Representation Learning - A Case Study

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Outline

Problem

"When solving a problem of interest, do not solve a more general problem as an intermediate step. Try to get the answer that you really need but not a more general one."

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"When solving a problem of interest, do not solve a more general problem as an intermediate step. Try to get the answer that you really need but not a more general one."

- Discriminative models are better than generative models.
- It was intended to justify trunsduction - label the unlabeled point only, not a full model.
- It neglected the structure of the data.

Problem

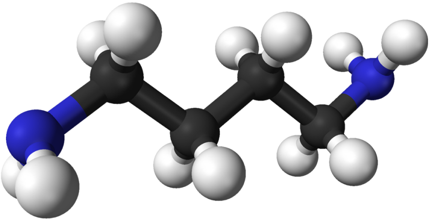
How do humans learn actually?

Problem

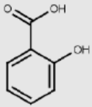
- Kids can recognize their parents.
- They cannot paint them yet.
- This model is far more useful than a perfect reproduction.

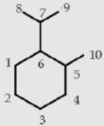
Attributes of representation

- Useful - It can do an inference on what is possible.
- Simple - it skips a lot of details.
- Accurate enough - it enables to recognize and identify novelty.



Neighbours matrix

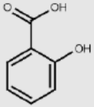


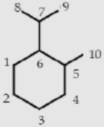


n	1	2	3	4	5	6	7	8	9	10
1	0	1	0	0	0	1	0	0	0	0
2		0	1	0	0	0	0	0	0	0
3			0	1	0	0	0	0	0	0
4				0	1	0	0	0	0	0
5					0	1	0	0	0	1
6						0	1	0	0	0
7							0	1	1	0
8								0	0	0
9									0	0
10										0

$$[A(G)]_{ij} = \begin{cases} 1; & i \neq j, \ e_{ij} \in E(G) \\ 0; & i = j, \ e_{ij} \notin E(G) \end{cases}$$

Distance matrix

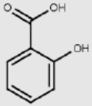


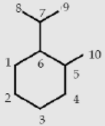


n	1	2	3	4	5	6	7	8	9	10
1	0	1	2	3	2	1	2	3	3	3
2		0	1	2	3	2	3	4	4	4
3			0	1	2	3	4	5	5	3
4				0	1	2	3	4	4	2
5					0	1	2	3	3	1
6						0	1	2	2	2
7							0	1	1	3
8								0	2	4
9									0	4
10										0

$$[D(G)]_{ij} = \begin{cases} d_{ij} \; ; \; i \neq j \\ 0 \; ; \; i = j \end{cases}$$

Connections matrix

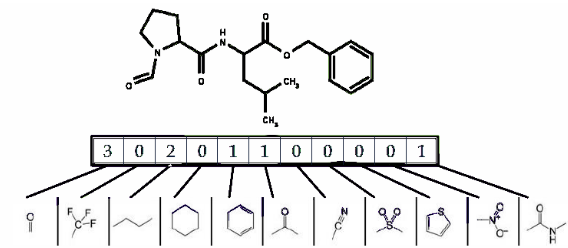




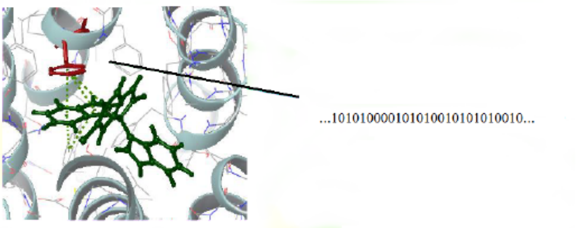
n	1	2	3	4	5	6	7	8	9	10
1	0	2				1				
2	2	0	1							
3		1	0	2						
4			2	0	1					
5				1	0	2				1
6	1				2	0	1			
7						1	0	1	2	
8							1	0	1	
9							2		0	
10					1					0

