struc2vec: Learning Node Representations from Structural Identity

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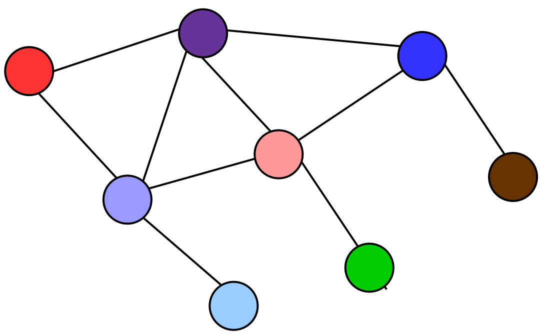
Node Representations

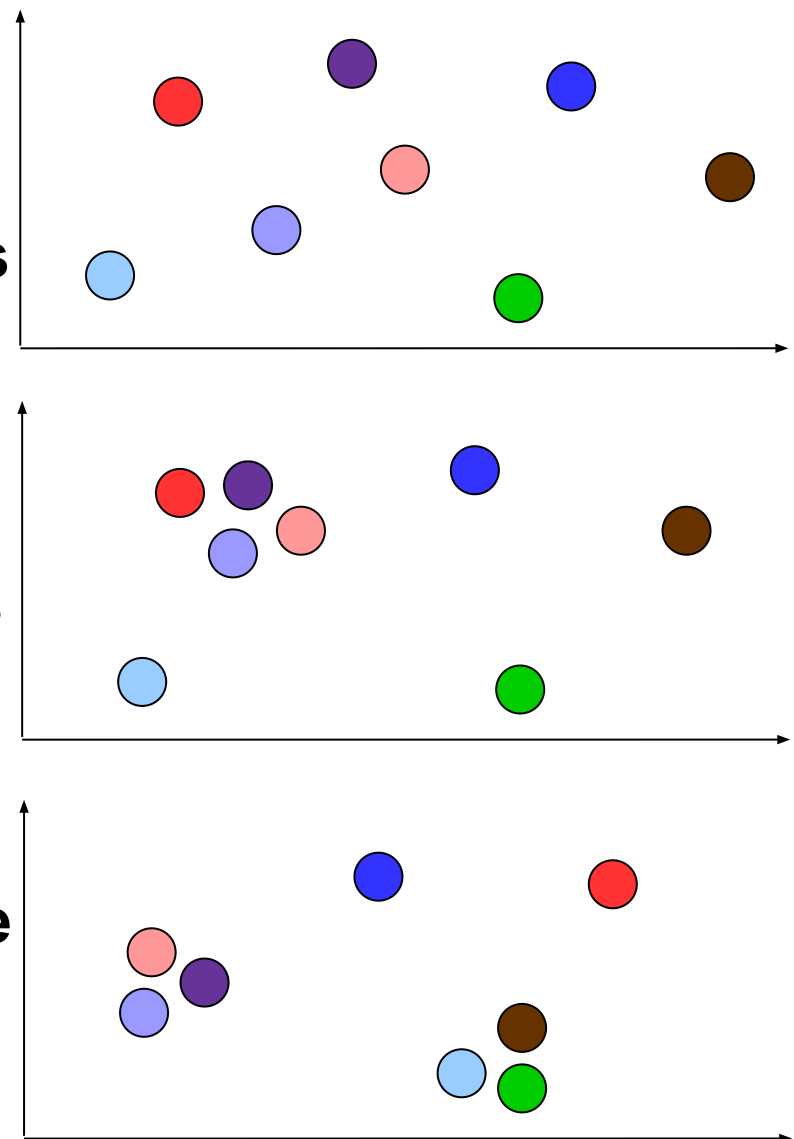
- Map network nodes into Euclidean space
  - aka. network embedding



preserve distances

find cliques

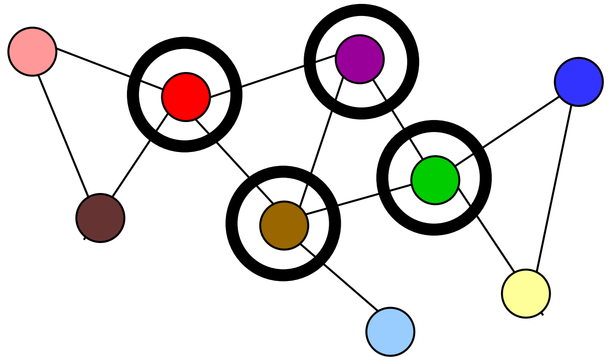
preserve degrees



- Many ways to embed nodes
- Right way depends on application

Structural Identity

- Nodes in networks have specific roles
  - eg., individuals, web pages, proteins, etc
- Structural identity
  - identification of nodes based on network structure (no other attribute)
  - often related to role played by node
- Automorphism: strong structural equivalence



- Red, Green: automorphism
- Purple, Brown: structurally similar

Related Work

- *word2vec*: framework to embed words (from sentences) into Euclidean space [arXiv'13]
- *deepwalk*: embed network nodes generating sentences through random walks [KDD'14]
- *node2vec*: use *biased* random walks to generate sentences [KDD'16]

Walk on original network to generate context

- *rolx*: use node-feature matrix to compute low rank matrix for roles [KDD'12]

