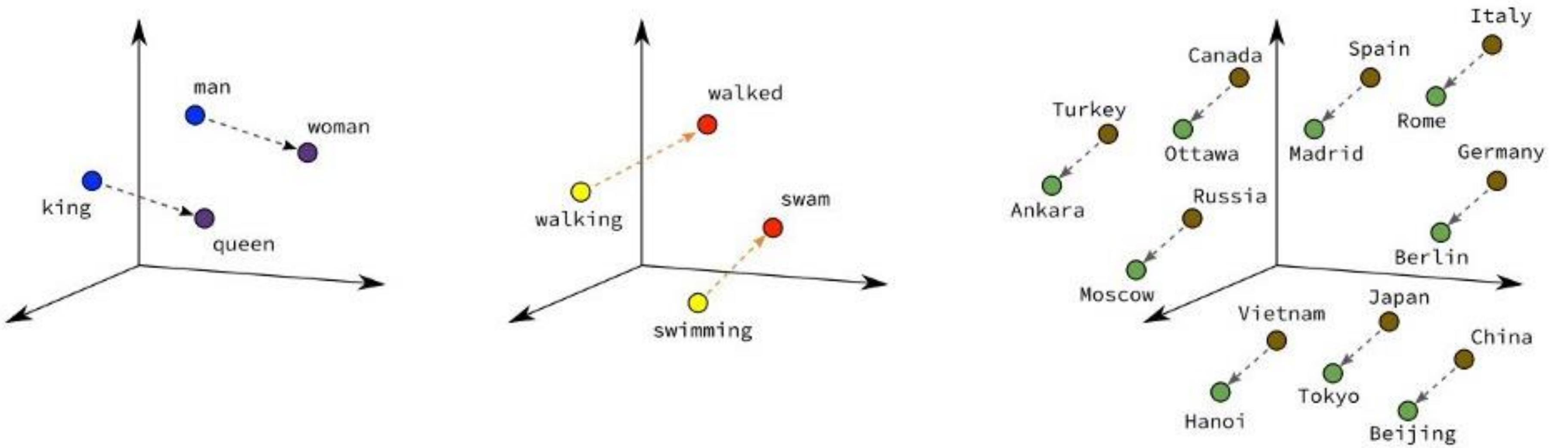
Michael Heck, 2019. The World of Vectors. Dialog Systems and Machine Learning.
Heinrich-Heine-Universität Düsseldorf.

Word embeddings

- A word embedding is a learned text representation where terms of the same meaning have an equal representation.
  - It can capture the context of a word in a document, semantic and syntactic similarity, relation with other words, etc.
- It is typically in the form of a real-valued vector that encodes the meaning of the word.

Word embeddings

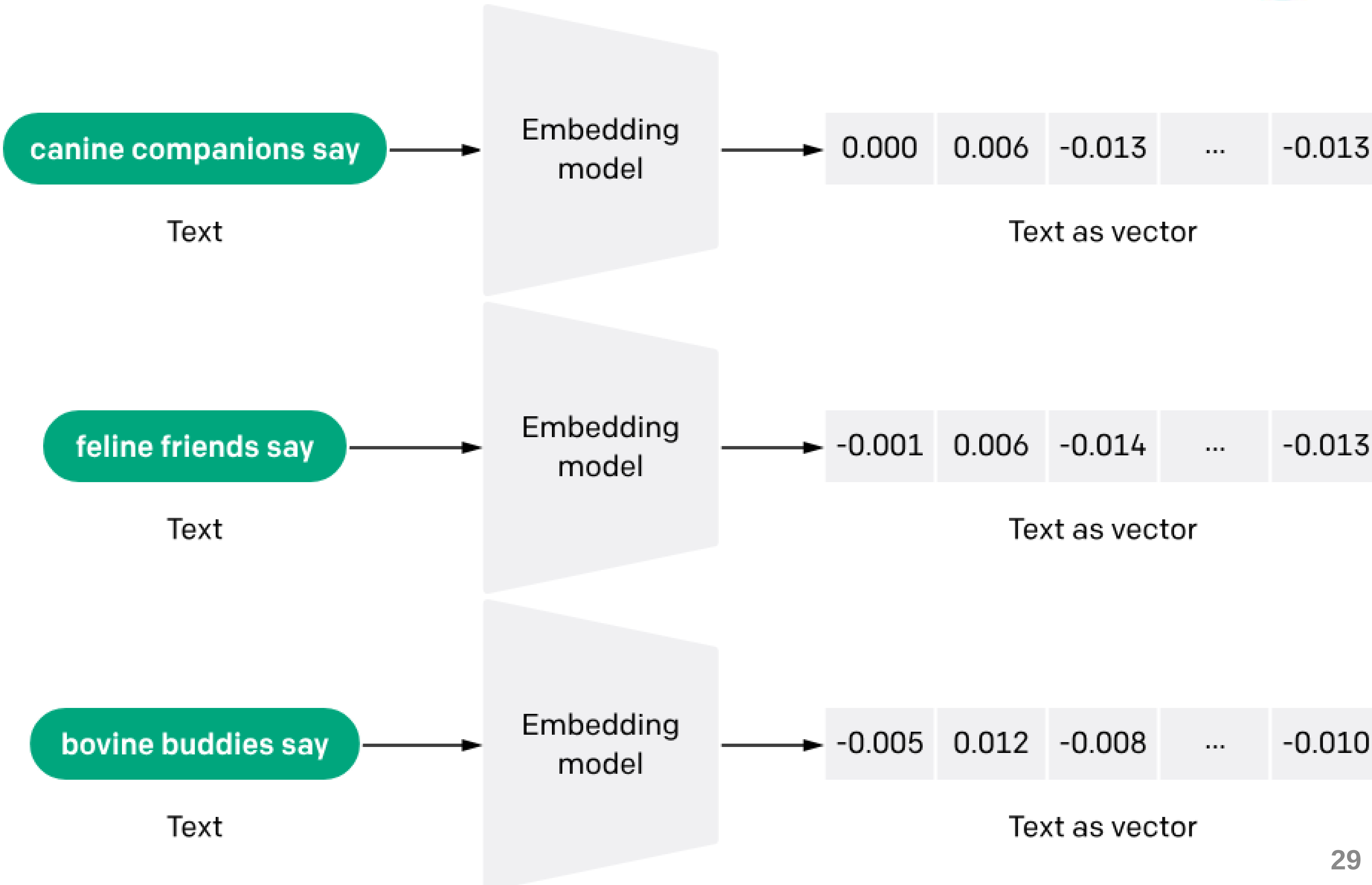
- **Key idea:** The embeddings of similar words are closer in the vector space than those of different ones.



