Towards Understanding the Geometry of Knowledge Graph Embeddings

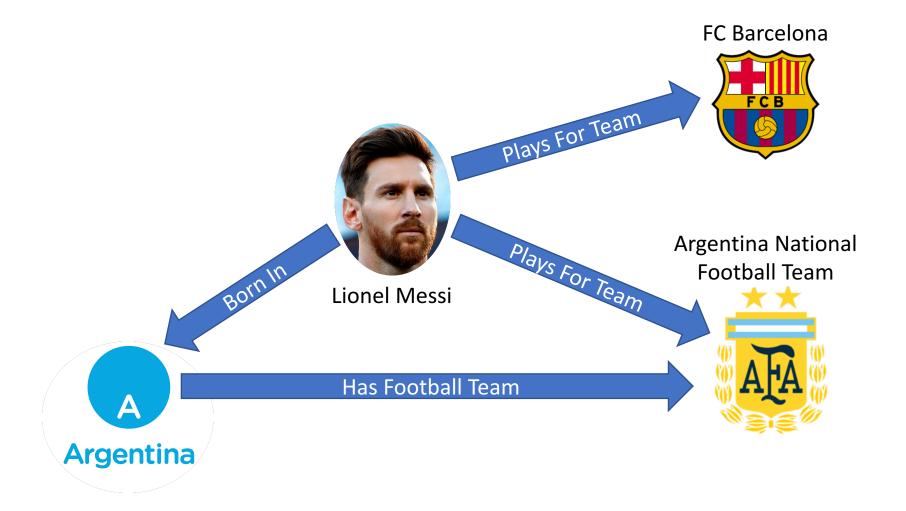
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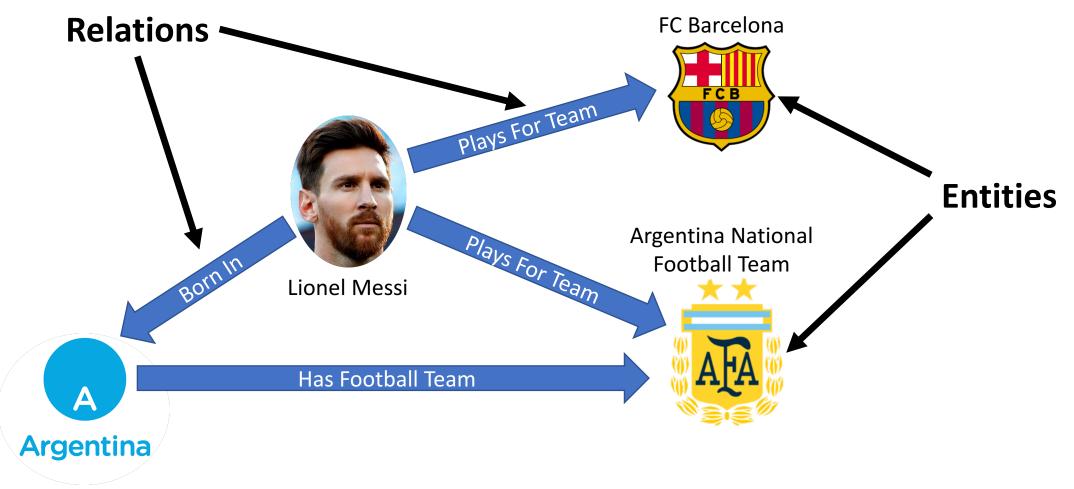












• Example KGs







• Example KGs





• Applications



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Barack Hussein Obama II is an American politician currently serving as the 44th and current President of the United States. He is the first African American to hold the office and the first president born outside the continental United States. Weignedia

k And Michele Obama Born: August 4, 1961 (age 55), Kapiolani M Children, Honolulu, Hawaii, United States Spouse: Michelle Obama (m. 1992)

Party: Democratic Party Children: Malia Ann Obama, <u>Natissha Obama</u> Parents: Ann Dunham, Barack Obama Sr. Siblings: Maya Seekoro-Ng, Auma Obama, David Ndesan

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• Example KGs







• Applications





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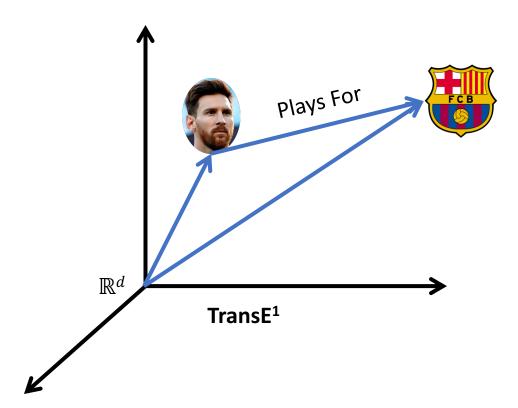


 Question Answering



KG Embeddings

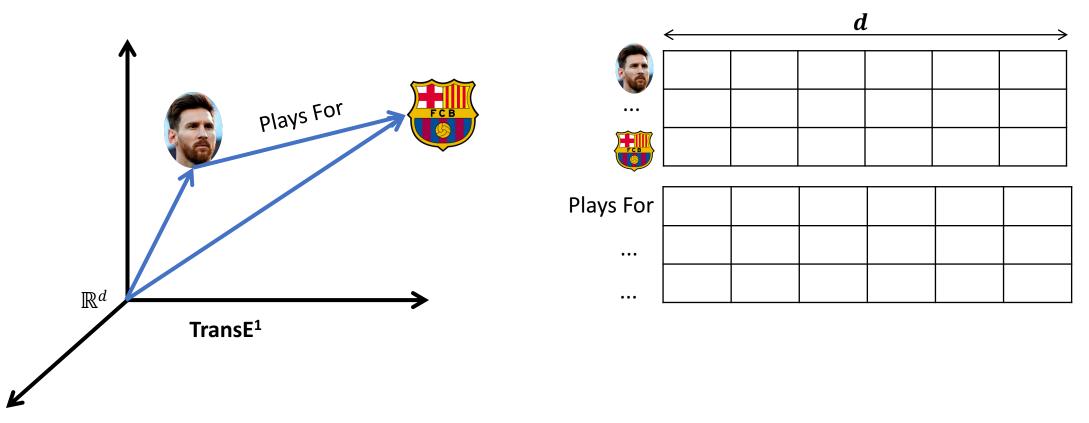
• Represents entities and relations as vectors in a vector space



1. Translating Embeddings for Modeling Multi-relational Data, Bordes et al.

KG Embeddings

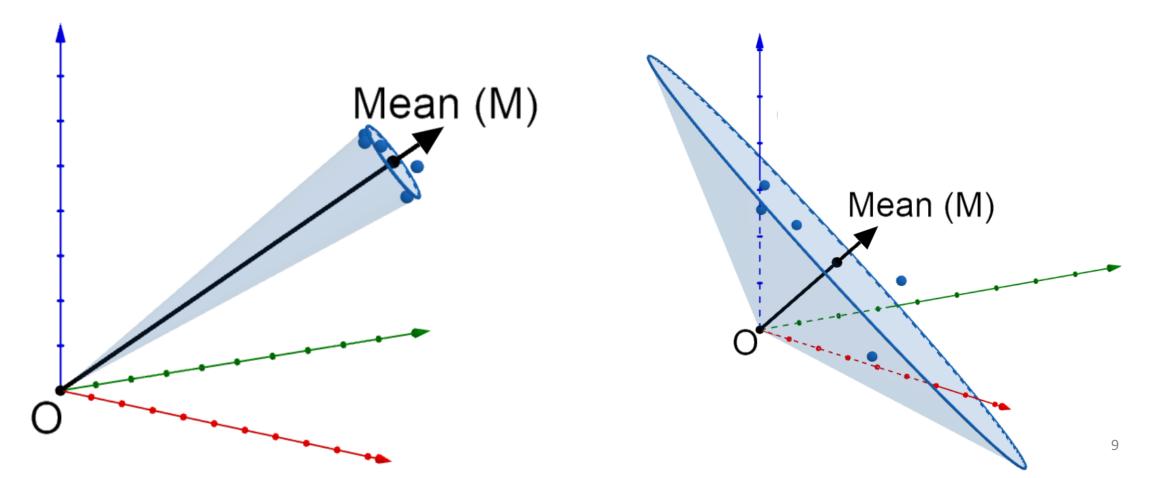
• Represents entities and relations as vectors in a vector space



1. Translating Embeddings for Modeling Multi-relational Data, Bordes et al. NIPS 2013.

Geometry of Embeddings

• Arrangement of vectors in the vector space.



