# Representation Learning For Computational Imagination 

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## Word2vec



## Machine Learning

Data $\rightarrow$ "feature vectors" $\rightarrow$ Task

## Deep Learning



Can we let the machine discover useful features?

## Representations live in a vector space.



## Can we interpret this literally, as a "space"?



## We can find meaningful semantic axes in the space



## "Geometry of Culture"

## ASA

## The Geometry of Culture: Analyzing the Meanings of Class through Word Embeddings <br> American Sociological Review 2019, Vol. 84(5) 905-949 © American Sociological Association 2019 DOI: 10.1177/0003122419877135 journals.sagepub.com/home/asr ©SAGE

Austin C. Kozlowski, ${ }^{\text {a }}$ (D) Matt Taddy, ${ }^{\text {b }}$ and James A. Evans ${ }^{\text {a,c ( }}$ (D)

## Abstrac

We argue word embedding models are a useful tool for the study of culture using a historical analysis of shared understandings of social class as an empirical case. Word embeddings represent semantic relations between words as relationships between vectors in a highdimensional space, spify a relational model of meaning consistent with contemporary dimensional space, specifying a relational model of meaning consistent with contemporary heories of culture. Dimensions induced by word differences (rich - poor) in these spaces correspond to dimensions of cultural meaning, and the projection of words onto these dimensions reflects widely shared associations, which we validate with surveys. Analyzing text from millions of books published over 100 years, we show that the markers of class
continuously shifted amidst the economic transformations of the twentieth century, yet continuously shifted amidst the economic transformations of the twentieth century, yet
the basic cultural dimensions of class remained remarkably stable. The notable exception is education, which became tightly linked to affluence independent of its association with cultivated taste.

A. C. Kozlowski, M. Taddy, and J. Evans, ASR, 2019 https://arxiv.org/abs/1806.05521

## Meaningful axes about material properties



## Meaningful axes about facial features



## Meaningful axes about facial features



# The representation space itself is interesting! 

## We think and imagine spatially



## We think and imagine spatially

## HAPPY IS UP; SAD IS DOWN



I'm feeling up. That boosted my spirits. My spirits rose. You're in high spirits. Thinking about her always gives me a lift. I'm feeling down. I'm depressed. He's really low these days. I fell into a depression. My spirits sank.

## We think and imagine spatially



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CONSCIOUS IS UP; UNCONSCIOUS IS DOWN
Get up. Wake up. I'm up already. He rises early in the morning. He fell asleep. He dropped off to sleep. He's under hypnosis. He sank into a coma.

## We think and imagine spatially



GEORGE LAKOFF AND MARK JOHNSON with a new afterworo

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HEALTH AND LIFE ARE UP; SICKNESS AND DEATH ARE DOWN
He's at the peak of health. Lazarus rose from the dead. He's in top shape. As to his health, he's way up there. He fell ill. He's sinking fast. He came down with the flu. His health is declining. He dropped dead.

## We think and imagine spatially



## HAPPY IS UP; SAD IS DOWN

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## GOOD IS UP; BAD IS DOWN

Things are looking up. We hit a peak last year, but it's been downhill ever since. Things are at an all-time low. He does high-quality work.

# Representation learning <br> $\sim$ matrix factorization 



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## Abstract

trends suggest that neural -inspired word embedding models orm traditional count-based distri1 models on word similarity and detection tasks. We reveal that

A recent study by Baroni et al. (2014) conducts a set of systematic experiments comparing word2vec embeddings to the more traditional distributional methods, such as pointwise mutual information (PMI) matrices (see Turney and Pantel (2010) and Baroni and Lenci (2010)

# How should we represent them? How to encode the "meaning"? 

## hello world!

01101000011001010110110001101100
01101111001000000111011101101111
01110010011011000110010000100001

# How should we represent them? How to encode the "meaning"? 


"Among all the individuals that are linked together by speech, some sort of average will be set up: all will reproduce - not exactly of course, but approximately - the same signs united with the same concepts."
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Distributional hypothesis: words that occur in the same contexts tend to have similar meanings.

We can study language by analyzing how it is used in a corpus.
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Distributional hypothesis: words that occur in the same contexts tend to have similar meanings.

We can study language by analyzing how it is used in a corpus.


## "You shall know a word by the company it keeps."

## Contexts ~ Meaning

The quick brown __ jumps over the lazy dog. He is cunning as $a \ldots$.

The___ was already in your chicken house.

## Contexts ~ Meaning

The quick brown __ jumps over the lazy dog. He is cunning as a $\qquad$
The ___ was already in your chicken house.

What do you mean by "contexts"?

