Artificial Intelligence - Knowledge Representation and Planning - Assignment 3

Lorenzo Soligo - 875566

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1 Requirements

Read this article presenting a way to improve the disciminative power of graph kernels. Choose one graph kernel among

- Shortest-path Kernel
- Graphlet Kernel
- Random Walk Kernel
- Weisfeiler-Lehman Kernel

Choose one manifold learning technique among

- Isomap
- Diffusion Maps
- Laplacian Eigenmaps
- Local Linear Embedding

Compare the performance of an SVM trained on the given kernel, with or without the manifold learning step, on the following datasets:

- PPI
- Shock

Note: the datasets are contained in Matlab files. The variable G contains a vector of cells, one per graph. The entry am of each cell is the adjacency matrix of the graph. The variable labels, contains the class-labels of each graph.

2 Graph Kernels

2.1 Graph Comparison Problem

Given two graphs G and G' from the space of graphs $\mathcal{G}$, the problem of graph comparison is to find a mapping

$$s : \mathcal{G} \times \mathcal{G} \to \mathbb{R}$$

such that $s(G, G')$ quantifies the similarity (or dissimilarity) of G and G'.

2.2 Graph isomorphism

Given two graphs G_1 and G_2, find a mapping f of the vertices of G_1 to the vertices of G_2 such that G_1 and G_2 are identical, i.e. (x, y) is an edge of G_1 iff $(f(x), f(y))$ is an edge of G_2. Then f is an isomorphism, and G_1 and G_2 are said to be isomorphic.
At the moment we do not know a polynomial time algorithm for graph isomorphism, but we also do not know whether the problem is NP-complete.
On the other hand, we know that subgraph isomorphism is NP-complete. Subgraph isomorphism checks whether there is a subset of edges and vertices of G_1 that is isomorphic to a smaller graph G_2.

2.3 Graph edit distances

3 Resources

- Professor's slides

- http://www.dsi.unive.it/~atorsell/AI/graph/Unfolding.pdf
- http://www.dsi.unive.it/~atorsell/AI/graph/kernels.pdf
- https://www.ethz.ch/content/dam/ethz/special-interest/bsse/borgwardt-lab/documents/slides/CA10_GraphKer
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