Graph Embedding in Vector Spaces

GbR'2011 Mini-tutorial

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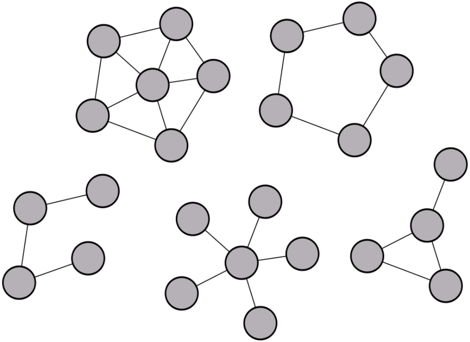
What do we understand by Graph Embedding?

Motivational problem

Given a set of graphs to be categorized, how do we process them?



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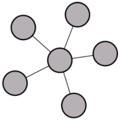
- The solution we are here interested in:
  Assign a feature vector to every graph.

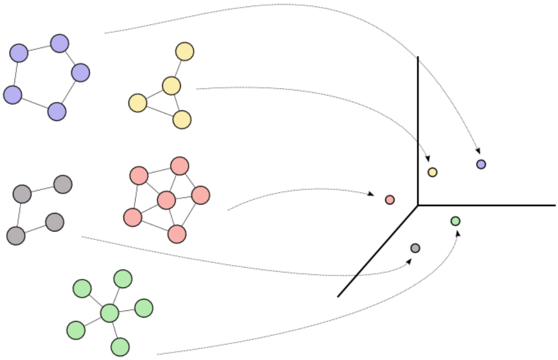


$v = (f_1, f_2, \ldots, f_n) \in \mathbb{R}^n$

What do we understand by Graph Embedding?

Formally, a graph embedding is a mapping from the set of graphs to a vectorial space

$$\begin{aligned} \phi : G &\longrightarrow \mathbb{R}^n \\ g &\longmapsto \phi(g) = (f_1, f_2, \ldots, f_n) \end{aligned}$$



Possible misunderstandings

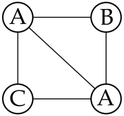
- We do not want to draw a graph in the 2D plane.

- Graph kernels are an implicit way of defining a graph embedding (more on that tomorrow).

Crucial Issue

Which features do we extract from graphs?

Simple features



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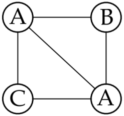

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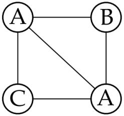

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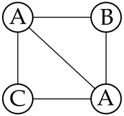

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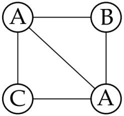

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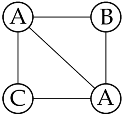

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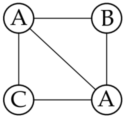

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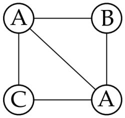

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Let us review the literature.

Literature Review

- Substructure finding methods
- Spectral methods
- Dissimilarity Representation

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- The truncated modal matrix is defined by

$$\phi_k = (\phi_k^1 \,|\, \phi_k^2 \,|\, \ldots \,|\, \phi_k^n)$$

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- Unary features:

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- Binary features:

  $\longrightarrow$ One feature for each pair of eigen-modes.

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- Unary features (among others)
  - Leading eigenvalues

    Consider all eigenvalues as features for the vectorial representation of G_k:

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  - Eigen-mode volume

    Let $D_k(i)$ be the degree of the node i in the graph G_k. The volume of the eigenmode w is defined as

    $$Vol_k(w) = \sum_{i \in V_k} \phi_k(i, w) D_k(i).$$

    As a feature vector for G_k, we define

    $$B_k = (Vol_k(1), Vol_k(2), \ldots, Vol_k(n))^T$$

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- Binary features
  - Inter-mode adjacency matrix

    Project the adjacency matrix onto the basis of eigenvectors

    $$U_k = \phi_k^T A_k \phi_k$$

    The vectorial representation of the graph G_k is defined by $B_k = (U_k(1,1), U_k(1,2), \ldots, U_k(n,n))$, where

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  - Inter-mode distance

    The leading node (most important) in the eigenmode u is defined by

    $$i_u^k = \underset{i \in V_k}{\operatorname{argmax}}\, \phi_k(i,u)$$

    The vectorial representation of the graph G_k is defined by $B_k = (d_{1,1}, d_{1,2}, \ldots, d_{n,n})$, where

    $$d_{u,v} = \underset{p}{\operatorname{argmin}} (A_k)^p (i_u^k, i_v^k).$$

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The proposed feature vectors are further reduced by PCA, ICA, MDS in order to perform graph visualization and clustering:

Fig. 8. MDS space clustering using the eigenvalues.