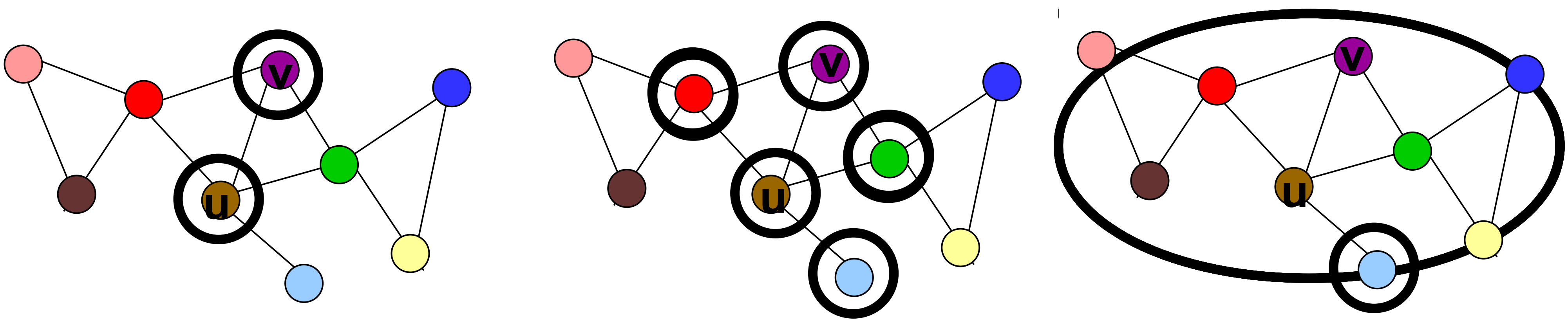
struc2vec

- Novel framework for node representations based on structural identity
  - structurally similar nodes close in space

- **Key ideas**
- Structural similarity does not depend on hop distance
  - neighbor nodes can be different, far away nodes can be similar
- Structural identity as a hierarchical concept
  - depth of similarity varies
- Flexible four step procedure
  - operational aspect of steps are flexible

Step 1: Structural Similarity

- Hierarchical measure for structural similarity between two nodes
- $R_k(u)$: set of nodes at distance k from u (ring)
- $s(S)$: ordered degree sequence of set S



$s(R_0(u)) = 4$

$s(R_0(v)) = 3$

$s(R_1(u)) = 1,3,4,4$

$s(R_1(v)) = 4,4,4$

$s(R_2(u)) = 2,2,2,2$

$s(R_2(v)) = 1,2,2,2,2$

Step 1: Structural Similarity

- $g(D_1,D_2)$: distance between two ordered sequences
  - cost of pairwise alignment: $\max(a,b) / \min(a,b) - 1$
  - optimal alignment by DTW in our framework

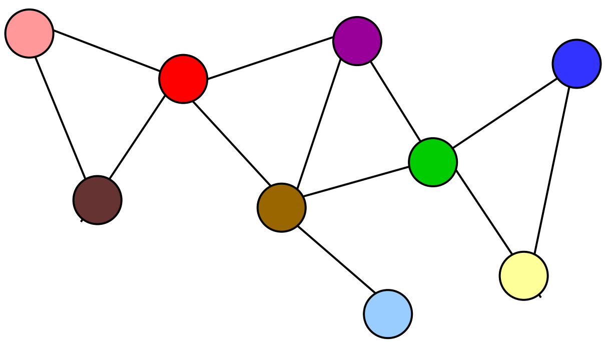
$s(R_0(u)) = 4$	$s(R_1(u)) = 1,3,4,4$	$s(R_2(u)) = 2,2,2,2$
$s(R_0(v)) = 3$	$s(R_1(v)) = 4,4,4$	$s(R_2(v)) = 1,2,2,2,2$
$g(. , .) = 0.33$	$g(. , .) = 3.33$	$g(. , .) = 1$

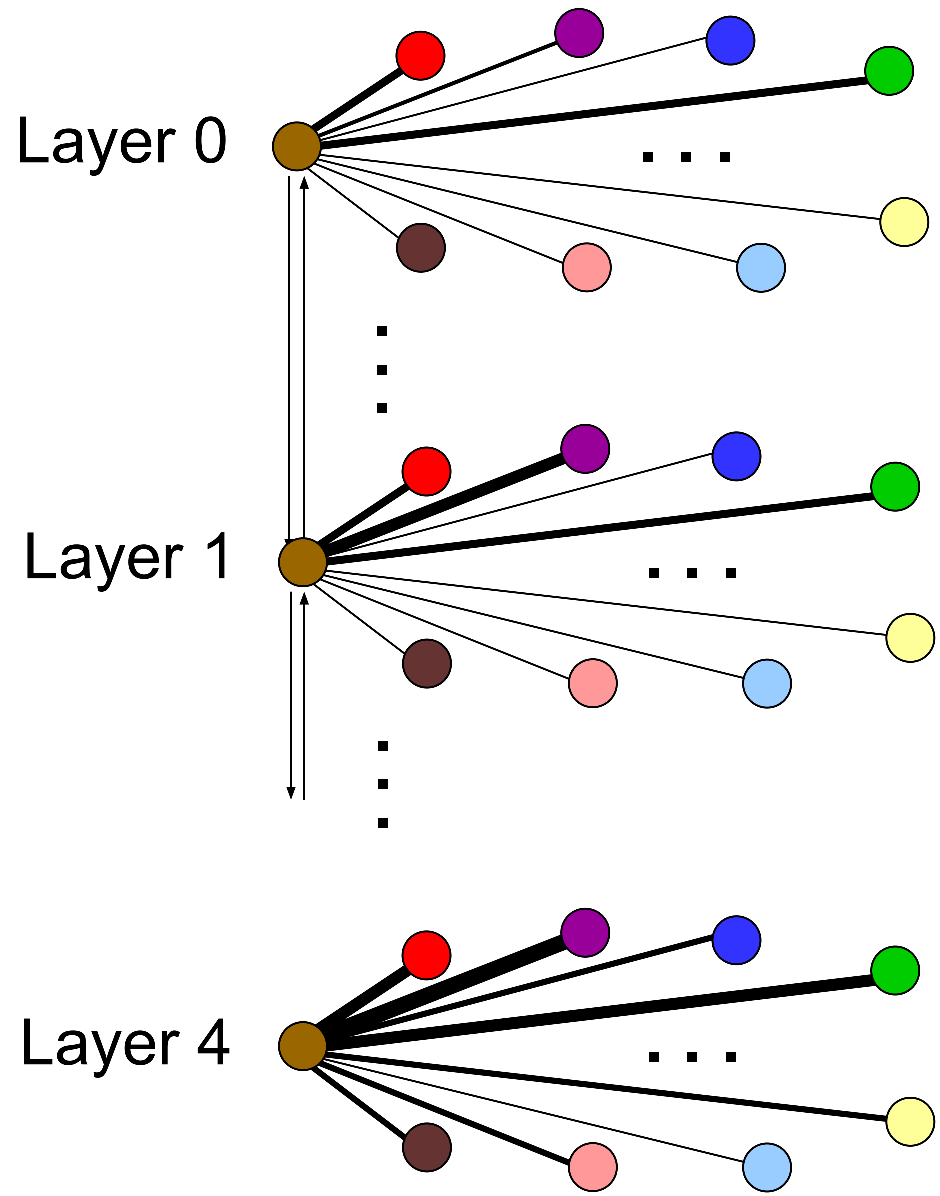
- $f_k(u,v)$: structural distance between nodes *u* and *v* considering first *k* rings
  - $f_k(u,v) = f_{k-1}(u,v) + g(s(R_k(u)), s(R_k(v)))$

