Intelligent Agents

Sequential Structures, Word Semantics, and Embeddings

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Motivation: Part Of Speech Tagging

- Annotate each word in a sentence with a part-ofspeech (POS) tags.
- Lowest level of syntactic analysis.

John saw the saw and decided to take it to the table. NNP VBD DT NN CC VBD TO VB PRP IN DT NN

- Useful for subsequent syntactic parsing and word sense disambiguation
- Topic modeling as discussed before could be extended to better consider POS tags



Abbreviations: https://sites.google.com/site/partofspeechhelp/home

Information Extraction

- Identify phrases in language that refer to specific types of entities and relations in text.
- Named entity recognition is the task of identifying names of people, places, organizations, etc. in text.
 people organizations places
 - Michael Dell is the CEO of Dell Computer Corporation and lives in Austin Texas.
- Extract pieces of information relevant to a specific application, e.g. used car ads:

make model year mileage price

For sale, 2002 Toyota Prius, 20,000 mi, \$15K or best offer.
 Available starting July 30, 2006.



Semantic Role Labeling

- For each clause, determine the semantic role played by each noun phrase that is an argument to the verb.
 agent patient source destination instrument
 John drove Mary from Austin to Dallas in his Toyota Prius.
 The hammer broke the window.
- Also referred to as "case role analysis," "thematic analysis," and "shallow semantic parsing"



Using Outputs as Inputs

- Better input features are usually the categories of the surrounding tokens, but these are not available yet.
- Can use category of either the preceding or succeeding tokens by going forward or back and using previous output.



Forward Classification





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Forward Classification





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- In LDA the order of documents does not matter
- Not appropriate for sequential corpora (e.g., that span hundreds of years)

Inaugural addresses

- Further, we may want to track how language changes over time
- Let the topics *drift* in a sequence.



My fellow citizens: I stand here today humbled by the task before us, grateful for the trust you have bestowed, mindful of the sacrifices borne by our ancestors...

2009



AMONG the vicissitudes incident to life no event could have filled me with greater anxieties than that of which the notification was transmitted by your order...



David M. Blei and John D. Lafferty. Dynamic topic models. In Proc. ICML '06. pp. 113-120. **2006**.



Topics drift through time



- Use a logit normal distribution to model topics evolving over time
- Embed it in a state-space model on the log of the topic distribution

$$\beta_{t,k} | \beta_{t-1,k} \sim \mathcal{N}(\beta_{t-1,k}, l\sigma^2)$$

 $p(w | \beta_{t,k}) \propto \exp{\{\beta_{t,k}\}}$

• Let us make inferences about sequences of documents



A **logistic function** or **logistic curve** is a common "S" shape (sigmoid curve), with equation:

$$f(x)=rac{L}{1+e^{-k(x-x_0)}}$$

where

- *e* = the natural logarithm base (also known as Euler's number),
- x₀ = the *x*-value of the sigmoid's midpoint,
- L = the curve's maximum value, and
- *k* = the steepness of the curve.^[1]





Logit Normal Distribution

Normal Distribution $f(x) = rac{1}{\sigma\sqrt{2\pi}}e^{-rac{1}{2}\left(rac{x-\mu}{\sigma} ight)^2}$

The probability density function (PDF) of a logit-normal distribution, for $0 \le x \le 1$, is:

$$f_X(x;\mu,\sigma) = rac{1}{\sigma \sqrt{2\pi}} \, rac{1}{x(1-x)} \, e^{-rac{(ext{logit}(x)-\mu)^2}{2\sigma^2}}$$

where μ and σ are the mean and standard deviation of the variable's logit (by definition, the variable's logit is normally distributed).



[Wikipedia]

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$\beta_{t,k}$ is a multinomial: Simplex again



- The **logistic normal** is a distribution on the simplex that can model dependence between components (Aitchison, 1980).
- The log of the parameters of the multinomial are drawn from a multivariate Gaussian distribution,

$$X \sim \mathcal{N}_{\mathcal{K}}(\mu, \Sigma)$$

 $\theta_i \propto \exp\{x_i\}.$



Original article

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Topic proportions

TECHVIEW: DNA SEQUENCING

Sequencing the Genome, Fast

James C. Mullikin and Amanda A. McMurray

. ..

....

Genome sequencing projects reveal the genetic makeup of an organism by reading off the sequence of the human genome, the largest amount of any center so far (3). We DNA bases, which encodes all of the information necessary for the life of the organism. The base sequence contains four nucleotides-adenine, thymidine, guanosine, and cytosine-which are linked together into long double-helical chains. Over the last two decades, automated DNA sequencers have made the process of obtaining the base-by-base sequence of DNA easier. By application of an electric field across a gel matrix, these sequencers separate fluorescently labeled DNA molecules that differ in size by one base. As the molecules move past a given point in the gel, laser excitation of a fluorescent dye specific to the base at the end of the molecule yields a base-specific signal that can be automatically recorded.

The latest sequencer to be launched is Perkin-Elmer's much-anticipated ABI Prism 3700 DNA Analyzer which, like the Molecular Dynamics MegaBACE 1000 launched last year, incorporates a capillary tube to hold the sequence gel rather than a traditional slab-shaped gel apparatus. Extra interest in the ABI 3700 has been generated because Craig Venter of Celera Genomics Corporation anticipates that ~230 of these machines (1) will enable the company to produce raw sequence for the entire 3 gigabases (Gb) of the human genome in 3 years. The specifications of the ABI 3700 machine say that with less than 1 hour of human labor per day, it can se-quence 768 samples per day. Assuming that each sample gives an average of 400 base pairs (bp) of usable sequence data (its read length) and any section from the entire human genome is covered by an aver-age of 10 overlapping independent reads (2), the 75 million samples that Celera must process will require ~100,000 ABI 3700 machine days. With ~230 machines, that works out to less than 2 years or about 434 days, which affords some margin of error for unexpected developments.