## Encoding contexts: term-document matrix

|  | cat | dog | fox | wolf | coyote | $\ldots$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| D1 | 15 | 10 | 0 | 0 | 8 | $\ldots$ |
| D2 | 2 | 6 | 2 | 2 | 0 | $\ldots$ |
| D3 | 0 | 1 | 16 | 15 | 6 | $\ldots$ |
| $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ | $\ldots$ |



$$
\text { Document } \rightarrow \text { term } \sim \text { Document } \rightarrow \text { Topic } \rightarrow \text { Term }
$$

Terms


Topics


Terms

## 

Non-negative Matrix Factorization

$$
\text { Document } \rightarrow \text { term } \sim \text { Document } \rightarrow \text { Topic } \rightarrow \text { Term }
$$

Terms


Topics


Terms

## 

## Non-negative Matrix Factorization

(Latent Dirichlet Allocation can be thought as a "softer" Bayesian method to do this.)

$$
\text { Document } \rightarrow \text { term } \sim \text { Document } \rightarrow \text { Topic } \rightarrow \text { Term }
$$

Terms


Topics


Terms


A word as a low-dimensional vector

Document $\rightarrow$ term $\sim$ Document $\rightarrow$ Topic $\rightarrow$ Term

# Using documents as "contexts" led to nice models and representations. 

Can we think of nearby words as contexts?

## Neural Language Model as a Matrix Factorization

Words

??


Words


A word as a low-dimensional vector

A word as a
low-dimensional vector

## Neural Language Model as a Matrix Factorization



## The idea of "language model"

## What is the probability of this sentence?

A good language model should assign high probability for real sentences and low probability for nonsensical sentences.

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$$

## The idea of "language model"

## What is the probability of this sentence?

A good language model should assign high probability for real sentences and low probability for nonsensical sentences.

$$
\begin{gathered}
P\left(w_{1}, w_{2}, \ldots, w_{n}\right)=? \\
P\left(w_{1}, w_{2}, \ldots, w_{n}\right)=P\left(w_{n} \mid w_{1}, \ldots, w_{n-1}\right) P\left(w_{n-1} \mid w_{1}, \ldots, w_{n-2}\right) \\
\times P\left(w_{n-2} \mid w_{1}, \ldots, w_{n-3}\right) \times \cdots \times P\left(w_{1}\right)
\end{gathered}
$$

## The idea of "language model"

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\begin{array}{r}
P\left(w_{1}, w_{2}, \ldots, w_{n}\right)=P\left(w_{n} \mid w_{1}, \ldots, w_{n-1}\right) P\left(w_{n-1} \mid w_{1}, \ldots, w_{n-2}\right) \\
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What is the probability of the next word?

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Target

## The idea of "language model"

$$
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P\left(w_{1}, w_{2}, \ldots, w_{n}\right)=P\left(w_{n} \mid w_{1}, \ldots, w_{n-1}\right) P\left(w_{n-1} \mid w_{1}, \ldots, w_{n-2}\right) \\
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\end{array}
$$

What is the probability of the next word?

$$
P\left(w_{t} \mid w_{1}, \ldots, w_{t-1}\right)=?
$$

## Target Context

A slightly different formulation

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What is the probability of the target zoord given the contexts around it?

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The quick brown ___ jumps over the lazy dog.

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## A slightly different formulation

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## A slightly different formulation

What is the probability of the target word given the contexts around it?


## Even the most sophisticated methods are still rooted in this simple core idea.

BERT:
predict the masked word

## GPT:

predict the next word


The quick brown fox jumps
word2vec: Skip-gram model (single-word context)

$$
P\left(w_{t} \mid w_{t-n}, \ldots, w_{t-1}\right)=?
$$

Can we just think about one word at a time ("skipping" the others)?
word2vec: Skip-gram model (single-word context)

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P\left(w_{t} \mid w_{t-n}, \ldots, w_{t-1}\right)=?
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# word2vec: Skip-gram model (single-word context) 

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$$



Can we just think about one word at a time ("skipping" the others)?

$$
P\left(w_{t} \mid w_{c}\right)=?
$$

## A single context word from the

n-gram window

## word2vec: Skip-gram model (single-word context)

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P\left(w_{t} \mid w_{t-n}, \ldots, w_{t-1}\right)=?
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Can we just think about one word at a time ("skipping" the others)?