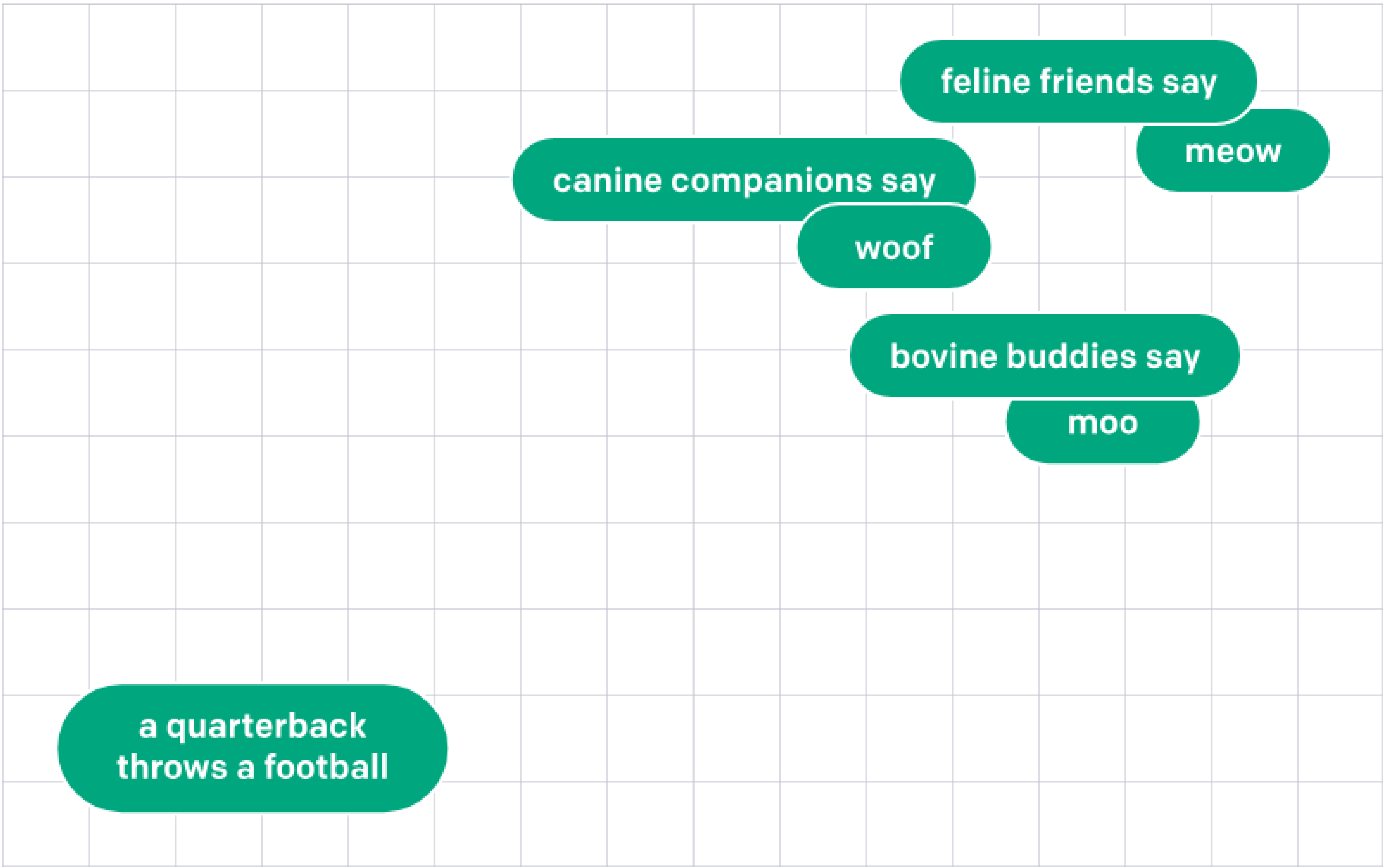
Male-Female Verb Tense Country-Capital

Image credit: Google Developer

Word embeddings: An example



Word embeddings: An example



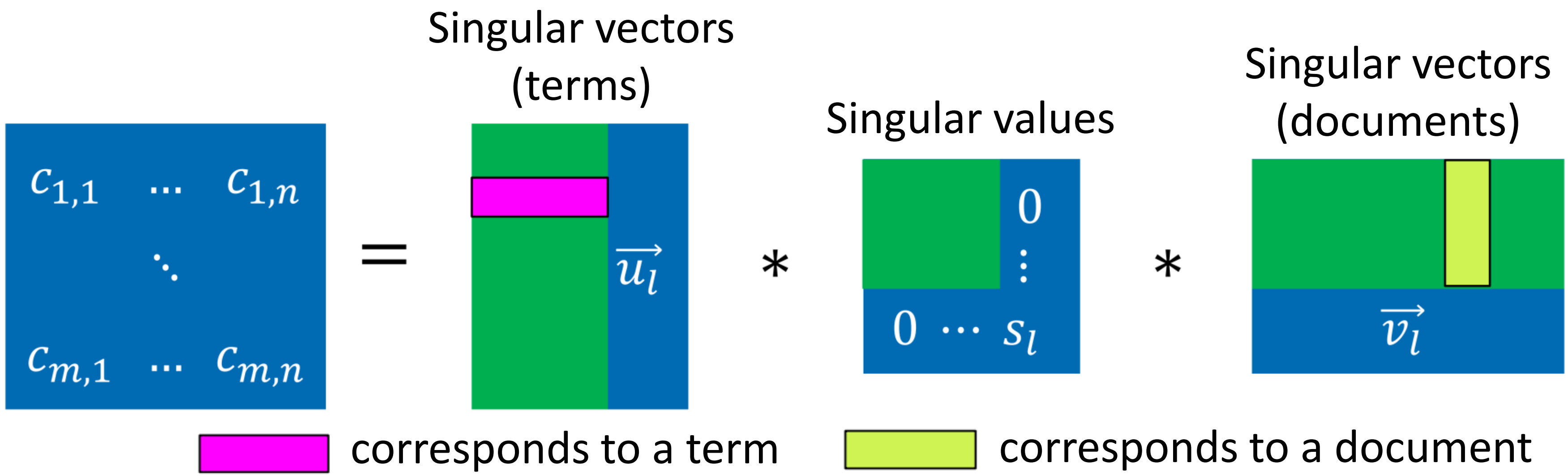
Word embeddings: Applications

Similarity analysis	Word clustering	Ambiguity resolution & Paraphrasing
Information retrieval & Data mining	Topic classification	Sentiment analysis

Latent semantic analysis (LSA)

- LSA computes a term-document matrix A by using SVD.

$$\boldsymbol{A} = \boldsymbol{U} * \boldsymbol{S} * \boldsymbol{V}^{\boldsymbol{T}}$$



- Dimensional reduction is done by omitting singular values.
- Term and document vectors are treated as semantic spaces.

Latent semantic analysis (LSA)	
Capture the meaning	Difficult to interpret

word2vec (2013)

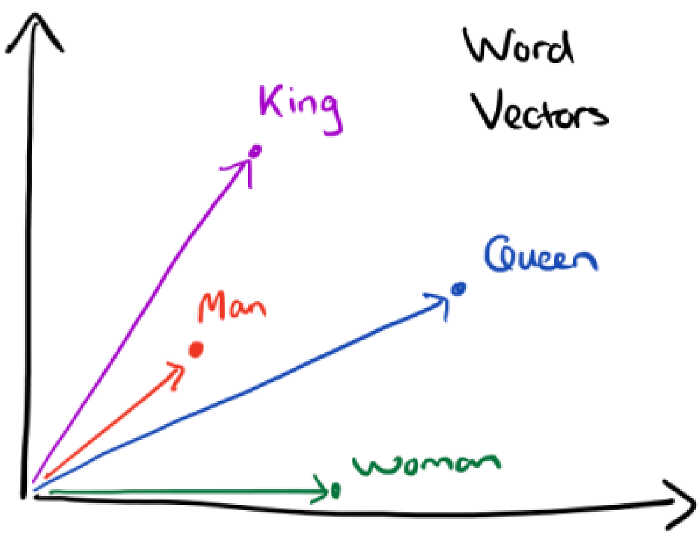
- word2vec uses a neural network to learn word associations from a large corpus.
  - Word embeddings are a by-product of solving a prediction task.
- Each distinct term in the corpus is assigned a corresponding vector in the space, typically of several hundred dimensions.

word2vec (2013)

- It performs operations with vectors to answer questions

$$A - B + C = ?$$

  - What is to C in the same sense as B is to A?
- Word closest by cosine distance is taken as answer.



