role2vec: Role-based Network Embeddings

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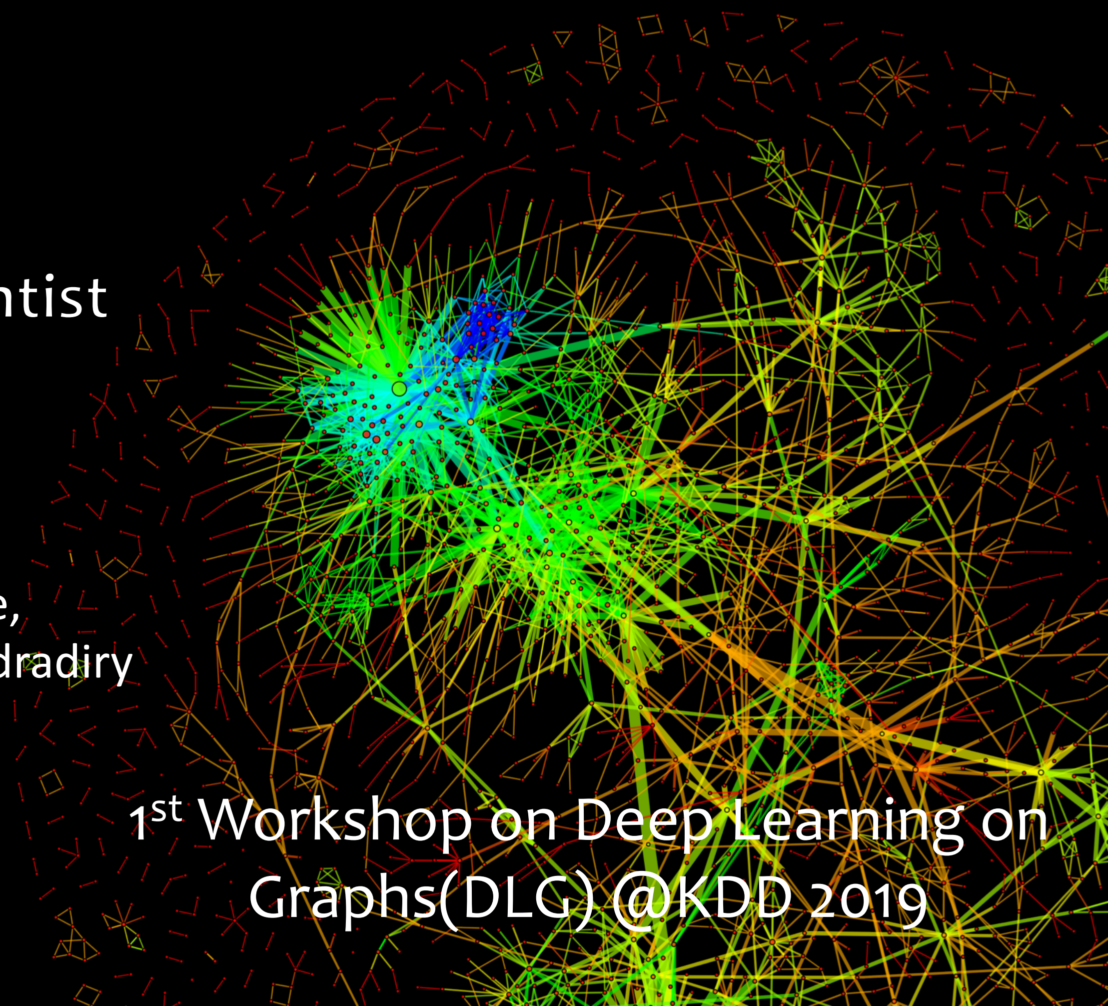

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Representation Learning in Graphs