At the Sanger Centre, we have finished 146 Mb of genomic sequence from a vari-

The authors are at The Sanger Centre, Wellcome Trust Genome Campus, Hinxton, Cambs, CB10 15A, UK.E-mail: jcm@sanger.ac.uk

taking approximately 16 hours before oper-ator intervention is required. This rate falls ator intervention is required. This rate fails short of the design specification of four 96-well plates in 12 hours. The main innovation of the ABI 3700 is the use of a sheath flow fluorescence detec tion system (4). Detection of the DNA frag-ments occurs 300 µm past the end of the capare aiming to sequence 1 Gb of human seillary within a fused silica cuvette. A laminar quence in rough-draft form by 2001, with a finished version by 2003. Our sequencfluid flows over the ends of the capillaries, drawing the DNA fragments as they emerge ing equipment includes 44 ABI 373XL, 61 ABI 377XL, and 31 ABI 377XL-96 slab from the capillaries through a fixed laser beam that simultaneously intersects with all of the samples. The emitted fluorescence is gel sequencers from Perkin-Elmer plus 6

throughput of 32,000 samples per day. Two ABI 3700 capillary sequencers-delivered

Fig. 1. Comparison of read-length histograms for sequences collected with the ABI 3700 capillary machine and the ABI 377XL-96 slab gel machine. The capillary machine under-performs the slab gel machine by about 200 bases. Both sets of reads are from runs with ABI Big Dye Terminator chemistries. Read length is computed as the number of bases per read where the predicted error rate is less than or equal to 1.0% ($Q \ge 20$). The "phred" Q value was recalible for our days many bases per read where the predicted error rate is less than or equal to 1.0% ($Q \ge 20$). The "phred" Q value was recalible for exceeding the prediction of the phred for exceeding the prediction of the predi brated for each type of read.

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into a floor-standing cabinet, which contains in its base all the reagents required for its operation. The reagent containers are readily accessible for replenishment, which is required every day under high-throughput operation. At bench height within the cabinet is a four-position bed, on which mi-crotiter plates of DNA samples are located. The operator places the prepared plates into position, closes the front of the machine and programs it by using a personal com-puter. A robotic arm transfers DNA sam-

www.sciencemag.org SCIENCE VOL 283 19 MARCH 1999

Molecular Dynamics MegaBACE 1000 capillary sequencers, allowing a maximum detected with a spectral CCD (charge-cou-pled device) detector. This arrangement means that there are no moving parts in the detection system, other than a shutter in front of the CCD detector. We have evaluated these machines for their performance, op-eration, ease of use, and reliability in comparison to the more commonly used slab gel seauencing machines. In automat-

ples from the plates into wells that open in-to the capillaries. This and the rest of the sequencing operation is fully automatic

The machine can currently process four 96-well plates of DNA samples unattended,



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to the Sanger Centre in December 1998— are desirable. In fact, a system that could are in our Research and Development de-partment for evaluation. Thus, the ABI 3700 will ultimately be added to our psystems cost the same. This is because assembling relatively fewer long-se-quenced fragments is easier than assem-bling many short ones. So, read length is an important parameter when evaluating new sequencing technologies.

We have directly compared the ABI 3700 sequencer to the ABI 377XL slab gel sequencer by evaluating the sequence data obtained from both machines with human DNA samples. These samples were subcloned into plasmid or m13 phage and prepared and sequenced with our standard protocols for Perkin-Elmer Big Dye Terminator chemistry

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Original article

TECHVIEW: DNA SEQUENCING

Sequencing the Genome, Fast

James C. Mullikin and Amanda A. McMurray

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are desirable. In fact, a system that could read twice as many bases but at half the speed of another system is preferable, if both systems cost the same. This is because assembling relatively fewer long-se-quenced fragments is easier than assembling many short ones. So, read length is an important parameter when evaluating new sequencing technologies.

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sequence genome genes sequences human gene dna sequencing chromosome regions analysis data genomic number

devices device materials current high gate light silicon material technology electrical fiber power based

Most likely words from top topics

data information network web computer language networks time software system words algorithm number internet







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OXYGEN FORCE LASER 0-0-0 NERVE 00 RELATIVITY NEURON 1880 1900 1920 1940 1980 1900 1980 1960 2000 1880 1920 1940 1960 2000

"Theoretical Physics"

"Neuroscience"



David M. Blei and John D. Lafferty. Dynamic topic models. In Proc. ICML '06. pp. 113-120. **2006**.

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Probabilistic Topic Models, David Blei, 2013

- Understand developments
- Distributions of topics over time
- Discretization of time might be a problem
 - Runtime increases dramatically
 - Continuous dynamic topic models
- Many applications
 - E.g., comparison of science areas, analysis of scientific work
- How can we compare distributions?



Recap: Huffman code example





М	code 1	ength	prob	Exp. len
А	000	3	0,125	0,375
В	001	3	0,125	0,375
С	01	2	0,250	0,500
D	1	1	0,500	0,500
averag	1,750			

If we need to send many messages (A,B,C or D) and they have this probability distribution and we use this code, then over time, the average bits/message should approach 1.75

Recap: Information Theory Background

- Assume that you need to send messages from a repertoire of n messages
- If there are n equally probable possible messages, then the probability p of each is 1/n or n = 1/p
- Information (number of bits) conveyed by a message is log(n) = log(1/p)= -log(p)
- E.g., if there are 16 messages, then log(16) = 4 and we need 4 bits to identify/send each message.
- In general, if we are given a probability distribution

 $P = (p_1, p_2, .., p_n)$

- Expected information induced by distribution P (aka entropy of P): $I(P) = -(p_1^*log(p_1) + p_2^*log(p_2) + ... + p_n^*log(p_n))$ $= -\sum_i p_i^*log(p_i) = \sum_i p_i^*log(1/p_i)$
- What if one used an erroneous distribution q?
 - One might use too many bits for more frequent messages



The KL Divergence

 The cross-entropy, or Kullback-Leibler divergence, between two distributions p and q measures the expected information gain (reduction in average number of bits per event) due to replacing the "wrong" distribution q with the "right" distribution p:

$$D^{KL}(\mathbf{p},\mathbf{q}) \equiv \sum_{i} p_i (\ln(1/q_i) - \ln(1/p_i)) = \mathbf{E}_{\mathbf{p}} [\ln(\mathbf{p}/\mathbf{q})]$$