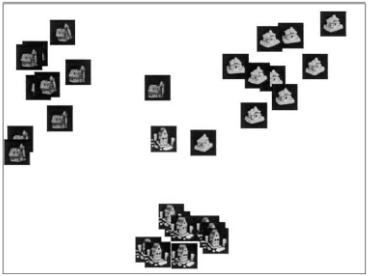

Fig. 10. ICA space clustering using the inter-mode adjacency matrix.

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Graph Characterization via Ihara Coefficients (Ren et al., Neural Networks 2011)

- Extract Ihara Coefficients from the Oriented line graph
- Important topological information

Spectral methods - Summary

Good points

- Solid theoretical insight into the meaning of the extracted features
- Rich and discriminative features (really good clustering examples)

Drawbacks

- Spectral analysis is sensitive to structural errors
- Restriction on the nature of the graphs

Graph Classification based on Vector Space Embedding

(Riesen and Bunke, IJPRAI 2009)

Dissimilarity based embedding

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The extracted features are based on distances to a set of prototype graphs:

Given a graph G and set of prototypes $\mathcal{P} = \{p_1, p_2, \ldots, p_n\}$, the dissimilarity based embedding is defined by

$$\varphi^{\mathcal{P}}(G) = (d(G, p_1), d(G, p_2), \ldots, d(G, p_n))$$

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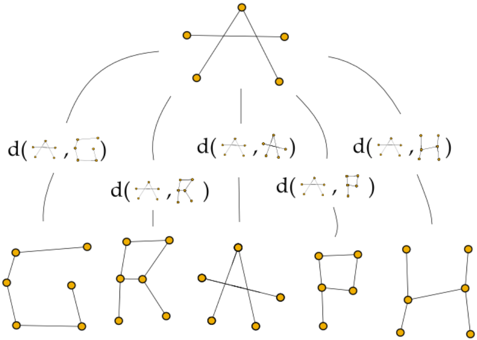

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  $\longrightarrow$ Random
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  $\longrightarrow$ k-Centres
  $\longrightarrow$ And many others...

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  $\longrightarrow$ And many others...

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  $\longrightarrow$ Cross-validated

$\longrightarrow$ The work is concerned with the classification of graphs using the dissimilarity features.

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Good behaviour of the vectors in the embedding space:

$$\begin{aligned}
\| \varphi^P(G_1) - \varphi^P(G_2) \|^2 &= \langle \varphi^P(G_1), \varphi^P(G_1) \rangle + \langle \varphi^P(G_2), \varphi^P(G_2) \rangle - 2 \langle \varphi^P(G_1), \varphi^P(G_2) \rangle \\
&= \sum_{i=1}^{n} d(G_1, p_i)^2 + \sum_{i=1}^{n} d(G_2, p_i)^2 - 2 \sum_{i=1}^{n} d(G_1, p_i) d(G_2, p_i) \\
&= \sum_{i=1}^{n} (d(G_1, p_i) - d(G_2, p_i))^2 \\
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&= \sum_{i=1}^{n} (d(G_1, p_i) - d(G_2, p_i))^2 \\
&\leq n \cdot d(G_1, G_2)^2
\end{aligned}$$

$\longrightarrow$ The Euclidean distance between feature vectors of graphs is equal to the sum of the squared differences between the edit distances of the graphs to the prototypes.

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Good behaviour of the vectors in the embedding space:

$$\begin{aligned}
\| \varphi^P(G_1) - \varphi^P(G_2) \|^2 &= \langle \varphi^P(G_1), \varphi^P(G_1) \rangle + \langle \varphi^P(G_2), \varphi^P(G_2) \rangle - 2\langle \varphi^P(G_1), \varphi^P(G_2) \rangle \\
&= \sum_{i=1}^{n} d(G_1, p_i)^2 + \sum_{i=1}^{n} d(G_2, p_i)^2 - 2\sum_{i=1}^{n} d(G_1, p_i) d(G_2, p_i) \\
&= \sum_{i=1}^{n} (d(G_1, p_i) - d(G_2, p_i))^2 \\
&\leq n \cdot d(G_1, G_2)^2
\end{aligned}$$

$\longrightarrow$ The Euclidean distance between feature vectors of graphs is equal to the sum of the squared differences between the edit distances of the graphs to the prototypes.

$\longrightarrow$ The Euclidean distance between feature vectors of graphs is upper-bounded by the edit distance of the graphs

Graph Classification based on Vector Space Embedding (Riesen and Bunke, IJPRAI 2009)

Good points

- Any kind of graphs can be plugged into this methodology (because of GED)
- Good behaviour of vectors in the embedding space, which leads to good classification rates

Drawbacks

- The distance measure (edit distance) is computationally challenging
- Validation of parameters has to be performed

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  - Spectral methods
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  - And others...

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$\longrightarrow$ We bridge the gap between the structural and the statistical pattern recognition fields.

Thanks for the attention!

Time for discussions?

In the next talk, we will present another graph embedding methodology.
Do not miss it!