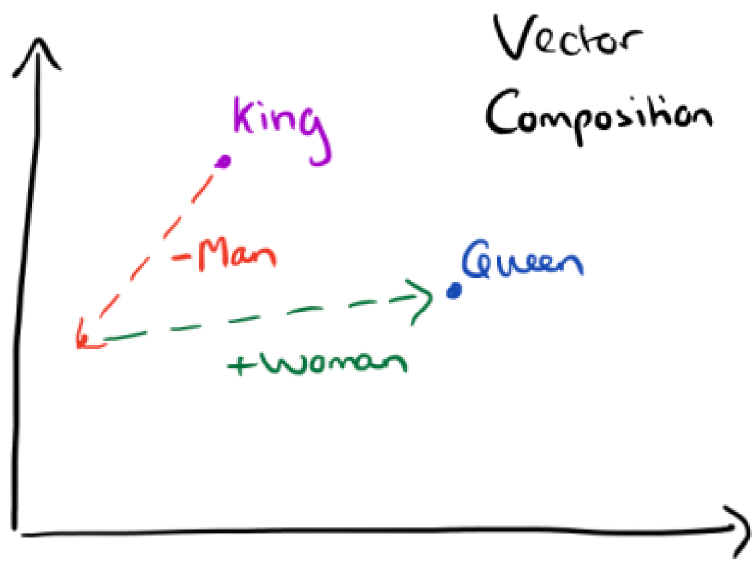
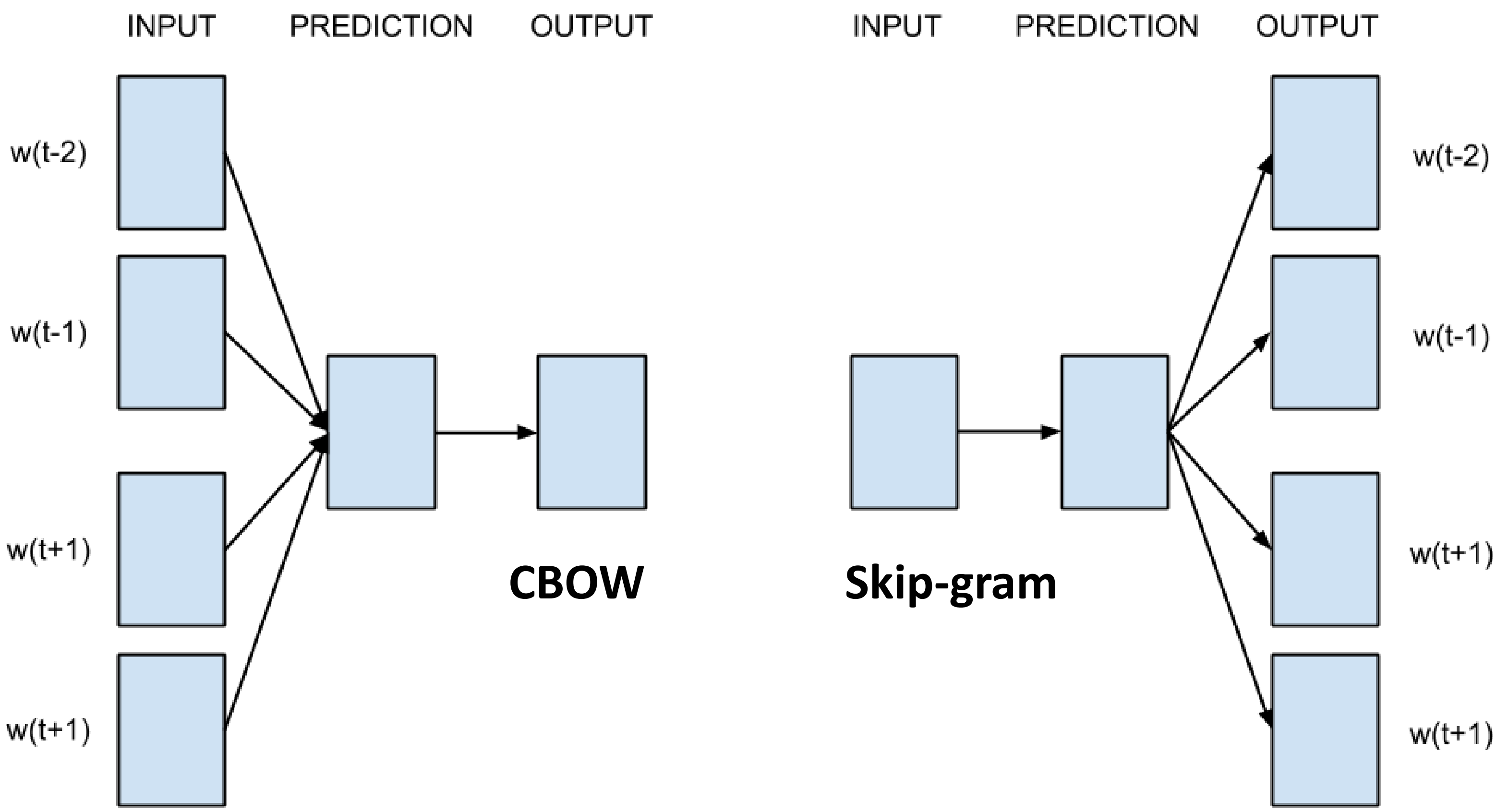


Image credit: [KDnuggets]

word2vec (2013)

- It utilizes either of the two architectures: continuously sliding bag-of-words (CBOW) or continuously sliding skip-gram.



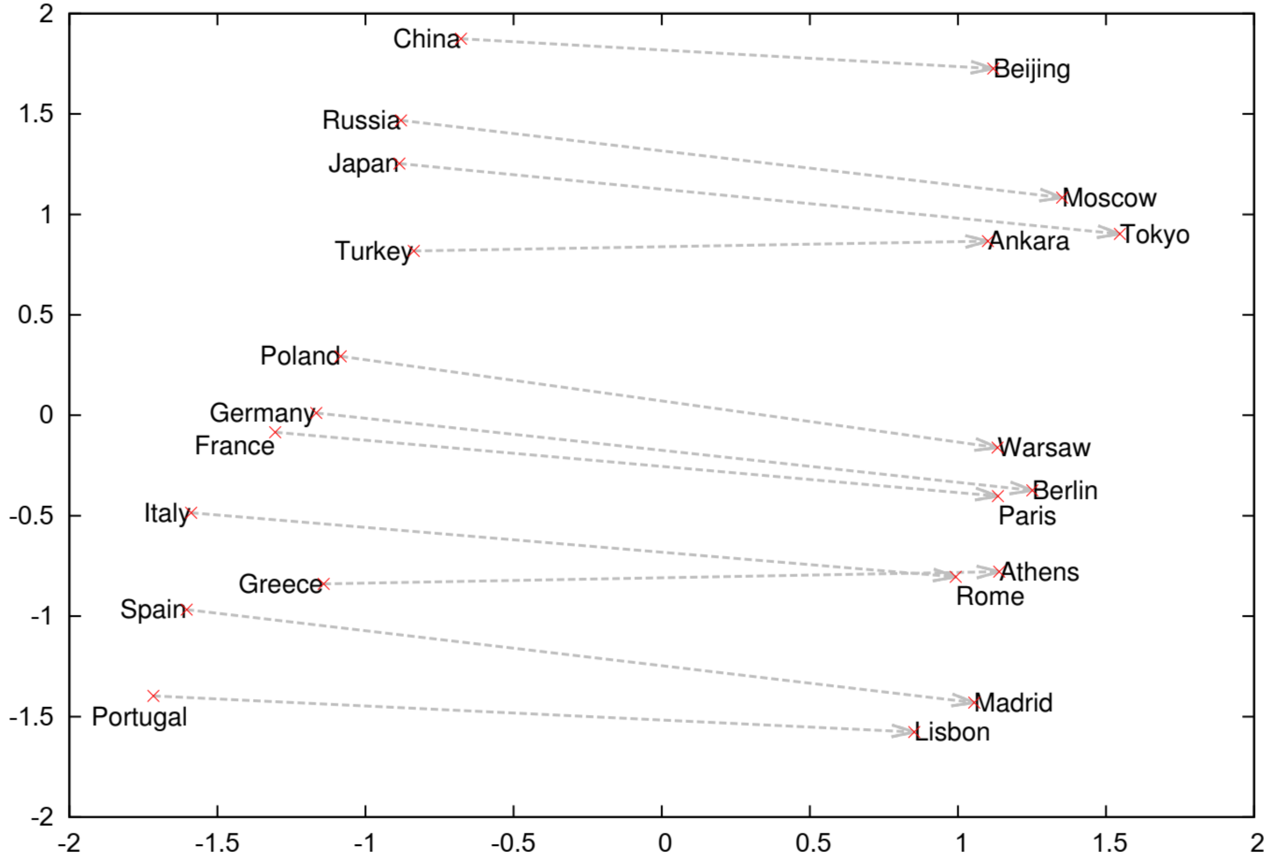
word2vec: Word pair relationships

Examples of the word pair relationships, using the best word vectors (Skip-gram model trained on 783M words with 300 dimensionality)