Geometry of Embeddings

- A recent work by (Mimno and Thompson, 2017)¹ presented an analysis of the geometry of word embeddings and revealed interesting results.
- However, geometrical understanding of KG embeddings is very limited, despite their popularity.

Problem

- Study the geometrical behavior of KG embeddings learnt by different methods.
- Study the effect of various hyper-parameters used during training on the geometry of KG embeddings.
- Study the correlation between the geometry and performance of KG embeddings.

• Learns d-dimensional vectors for entities ${m {\cal E}}$ and relations ${m {\cal R}}$ in a KG.

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- A score function $\sigma : \mathcal{E} \times \mathcal{R} \times \mathcal{E} \rightarrow \mathbb{R}$ distinguishes correct triples T^+ from incorrect triples T^- . For example, σ (Messi, plays-for-team, Barcelona) > σ (Messi, plays-for-team, Liverpool)

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- A loss function $L(T^+, T^-)$ is used for training the embeddings (usually logistic loss or margin-based ranking loss).



• Additive Methods

$$\sigma(h, r, t) = - \left\| M_r^1 \mathbf{h} + \mathbf{r} - M_r^2 \mathbf{t} \right\|_1$$

• Multiplicative Methods

$$\sigma(h, r, t) = \mathbf{r}^{\top} f(\mathbf{h}, \mathbf{t})$$

• Neural Methods

Туре	Model	Score Function $\sigma(h, r, t)$
Additive	TransE (Bordes et al., 2013)	$\ - \ \mathbf{h} + \mathbf{r} - \mathbf{t} \ _1$
	TransR (Lin et al., 2015)	$\ - \ M_r \mathbf{h} + \mathbf{r} - M_r \mathbf{t} \ _1$
	STransE (Nguyen et al., 2016)	$- \left\ M_r^1 \mathbf{h} + \mathbf{r} - M_r^2 \mathbf{t} \right\ _1$
Multiplicative	DistMult (Yang et al., 2014)	$\mathbf{r}^{ op}(\mathbf{h}\odot\mathbf{t})$
	HolE (Nickel et al., 2016)	$\mathbf{r}^{ op}(\mathbf{h} \star \mathbf{t})$
	ComplEx (Trouillon et al., 2016)	$\mathbf{Re}(\mathbf{r}^{ op}(\mathbf{h}\odotar{\mathbf{t}}))$

 \star Circular correlation

• Average Vector Length

$$AVL(\mathbf{V}) = \frac{1}{|\mathbf{V}|} \sum_{\mathbf{v} \in \mathbf{V}} \|\mathbf{v}\|_2$$

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• Alignment to Mean

$$ATM(\mathbf{v}, \mathbf{V}) = cosine\left(\mathbf{v}, \frac{1}{|\mathbf{V}|} \sum_{\mathbf{x} \in \mathbf{V}} \mathbf{x}\right)$$

• Conicity

$$Conicity(\mathbf{V}) = \frac{1}{|\mathbf{V}|} \sum_{\mathbf{v} \in \mathbf{V}} ATM(\mathbf{v}, \mathbf{V})$$

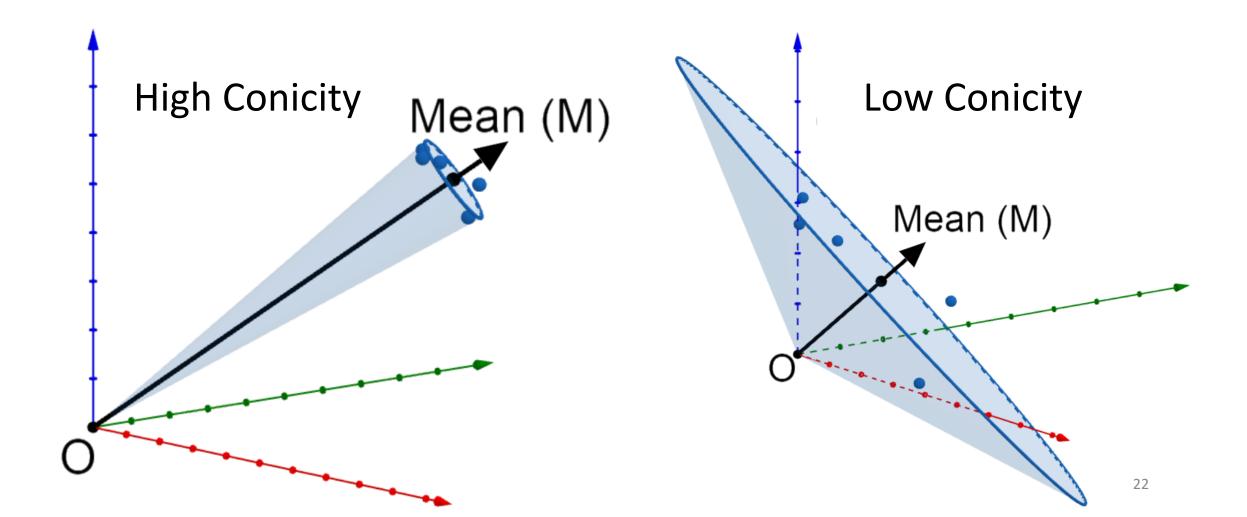
• Conicity

$$\operatorname{Conicity}(\mathbf{V}) = \frac{1}{|\mathbf{V}|} \sum_{\mathbf{v} \in \mathbf{V}} \operatorname{ATM}(\mathbf{v}, \mathbf{V})$$

• Vector Spread

$$VS(\mathbf{V}) = \frac{1}{|\mathbf{V}|} \sum_{\mathbf{v} \in \mathbf{V}} \left(ATM(\mathbf{v}, \mathbf{V}) - Conicity(\mathbf{V}) \right)^2$$