• Not symmetric



Hellinger Distance

 The Hellinger distance is a symmetric measure of distance between two distributions that is popular in machine learning applications:

$$D^{HEL}(\mathbf{p}, \mathbf{q}) \equiv \|\sqrt{\mathbf{p}} - \sqrt{\mathbf{q}}\|_2 = \left(\sum_{j=1}^n \left(\sqrt{p_j} - \sqrt{q_j}\right)^2\right)$$
$$\in [0, \sqrt{2}]$$

• Sometimes value should be in [0, 1]

For two discrete probability distributions $P=(p_1,\ldots,p_k)$ and $Q=(q_1,\ldots,q_k)$, their Hellinger distance is defined as

$$H(P,Q) = rac{1}{\sqrt{2}}\; \sqrt{\sum_{i=1}^k (\sqrt{p_i} - \sqrt{q_i})^2},$$
 [Wikipedia]

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- Time-corrected similarity shows a new way of using the posterior
- Consider the expected Hellinger distance between the topic proportions of two documents,

$$d_{ij} = \mathrm{E}\left[\sum_{k=1}^{K} (\sqrt{\theta_{i,k}} - \sqrt{\theta_{j,k}})^2 |\mathbf{w}_i, \mathbf{w}_j\right]$$

- Uses the latent structure to define similarity
- Time has been factored out because the topics associated to the components are different from year to year
- Similarity of documents based only on topic proportions



SCIENCE.

The Brain of the Orang (1880)

F. Barker, Professor O. C. Marsh

THE BRAIN OF THE ORANG.*

BY HENRY C. CHAPMAN, M.D.

The brain of the Orang has been figured by Tiede The brain of the Orang has been figured by Toled-man, Sandiffort, Konceler van der Kolk and Vroik, Gratistiet, Relleston, etc. On account, however, of the few illustrations excatut, and of the importance of the subject, I avail myself of the copportunity of presenting several views of my Orang's brain (Figures, to c), which was removed from the skull only a few hours after death. The membranes were in a bigh state of coggen-tion, and a little of the surface of the left hemisphere had here disconstructions of the later of the left hemisphere had here disconstructions. en disorganized by disease, otherwise the brain was in usorganized by disease, otherwise the orath was in condition. It weighed exactly ten ounces. The of the Orang in its general contour resembled that an more than those of either of the Chimpanzees I examined. In these the brain was more elong-The general character of the folds and fissures in



and man all three. The fissure of Sylvius in and down the posterior branch pur-tly backward direction; the anterior The fissure of Rolando, or central fis-The par occipital fising the parietal from the occipal lober

demy of Natural S ces, Phila, 1880.

in these cases, which were submitted to the in the Orang, the parteto-occidital fasure does not reast the destination of the d Gorilla, and se is to be i In the female Chir



F1G. # proc. a. proc. b. proc. b. proc. a. The precuneus, or the space on the mesial e parietal lobe between the parieto-occipital portions. The side of the par





Representation of the Visual Field on the Medial Wall of Occipital-Parietal Cortex in the Owl Monkey (1976)





Dynamic Topic Models: Summary

- Can model changes of topics (= word distributions) in corpora over time
- Uses a technique for modeling temporal influences
- As a by-product we have discussed techniques for comparing distributions



Word-Word Associations in Document Retrieval

Recap

- LSI: Documents as vectors, dimension reduction
- Topic Modeling

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- Topic = Word distribution
- From LDA-Model: P(Z | w)
- Assumption: Bag of words model
 - (independence, naïve Bayes, unigram distribution)

Words are not independent of each other

- Word similarity measures
- Extend query with similar words automatically
- Extend query with most frequent followers/predecessors
- Insert words in anticipated gaps in a string query Need to represent more aspects of word semantics

Approaches for Representing Word Semantics

Beyond bags of words

 Distributional Semantics	 Word Embeddings (Predict) Inspired by deep learning word2vec				
(Count) Used since the 90's Sparse word-context	(Mikolov et al., 2013) GloVe				
PMI/PPMI matrix Decomposed with SVD	(Pennington et al., 2014)				
Underlying Theory: The Distributional Hypothesis (<i>Harris, '54; Firth, '57</i>) "Similar words occur in similar contexts"					

https://www.tensorflow.org/tutorials/word2vec https://nlp.stanford.edu/projects/glove/



Point(wise) Mutual Information: PMI

Measure of association used in information theory and statistics

$$ext{pmi}(x;y) \equiv \log rac{p(x,y)}{p(x)p(y)} = \log rac{p(x|y)}{p(x)} = \log rac{p(y|x)}{p(y)}$$

- Positive PMI: PPMI(x, y) = max(pmi(x, y), 0)
- Quantifies the discrepancy between the probability of their coincidence given their joint distribution and their individual distributions, assuming independence
- Finding collocations and associations between words
- Countings of occurrences and co-occurrences of words in a text corpus can be used to approximate the probabilities p(x) or p(y) and p(x,y) respectively



Kenneth Ward Church and Patrick Hanks. "Word association norms, mutual information, and lexicography". Comput. Linguist. 16 (1): 22–29. **1990**.

PMI – Example

word 1	word 2	count word 1	count word 2	count of co-occurrences	PMI
puerto	rico	1938	1311	1159	10.0349081703
hong	kong	2438	2694	2205	9.72831972408
los	angeles	3501	2808	2791	9.56067615065
carbon	dioxide	4265	1353	1032	9.09852946116
prize	laureate	5131	1676	1210	8.85870710982
san	francisco	5237	2477	1779	8.83305176711
nobel	prize	4098	5131	2498	8.68948811416
ice	hockey	5607	3002	1933	8.6555759741
star	trek	8264	1594	1489	8.63974676575
car	driver	5578	2749	1384	8.41470768304
it	the	283891	3293296	3347	-1.72037278119
are	of	234458	1761436	1019	-2.09254205335
this	the	199882	3293296	1211	-2.38612756961
is	of	565679	1761436	1562	-2.54614706831
and	of	1375396	1761436	2949	-2.79911817902
а	and	984442	1375396	1457	-2.92239510038
in	and	1187652	1375396	1537	-3.05660070757
to	and	1025659	1375396	1286	-3.08825363041
to	in	1025659	1187652	1066	-3.12911348956
of	and	1761436	1375396	1190	-3.70663100173

- Counts of pairs of words getting the most and the least PMI scores in the first 50 millions of words in Wikipedia (dump of October 2015)
- Filtering by 1,000 or more co-occurrences.
 - The frequency of each count can be obtained by dividing its value by 50,000,952. (Note: natural log is used to calculate the PMI values in this example, instead of log base 2)



The Contributions of Word Embeddings

Novel Algorithms

(objective + training method)

- Skip Grams + Negative Sampling
- CBOW + Hierarchical Softmax
- Noise Contrastive Estimation
- GloVe
- ..