Relationship	Example 1	Example 2	Example 3
France - Paris	Italy: Rome	Japan: Tokyo	Florida: Tallahassee
big - bigger	small: larger	cold: colder	quick: quicker
Miami - Florida	Baltimore: Maryland	Dallas: Texas	Kona: Hawaii
Einstein - scientist	Messi: midfielder	Mozart: violinist	Picasso: painter
Sarkozy - France	Berlusconi: Italy	Merkel: Germany	Koizumi: Japan
copper - Cu	zinc: Zn	gold: Au	uranium: plutonium
Berlusconi - Silvio	Sarkozy: Nicolas	Putin: Medvedev	Obama: Barack
Microsoft - Windows	Google: Android	IBM: Linux	Apple: iPhone
Microsoft - Ballmer	Google: Yahoo	IBM: McNealy	Apple: Jobs
Japan - sushi	Germany: bratwurst	France: tapas	USA: pizza

Mikolov, T., Chen, K., Corrado, G. and Dean, J., 2013. Efficient estimation of word representations in vector space. arXiv preprint arXiv:1301.3781.

word2vec (2013)



Two-dimensional PCA projection of the 1000-dimensional Skip-gram vectors of countries and their capital cities.

Mikolov, T., Sutskever, I., Chen, K., Corrado, G.S. and Dean, J., 2013. Distributed representations of words and phrases and their compositionality. Advances in neural information processing systems, 26.

word2vec: Vector compositionality

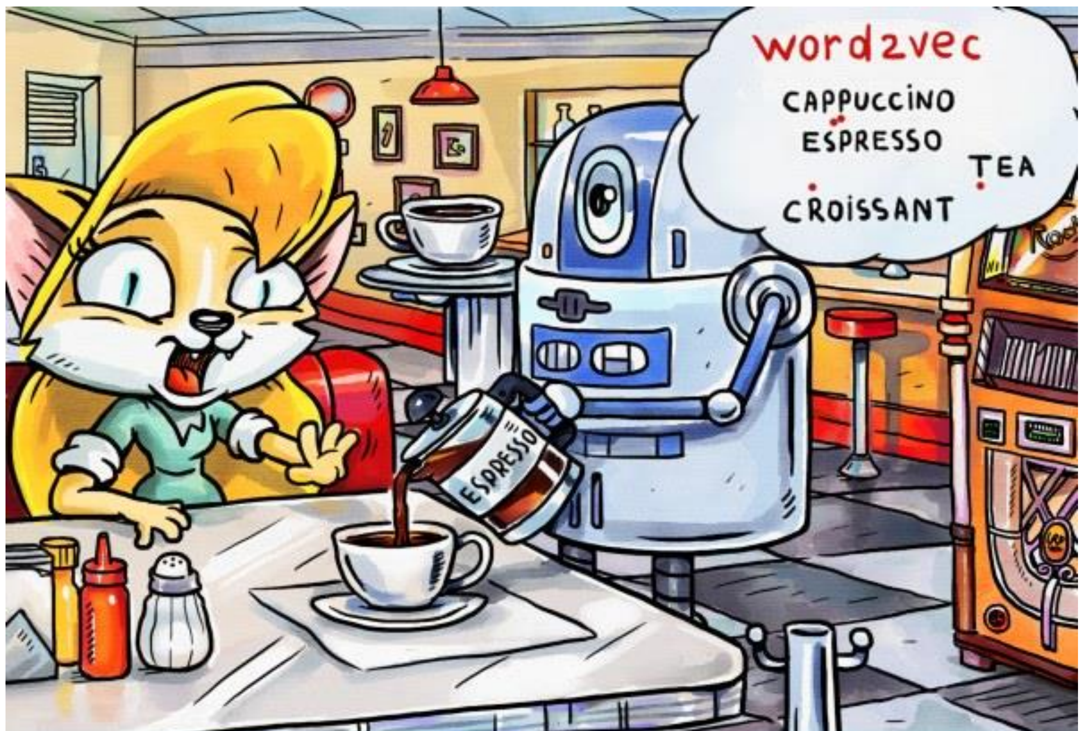
Vector compositionality using element-wise addition. Four closest tokens to the sum of two vectors are shown, using the best Skip-gram model.

Czech + currency	Vietnam + capital	German + airlines	Russian + river	French + actress
Koruna	Hanoi	airline Lufthansa	Moscow	Juliette Binoche
Check crown	Ho Chi Minh City	carrier Lufthansa	Volga River	Vanessa Paradis
Polish zloty	Viet Nam	flag carrier Lufthansa	upriver	Charlotte Gainsbourg
CTK	Vietnamese	Lufthansa	Russia	Cecile De

Mikolov, T., Sutskever, I., Chen, K., Corrado, G.S. and Dean, J., 2013. Distributed representations of words and phrases and their compositionality. Advances in neural information processing systems, 26.

Latent semantic analysis (LSA)	
Capture the meaning	Difficult to interpret

word2vec	
Intuitive	Local context



- Espresso? But I ordered a cappuccino!
- Don't worry, the cosine distance between them is so small that they are almost the same thing.

GloVe – Global Vectors (2014)

- GloVe considers the global context by using a co-occurrence matrix to capture overall statistics.
- **Intuition:** The ratio of word-word co-occurrence probabilities has the potential for encoding some form of meaning.

Co-occurrence probabilities for target words **ice** and **steam** with selected context words from a corpus of 6 billion token.

Probability and Ratio	$k = solid$	$k = gas$	$k = water$	$k = fashion$
$P(k\|ice)$	1.9×10^{-4}	6.6×10^{-5}	3.0×10^{-3}	1.7×10^{-5}
$P(k\|steam)$	2.2×10^{-5}	7.8×10^{-4}	2.2×10^{-3}	1.8×10^{-5}
$P(k\|ice)/P(k\|steam)$	8.9	8.5×10^{-2}	1.36	0.96

Pennington, J., Socher, R. and Manning, C.D., 2014. Glove: Global vectors for word representation. In Proceedings of EMNLP (pp. 1532-1543).

GloVe (2014)

- It is essentially a log-bilinear model with a weighted least-squares objective.

co-occurrence probabilities

$$\boldsymbol{J = \sum_{i,j=1}^{V} \left(w_i^T \widetilde{w_j} - log\left(P_{ij}\right)\right)^2}$$

product of word vector and context word vector

- **Goal:** Learn word vectors such that their product equals the log of their co-occurrence probability
  - J associates co-occurrence probability ratios with vector differences $\rightarrow$ the meaning is also encoded in the vector differences.