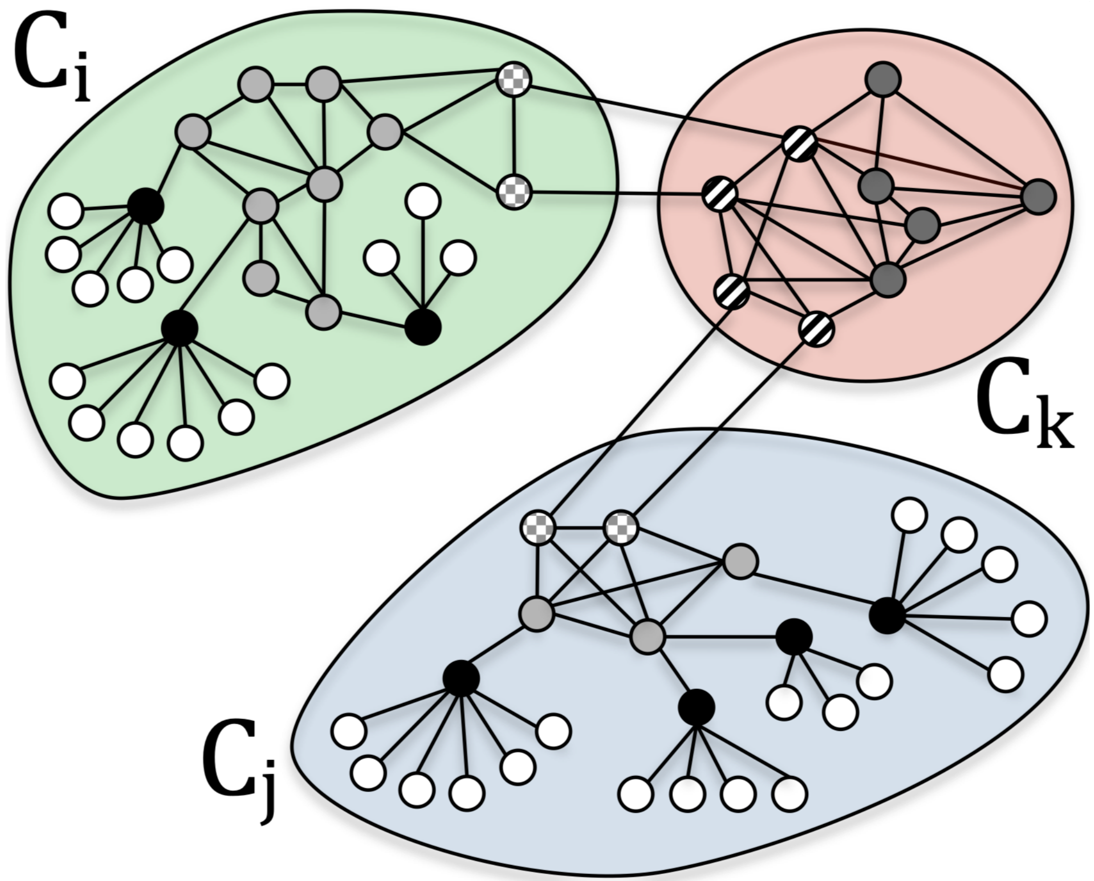
- **Goal:** Learn representation (features) for a set of graph elements (nodes, edges, etc.)

$$\text{Given } G = (V, E)$$
$$\text{Learn a function } f : V \rightarrow \mathbb{R}^d$$