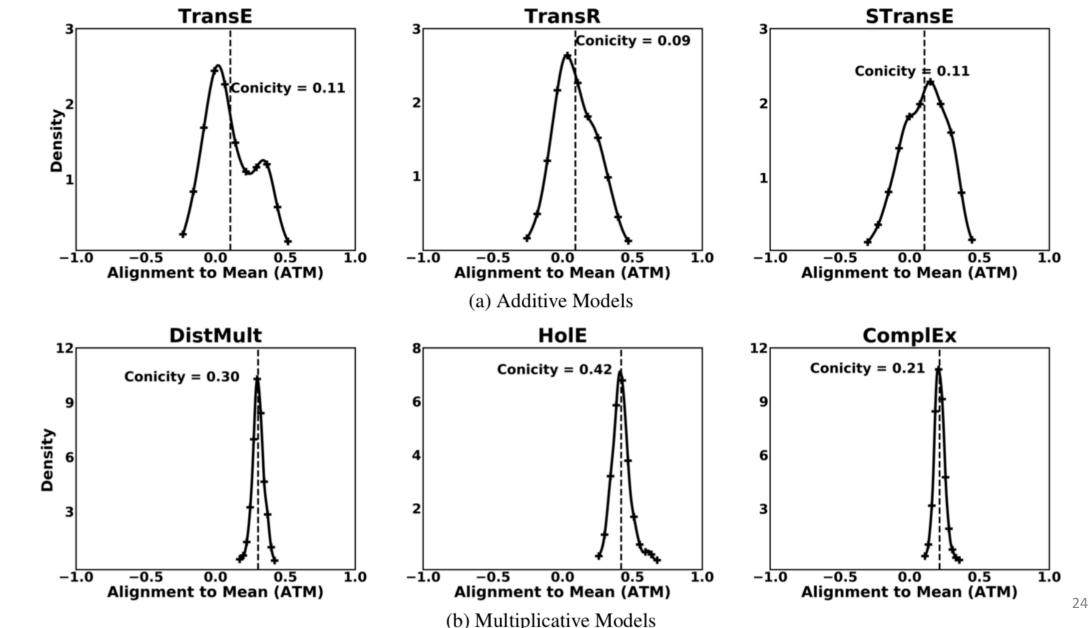
Geometry of Embeddings



Experiments

- We study the effect of following factors on the geometry of KG Embeddings
 - Type of method (Additive or Multiplicative)
 - Number of Negative Samples
 - Dimension of Vector Space
- We also study the correlation of performance and geometry.
- For experiments, we used FB15k dataset.

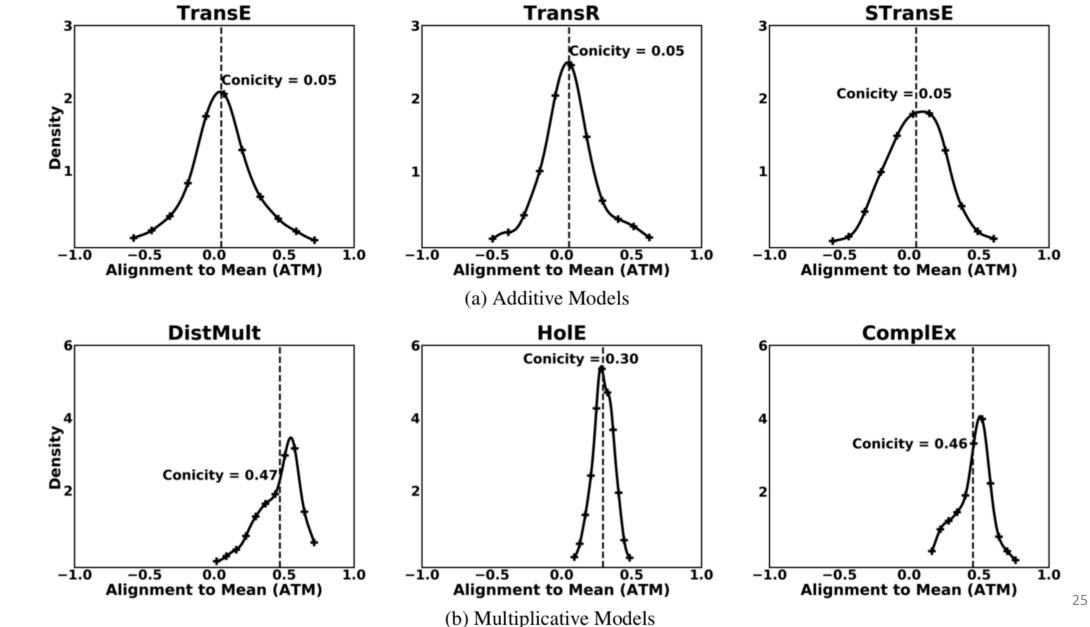
Additive vs Multiplicative (Entity Vectors)



Additive

Multiplicative

Additive vs Multiplicative (Relation Vectors)