$f_0(u,v) = 0.33$	$f_1(u,v) = 3.66$	$f_2(u,v) = 4.66$

Step 2: Multi-layer graph

- Encodes structural similarity between all node pairs





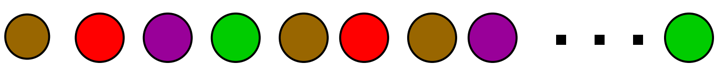
- Each layer is weighted complete graph
  - corresponds to similarity hierarchies
- Edge weights in layer *k*
  - $w_k(u,v) = \exp\{-f_k(u,v)\}$
- Connect corresponding nodes in adjacent layers

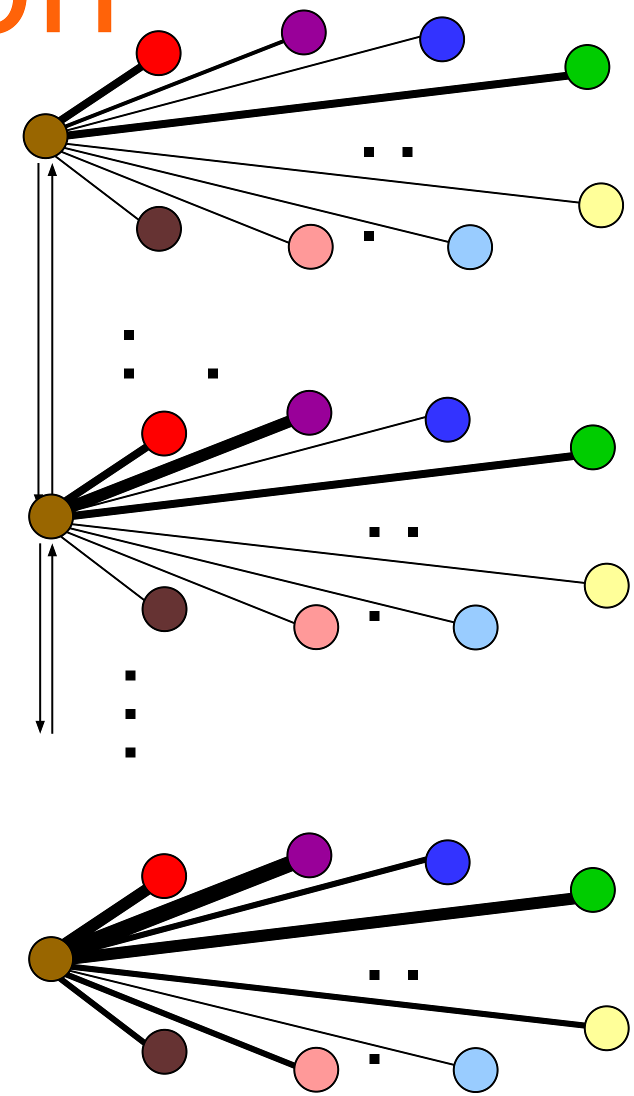
Step 3: Generate Context

- Context generated by biased random walk
  - walking on multi-layer graph
- Walk in current layer with probability *p*
  - choose neighbor according to edge weight
  - RW prefers more similar nodes
- Change layer with probability *1-p*
  - choose up/down according to edge weight
  - RW prefer layer with less similar neighbors

Step 4: Learn Representation

- For each node, generate set of independent and relative short random walks
  - context for node; sentences of a language