New Hyperparameters

(preprocessing, smoothing, etc.)

- Subsampling of Frequent Words
- Dynamic Context Windows
- Context Distribution Smoothing
- Adding Context Vectors

What's really improving performance?

. . .



Improving Distributional Similarity with Lessons Learned from Word Embeddings, Omer Levy, Yoav Goldberg, Ido Dagan, Transactions of the Association for Computational Linguistics, Volume 3, **2015**.

Embedding Approaches

- Represent each word with a low-dimensional vector
- Word similarity = vector similarity
- Key idea: Predict surrounding words of every word
- Faster and can easily incorporate a new sentence/document or add a word to the vocabulary


Represent the meaning of a **word** – word2vec

- 2 basic network models:
 - Continuous Bag of Word (CBOW): use a window to predict the middle word
 - Skip-gram (SG): use a word to predict the surrounding ones in window.





Word2vec – Continuous Bag of Words

- E.g. "The cat sat on floor"
 - Window size = 2



Distributed Representations of Words and Phrases and their Compositionality Tomas Mikolov, Ilya Sutskever, Kai Chen, Greg Corrado, Jeffrey Dean, NIPS **2013**























Logistic function

A **logistic function** or **logistic curve** is a common "S" shape (sigmoid curve), with equation:

$$f(x)=rac{L}{1+e^{-k(x-x_0)}}$$

where

- *e* = the natural logarithm base (also known as Euler's number),
- x₀ = the *x*-value of the sigmoid's midpoint,
- L = the curve's maximum value, and
- *k* = the steepness of the curve.^[1]





softmax(z)

The **softmax function**, or **normalized exponential function**, is a generalization of the logistic function that "squashes" a *K*-dimensional vector \mathbf{z} of arbitrary real values to a *K*-dimensional vector $\sigma(\mathbf{z})$ of real values in the range [0, 1] that add up to 1. The function is given by

$$egin{aligned} &\sigma: \mathbb{R}^K o [0,1]^K \ &\sigma(\mathbf{z})_j = rac{e^{z_j}}{\sum_{k=1}^K e^{z_k}} & ext{for } j = 1, \, ..., \, K. \end{aligned}$$

In probability theory, the output of the softmax function can be used to represent a categorical distribution – that is, a probability distribution over K different possible outcomes.







Objective: Given $w_{c-k} \dots, w_{c-1}, w_{c+1}, \dots, w_{c+k}$, predict w_c

Training data: Given sequence of words $\langle w_1, w_2, ..., w_n \rangle$, extract context and target: $(w_{c-k} ..., w_{c-1}, w_{c+1}, ..., w_{c+k}; w_c)$

Knowns:

- Training data { $(w_{c-k} \dots, w_{c-1}, w_{c+1}, \dots, w_{c+k}; w_c)$ }
- Vocabulary $\{w_1, w_2, \dots, w_V\}$ of the training corpus

Unknowns:

- Word embedding matrices $W_{V \times N}$ and $W'_{N \times V}$ with N being a hyperparameter



Loss Function for Learning

- How to determine word embedding matrices?
- Cross entropy for comparing probability distributions

$$- H(\hat{y}, y) = -\sum_{j=1}^{V} y_j \log(\hat{y}_j)$$

• *y* is a one-hot vector with a "one" at position *c*

$$-H(\hat{y}, y) = -y_c \log(\hat{y}_c) = -\log(\hat{y}_c)$$

In this formulation, *c* is the index where the correct word's one hot vector is 1. We can now consider the case where our prediction was perfect and thus $\hat{y}_c = 1$. We can then calculate $H(\hat{y}, y) =$ $-1 \log(1) = 0$. Thus, for a perfect prediction, we face no penalty or loss. Now let us consider the opposite case where our prediction was very bad and thus $\hat{y}_c = 0.01$. As before, we can calculate our loss to be $H(\hat{y}, y) = -1 \log(0.01) \approx 4.605$. We can thus see that for probability distributions, cross entropy provides us with a good measure of distance.



Minimize $-\log P(w_c | w_{c-k}, ..., w_{c-1}, w_{c+1}, ..., w_{c+k})$ $= -\log P(W'[c] | \hat{v})$ (and due to the softmax) $= -\log \frac{e^{W'[c]^T \hat{v}}}{\sum_{i=1}^{V} e^{W'[c]^T_j \hat{v}}}$ $= -W'[c]^T\hat{v} + \log\sum_{j=1}^V e^{W'[j]'\hat{v}}$ where Use gradient descent to update word $\hat{v} = (2k)^{-1} \sum_{i=-k}^{k} W^{T} W_{c+i}$ vectors





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Intrinsic Evaluation

Word Analogies

Test for linear relationships, examined by Mikolov et al. (2014)





Word analogies



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Word Analogies (Tense)





Extrinsic Evaluation

- Evaluate in applications
 - Sentiment analysis





CBOW







We would prefer \hat{y} close to z



N will be the size of word vector



Objective: Given w_c , predict $w_{c-k} \dots, w_{c-1}, w_{c+1}, \dots, w_{c+k}$

Training data: Given sequence of words $\langle w_1, w_2, ..., w_n \rangle$, extract input and output: $(w_c; w_{c-k}, ..., w_{c-1}, w_{c+1}, ..., w_{c+k})$

Knowns:

- Training data { $(w_c; w_{c-k} \dots, w_{c-1}, w_{c+1}, \dots, w_{c+k})$ }
- Vocabulary $\{w_1, w_2, \dots, w_V\}$ of the training corpus

Unknowns:

- Word embedding matrices $W_{V \times N}$ and $W'_{N \times V}$ with N being a hyperparameter



