

KONG: Kernels for ordered-neighborhood graphs

NeurIPS conference (poster #122)

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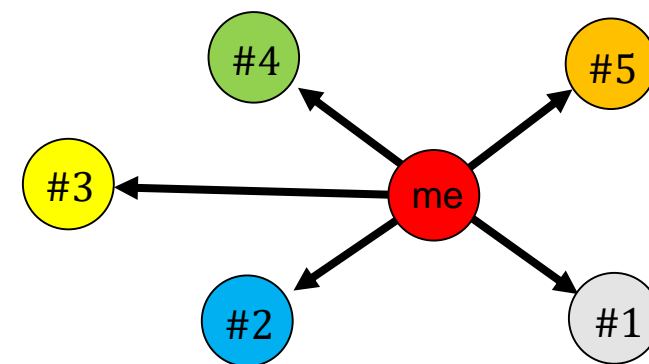


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Background

- Graphs are **highly complex objects**
 - Combinatorial nature of the object
 - Many relevant features
 - size, connectivity, density, hubs, periphery, short range patterns, large-scale structure, cliques, connected components, spectral characteristics...
 - **How to make it usable for ML problems?**
- Additional information: **ordered neighborhoods**
 - All edges may not be as important (e.g. friends on a social network)
 - Networks are often dynamic objects, changing through time
 - We may have a **ranking among neighbors**
 - Time of creation, importance, objective value, distance,...
 - **How to account for this information?**



The KONG algorithmic framework

- **A scalable kernel representation for graphs**

- 1) **Iterative** algorithm for node representation

- Weisfeiler-Lehman, breadth-first search...

- 2) Ordered neighborhood representation using **string kernels**

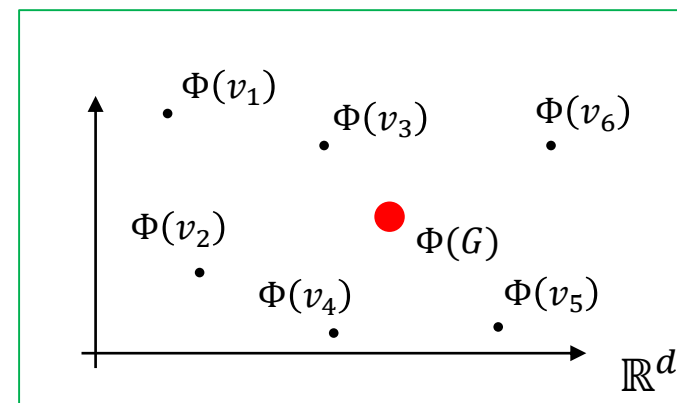
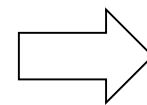
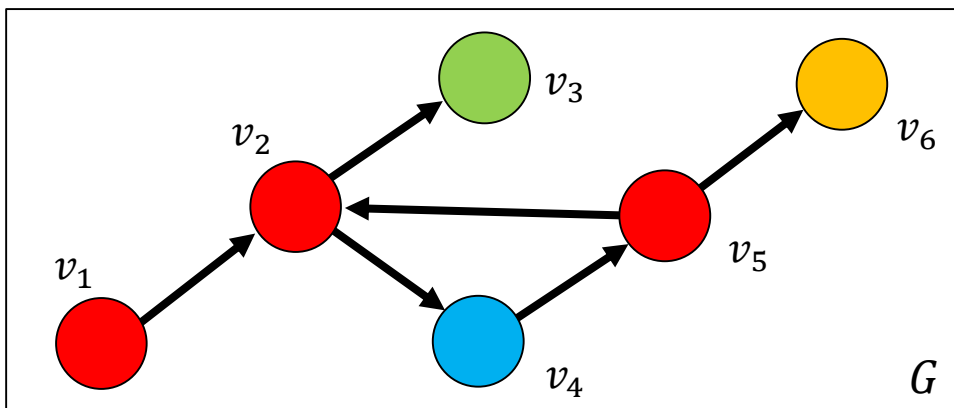
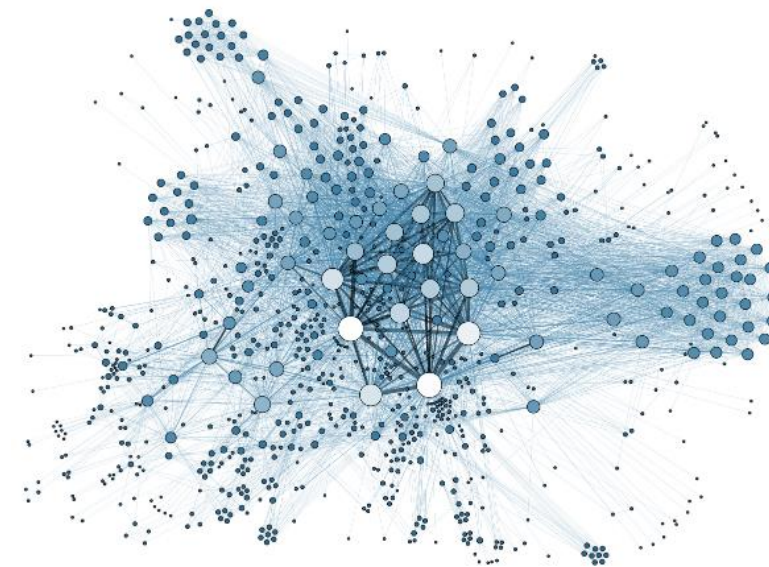
- K-gram counting approach, order captured by selection process