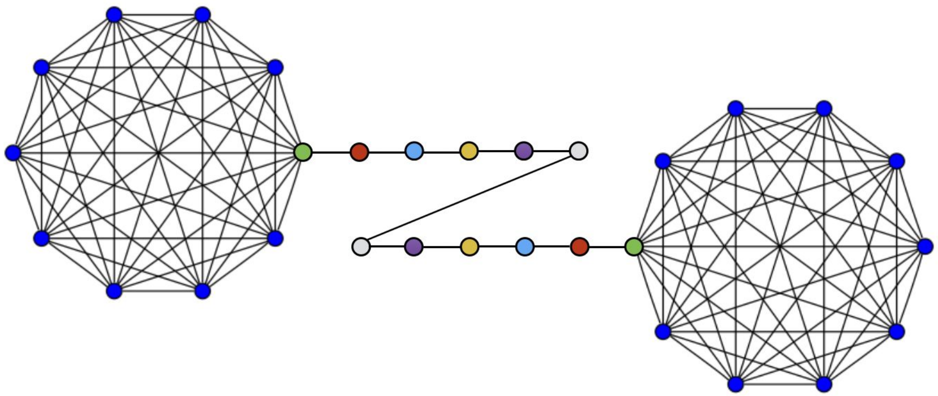


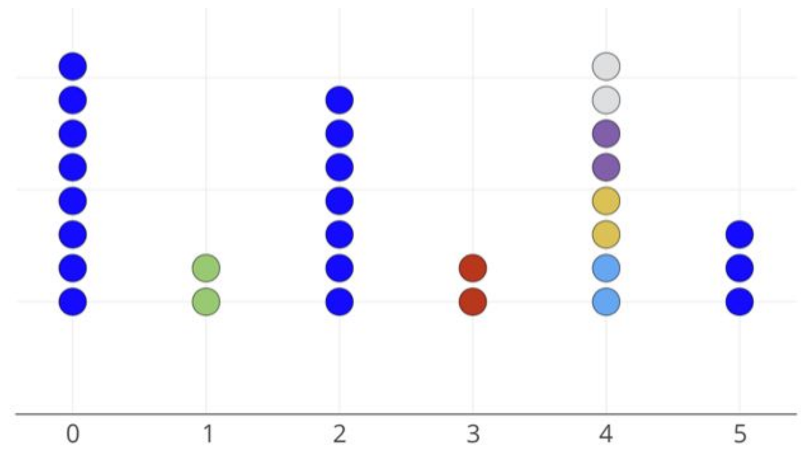
- Train a neural network to learn latent representation for nodes
  - maximize probability of nodes within context
  - Skip-gram (Hierarchical Softmax) adopted

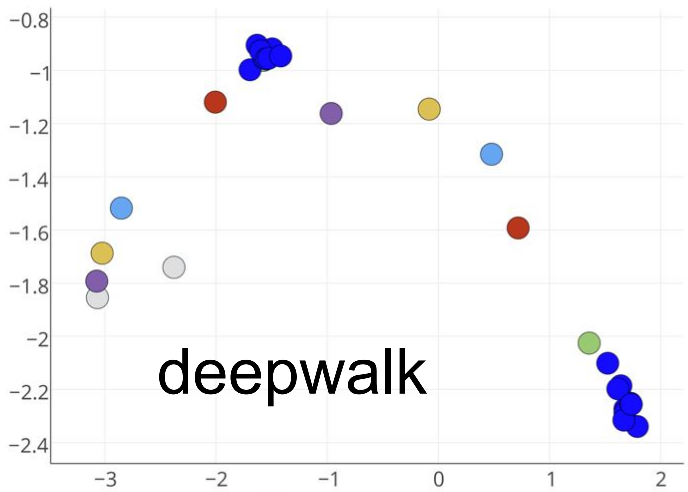
Optimization

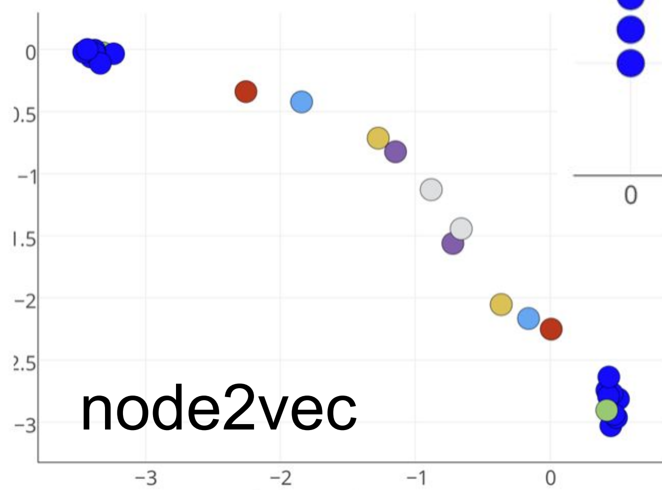
- Reduce time to generate/store multi-layer graph and context for nodes
- OPT1: Reduce length of degree sequences
  - use pairs (degree, number of occurrences)
- OPT2: Reduce number of edges in multi-layer graph
  - only *log n* neighbors per node
- OPT3: Reduce number of layers in multi-layer graph
  - fixed (small) number of layers
- Scales quasi-linearly
  - over 1 million nodes