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P\left(w_{t} \mid w_{c}\right)=?
$$

$$
P\left(w_{t} \mid \text { context }\right) \approx \prod_{c \in C} P\left(w_{t} \mid w_{c}\right)
$$

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$$

## A single context word from the

$$
C=\{t-w, \ldots, t-1, t+1, \ldots, t+w\}
$$

word2vec: Skip-gram model (single-word context)


$$
\begin{gathered}
P\left(w_{t} \mid \text { context }\right) \approx \prod_{c \in C} P\left(w_{t} \mid w_{c}\right) \\
P\left(w_{1}, \ldots, w_{n}\right) \approx \prod_{t} \prod_{c \in C} P\left(w_{t} \mid w_{c}\right) \\
\text { Maximize: } \frac{1}{T} \sum_{t}^{T} \sum_{c \in C} \log P\left(w_{t} \mid w_{c}\right)
\end{gathered}
$$

word2vec: using two vectors to evaluate the language model

$$
\frac{1}{T} \sum_{t}^{T} \sum_{c \in C} \log P\left(w_{t} \mid w_{c}\right) \quad P\left(w_{t} \mid w_{c}\right)=?
$$

Let's assume that we have really good (two) vector representations for each word.
$\left(\mathbf{q}_{i}, \mathbf{k}_{i}\right)$ Each word has a 'query' and a 'key' vector $P\left(w_{t} \mid w_{c}\right) \approx f\left(\mathbf{k}_{t}, \mathbf{q}_{c}\right)$ that approximates the conditional probability.

$$
P\left(w_{t} \mid w_{c}\right) \approx \frac{\exp \left(\mathbf{k}_{t} \cdot \mathbf{q}_{c}\right)}{\sum_{i} \exp \left(\mathbf{k}_{i} \cdot \mathbf{q}_{c}\right)}
$$

## word2vec



Representations that produce a good language model also capture "meaning"!

Correspondence between word2vec model and the gravity law of mobility

## Gravity law of mobility

"You are less likely to go somewhere farther away than somewhere close."


$$
F_{1}=F_{2}=G \frac{m_{1} \times m_{2}}{r^{2}}
$$





## Data: Scientific mobility (2008-2019), and several others

 <br> \title{
1 Clarivate <br> \title{
1 Clarivate Analytics
} Analytics
}


Derive flux between organizations from scientists' trajectories


## Does this embedding better explains flows than geographic distance? Yes!



## U.S. Flight Itineraries

## Reservation



## Embedding explains the flux best



Murray, Dakota, Jisung Yoon, Sadamori Kojaku, Rodrigo Costas, Woo-Sung Jung, Staša Milojević, and Yong-Yeol Ahn. "Unsupervised embedding of trajectories captures the latent structure of mobility." arXiv preprint arXiv:2012.02785 (2020)

Why?

## Let's go back to the word2vec model

$\left(\mathbf{q}_{i}, \mathbf{k}_{i}\right)$ Each Word Has a 'Query' and a 'Key' Vector $P\left(w_{t} \mid w_{c}\right) \approx f\left(\mathbf{k}_{t}, \mathbf{q}_{c}\right)$
That Approximates the Conditional Probability.

A Simple Choice: $\quad P\left(w_{t} \mid w_{c}\right) \approx \frac{\exp \left(\mathbf{k}_{t} \cdot \mathbf{q}_{c}\right)}{\sum_{i} \exp \left(\mathbf{k}_{i} \cdot \mathbf{q}_{c}\right)}$

$$
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$$

Negative sampling! Let's formulate a classification task.

$$
P\left(w_{t} \mid w_{c}\right) \approx \frac{\exp \left(\mathbf{k}_{t} \cdot \mathbf{q}_{c}\right)}{\sum_{i} \exp \left(\mathbf{k}_{i} \cdot \mathbf{q}_{c}\right)} \longleftarrow \text { nasty! }
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Negative sampling! Let's formulate a classification task.

$$
P^{\mathrm{NS}}\left(Y_{j}=1 ; \boldsymbol{v}_{i}, \boldsymbol{u}_{j}\right)=\frac{1}{1+\exp \left(-\boldsymbol{u}_{j} \cdot \boldsymbol{v}_{i}\right)},
$$

$$
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\mathcal{J}^{\mathrm{NS}}=\sum_{i \in \mathcal{F}} \sum_{j \in \mathcal{D}}\left[Y_{j} \log P^{\mathrm{NS}}\left(Y_{j}=1 ; \boldsymbol{v}_{i}, \boldsymbol{u}_{j}\right)+\left(1-Y_{j}\right) \log P^{\mathrm{NS}}\left(Y_{j}=0 ; \boldsymbol{v}_{i}, \boldsymbol{u}_{j}\right)\right],
\end{gathered}
$$

## Noise contrastive estimation and negative sampling

"Noise Contrastive Estimation" [Gutmann \& Hyvärinen, 2010], an unbiased estimator, is subtly different.

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$$

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\end{aligned}
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## SGNS word2vec actually optimzes...

$$
P^{N S}(j \mid i)=P_{m}^{N S}\left(\boldsymbol{u}_{j} \cdot \boldsymbol{v}_{i}\right)=\frac{P^{\gamma}(j) \exp \left(\boldsymbol{u}_{j} \cdot \boldsymbol{v}_{i}\right)}{Z_{i}^{\prime}}
$$

Sadamori Kojaku

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## What happens if we apply word2vec to mobility trajectories?