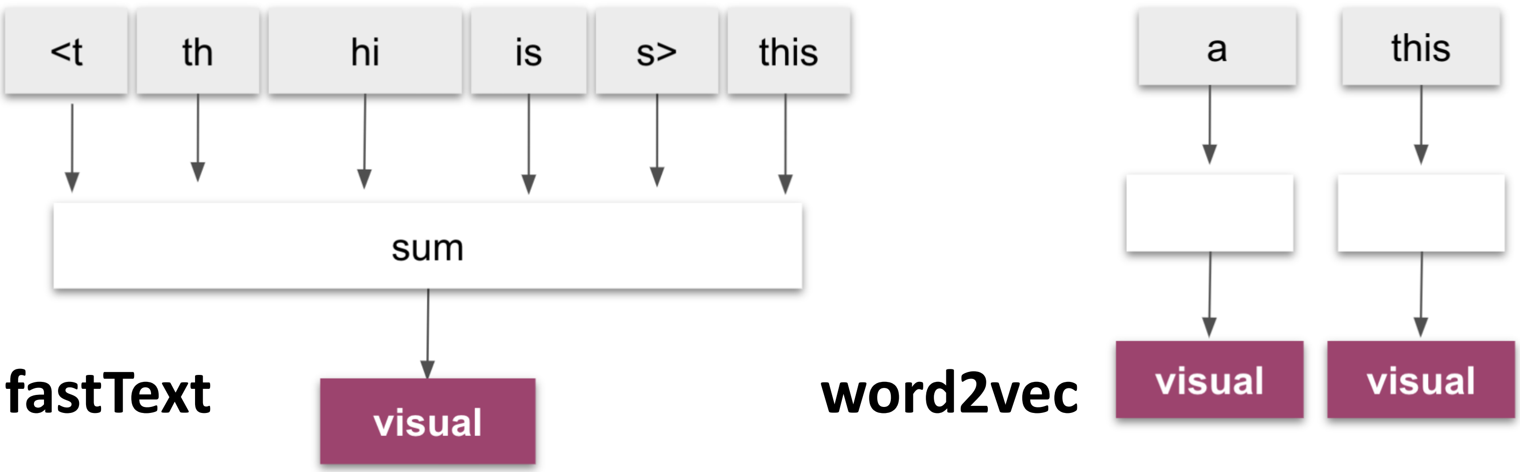
Latent semantic analysis (LSA)	
Capture the meaning	Difficult to interpret

word2vec	
Intuitive	Local context

GloVe	
Global context	No Out-of-Vocabulary handling

fastText (2017)

- fastText views words as compositions of character n-grams.
  - word2vec and GloVe consider “words” as smallest units.



- It creates better embeddings for rare words and constructs vectors for unseen (OOV) words.
- Hyperparameter choice is critical for performance

fastText (2017): An example

- An example that demonstrates the importance of sub-word information.

typo

word2vec:	fastText:
Query word? accomodation	Query word? accomodation
sunnhordland 0.775057	accomodations 0.96342
accomodations 0.769206	accommodation 0.942124
administrational 0.753011	accommodations 0.915427
laponian 0.752274	accommodative 0.847751
ammenities 0.750805	accommodating 0.794353
dachas 0.75026	accomodated 0.740381
vuosaari 0.74172	amenities 0.729746
hostelling 0.739995	catering 0.725975
greenbelts 0.733975	accomodate 0.703177
asserbo 0.732465	hospitality 0.701426

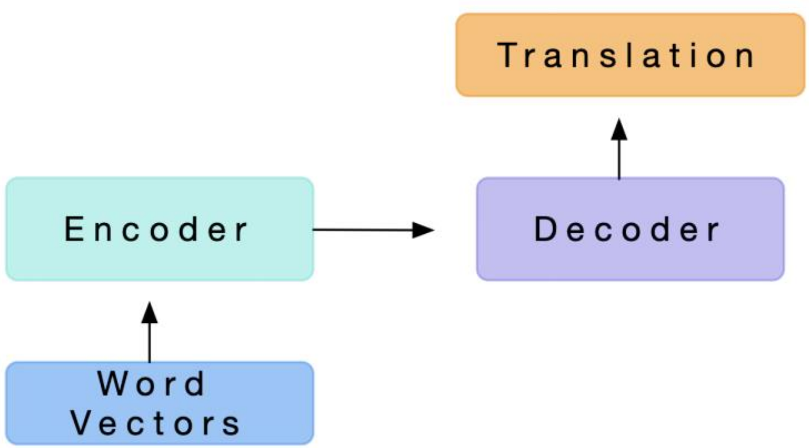
Image credit: https://fasttext.cc

Bojanowski, P., Grave, E., Joulin, A. and Mikolov, T., 2017. Enriching word vectors with subword information. Transactions of the association for computational linguistics, 5, pp.135-146.

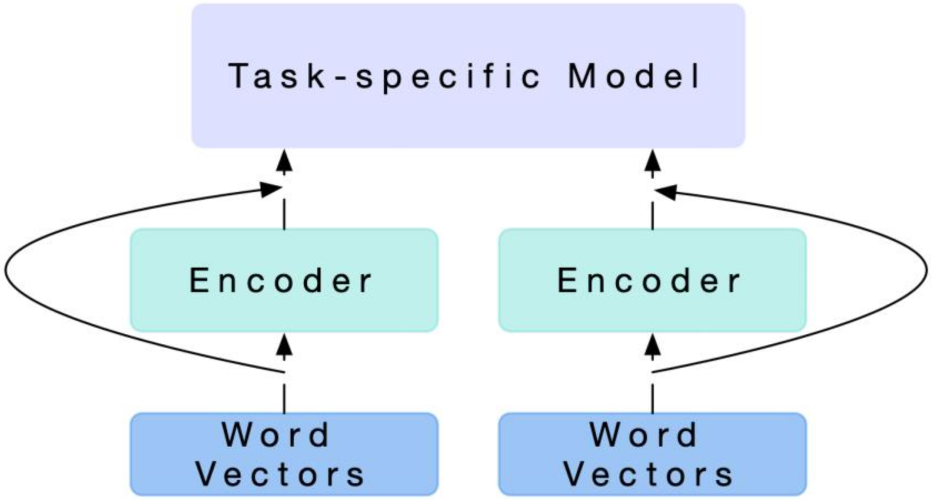
Latent semantic analysis (LSA)	
Capture the meaning	Difficult to interpret
word2vec	
Intuitive	Local context
GloVe	
Global context	No Out-of-Vocabulary handling
fastText	
OOV handling	Not contextual

CoVe (2017)

- **Co**ntextualized word **Ve**ctors are attained by leveraging machine translation (MT).
  - MT is assumed to be general enough to get the words' meanings.
- This enables sense-specific representations for homographs.



Training of encoder-decoder architecture for MT



Encoders are utilized to generate word vectors

CoVe (2017)

- The sequence of context vectors produced by encoder is

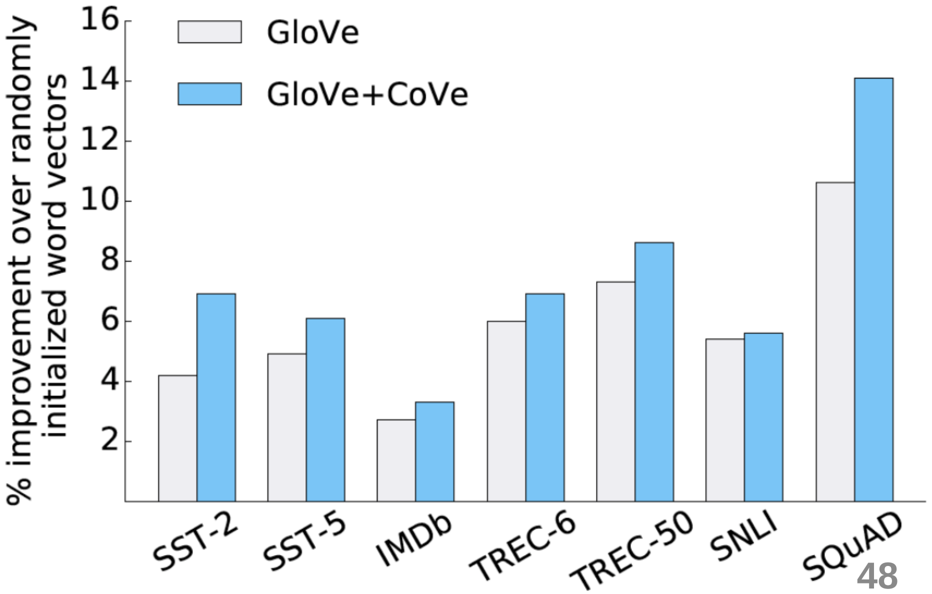
$$\mathbf{CoVe}(\boldsymbol{w}) = \mathbf{MT-LSTM}\left(\mathbf{GloVe}(\boldsymbol{w})\right)$$

sequence of words

sequence of GloVes

- It serves as input for downstream tasks

$$\tilde{\boldsymbol{w}} = [\mathbf{GloVe}(\boldsymbol{w}); \mathbf{CoVe}(\boldsymbol{w})]$$



McCann, B., Bradbury, J., Xiong, C. and Socher, R., 2017. Learned in translation: Contextualized word vectors. Advances in neural information processing systems, 30.