$$[B(G)]_{ij} = \begin{cases} b_{ij}\ ;\ i \neq j \\ 0\ ;\ i = j \end{cases}$$

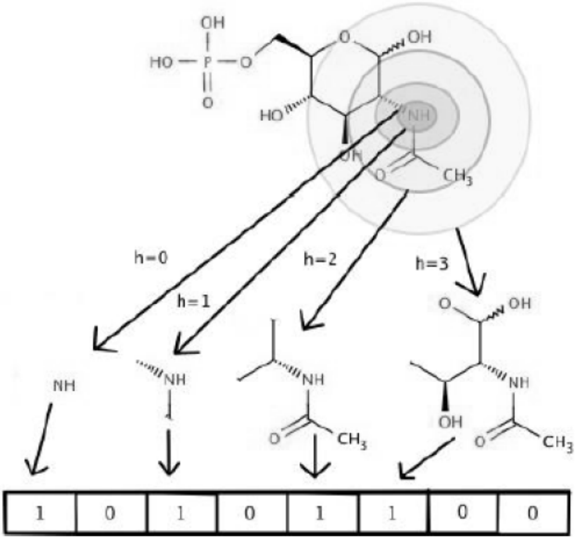
Substructural fingerprint



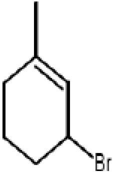
Structural interaction fingerprint



Hashed fingerprint

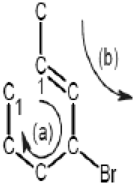


SMILES



(a) CC1=CC(Br)CCC1

(b) CC1=CC(CCC1)Br



SDF

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Mrv0541 01151319442D

 10 10  0  0  0  0            999 V2000
   -1.6721   -0.1120    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9576   -0.5245    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9576   -1.3495    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6721   -1.7620    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3866   -1.3495    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3866   -0.5245    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.6721    0.7130    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.3866    1.1255    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.9576    1.1255    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.2432   -0.1120    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1  6  2  0  0  0  0
  2  3  2  0  0  0  0
  3  4  1  0  0  0  0
  4  5  2  0  0  0  0
  5  6  1  0  0  0  0
  1  7  1  0  0  0  0
  7  8  2  0  0  0  0
  7  9  1  0  0  0  0
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M  END
>  <CdId>
5