Skip-Gram: Derivation of Learning Procedure

$$\begin{aligned} \text{Minimize} &-\log P(w_{c-m}, \dots, w_{c-1}, w_{c+1}, \dots, w_{c+m} | w_{c}) \\ &= -\log \prod_{j=0, j \neq m}^{2m} P\left(w_{c-m+j} | v_{c}\right) \quad (\text{and due to softmax}) \\ &= -\log \prod_{j=0, j \neq m}^{2m} \frac{e^{W_{c-m+j} v_{c}}}{\sum_{k=1}^{V} e^{W_{k} v_{c}}} \\ &= -(\sum_{j=0, j \neq m}^{2m} W_{c-m+j} v_{c}) \quad + 2m \log \sum_{k=1}^{V} e^{W_{k} v_{c}} \\ &\text{where } v_{c} = W' w_{c} \\ &\text{(no averaging for skip-gram)} \end{aligned}$$



word2vec Explained: Deriving Mikolov et al.'s Negative-Sampling Word-Embedding Method, Yoav Goldberg and Omer Levy, arxiv, **2014**.

What is word2vec?

- word2vec is **not** a single algorithm
- It is a software package for representing words as vectors, containing:
 - Two distinct models
 - CBoW
 - Skip-Gram
 - Various training methods
 - Softmax is a bottleneck (discussed next)
 - A rich preprocessing pipeline
 - Dynamic Context Windows
 - Subsampling of Frequent Words
 - Deleting Rare Words (left out)



Softmax is a Bottleneck (CBOW and Skip-Gram)

- The denominator is a sum across entire vocabulary
- $-(\sum_{j=0, j \neq m}^{2m} W_{c-m+j} v_c) + 2m \log \sum_{k=1}^{V} e^{W_k v_c}$
- To be computed for every window
 - Too expensive
 - Single update of parameters requires iteration of entire vocabulary (which usually is in millions)
- Various optimized training methods
 - Hierarchical Softmax (use binary tree)
 - Probability of a word is calculated through the product of probabilities on each edge on the path to that node
 - Noise Contrastive Estimation (left out)



Rong, X. word2vec Parameter Learning Explained (cite arxiv:1411.2738). **2014**.

Tree for Computing Word Probabilities





Marco saw a furry little wampimuk hiding in the tree.

Distributed Representations of Words and Phrases and their Compositionality Tomas Mikolov, Ilya Sutskever, Kai Chen, Greg Corrado, Jeffrey Dean, NIPS **2013**



Marco saw a furry little wampimuk hiding in the tree.

<u>words</u>

wampimuk wampimuk wampimuk wampimuk

contexts furry little hiding D (data) in



"word2vec Explained..." Goldberg & Levy, arXiv 2014

- SGNS finds a vector \vec{w} for each word w in our vocabulary V_W
- Each such vector has d latent dimensions (e.g. d = 100)
- Effectively, it learns a matrix W whose rows represent V_W
- Key point: it also learns a similar auxiliary matrix C of context vectors
- In fact, each word has two embeddings



d was called N before



"word2vec Explained..." Goldberg & Levy, arXiv 2014

Coming back to Negative Sampling

- Given (*w*, *c*): word and context
- Let P(D = 1 | w, c) be the probability that (w, c) came from the corpus data
- P(D = 0 | w, c) = probability that (w, c) are not from the corpus data
- Let us model P(D = 1 | w, c) with *sigmoid*
- $P(D = 1 | w, c) = sigmoid(u_w^T v_c) = \frac{1}{1 + e^{-u_w^T v_c}}$ $u_v = Ww \ v_c = Cc$
- Objective:
 - Maximize P(D = 1 | w, c) if (w, c) is in the corpus data
 - MinimizeP(D = 1 | w, c) if (w, c) not in the corpus data

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• Maximize: $\sigma(\vec{w} \cdot \vec{c})$		
 c was observed with 		
W		
<u>words</u>	<u>contexts</u>	
wampimuk	furry	
wampimuk	little	
wampimuk	hiding	
wampimuk	in	



"word2vec Explained..." Goldberg & Levy, arXiv 2014

• Maximize: $\sigma(\vec{w} \cdot \vec{c})$ - <i>c</i> was observed with <i>w</i>		• Minimize: $\sigma(\vec{w} \cdot \vec{c}')$ - c' was hallucinated with w	
<u>words</u>	<u>contexts</u>	<u>words</u>	<u>contexts</u>
wampimuk	furry	wampimuk	Australia
wampimuk	little	wampimuk	cyber
wampimuk	hiding	wampimuk	the
wampimuk	in	wampimuk	1985



"word2vec Explained..." Goldberg & Levy, arXiv 2014

Math behind Negative Sampling

Maximum Likelihood approach for learning $\theta = (W, C)$

$$\begin{aligned} \theta &= \operatorname*{argmax}_{\theta} \prod_{(w,c)\in D} P(D=1|w,c,\theta) \prod_{(w,c)\in \tilde{D}} P(D=0|w,c,\theta) \\ &= \operatorname*{argmax}_{\theta} \prod_{(w,c)\in D} P(D=1|w,c,\theta) \prod_{(w,c)\in \tilde{D}} (1-P(D=1|w,c,\theta)) \\ &= \operatorname*{argmax}_{\theta} \sum_{(w,c)\in D} \log P(D=1|w,c,\theta) + \sum_{(w,c)\in \tilde{D}} \log(1-P(D=1|w,c,\theta)) \\ &= \operatorname*{argmax}_{\theta} \sum_{(w,c)\in D} \log \frac{1}{1+\exp(-u_w^T v_c)} + \sum_{(w,c)\in \tilde{D}} \log(1-\frac{1}{1+\exp(-u_w^T v_c)}) \\ &= \operatorname*{argmax}_{\theta} \sum_{(w,c)\in D} \log \frac{1}{1+\exp(-u_w^T v_c)} + \sum_{(w,c)\in \tilde{D}} \log(1-\frac{1}{1+\exp(-u_w^T v_c)}) \end{aligned}$$

$$u_v = Ww \quad v_c = Cc$$

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Math behind Negative Sampling