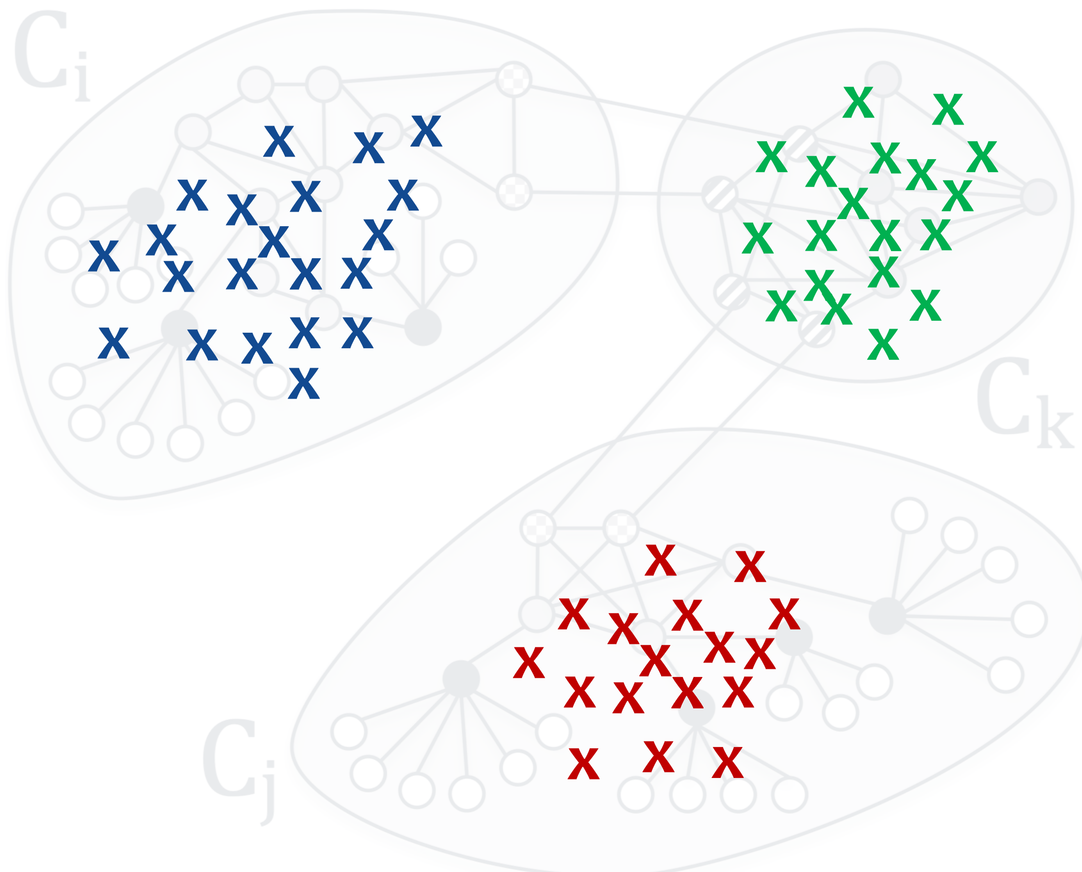
- **Key intuition**: Map the graph elements (e.g., nodes) to the d-dimension space
- Use the features for any downstream prediction task

Many examples: deepWalk, node2vec, GCN … etc

Two Complimentary Notions in Graphs: Proximity vs. Structural Similarity



Most Existing Work Focus on Modeling Graph Proximity



No guarantee that nearby vertices are ***structurally similar***

e.g., Deepwalk, GraRep, node2vec, Line, etc.