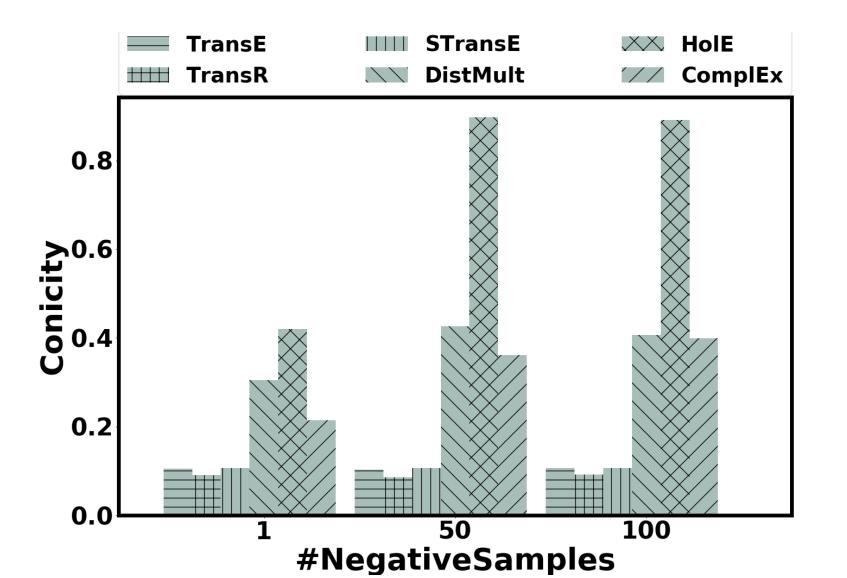


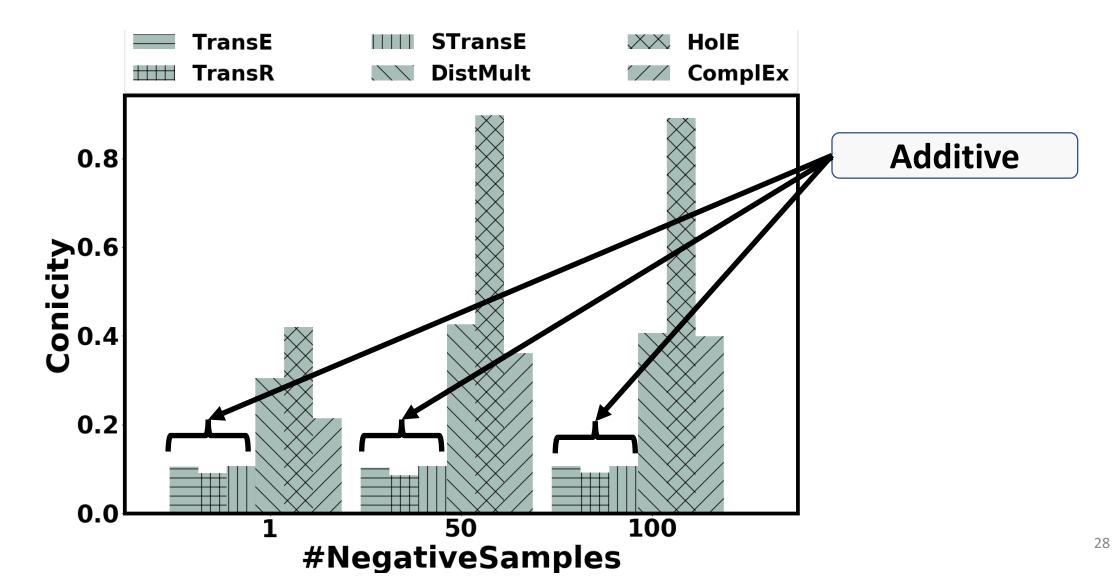
Additive

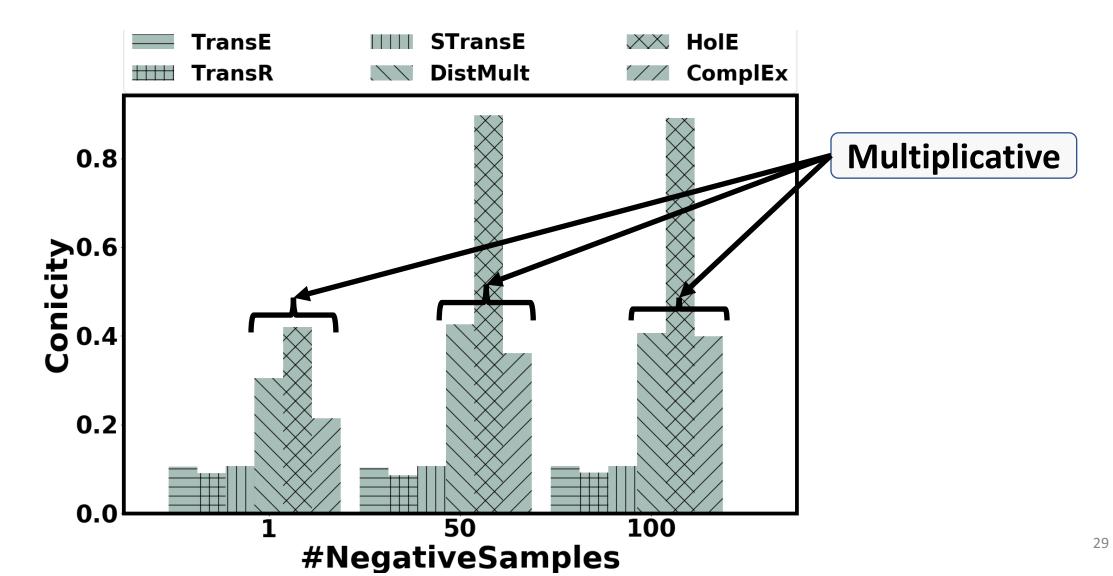
Multiplicative

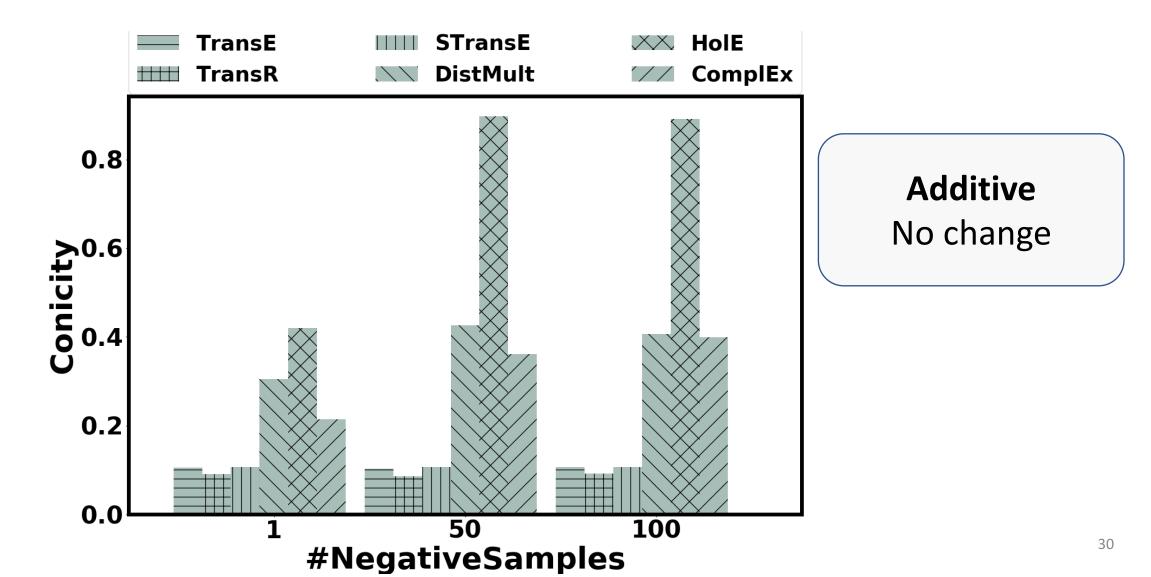
Additive vs Multiplicative

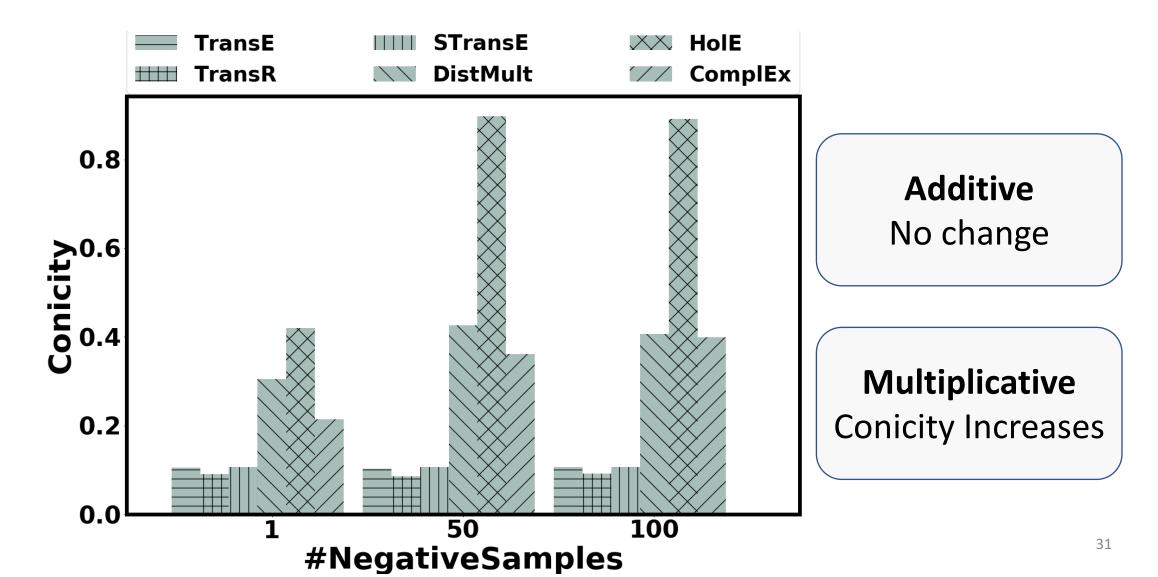
Model Type	Conicity	Vector Spread
Additive	Low	High
Multiplicative	High	Low