- 3) Refined k-gram counting using **polynomial** or **cosine** kernels

- More powerful representation

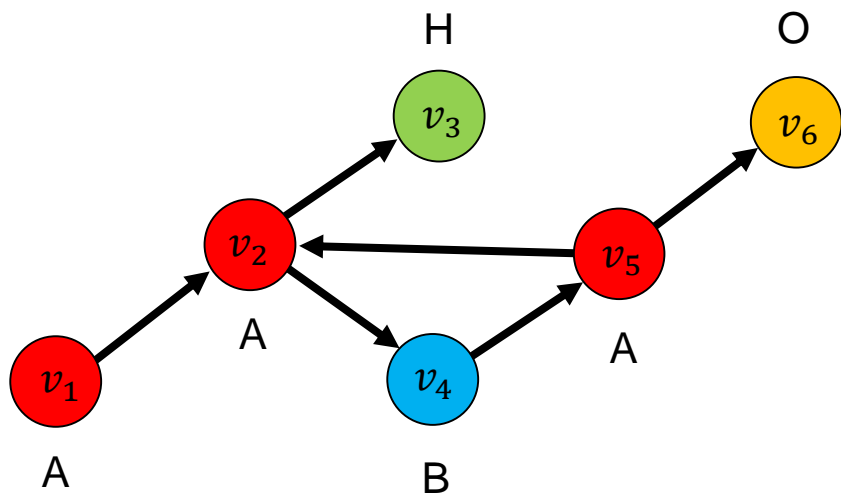
- 4) **Sketching** method for kernel approximation