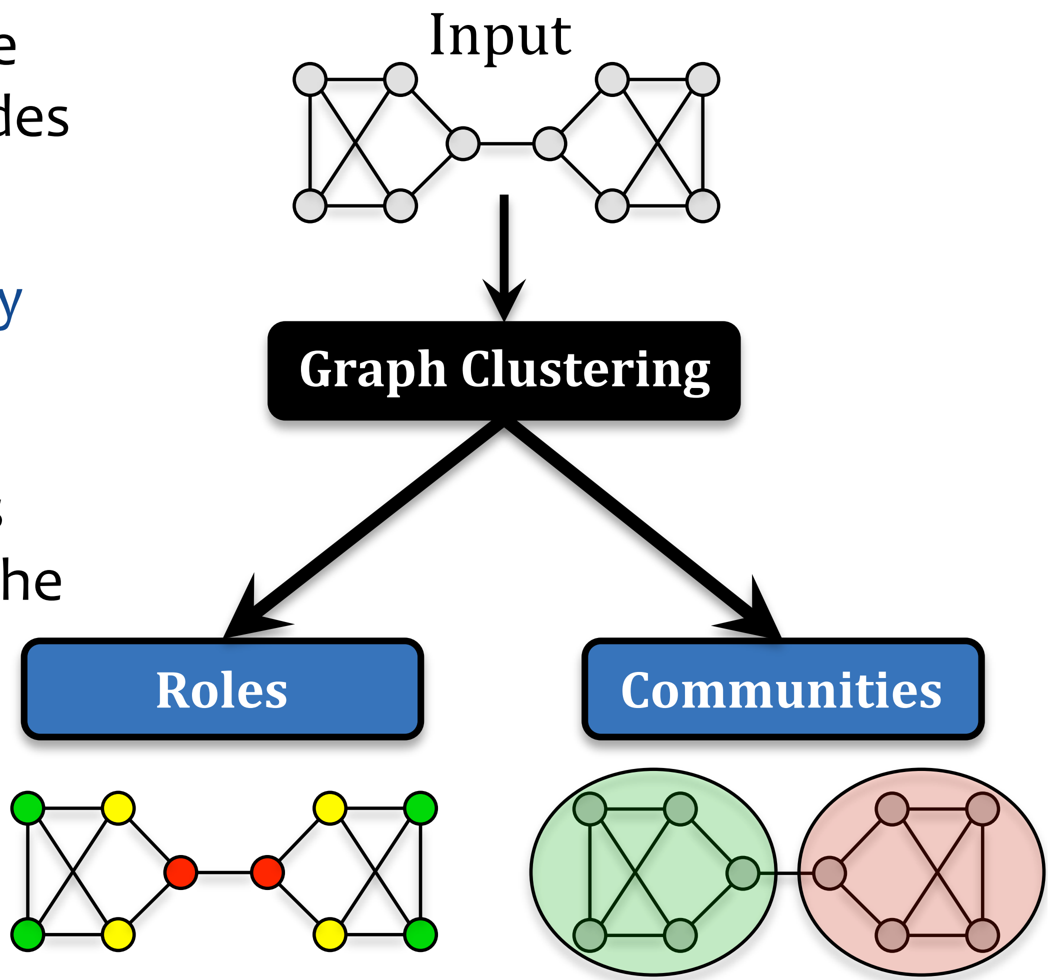
Communities and Roles

Roles are sets of nodes that are more structurally similar to nodes inside the set than outside