Maximize log likelihood = minimize –log likelihood

$$-\sum_{(w,c)\in D}\log\frac{1}{1+\exp(-u_w^Tv_c)} - \sum_{(w,c)\in \tilde{D}}\log(\frac{1}{1+\exp(u_w^Tv_c)})$$

Sigmoid

- \widetilde{D} is the negative corpus with wrong contexts
- Generate \widetilde{D} on the fly by randomly sampling from the vocabulary
- New objective function for observing context word w_{c-m+j} (j = 0..2m) given the center word w_c would be

$$-\log \sigma(u_{c-m+j}^{T} \cdot v_{c}) - \sum_{k=1}^{K} \log \sigma(-\tilde{u}_{k}^{T} \cdot v_{c}) - \sum_{k=1}^{|V|} \log \sigma(-\tilde{u}_{k}^{T} \cdot v_{c})$$
regular softmax loss for skip-gram
$$-\sum_{j=0, j \neq m}^{2m} W_{c-m+j} v_{c} + 2m \log \sum_{k=1}^{|V|} e^{W_{k} v_{c}}$$
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- "Negative Sampling"
- SGNS samples k contexts c' at random as negative examples
- "Random" = unigram distribution

$$P(c) = \frac{\#c}{\sum_{c' \in V_C} (\#c')}$$

• Changing this distribution has a significant effect

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Context Distribution Smoothing

 In practice, it's a smoothed unigram distribution

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$$P^{0.75}(c) = \frac{(\#c)^{0.75}}{\sum_{c' \in V_C} (\#c')^{0.75}}$$



• This little change makes a big difference

Context Distribution Smoothing

- We can **adapt** context distribution smoothing to PMI!
- Replace P(c) with $P^{0.75}(c)$ $PMI^{0.75}(w,c) = \log \frac{P(w,c)}{P(w) \cdot P^{0.75}(c)}$
- Consistently improves
 PMI on every task
- Always use Context Distribution Smoothing!




Math behind CBOW with Negative Sampling

- Likewise for CBOW $\hat{v} = \frac{v_{c-m} + v_{c-m+1} + \dots + v_{c+m}}{2m}$
- Objective: $-\log \sigma(u_c^T \cdot \hat{v}) - \sum_{k=1}^{K} \log \sigma(-\tilde{u}_k^T \cdot \hat{v})$

where $\{\tilde{u}_k \mid k = 1..K\}$ is sampled from vocabulary (also use context distribution smoothing)

• Rather than:

$$-u_c^T \hat{v} + \log \sum_{j=1}^{|V|} \exp(u_j^T \hat{v})$$
 regular softmax loss for CBOW



• Take SGNS's embedding matrices (*W* and *C*)





- Take SGNS's embedding matrices (*W* and *C*)
- Multiply them
- What do you get?





- A $V_W \times V_C$ matrix
- Each cell describes the relation between a specific word-context pair

$$\vec{w} \cdot \vec{c} = ?$$





 Levy&Goldberg [2014] proved that for large enough d and enough iterations ...





- Levy&Goldberg [2014] proved that for large enough d and enough iterations ...
- ... one obtains the word-context PMI matrix





- Levy&Goldberg [2014] proved that for large enough d and enough iterations ...
- ... one obtains the word-context PMI matrix ...
- shifted by a global constant



where k is the number of negative examples



- SGNS is doing something very similar to the older approaches
- SGNS factorizes the traditional word-context PMI matrix
- So does SVD!



But embeddings are still better, right?

- Plenty of evidence that embeddings outperform traditional methods
 - "Don't Count, Predict!" (Baroni et al., ACL 2014)
 - GloVe (Pennington et al., EMNLP 2014)
- How does this fit with our story?

Marco Baroni, Georgiana Dinu, Germán Kruszewski. Don't count, predict! A systematic comparison of context-counting vs. context-predicting semantic vectors. In: Proc. ACL-14, 238–247, **2014**.

Jeffrey Pennington, Richard Socher, Christopher Manning. GloVe: Global Vectors for Word Representation. In: Proc. EMNLP-.14, 1532–1543, **2014**.



The Big Impact of "Small" Hyperparameters

- word2vec & GloVe are more than just algorithms...
- Introduce new hyperparameters
- May seem minor, but **make a big difference** in practice



New Hyperparameters

Preprocessing

- Dynamic Context Windows
- Subsampling of Frequent Words
- Deleting Rare Words

Postprocessing

- Adding Context Vectors

Association Metric

- Shifted PMI
- Context Distribution Smoothing

(word2vec)

(GloVe)

(SGNS)



Dynamic Context Windows

Marco saw a furry little wampimuk hiding in the tree.



Dynamic Context Windows

saw a furry little wampimuk hiding in the tree



saw a furry little wampimuk hiding in the tree

Word2vec:	$\frac{1}{4}$	$\frac{2}{4}$	3 4	$\frac{4}{4}$	$\frac{4}{4}$	3 4	2 4	$\frac{1}{4}$	
GloVe:	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{1}{1}$	$\frac{1}{1}$	1 2	$\frac{1}{3}$	$\frac{1}{4}$	
Aggressive:	$\frac{1}{8}$	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{1}{1}$	$\frac{1}{1}$	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{8}$	

The Word-Space Model (Sahlgren, 2006)



Magnus Sahlgren, The Word-Space Model, Dissertation, Stockholm Univ., **2006**.

Subsampling of Frequent Words

- Counter imbalance of rare and frequent words
- Each word in the training set is discarded with a probability computed by

$$P(w_i) = 1 - \sqrt{\frac{t}{f(w_i)}}$$

 where f(w_i) is the number of occurrences of word w_i and t is a chosen threshold

> Distributed Representations of Words and Phrases and their Compositionality Tomas Mikolov, Ilya Sutskever, Kai Chen, Greg Corrado, Jeffrey Dean, NIPS **2013**



Adding Context Vectors

- SGNS creates word vectors \vec{w}
- SGNS creates auxiliary context vectors \vec{c}
 - So do GloVe and SVD
- Instead of just \vec{w}
- Represent a word as: $\vec{w} + \vec{c}$
- Introduced by Pennington et al. (2014)
- Only applied to GloVe



Don't Count, Predict! ?