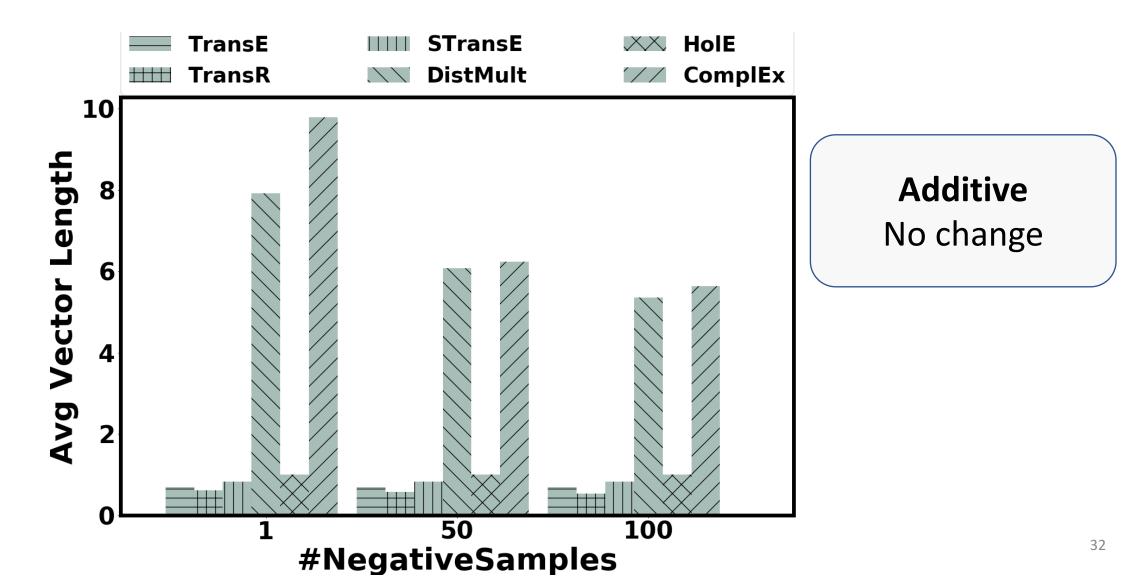


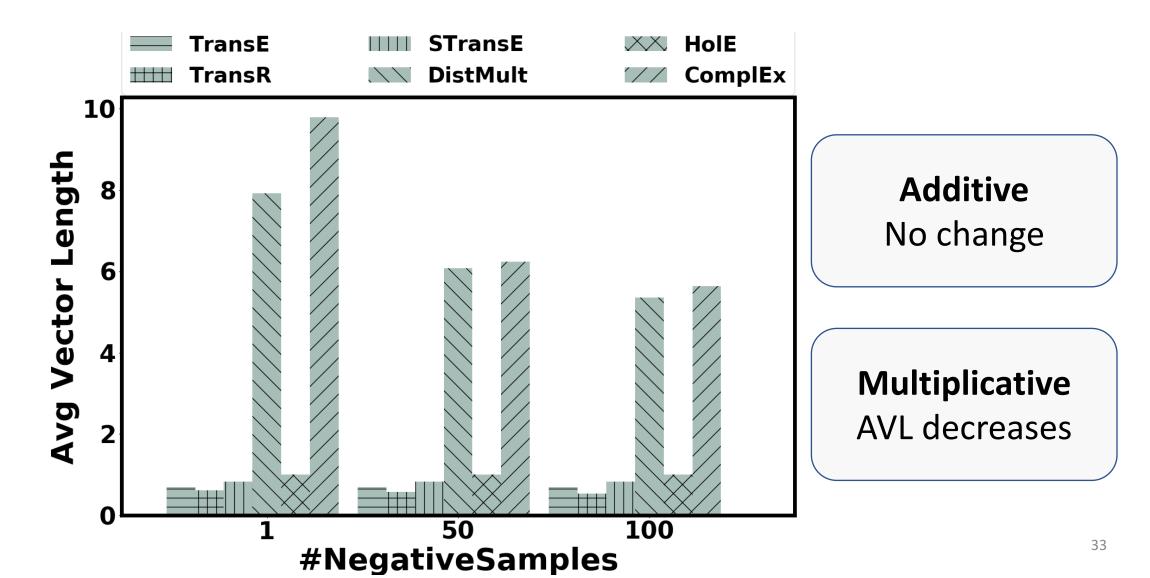












Effect of #Negative Samples

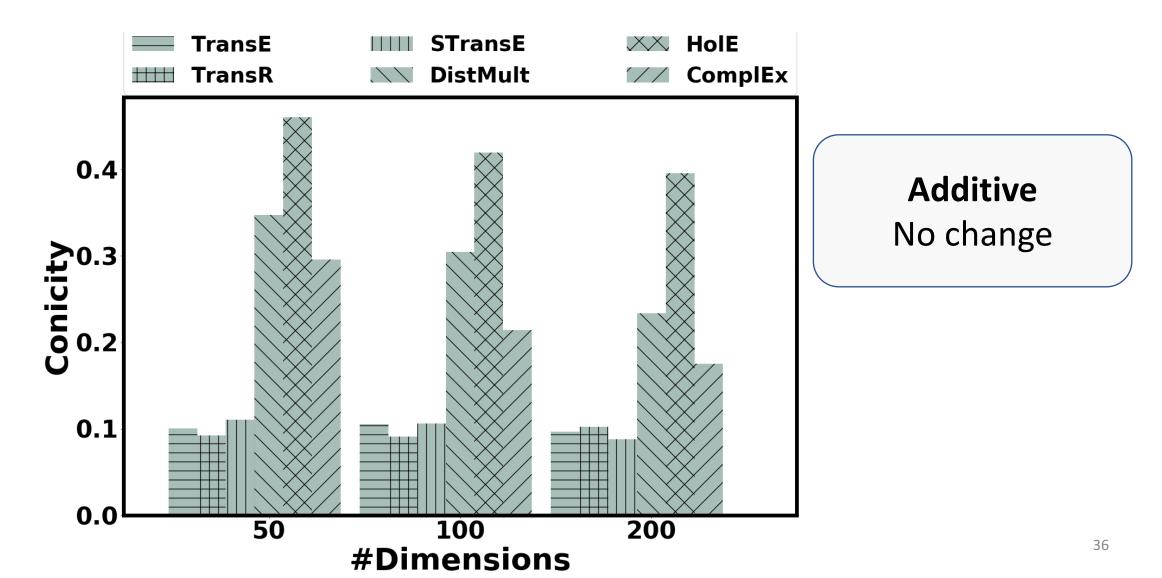
Model Type	Vector Type	Conicity	AVL
A dditiyo	Entity	No Change	No Change
Additive	Relation	No Change	No Change
	Entity	Increases	Decreases
Multiplicative	Relation	Decreases	No Change except HolE

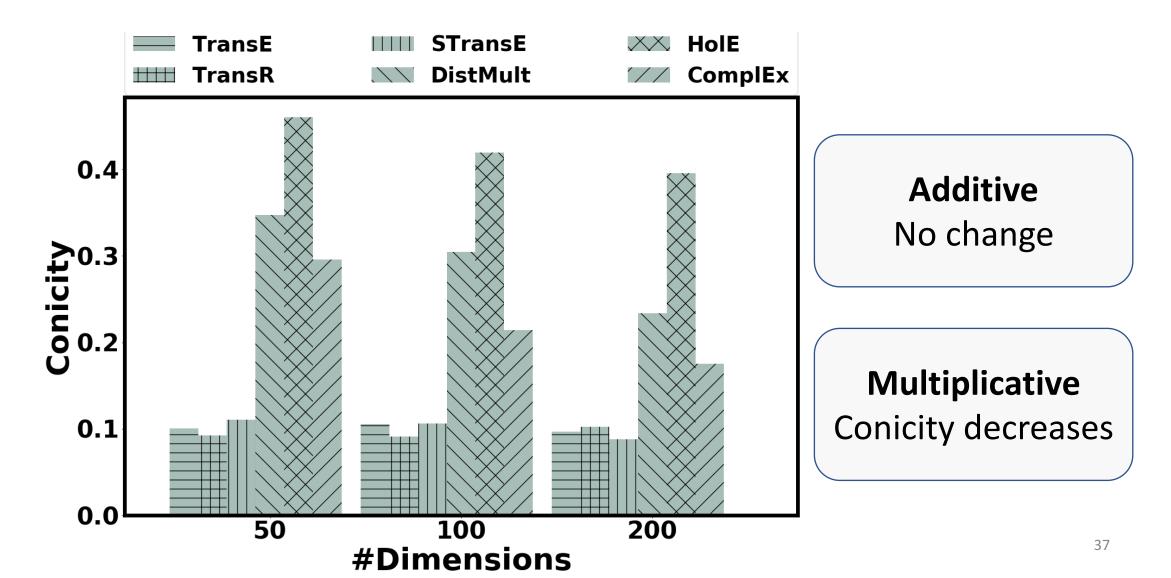
SGNS (Word2Vec¹) as Multiplicative Model