→ Based on structural similarity

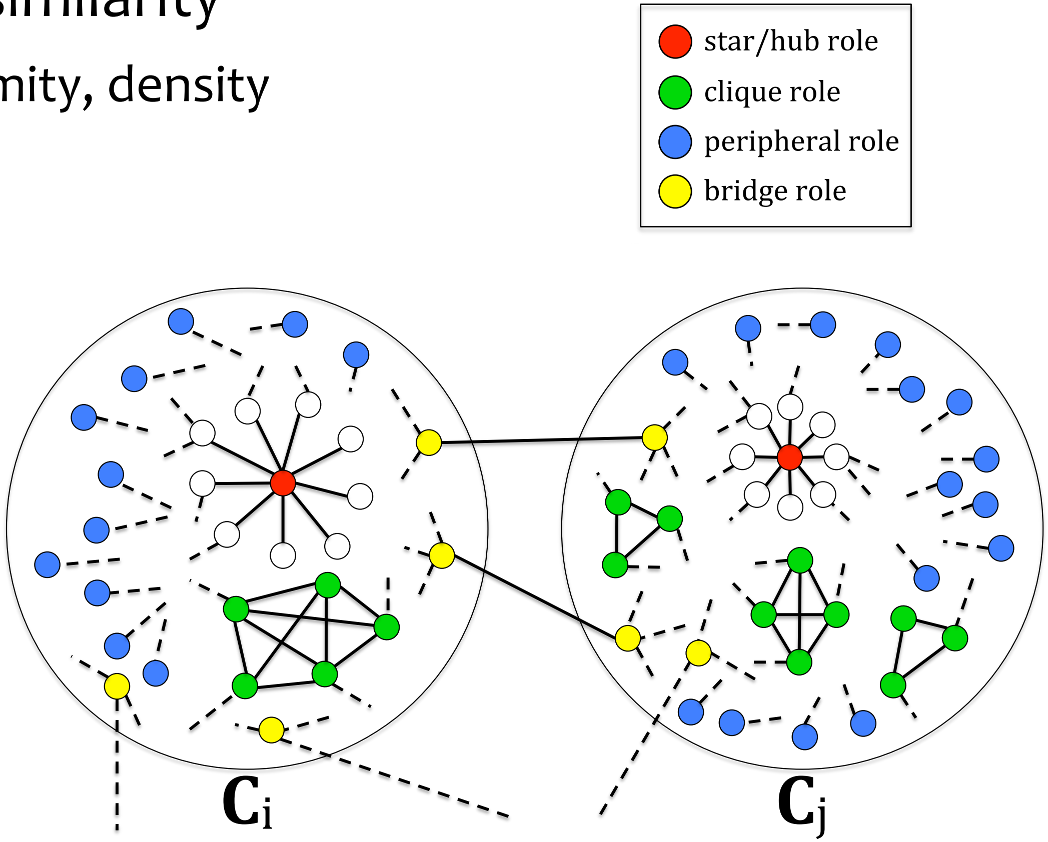
Communities are sets of nodes with more connections inside the set than outside.

→ Based on proximity, density



Roles and Communities are *Complimentary*

- Roles based on structural similarity
  - Communities based on proximity, density
- Roles globally distributed
  - Communities are local
- Roles generalize
  - Communities do not generalize across graphs (for graph transfer learning tasks)



Problem:
Learn Role-based Embeddings

Goal: Find d-dimensional embeddings of nodes that preserve *structural* similarity

Based on structural properties of nodes + attributes (if any)

Properties warranted by approach:

- General & unifying framework
- Methods generalized via framework are representationally more powerful
- Space-efficient

role2vec: Learning Role-based Graph Embeddings

- **Step 1:** Mapping vertices to vertex-roles.

$$\Phi \; : \; \mathbf{x} \; \rightarrow \; w$$

- **Step 2:** Sample Feature-based/Attributed Random walks.

A feature-based/attributed walk of length *L* is a sequence of adjacent vertex-roles

$$\Phi(\mathbf{x}_{v_0}), \ldots, \Phi(\mathbf{x}_{v_t}), \Phi(\mathbf{x}_{v_{t+1}}), \ldots, \Phi(\mathbf{x}_{v_{L-1}})$$

induced by a randomly chosen sequence of indices

$$(v_t : t = 0, 1, ..., L-1)$$

generated by a random walk of length *L* and a function Φ

- **Step 3:** Model the conditional probability that relate each vertex-role to the roles of its context.

$$\mathbb{P}\Big[\Phi\langle\mathbf{x}_{c_i}\rangle|\Phi\langle\mathbf{x}_i\rangle\Big] = \prod_{j\in c_i} \mathbb{P}(\Phi\langle\mathbf{x}_j\rangle \; |\Phi\langle\mathbf{x}_i\rangle)$$