- "word2vec is better than count-based methods" [Baroni et al., 2014]
- Hyperparameter settings account for most of the reported gaps in count-based approaches
- Embeddings do **not** really outperform count-based methods
- No unique conclusion available



Marco Baroni, Georgiana Dinu, Germán Kruszewski. Don't count, predict! A systematic comparison of context-counting vs. contextpredicting semantic vectors. In: Proc. ACL-14, 238–247, **2014**.

Problem

- Learn low-dimensional, dense representations (or embeddings) for documents.
- Document embeddings can be used off-the-shelf to solve many IR applications such as,
 - Document Classification
 - Document Retrieval
 - Document Ranking



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Power of 2Vec Representations

- Bag-of-words (BOW) or Bag-of-n-grams
 - Data sparsity
 - High dimensionality
 - Not/hardly capturing word order
- Latent Dirichlet Allocation (LDA)
 - Computationally inefficient for larger dataset.
- Paragraph Vector
 - Dense representation
 - Compact representation
 - Captures word order
 - Efficient to estimate



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Represent the meaning of sentence/paragraph/doc

- Paragraph Vector (Le and Mikolov, 2014)
 - Extend word2vec to text level
 - Also two models: add paragraph vector as the input





Quoc Le and Tomas Mikolov. Distributed representations of sentences and documents. In Proceedings ICML'14. **2014**.

Paragraph Vector

- Learn document embedding by predicting the next word in the document using the context of the word and the ('unknown') document vector as features.
- Resulting vector captures the topic of the document.
- Update the document vectors, but not the word vectors
 [Le et al.]
- Update the document vectors, along with the word vectors [Dai et al.]
 - Improvement in the accuracy for document similarity tasks.

Quoc Le and Tomas Mikolov. Distributed representations of sentences and documents. In Proceedings ICML'14. **2014**.

Dai, A.M., Olah, C., Le, Q.V., Corrado, G.S.: Document embedding with paragraph vectors. In: NIPS Deep Learning Workshop. **2014**

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Doc2Sent2Vec Idea - Being granular helps

- Should we learn the document embedding from the word context directly?
- Can we learn the document embedding from the sentence context?
 - Explicitly exploit the sentence-level and word-level coherence to learn document and sentence embedding respectively.



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Notation

- **Document Set:** $D = \{d_1, d_2, ..., d_M\}$; 'M' documents;
- **Document:** $d_m = \{s(m,1), s(m,2), ..., s(m,T_m)\}; T_m' \text{ sentences};$
- Sentence: $s(m,n) = \{w(n,1), w(n,2), ..., w(n,T_n)\}; T_n' words;$
- Word: w(n,t);

Doc2Sent2Vec's goal is to learn low-dimensional representations of words, sentences and documents as a continuous feature vector of dimensionality D_w , D_s and D_d respectively.



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Architecture Diagram



words within sentence (word-level coherence)



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Phase 1: Learn Sentence Embedding

Idea: Learn sentence representation from the word sequence within the sentence.

Input Features:

- Context words for target word w(n,t): w(n,t-c_w), ..., w(n,t-1), w(n,t+1), ..., w(n,t+c_w) (where 'c_w' is the word context size)
- Target Sentence: s(m,n) (where 'm' is the document id)

Output: w(n,t)

Task: Predict the target word using the concatenation of word vectors of context words along with the sentence vector as features.

Maximize the word likelihood:

 $L_{word} = P(w(n,t)|w(n,t-c_w), ..., w(n,t-1), w(n,t+1), ..., w(n,t+c_w), s(m,n))$



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Phase 2: Learn Document Embedding

Idea: Learn document representation from the sentence sequence within the document.

Input Features:

- Context sentences for target sentence s(m,t): s(m,t-c_s), ..., s(m,t-1), s(m,t+1), ..., s(m,t+c_s) (where 'c_s' is the sentence context size)
- Target Document: d(m)

Output: s(m,t)

Novel Task: Predict the target sentence using the concatenation of sentence vectors of context sentences along with the document vector as features.

Maximize the sentence likelihood:

 $L_{sent} = P(s(m,t)|s(m,t-c_s), ..., s(m,t-1), s(m,t+1), ..., s(m,t+c_s), d(m))$



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Training

- Overall objective function: $L = L_{word} + L_{sent}$
- Use Stochastic Gradient Descent (SGD) to learn parameters
- Use Hierarchical Softmax (Mikolov et al.) to facilitate faster training



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Latent Relational Structures

Processing natural language data:

- ✓ Tokenization/Sentence Splitting
- ✓ Part-of-speech (POS) tagging
- Phrase chunking
- Named entity recognition
- Coreference resolution
- Semantic role labeling



Ronan Collobert and Jason Weston. A unified architecture for natural language processing: deep neural networks with multitask learning. In Proceedings ICML '08. pp. 160–167. **2008**.

Phrase Chunking

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• Identifies phrase-level constituents in sentences

[NP Boris] [ADVP regretfully] [VP told] [NP his wife][SBAR that] [NP their child] [VP could not attend] [NP night school] [PP without] [NP permission].

- Useful for filtering: identify e.g. only noun phrases, or only verb phrases
- Used as source of features, e.g. distance, (abstracts away determiners, adjectives, for example), sequence,...
 - More efficient to compute than full syntactic parse
 - Applications in e.g. Information Extraction getting (simple) information about concepts of interest from text documents
- Hand-crafted chunkers (regular expressions/finite automata)
- HMM/CRF-based chunk parsers derived from training data

Named Entity Recognition

- Identifies and classifies strings of characters representing proper nouns
- [PER Neil A. Armstrong], the 38-year-old civilian commander, radioed to earth and the mission control room here: "[LOC Houston], [ORG Tranquility] Base here; the Eagle has landed."
- Useful for filtering documents
 - "I need to find news articles about organizations in which Bill Gates might be involved..."
- Disambiguate tokens: "Chicago" (team) vs. "Chicago" (city)
- Source of abstract features
 - E.g. "Verbs that appear with entities that are Organizations"
 - E.g. "Documents that have a high proportion of Organizations"