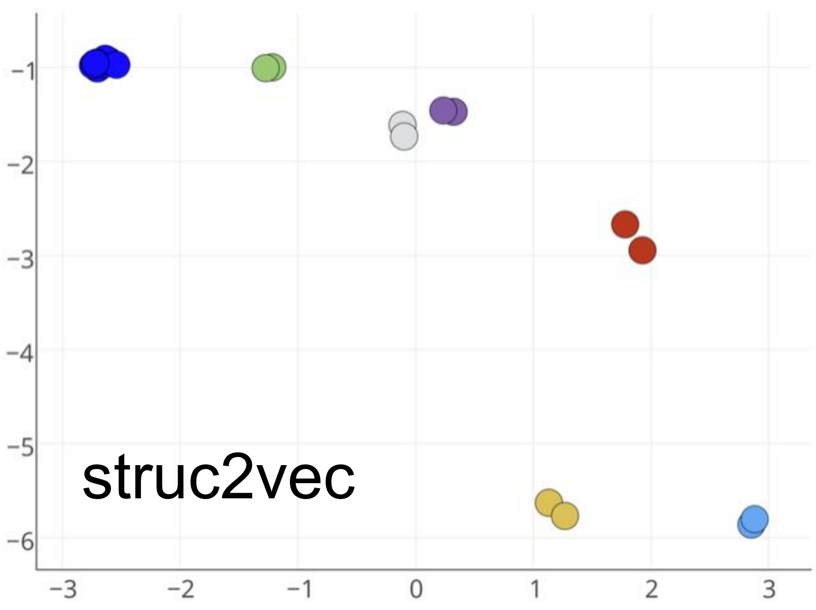
Barbell Network





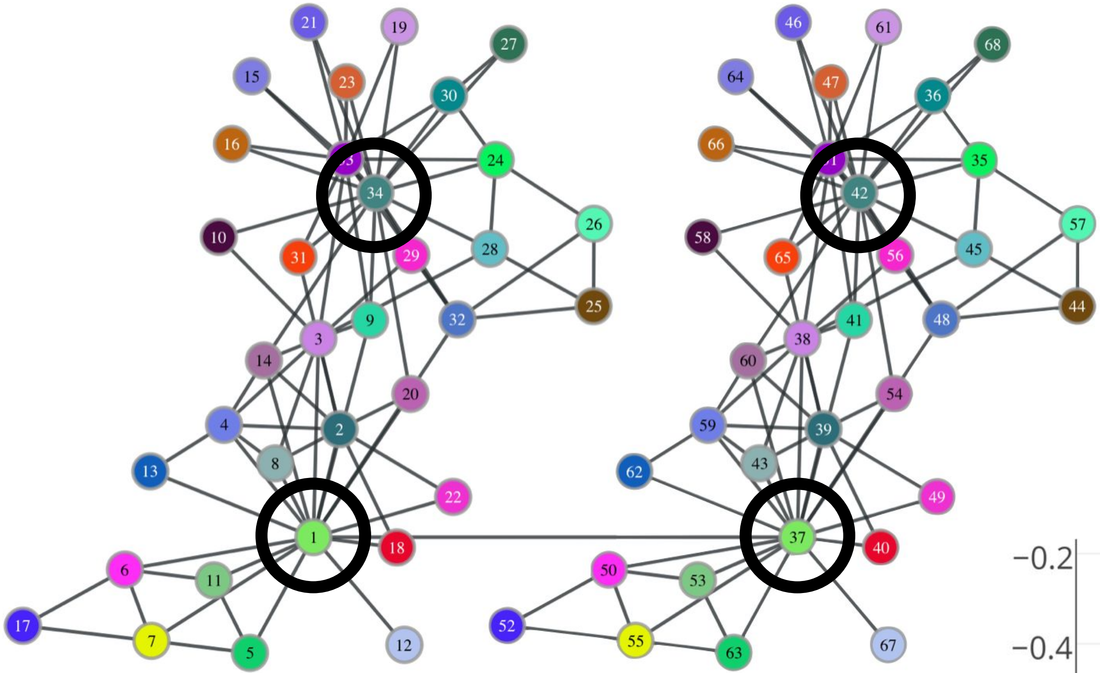


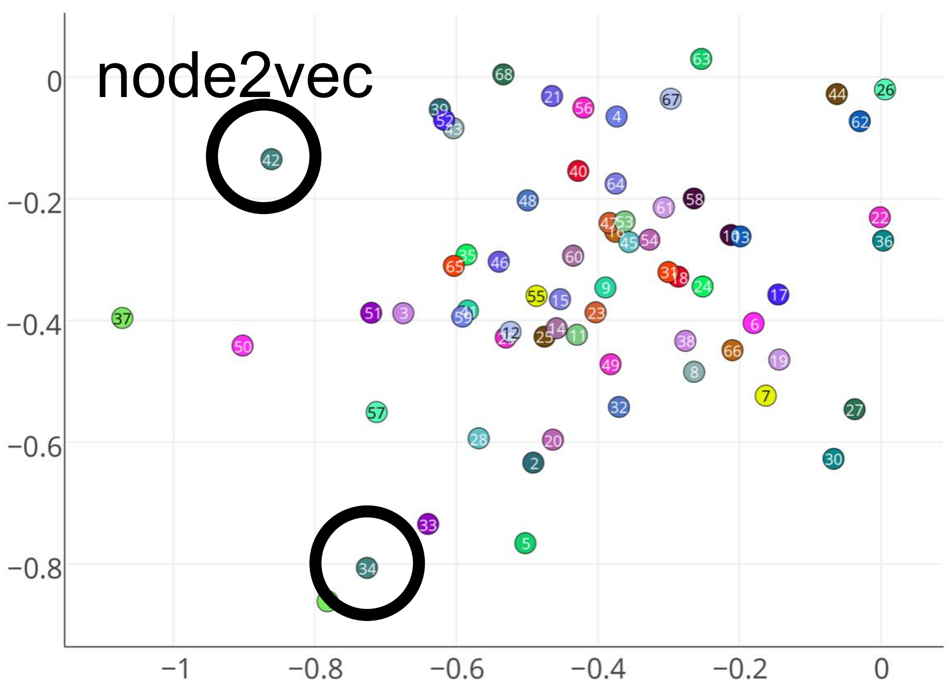


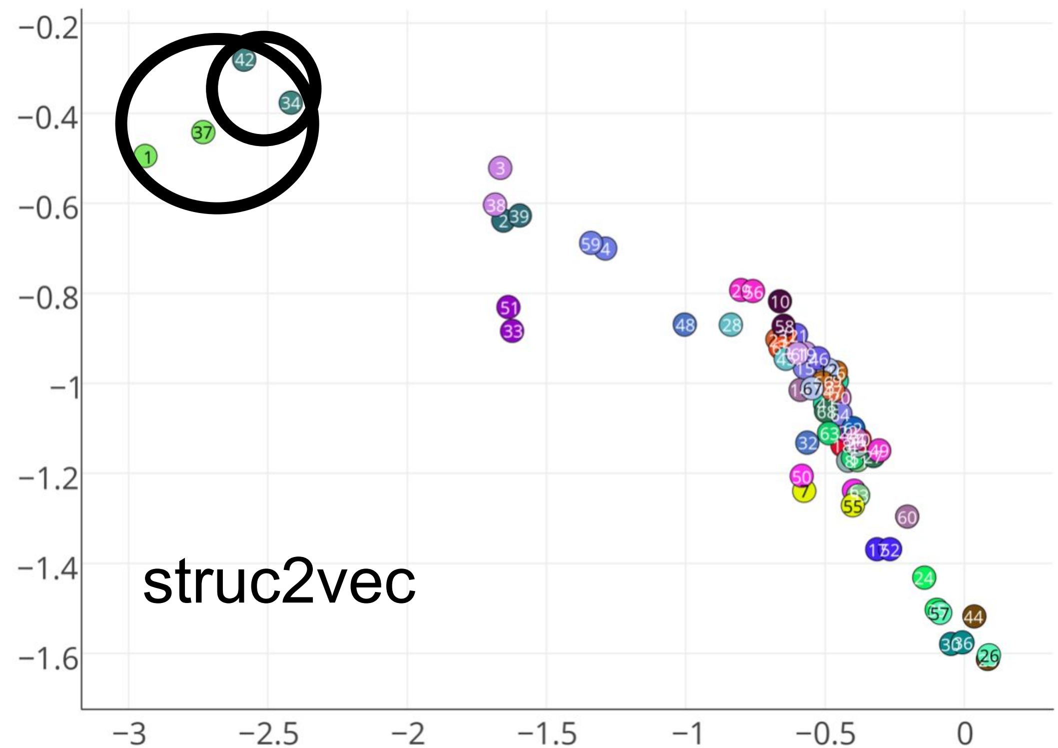


- Isomorphic nodes very close in space
  - similar with OPTs

Mirrored Karate Network







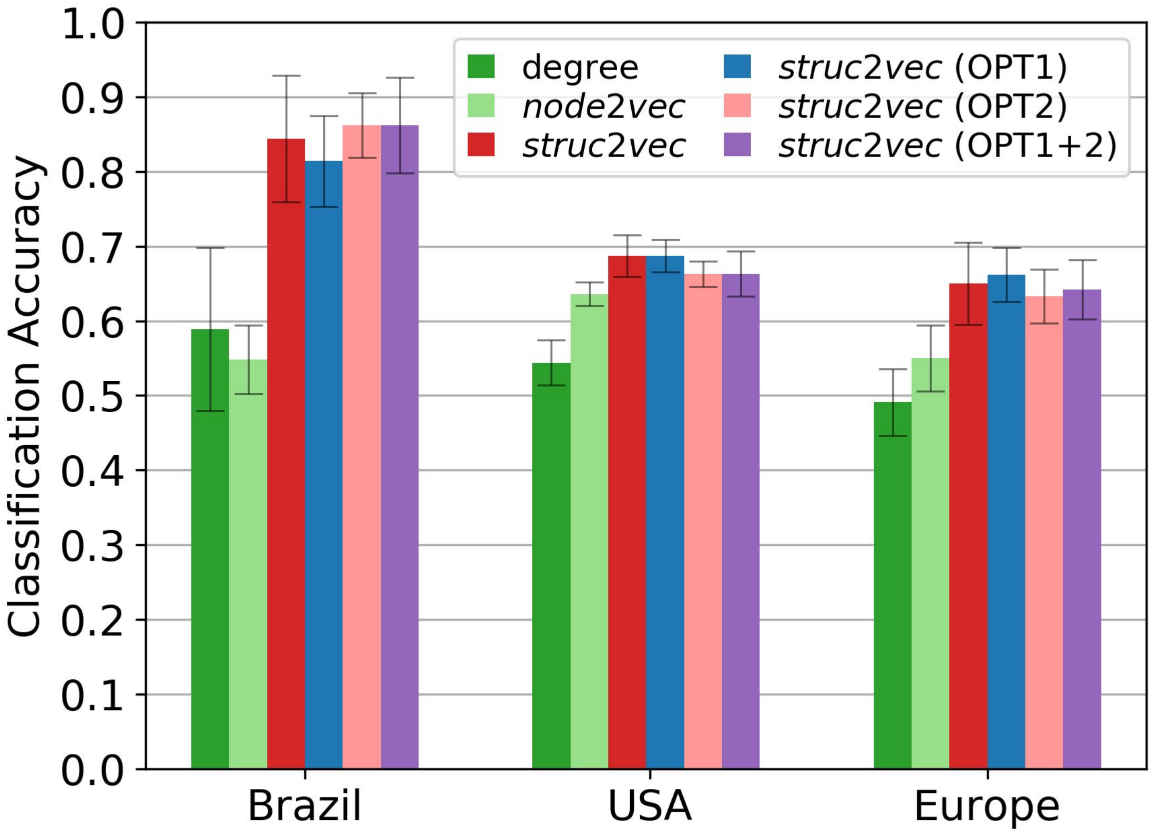
- Similar roles close in space

Airport Classification

- struc2vec helps classification if labels related to role of nodes
- Air traffic network: airports, commercial flights
  - Brazilian, USA, European (collected from public data)
  - airport activity measured in number of flights or movement of people
  - four labels according to quartiles of activity
- struc2vec (and others) learn node representation from network
  - no labels or activity used here

Airport Classification

- Node representations used to train classifier
  - logistic regression, L2 normalization



- struc2vec superior performance
- 50% improvement in Brazilian network
- Activity related to structure more than neighbors or degree

Conclusion

- Structural identity: symmetry concept based on network, related to node roles
- *struc2vec*: flexible framework to learn representations for structural identity
  - multi-layer graph encodes structural similarity
- *struc2vec* helps classification based on roles
- Yet another useful kind of embedding
  - not necessarily a substitute for others

Find the right embedding for your task!