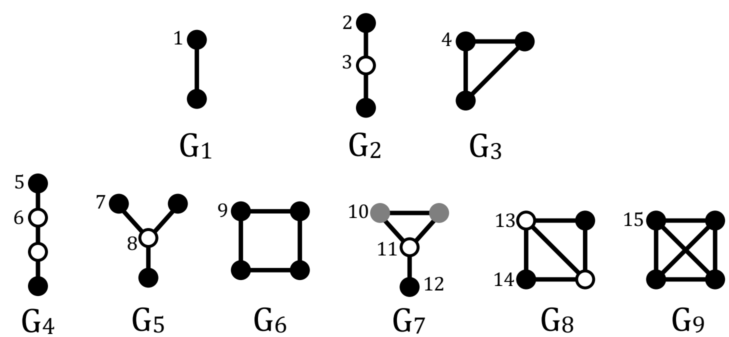
Generalize Existing Methods via Framework

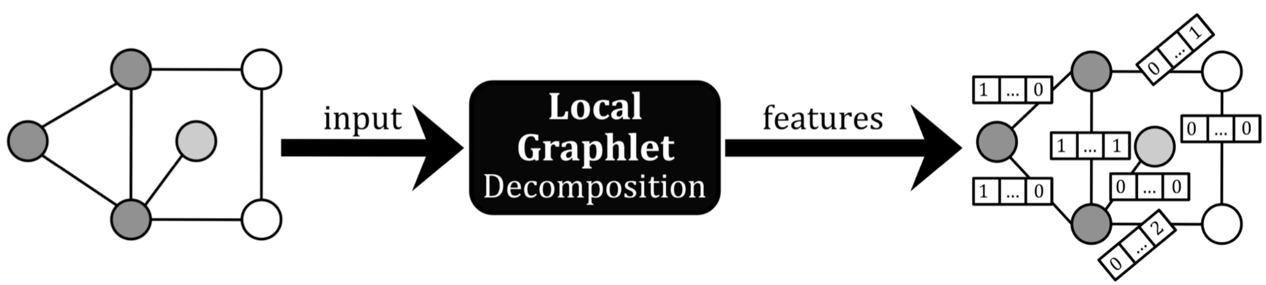
- Embeddings can be learned using basic Skip-gram model
- Other existing or future RW-based embedding methods can be easily generalized via the proposed framework

Examples: DeepWalk, node2vec, metapath2vec, struct2vec, and deep graph models, e.g., GRAM