Named Entity Recogniton: Definition

- NE involves identification of proper names in texts, and classification into a set of predefined categories of interest
 - Three universally accepted categories: person, location and organisation
 - Other common tasks: recognition of date/time expressions, measures (percent, money, weight etc), email addresses etc.
 - Other domain-specific entities: names of drugs, medical conditions, names of ships, bibliographic references etc
- NER ist not easy



Named Entity Classification

- Category definitions are intuitively quite clear, but there are many grey areas.
- Many of these grey areas are caused by metonymy.
 - Person vs. Artefact: "The ham sandwich wants his bill." vs "Bring me a ham sandwich."
 - Organisation vs. Location : "England won the World Cup" vs. "The World Cup took place in England".
 - Company vs. Artefact: "shares in MTV" vs. "watching MTV"
 - Location vs. Organisation: "she met him at Heathrow" vs.
 "the Heathrow authorities"



Basic Problems in NE

- Variation of NEs e.g. John Smith, Mr Smith, John.
- Ambiguity of NE types
 - John Smith (company vs. person)
 - May (person vs. month)
 - Washington (person vs. location)
 - 1945 (date vs. time)
- Ambiguity with common words, e.g. "may"



More complex problems in NER

- Issues of style, structure, domain, genre etc.
 - Punctuation, spelling, spacing, formatting,all have an impact

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> Tell me more about Leonardo> Da Vinci



List Lookup Approach

- System that recognises only entities stored in its lists (gazetteers).
- Advantages Simple, fast, language independent, easy to retarget
- Disadvantages collection and maintenance of lists, cannot deal with name variants, cannot resolve ambiguity



Shallow Parsing Approach

 Internal evidence – names often have internal structure. These components can be either stored or guessed.

location:

CapWord + {City, Forest, Center}

e.g. Sherwood Forest

Cap Word + {Street, Boulevard, Avenue, Crescent, Road} e.g. *Portobello Street*



Shallow Parsing Approach

 External evidence - names are often used in very predictive local contexts

Location:

"to the" COMPASS "of" CapWord e.g. *to the south of* **Loitokitok** "based in" CapWord e.g. *based in* **Loitokitok** CapWord "is a" (ADJ)? GeoWord e.g. **Loitokitok** is a friendly city



Difficulties in Shallow Parsing Approach

- Ambiguously capitalised words (first word in sentence)
 [All American Bank] vs. All [State Police]
- Semantic ambiguity

"John F. Kennedy" = airport (location) "Philip Morris" = organisation

Structural ambiguity

[Cable and Wireless] vs. [Microsoft] and [Dell]

[Center for Computational Linguistics] vs. message from [City Hospital] for [John Smith].



Coreference

- Identify all phrases that refer to each entity of interest i.e., group mentions of concepts
- [Neil A. Armstrong], [the 38-year-old civilian commander], radioed to [earth]. [He] said the famous words, "[the Eagle] has landed"."
- The Named Entity Recognizer only gets us part-way...
- ...if we ask, "what actions did Neil Armstrong perform?", we will miss many instances (e.g., "He said...")
- Coreference resolver abstracts over different ways of referring to the same person
 - Useful in feature extraction, information extraction



Semantic Role Labeling (SRL)

Input Text:

A car bomb that exploded outside the U.S. military base in Beniji killed 11 Iraqi citizens.

Result: Complete!

General Explanation of Argument Labels



- SRL reveals relations and arguments in the sentence (where relations are expressed as verbs)
- Cannot abstract over variability of expressing the relations – e.g. kill vs. murder vs. slay…



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An Introduction to Machine Learning and Natural Language Processing Tools, , V. Srikumar, M. Sammons, N. Rizzolo

Why is SRL Important – Applications

- Question Answering
 - Q: When was Napoleon defeated?
 - Look for: [PATIENT Napoleon] [PRED defeat-synset] [ARGM-TMP *ANS*]
- Machine Translation

English (SVO) [AGENT The little boy] [PRED kicked] [THEME the red ball] [ARGM-MNR hard] Farsi (SOV)

[AGENT pesar koocholo] boy-little[THEME toop germezi] ball-red[ARGM-MNR moqtam] hard-adverb[PRED zaad-e] hit-past

- Document Summarization
 - Predicates and Heads of Roles summarize content

Information Extraction

SRL can be used to construct useful rules for IE



Some History

- Minsky 74, Fillmore 1976: Frames describe events or situations
 - Multiple participants, "props", and "conceptual roles"
 - E.g., agent, instrument, target, time, ...
- Levin 1993: verb class defined by sets of frames (meaningpreserving alternations) a verb appears in
 - {break,shatter,..}: Glass X's easily; John Xed the glass, ...
 - *Cut* is different: *The window broke; *The window cut.*
- FrameNet, late '90s: based on Levin's work: large corpus of sentences annotated with *frames*
- PropBank

Marvin Minky. A Framework for Representing Knowledge Marvin Minsky, MIT-AI Laboratory Memo 306, June, **1974**.

Charles J. Fillmore, Frame semantics and the nature of language Annals of the New York Academy of Sciences 280(1):20 – 32, **1976**.

Levin, B. English Verb Classes and Alternations: A Preliminary Investigation, University of Chicago Press, Chicago, IL. **1993**.

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Automatic Semantic Role Labeling, S. Wen-tau Yih, K. Toutanova

FrameNet



[Agent Kristina] hit [Target Scott] [Instrument with a baseball] [Time yesterday].



Gildea, Daniel; Jurafsky, Daniel. "Automatic Labeling of Semantic Roles". Computational Linguistics. 28 (3): 245–288. **2002**.

Proposition Bank (PropBank)

- Transfer sentences to propositions

 Kristina hit Scott → hit(Kristina,Scott)
- Penn TreeBank \rightarrow PropBank
 - Add a semantic layer on Penn TreeBank
 - Define a set of semantic roles for each verb
 - Each verb's roles are numbered
 - ...[A0 the company] to ... offer [A1 a 15% to 20% stake] [A2 to the public]
 - ...[A0 Sotheby's] ... offered [A2 the Dorrance heirs] [A1 a money-back guarantee]
 - ...[A1 an amendment] *offered* [A0 by Rep. Peter DeFazio] ...
 - ...[A2 Subcontractors] will be offered [A1 a settlement] ...



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