- Approximate embedding of counting vectors preserving scalar products

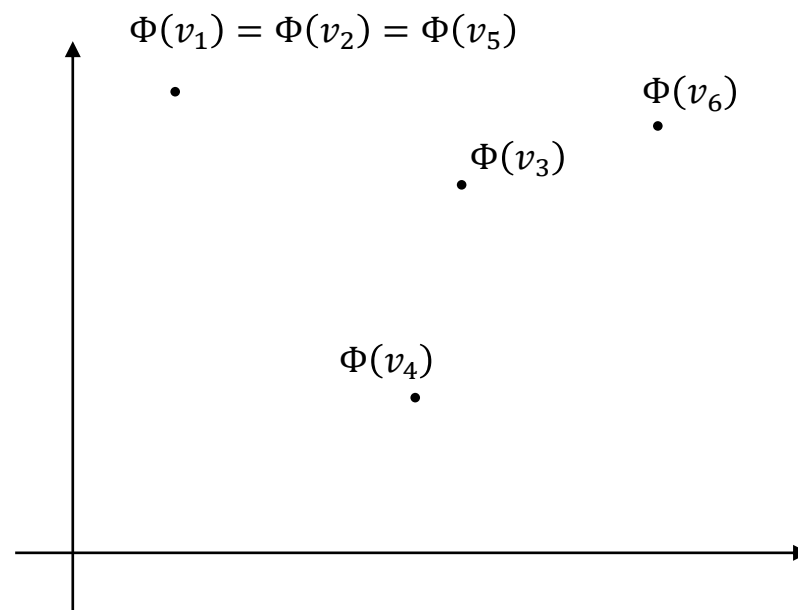


Simple example

Graph with string representations

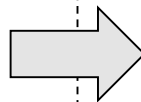
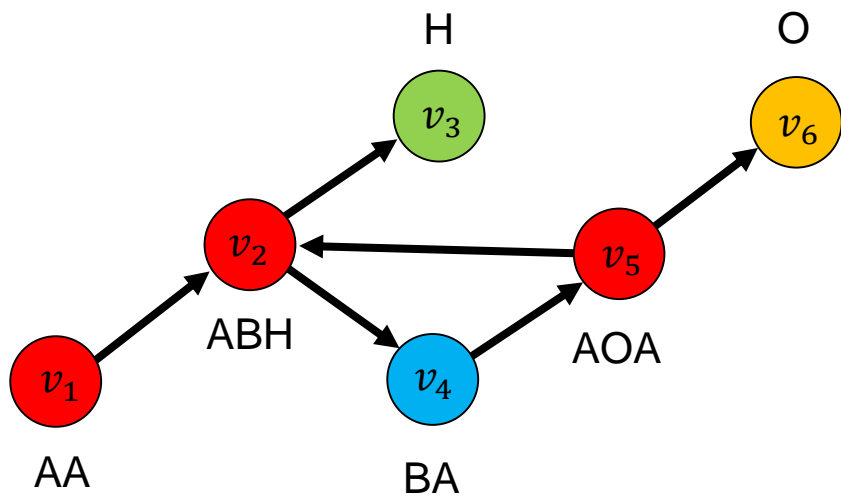


Sketching representation in \mathbb{R}^d

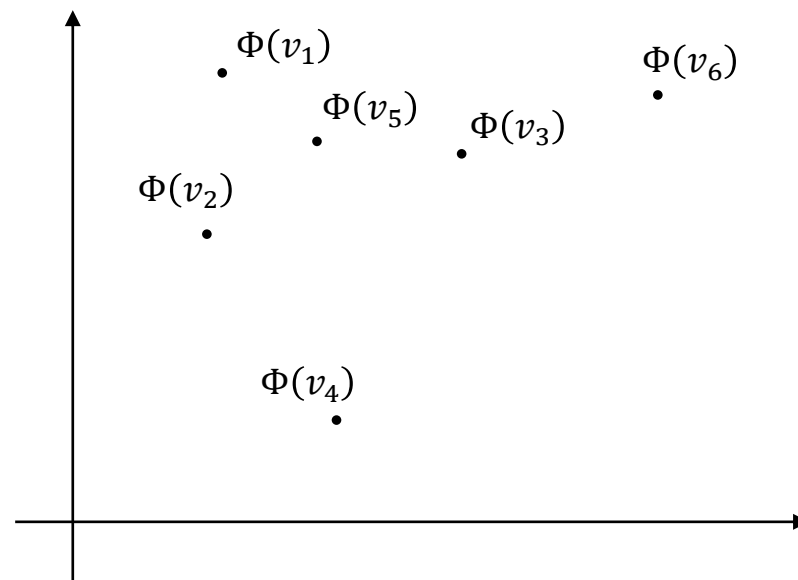


Simple example

Graph with string representations

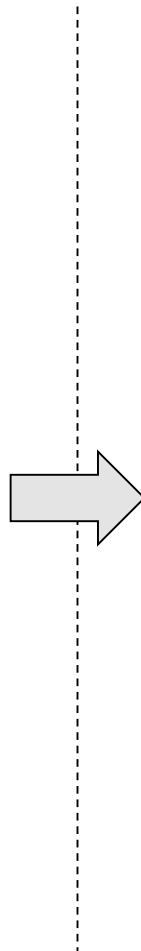
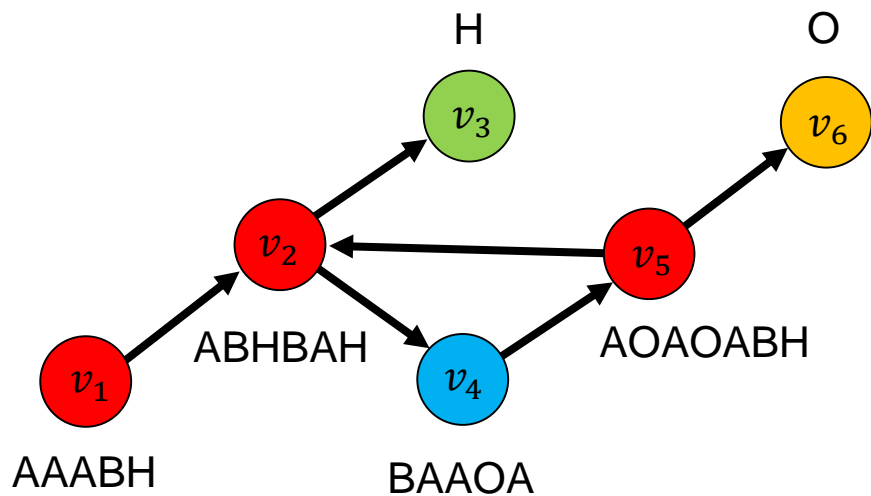