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P\left(w_{t} \mid w_{c}\right) \approx \frac{p_{n}(t) \exp \left(\mathbf{k}_{t} \cdot \mathbf{q}_{c}\right)}{\sum_{i} p_{n}(i) \exp \left(\mathbf{k}_{i} \cdot \mathbf{q}_{c}\right)}
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$$



$$
\hat{T}_{i j} \propto P(j \mid i) P(i) \propto \frac{P(i) P(j) \exp \left(\mathbf{k}_{j} \cdot \mathbf{q}_{i}\right)}{\sum_{j^{\prime}} P\left(j^{\prime}\right) \exp \left(\mathbf{k}_{j^{\prime}} \cdot \mathbf{q}_{i}\right)}
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$$



$$
\hat{T}_{i j} \propto P(j \mid i) P(i) \propto \frac{P(i) P(j) \exp \left(\mathbf{k}_{j} \cdot \mathbf{q}_{i}\right)}{\sum_{j^{\prime}} P\left(j^{\prime}\right) \exp \left(\mathbf{k}_{j^{\prime}} \cdot \mathbf{q}_{i}\right)}
$$

What happens if we apply word2vec to mobility trajectories?

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## word2vec model ~ gravity law



The space where the institutions are arranged so that the flux and distance between them satisfies the gravity law of mobility!

## Implications in Graph Embedding



Random walk $\rightarrow$ "Sentences" (DeepWalk, node2vec, etc.)

## Random walk is biased

Friendship paradox. When we follow an edge, the expected degree is proportional to the degree

$$
\sim p(k)
$$

$$
\sim k p(k)
$$

## Random walk is biased



Fraction of core nodes in the graph


Time spent in core node


What's the Implication?

## Random Walk Bias $\rightarrow$ Biased Embedding Space



DeepWalk


## But word2vec's bias negates this random walk bias!

$$
\text { Recall } P\left(w_{t} \mid w_{c}\right) \approx \frac{p_{n}(t) \exp \left(\mathbf{k}_{t} \cdot \mathbf{q}_{c}\right)}{\sum_{i} p_{n}(i) \exp \left(\mathbf{k}_{i} \cdot \mathbf{q}_{c}\right)}
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If negative samples are proportionally sampled based on their degree, SGNS negates the bias of the random walker!

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If negative samples are proportionally sampled based on their degree, SGNS negates the bias of the random walker!
(3) Can we remove other statistical biases as well?

## Residual2vec

We can extract out the expected conditional probability based on a null model.


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## We can extract out the expected conditional probability based on a null model.



Sadamori Kojaku, Jisung Yoon, Isabel Constantino, Yong-Yeol, "Residual2Vec: Debiasing graph embedding with random graphs", NeurIPS'21

## It also allows us to remove specific structural biases



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- We can further leverage this to remove specific biases from a model.
- Simple models, when understood well, can take us quite far.
- What could be the ways to obtain useful, compact representation of dynamic, functional brain networks?


# How about dense representation of dynamic neural networks? 


https://twitter.com/spornslab/status/1319390214767378432

Olaf Sporns
@spornslab
A short thread on this new pub: pnas.org/content/early/...

Movie below shows functional connectivity unwrapped into 'edge time series' (data: single rs-fMRI scan, 200 nodes, 1100 frames, $\mathrm{TR}=720 \mathrm{~ms}$ )

Note: the mean of all frames is exactly equal to 'classic' FC



3:28 PM • Oct 22, 2020 • Twitter Web App
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Can we identify universal \& individual

## cofluctuation patterns?

## Representation learning as Matrix Factorization



## Representation learning as Matrix Factorization



## Higher-Rank Tensor?



Rank 0
Tensor
scalar

Rank 1
Tensor
vector


Rank 2
Tensor
matrix


Rank 3
Tensor


Rank 4 Tensor

## Tensor Decomposition



## Edge co-fluctuation components from tensor decomposition



What could be the useful, compact representations of the brain's dynamics?

Can we imagine it as a meaningful space?

## Thanks!



Jisun An


Jaehyuk Park


Haewoon Kwak


Fabio Rojas

Sadamori Kojaku


Hao Peng


Isabel Constantino


Jisung Yoon



Qing Ke


Ceren Budak


Supun Nakandala


Dakota Murray


Giovanni Luca Ciampaglia


Daniel Romero


Norman Makoto Su

Other Science Genome \& CADRE team: Alessandro Flammini, Filippo Menczer, Sriraam Natarajan, Attila Varga, Xiaoran Yan, Filipi Silva, Clara Boothby, Valentin Pentchev, Matthew Hutchinson, Chathuri Peli Kankanamalage


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