We use small subgraphs called motifs as structural features

$$\Phi(\mathbf{x}) = x_1 \circ x_2 \circ \cdots \circ x_K$$





Prediction

Average improvement in AUC of 16.5%

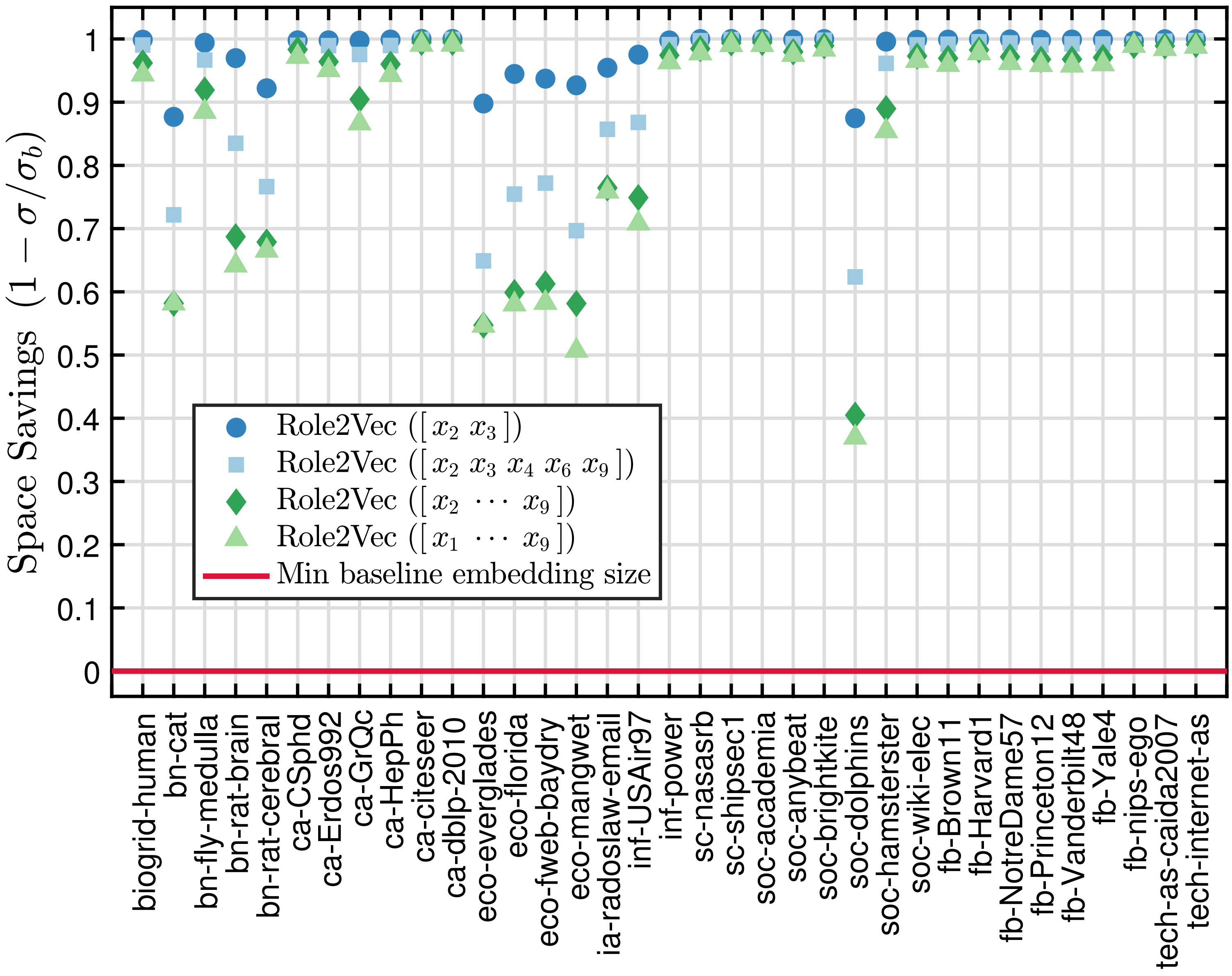
Experimental setup: 10-fold cross-validation, repeated for 10 random trials, D=128, Predict link existence via Logistic Regression

Table 1: AUC scores for various methods using $(\alpha_i + \alpha_j)/2$. **N2V**=node2vec, **DW**=DeepWalk and **S2V**=struc2vec.

GRAPH	R2V	R2V-DW	N2V	DW	LINE	S2V
bn–cat	**0.710**	0.688	0.627	0.627	0.672	0.669
bn–rat–brain	**0.748**	0.731	0.716	0.716	0.691	0.729
bn–rat–cerebral	**0.867**	0.846	0.813	0.811	0.709	0.858
ca–CSphd	**0.838**	**0.838**	0.768	0.735	0.620	0.791
eco–fweb–baydry	**0.681**	0.656	0.655	0.627	0.660	0.623
ia–radoslaw–email	**0.867**	0.847	0.756	0.745	0.769	0.857
soc–anybeat	**0.961**	0.960	0.854	0.848	0.850	0.883
soc–dolphins	**0.656**	0.597	0.580	0.498	0.551	0.590
fb–Yale4	**0.793**	**0.793**	0.742	0.728	0.763	0.758
web–EPA	**0.926**	0.925	0.804	0.738	0.768	0.861

Space-Efficiency

role2vec requires on average 850x less space



Conclusion

- Introduced notion of feature-based/attributed walks
- Proposed a generic framework for learning role-based embeddings based on this notion
- Learns universal functions that can generalize across networks/graphs → Useful for inductive & graph-based transfer learning
- role2vec achieves a mean gain in AUC of 16.5% while requiring 850x less space than existing methods

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Thank You!
Questions?

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