Sketching representation in \mathbb{R}^d

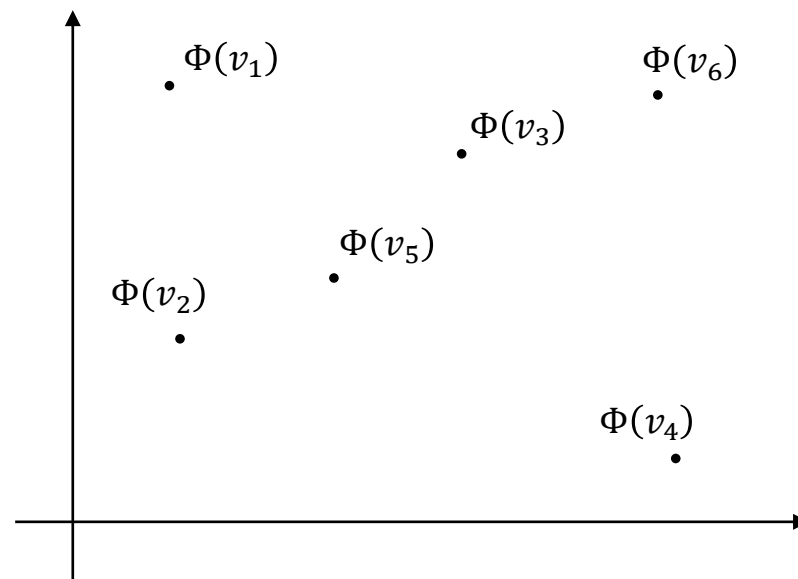


Simple example

Graph with string representations

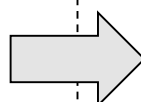
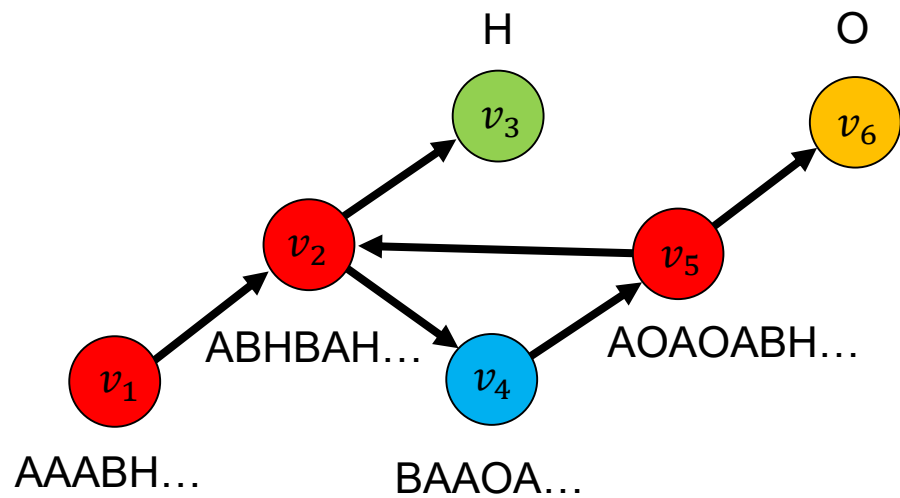