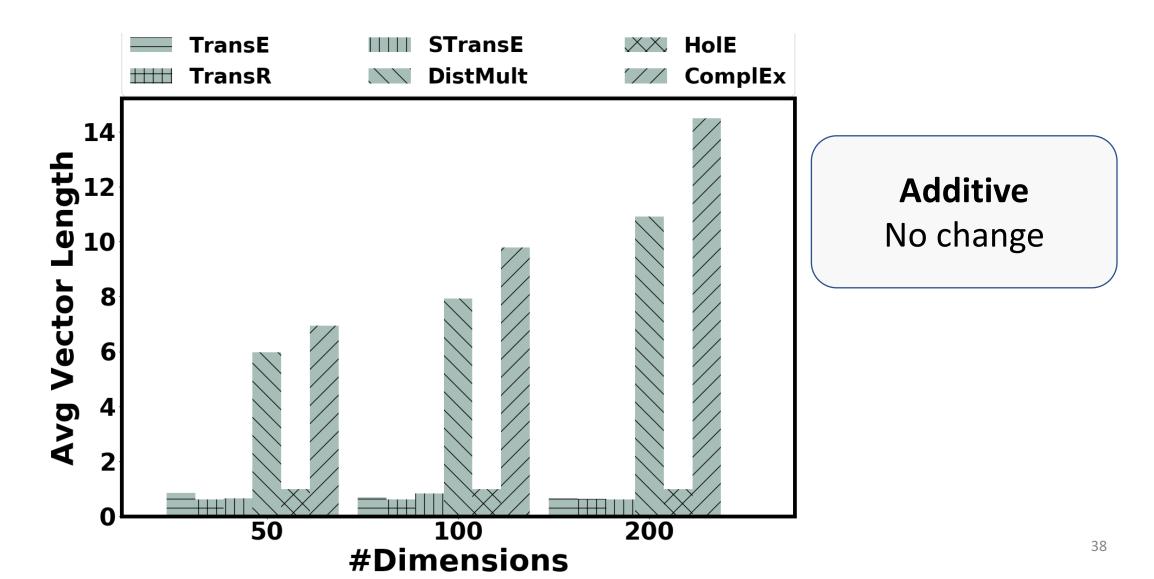
- Similar observation was made by (Mimno and Thompson, 2017)² for SGNS based word embeddings where higher #negatives resulted in higher conicity.
- Word2Vec¹ maximizes word and context vector dot product for positive word-context pairs.
- This behavior is consistent with that of multiplicative models.

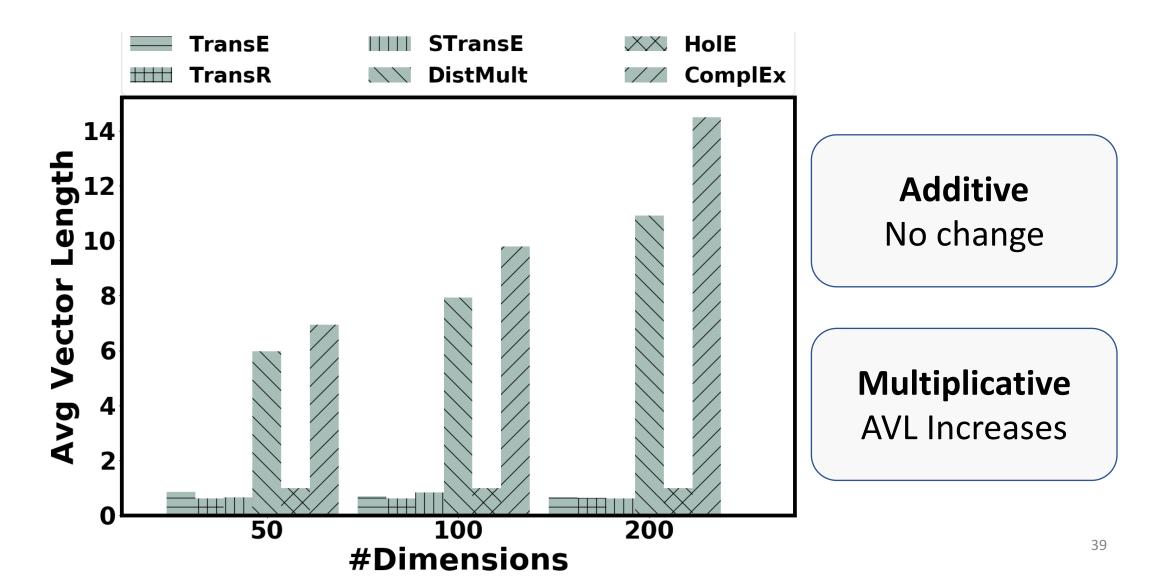
Distributed representations of words and phrases and their compositionality, Mikolov et al. NIPS 2013
 The strange geometry of skip-gram with negative sampling, Mimno and Thompson, EMNLP 2017

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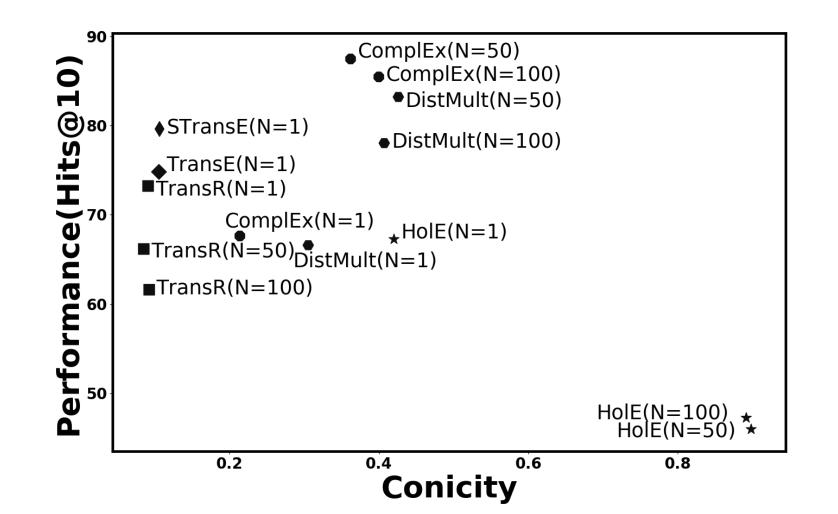