Method	Strength	Weakness
Latent semantic analysis (LSA)	Capture the meaning	Difficult to interpret
word2vec	Intuitive	Local context
GloVe	Global context	No Out-of-Vocabulary handling
fastText	OOV handling	Not contextual
CoVe	Contextual	Supervised

ELMo (2018)

- **E**mbeddings from **L**anguage **Mo**del learns word embeddings through building bidirectional language models (LMs).
- It is a deep contextualized word representation with various levels of knowledge.
  - Each token is described as a function of the entire input sentence.
- No labels needed $\rightarrow$ Unsupervised learning problem
- Out-of-vocabulary words can be accepted as input.

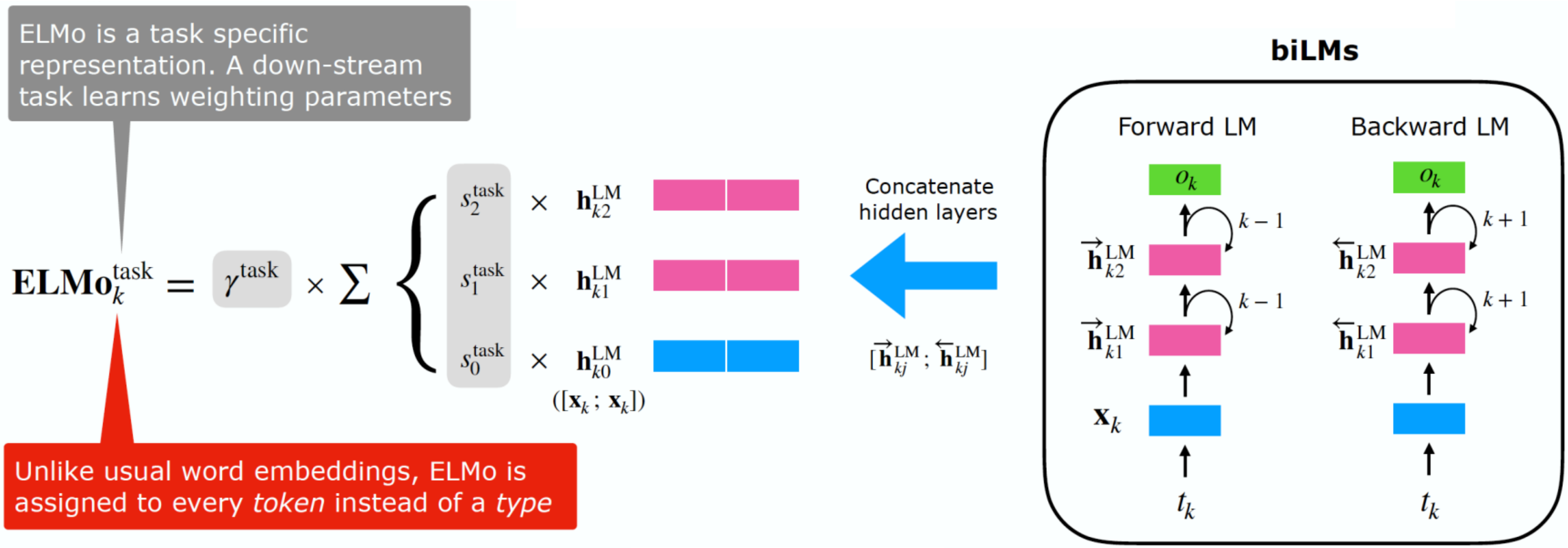
Peters, M. E., Neumann, M., Iyyer, M., Gardner, M., Clark, C., Lee, K., & Zettlemoyer, L. (2018). Deep contextualized word representations. In NAACL-HLT (pp. 2227–2237)

ELMo (2018): Bidirectional LM

- A bidirectional language model (biLM) includes the forward and backward language models.
  - Forward: $p(t_1, t_2, \ldots, t_N) = \prod_{k=1}^{N} p(t_1 | \, t_1, t_2, \ldots, t_{k-1})$
  - Backward: $p(t_1, t_2, \ldots, t_N) = \prod_{k=1}^{N} p(t_k | \, t_{k+1}, t_{k+2}, \ldots, t_N)$
    - t_k is the k^{th} term (token) in a sentence of N terms.
- A word t_k is defined as a linear combination of hidden layers.
- biLM parameters are fixed, weighting & scaling is learned
- Higher layers seem to capture semantics, lower layers for syntactics

ELMo (2018): Build bidirectional LMs

- We can build a bidirectional LM with two LSTMs predicting the next words in both directions.

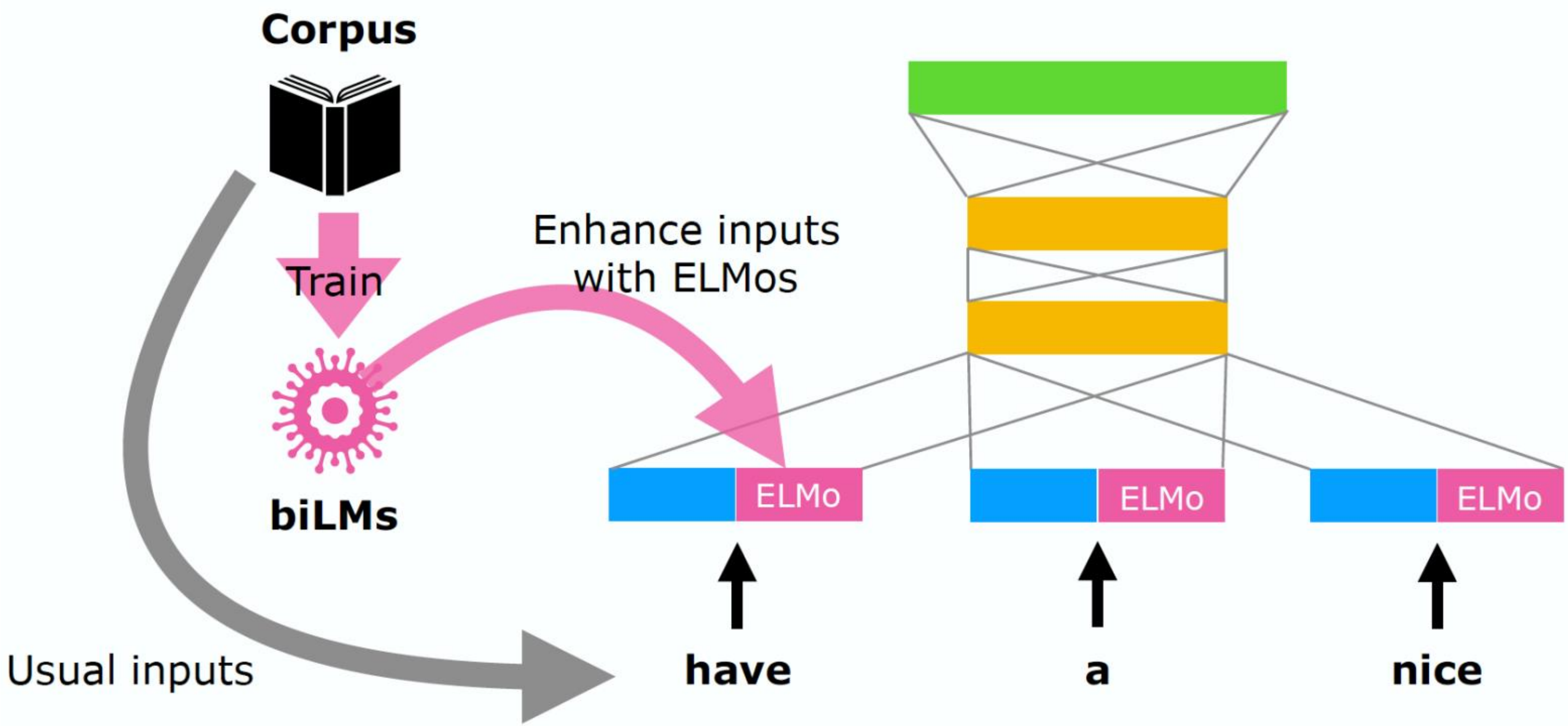


A Review of Deep Contextualized Word Representations. Yada, Shuntaro (2018)

Image credit: SlideShare

ELMo (2018): Usage

- ELMo vectors are used as additional features in NLP tasks with simple concatenation to the embedding layer.