>  <Mol Weight>
138.1207

>  <Formula>
C7H6O3

$$$$
```

header

atomic coordinates

connection table

properties

Moments

- Moments are scalar quantities used to characterize a function and to capture its significant features.

Moments

Definition

General moment $M_{pq}^{(f)}$ of an image f(x, y), gdzie p, q re non-negative integers and $r = p + q$ is called the order of the moment, defined as

$$M_{pq}^{(f)} = \iint p_{pq}(x, y) f(x, y) \mathrm{d}x \mathrm{d}y,$$

where $p_{00}(x, y), p_{10}(x, y), \ldots, p_{kj}(x, y), \ldots$ are polynomial basis functions defined on D.

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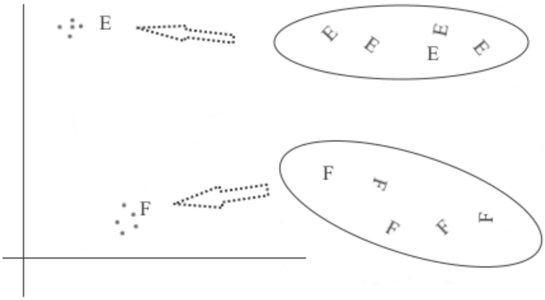
where $p_{00}(x, y), p_{10}(x, y), \ldots, p_{kj}(x, y), \ldots$ are polynomial basis functions defined on D.
Depending on the polynomial basis used, we recognize various systems of moments.

Geometric moments

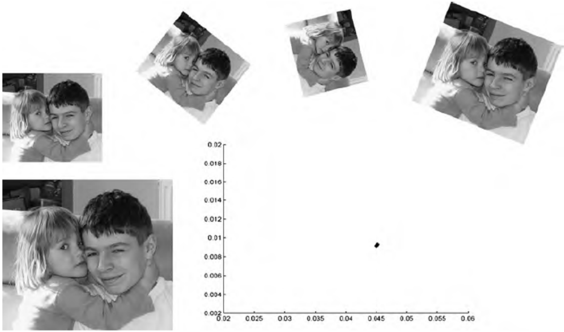
$p_{kj}(x, y) = x^k y^j$ leads to geometric moments.

$$m_{pq} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x^p y^q f(x, y) \mathrm{d}x \mathrm{d}y.$$

Vector of invariants (Hu, 1962)



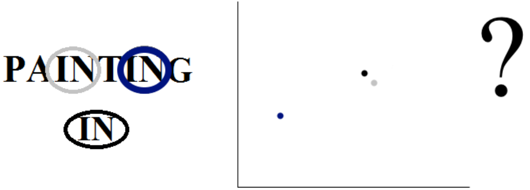
Vector of invariants



Hu invariants - drawbacks

- mutual dependence;
- restriction to second- and third-order moments only.

Research motivation



- Piotr Bojanowski, Edouard Grave, Armand Joulin, Tomas Mikolov: *Enriching Word Vectors with Subword Information*, arXiv, 2016.
- Tomas Mikolov, Kai Chen, Greg Corrado, and Jeffrey Dean: *Efficient estimation of word representations in vector space*, arXiv, 2013.

Background

- Scott Deerwester, Susan T. Dumais, George W. Furnas, Thomas K. Landauer, and Richard Harshman: *Indexing by latent semantic analysis*. Journal of the American Society for Information Science, 1990.
- neural networks
- Hinrich Schütze: *Dimensions of meaning*. Proceedings of the 1992 ACM/IEEE Conference on Supercomputing, 1992.
- N. Sakamoto, K. Yamamoto, and S. Nakagawa: *Combination of syllable based n-gram search and word search for spoken term detection through spoken queries and iv/oov classification*. Automatic Speech Recognition and Understanding (ASRU), 2015.

Model

- We extended the method introduced by Bojanowski et al.
- The model demonstrated by Bojanowski is derived from continuous Skip-gram (SG) model proposed by Mikolov et al.

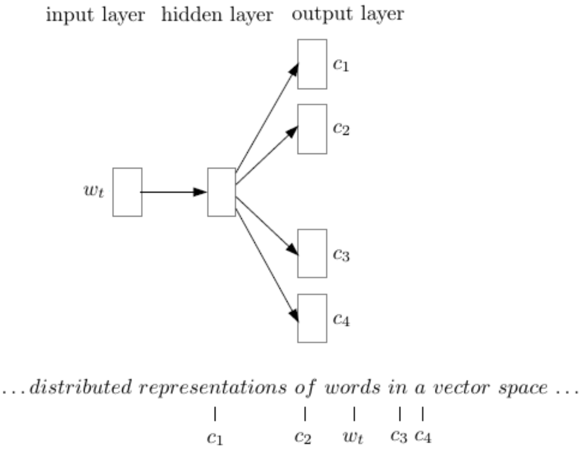
Skip-gram model

- The goal of Skip-gram model is to find word representation that is useful for predicting the surrounding words in a corpus.
- Let us denote the sequence of training words - vocabulary, $W = \{w_1, w_2, \ldots, w_S\}$, where S is the size of vocabulary.
- Skip-gram model maximizes the average log probability

$$l(W) = \sum_{t=1}^{S} \sum_{c \in C_t} \log p(w_c | w_t),$$

where C_t is the context.

Skip-gram model



Skip-gram model

- The probability of observing a context word w_c given w_t is parametrized using the word vectors.
- Given a scoring function s, which maps pairs of (word, context) to value in $\mathbb{R}$, a possible choice to define the probability of a context word is the softmax.

$$p(Context|Word) = y_c = \frac{e^{w_c^\top w_t}}{\sum_{j=1}^{S} e^{w_j^\top w_t}},$$

  where w_c, w_t, w_j are vector representations of words and y_c is the output of the c-th neuron of the output layer.
- The parametrization for the scoring function is done by taking the scalar product between word and context embeddings: $s(Word, Context) = w_t^\top w_c$.

Subword model by Bojanowski et al.

- The Skip-gram model ignores the internal structure of words.
- They introduced a different scoring function s

$$s(w, c) = \sum_{g \in G_w} z_g^\top v_c,$$

where $G_w = \{1, \ldots, G\}$ is the set of letter n-grams which appear in w.

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  where $G_w = \{1, \ldots, G\}$ is the set of letter n-grams which appear in w.
- Limitations:
  - n-grams with a length greater or equal than 3 and smaller or equal than 6 were considered.
  - We claim it may be insufficient for short and rare words.

Fragmentation model

- Let us denote by $G_w = \{1, \ldots, G\}$ the set of letter n-grams which appear in w and $H_w = \{1, \ldots, H\}$ to be the set of syllable n-grams which appear in w.

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$$z_{new} = [z_g, z_h].$$

- The scoring function is

$$s(w, c) = \sum_{new \in G_w \cup H_w} z_{new}^{\top} v_c.$$

- The upgraded model makes use of n-grams of varied length n.

Conclusions

- Invariance based methods are being tested in order to be applied to objects described by many features.
- The Skip-Gram based method outperforms state-of-the-art approaches on dense languages when tasks such as word similarity ranking or syntactic and semantic analogies are taken into consideration.

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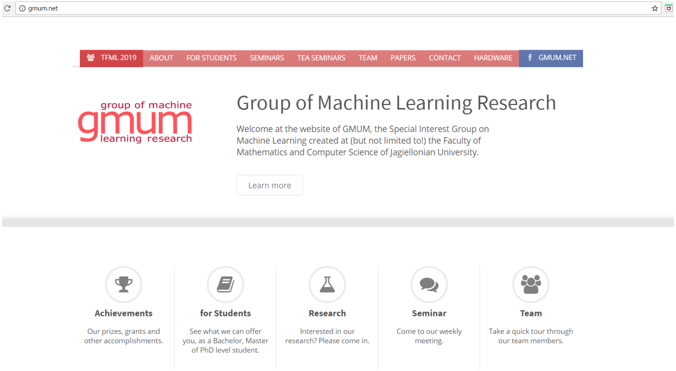
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Seminar
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Team
Take a quick tour through our team members.

Thank you.