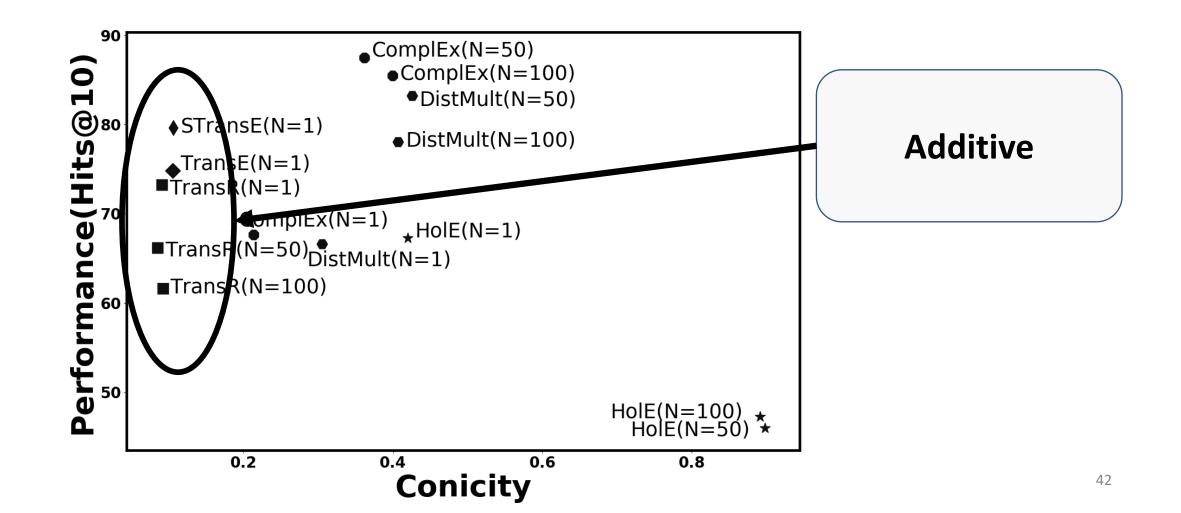


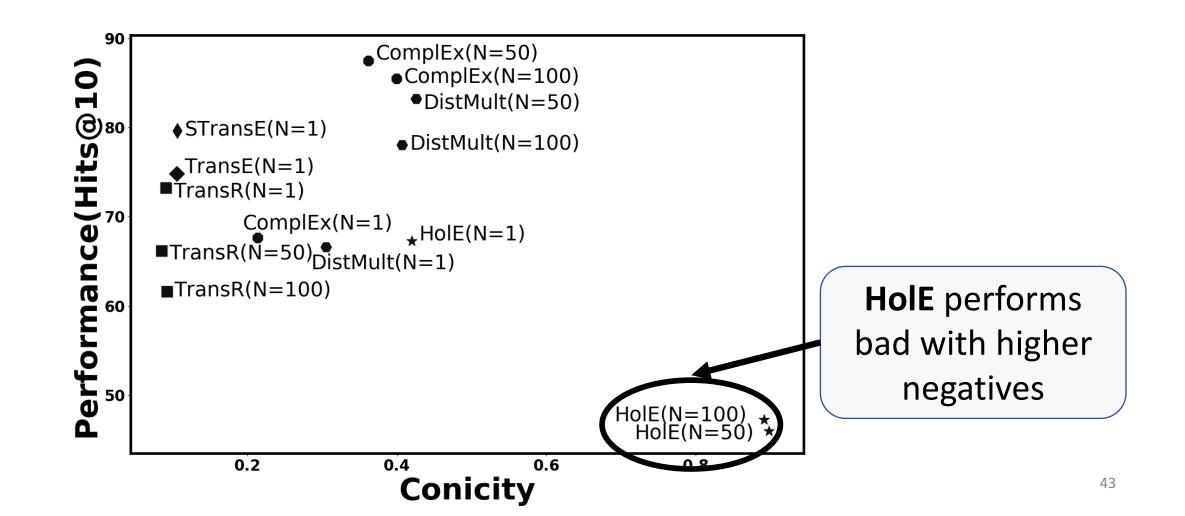


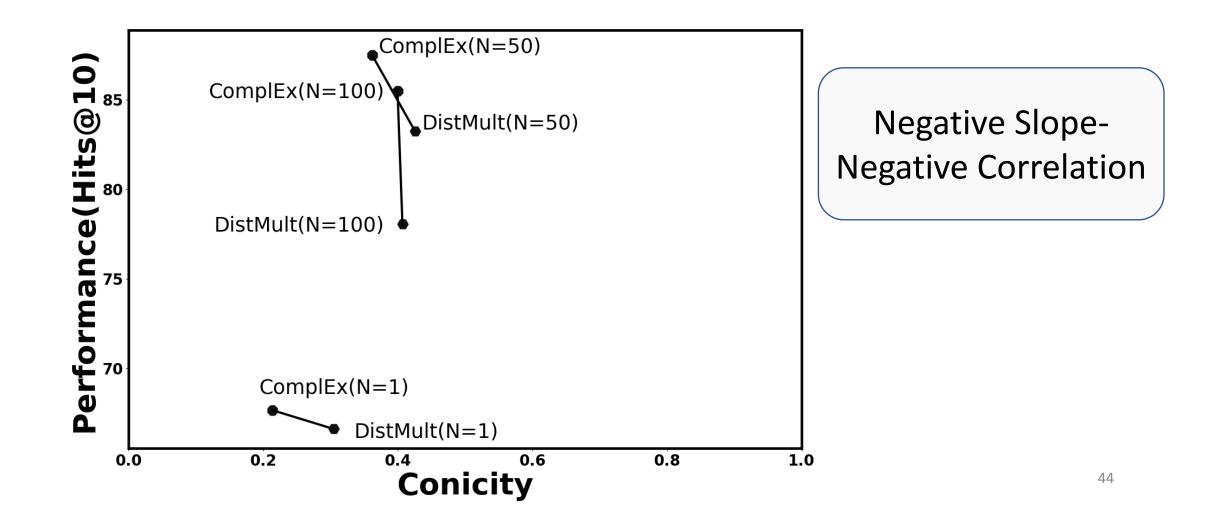
Effect of #Dimensions

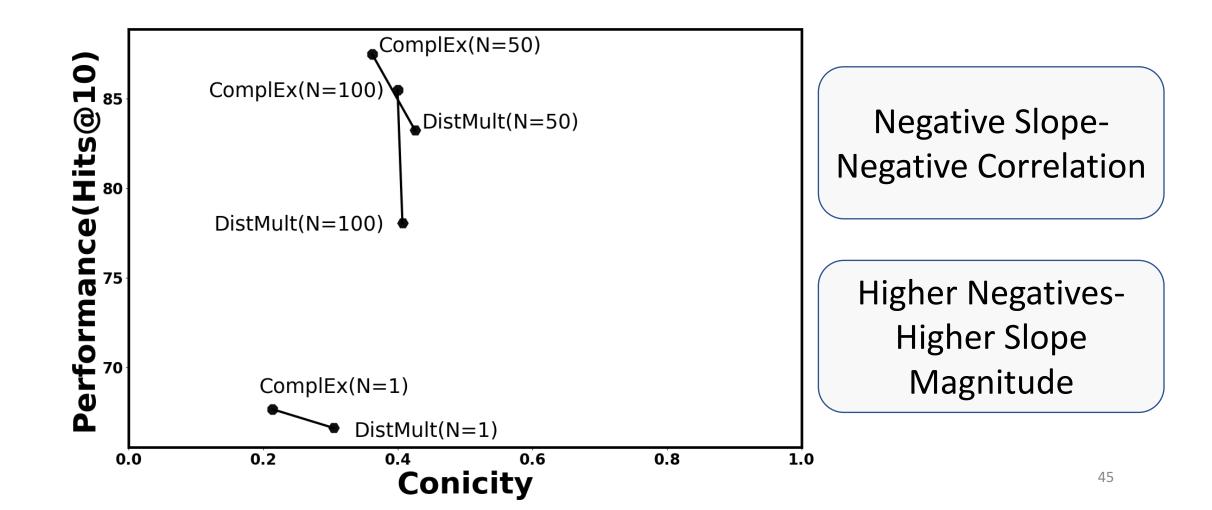
Model Type	Vector Type	Conicity	AVL
Additive	Entity	No Change	No Change
	Relation	No Change	No Change
Multiplicative	Entity	Decreases	Increases
	Relation	Decreases	Increases