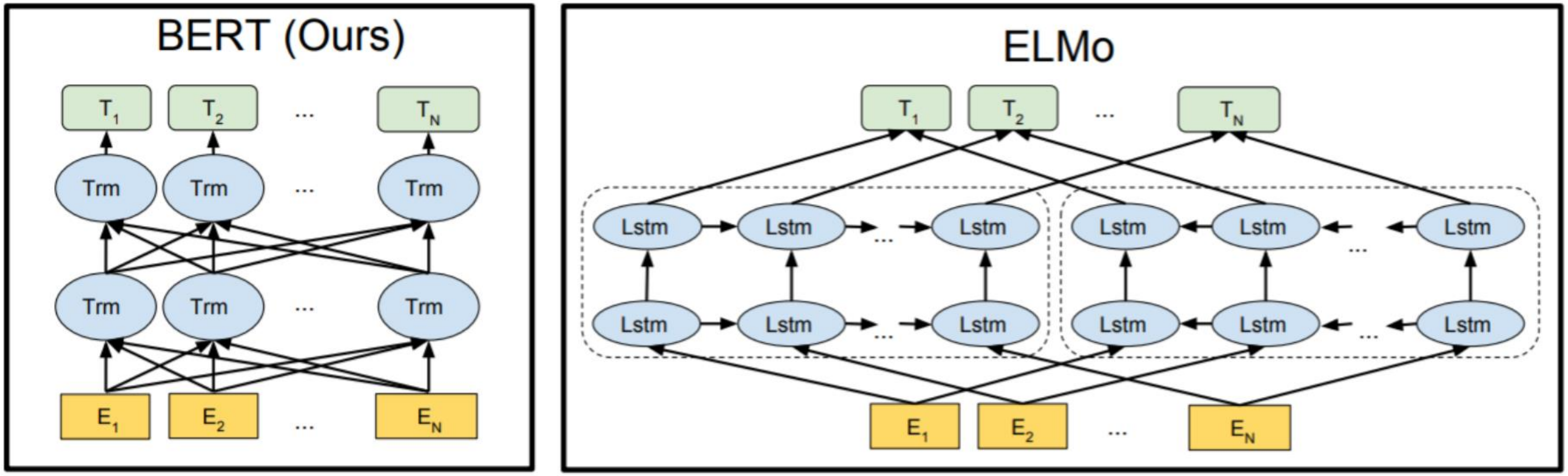
A Review of Deep Contextualized Word Representations. Yada, Shuntaro (2018)

Image credit: SlideShare

Latent semantic analysis (LSA)	
Capture the meaning	Difficult to interpret
word2vec	
Intuitive	Local context
GloVe	
Global context	No Out-of-Vocabulary handling
fastText	
OOV handling	Not contextual
CoVe	
Contextual	Supervised
ELMo	
Unsupervised	Not truly bidirectional

BERT (2018)

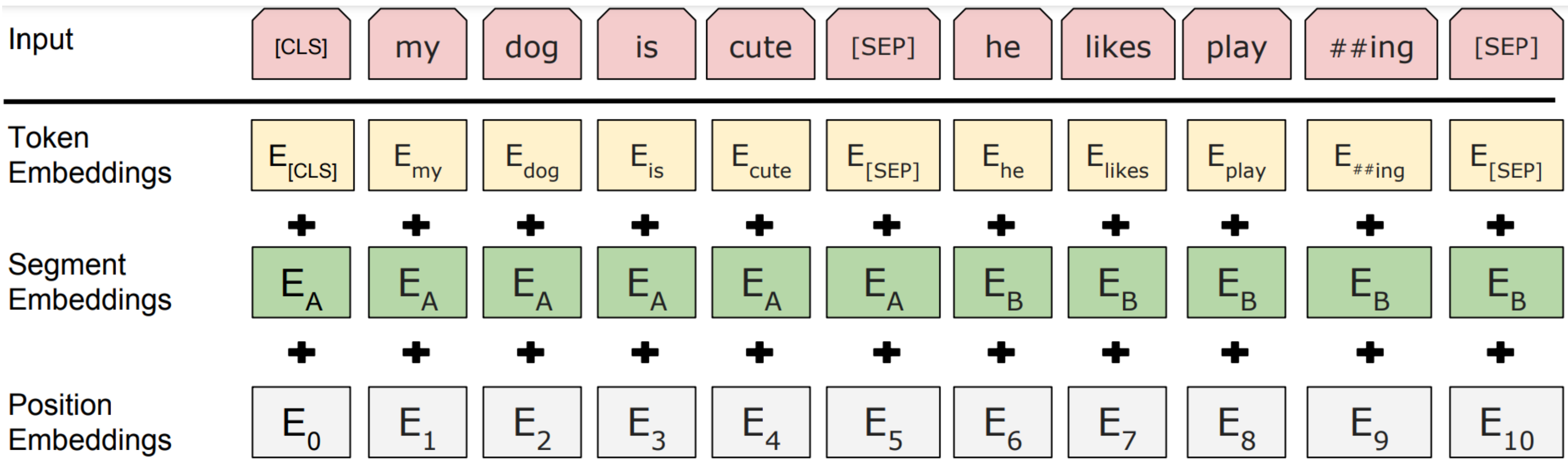
- **B**i-directional **E**ncoder **R**epresentations from **T**ransformers
- The representations are jointly conditioned on left and right context in all layers.



BERT uses a bidirectional Transformer, while ELMo uses the concatenation of independently trained left-to-right and right-to-left LSTMs.

BERT (2018): Input representation

- An input embedding is the sum of the token embedding, segmentation embedding and position embedding.



Devlin, J., Chang, M.W., Lee, K. and Toutanova, K., 2018. Bert: Pre-training of deep bidirectional transformers for language understanding. arXiv preprint arXiv:1810.04805.

BERT (2018): Pre-training

- **Pre-training Task 1 Masked LM**
- Mask 15% of all tokens in each sequence at random
  - Input: the man went to the [MASK1] . he bought a [MASK2] of milk
  - Label: [MASK1] = went – [MASK2] = gallon
- The data generator does not always replace the chosen words with [MASK], instead it will
  - 80% of the time: Replace the word with the [MASK] token
    - E.g., my dog is hairy → my dog is [MASK]
  - 10% of the time: Replace the word with a random word
    - E.g., my dog is hairy → my dog is apple
  - 10% of the time: Keep the word unchanged
    - E.g., my dog is hairy → my dog is hairy
    - This is to bias the representation towards the actual observed word.