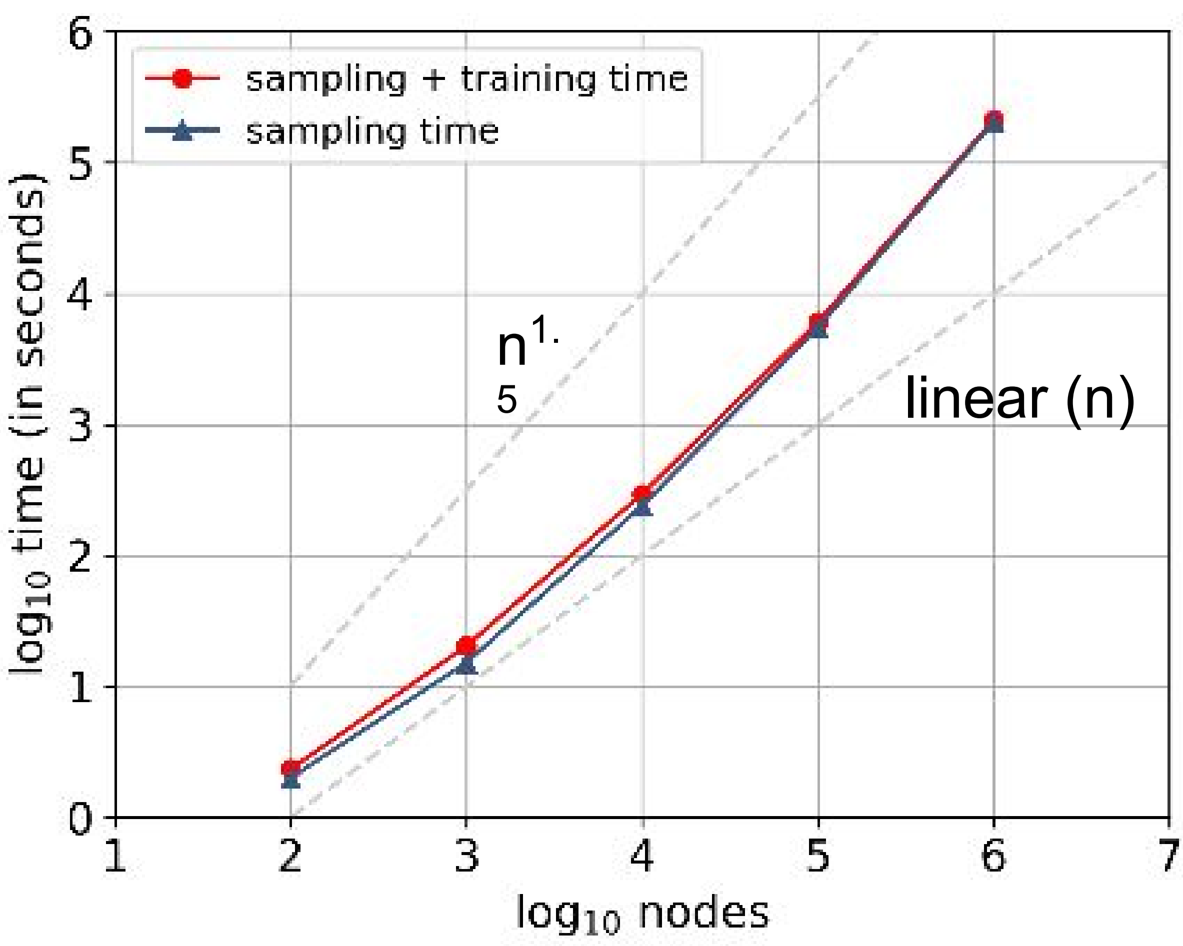
Thank You!

- Questions and comments?

- *struc2vec* (source code and datasets)
  https://github.com/leoribeiro/struc2vec