Sketching representation in \mathbb{R}^d

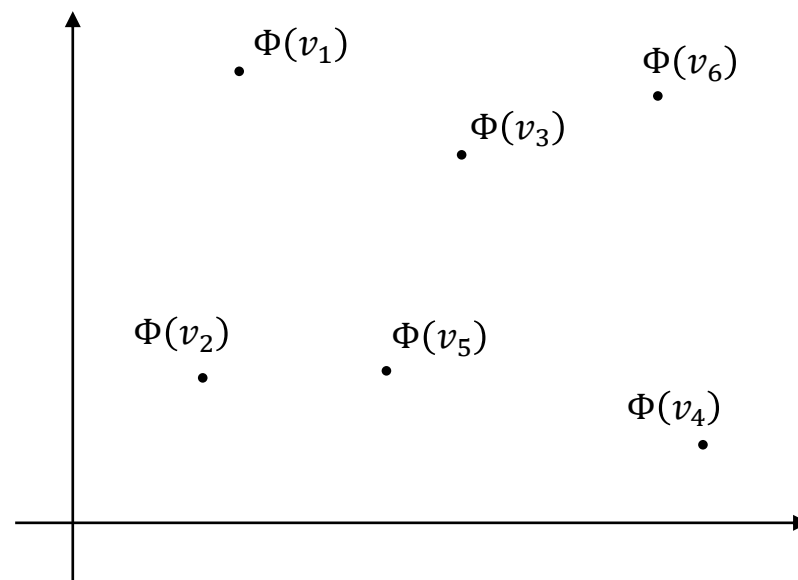


Simple example

Graph with string representations

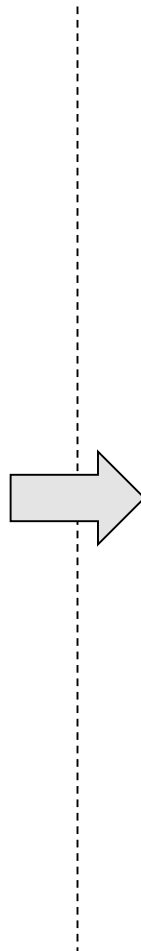
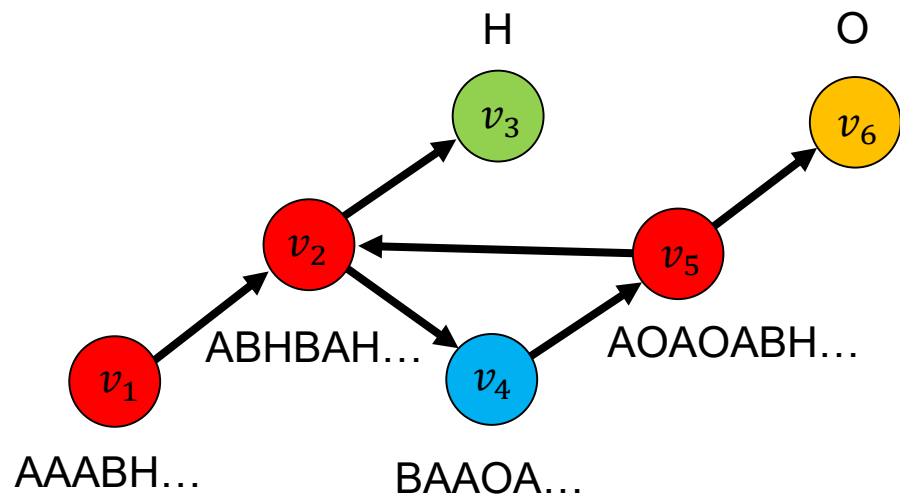


Sketching representation in \mathbb{R}^d

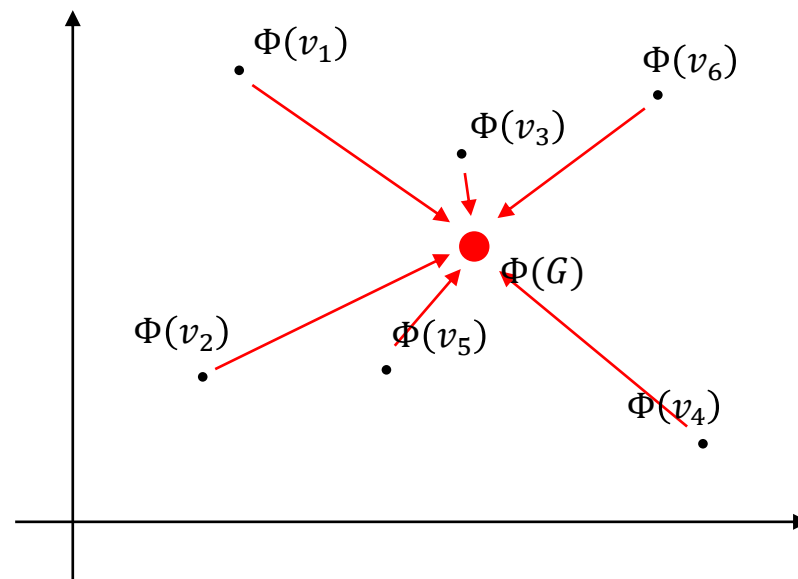


Simple example

Graph with string representations



Sketching representation in \mathbb{R}^d



Conclusion

- **The KONG framework: a new scalable algorithm for graphs kernels**
 - First method using **ordered neighborhoods**,
 - **Highly scalable** approach that can handle graphs with millions of nodes in seconds on a laptop in a single-threaded implementation,
 - **Flexibility** in the choice of the kernel function,
 - Outputs **vector representations**
 - Can be used by any ML algorithm for regression, classification, clustering, etc...
 - Excellent results on datasets from various domains, including
 - Anomaly detection in network flow graphs,
 - Gender prediction in recommender systems,
 - Affluence prediction in customer purchase graphs.



Poster #122