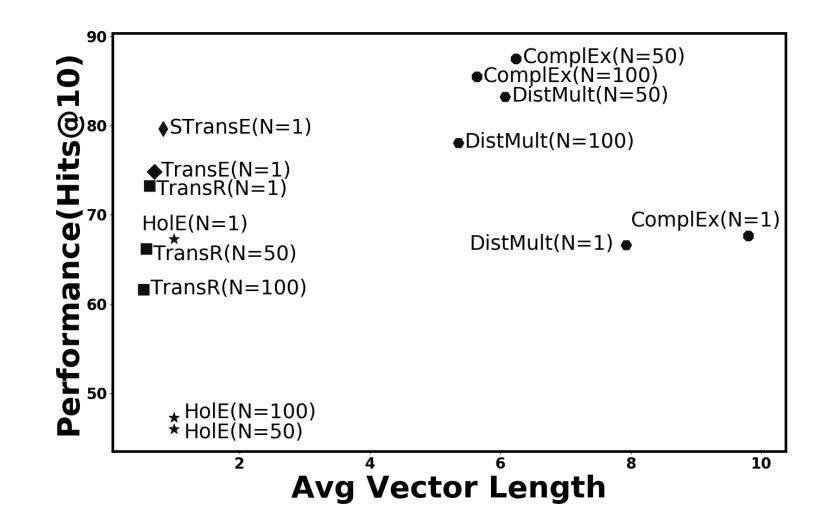


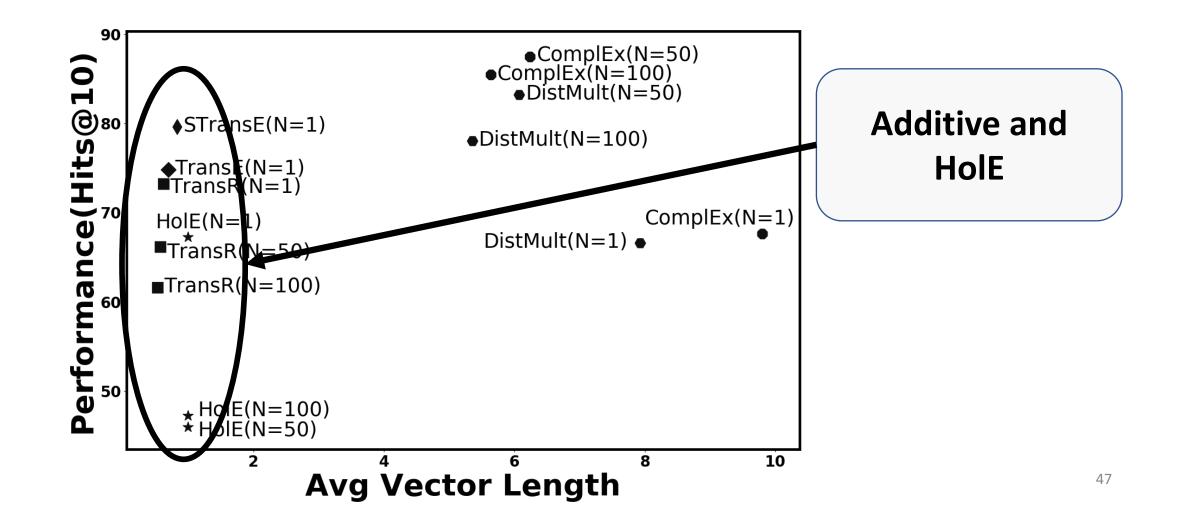


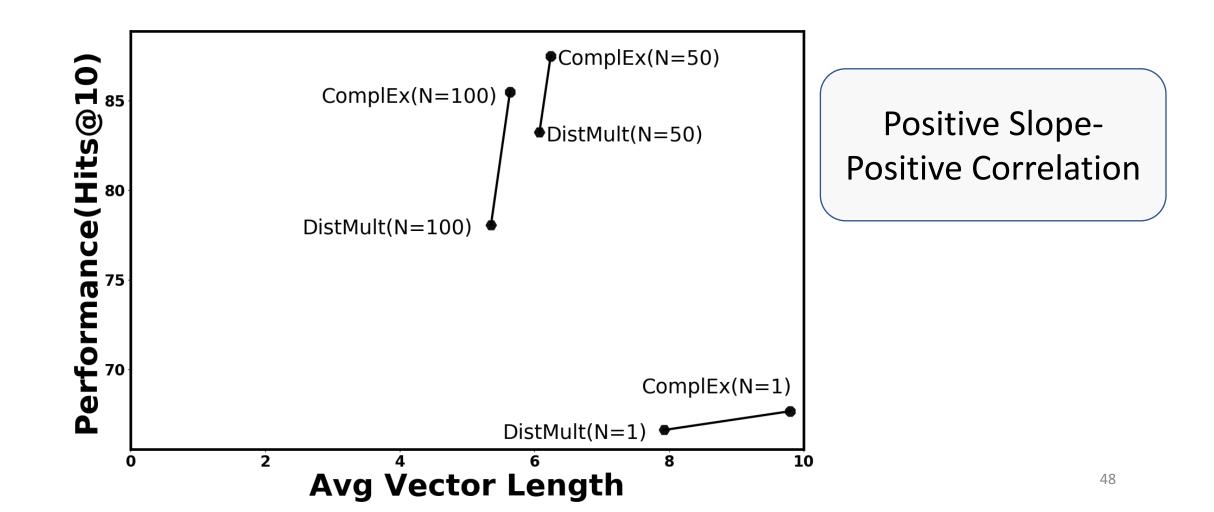


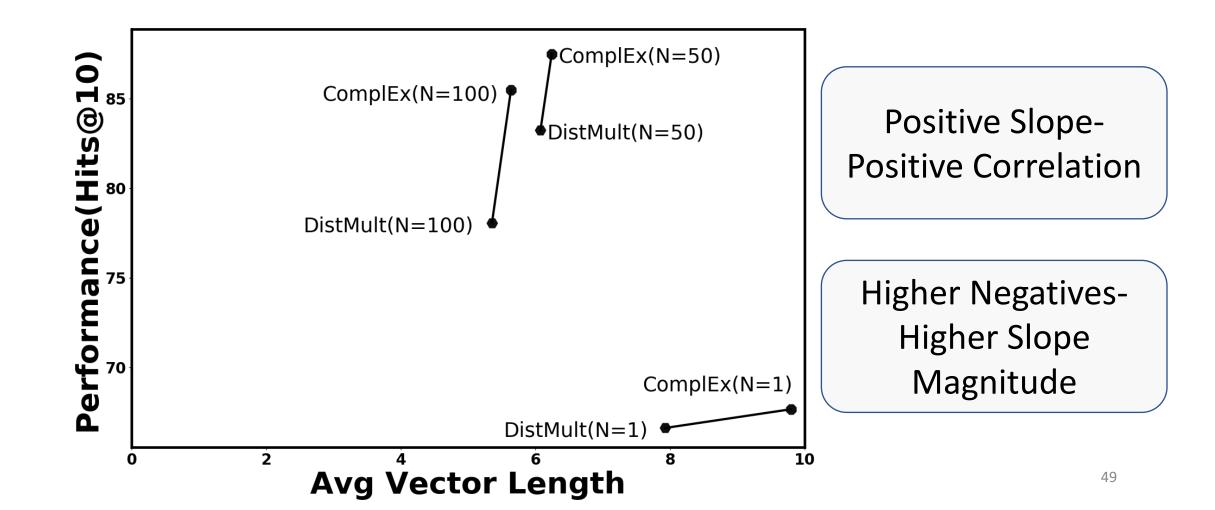












• Additive:

No correlation between geometry and performance.

• Multiplicative:

For fixed number of negative samples,

- Conicity has negative correlation with performance
- AVL has positive correlation with performance

Conclusion and Future Works

- We initiated the study of geometrical behavior of KG embeddings and presented various insights.
- Explore whether other entity/relation features (eg entity category) have any correlation with geometry.
- Explore other geometrical metrics which have better correlation with performance and use it for learning better KG embeddings.

Acknowledgements

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Thank you