BERT (2018): Pre-training

- **Pre-training Task 2 Next Sentence Prediction**
- An LM does not always understand relationships between sentences, which is important for many NLP tasks.
- BERT pre-train a binarized next sentence prediction task.
- Input: the man went to the store [SEP] he bought a gallon of milk

  $\rightarrow$ Label: IsNext
- Input: the man went to the store [SEP] penguins are flightless birds

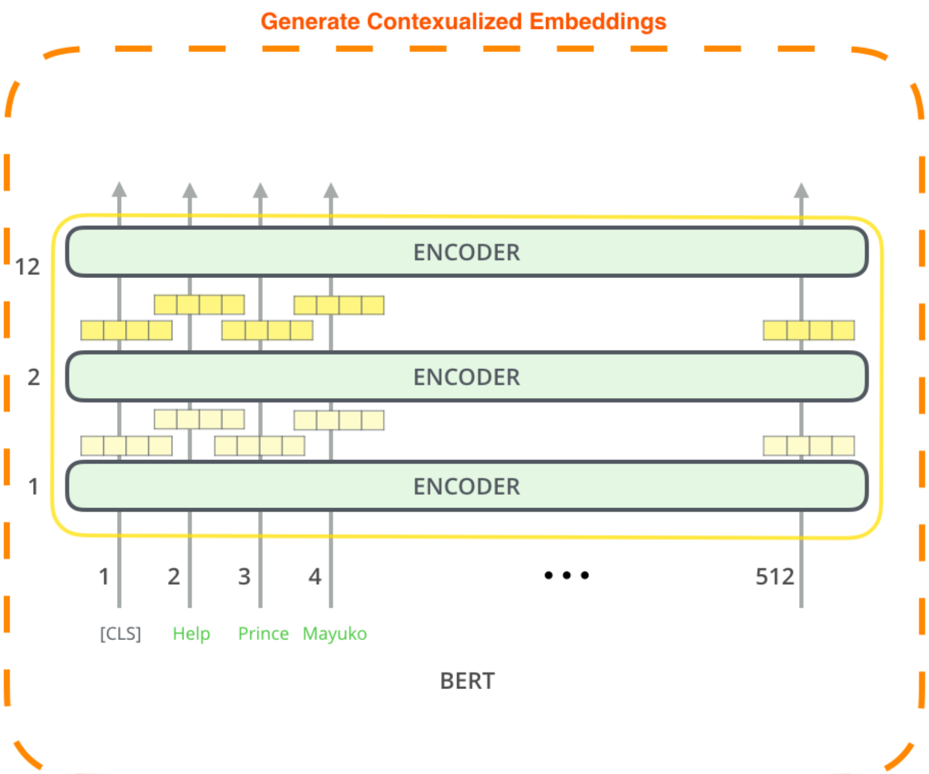
  $\rightarrow$ Label: NotNext

BERT (2018): Fine-tuning

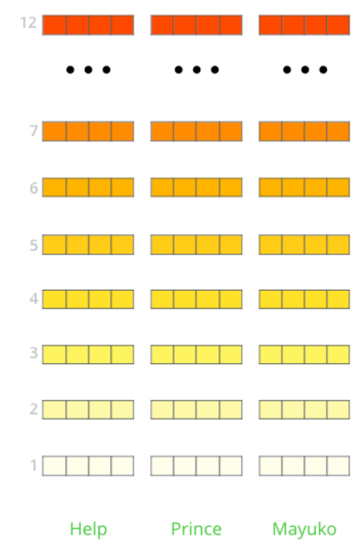
- The final hidden state for the first token [cls] in the input is taken as the representation of the input sequence.
- During fine-tuning, we only add new parameters for the classification layer.
- All the parameters are fine-tuned jointly to maximize the log-probability of the correct label.

BERT (2018): Feature extraction

- Pre-trained embeddings can be fed to an existing model.
- The results are not far behind fine-tuning BERT on a task such as named-entity recognition.



The output of each encoder layer along each token's path can be used as a feature representing that token.



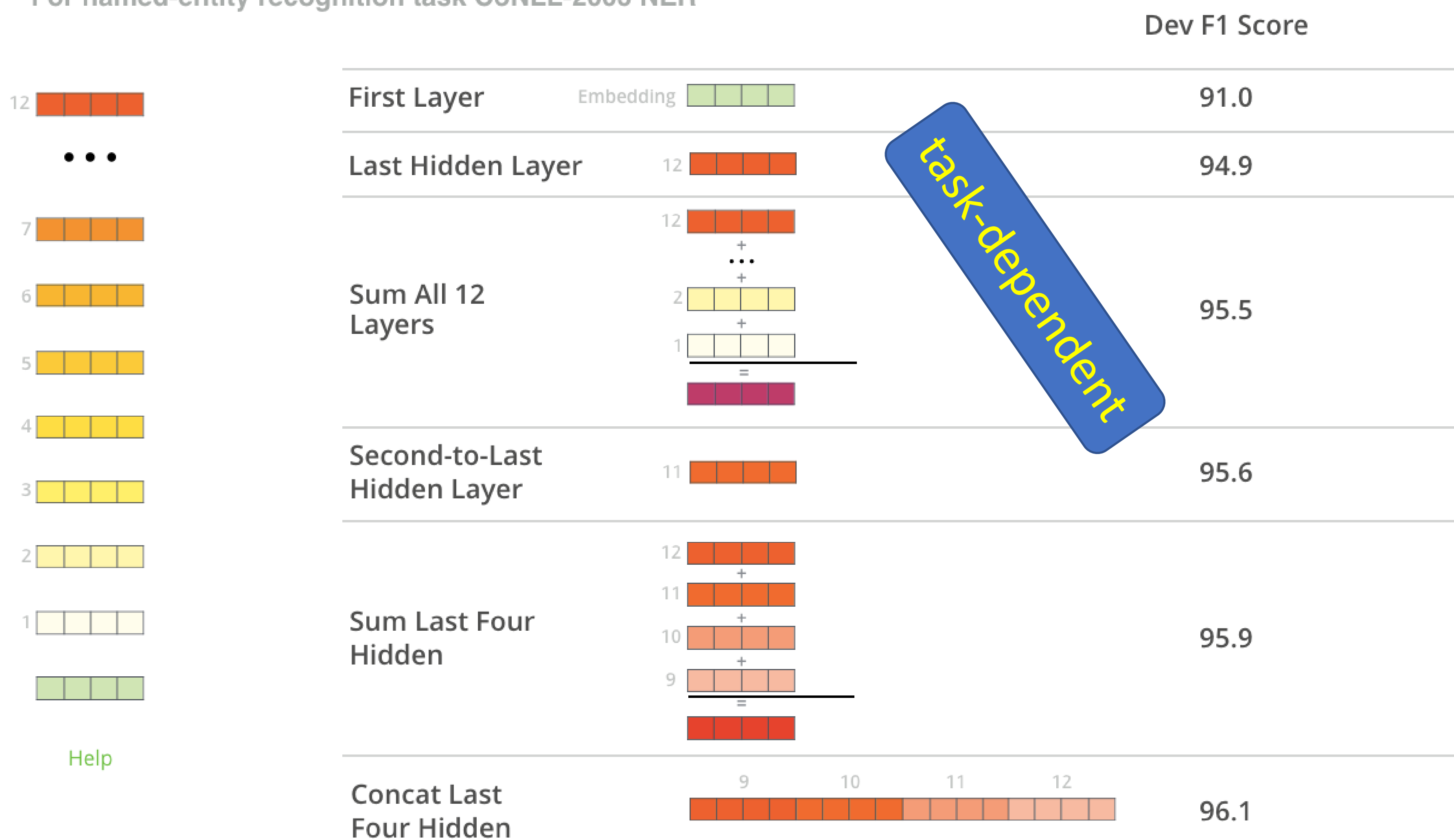
But which one should we use?

Image credit: jalammar.github.io

BERT (2018): Feature extraction

What is the best contextualized embedding for "Help" in that context?

For named-entity recognition task CoNLL-2003 NER



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CoVe	Contextual	Supervised
ELMo	Unsupervised	Not truly bidirectional
BERT	Bidirectional	Computationally expensive

Quiz 02: Large language models

- Distinguish these terminologies: language models (LMs) and large language models (LLMs).
- Classify the following models to either LM or LLM:
  - PaLM
  - Skip-gram
  - Word2Vec
  - GPT-4
  - BERT
  - LLaMA
  - PaLM

References

- Michael Heck, 2019. The World of Vectors. Dialog Systems and Machine Learning. Heinrich-Heine-Universität Düsseldorf.
- Wikipedia: tf-idf (link)
- GloVe: Global Vectors for Word Representation (link)
- A Visual Guide to FastText Word Embeddings (link)
- The Illustrated BERT, ELMo, and co. (How NLP Cracked Transfer Learning) (link)


...the end.