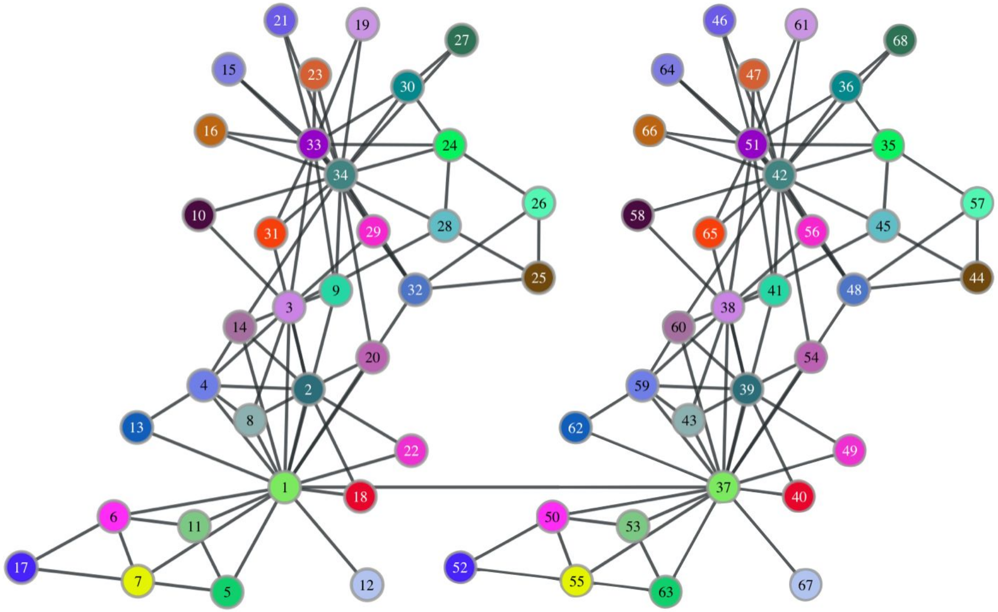
Scalability

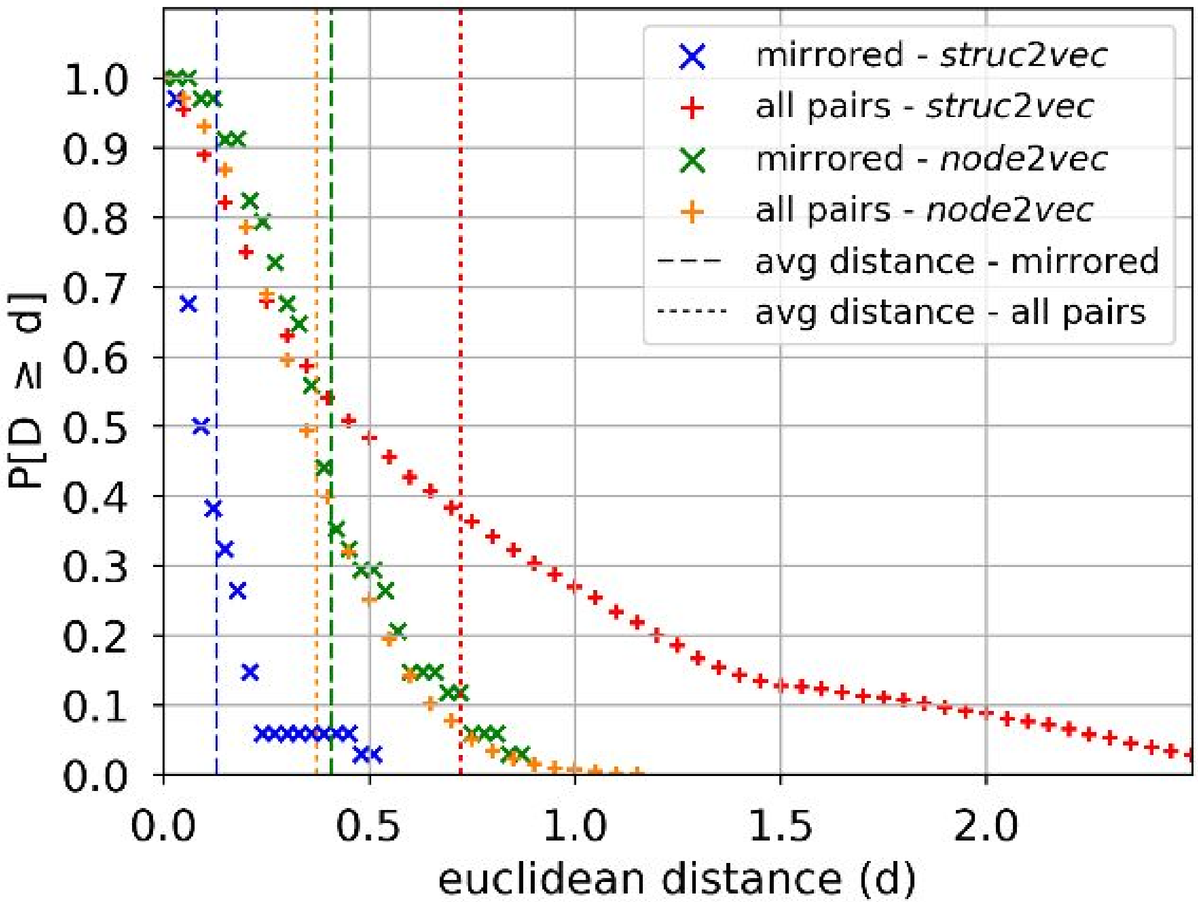
- G(n,p) network model, avg. deg 10
  - avg running time over 10 networks, OPTs on



- Time dominated by computing degree sequences of rings (yet to be optimized)

Distances

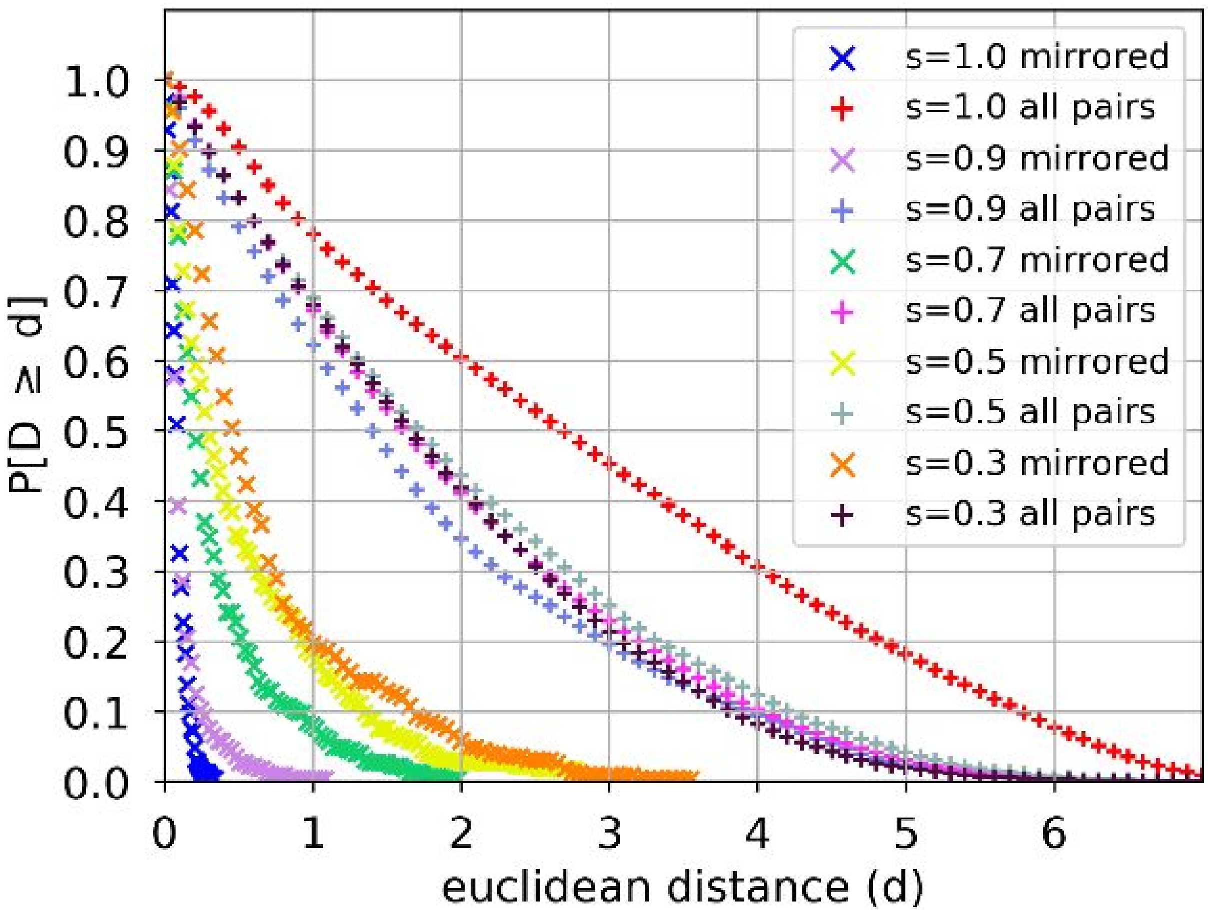




- Euclidean distance distribution in mirrored Karate network
- mirrored pairs much closer than all pairs
- not for node2vec

Robustness

- Structural similarity under edge removal
  - G is a social network
  - each edge present in $G_{1,2}$ with prob *s*



- Euclidean distance distribution
- Corresponding pairs much closer
- Even when *s* is moderate