Developing and evaluating a Cytoscape app for graph-based clustering

Philipp Spohr

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Abstract

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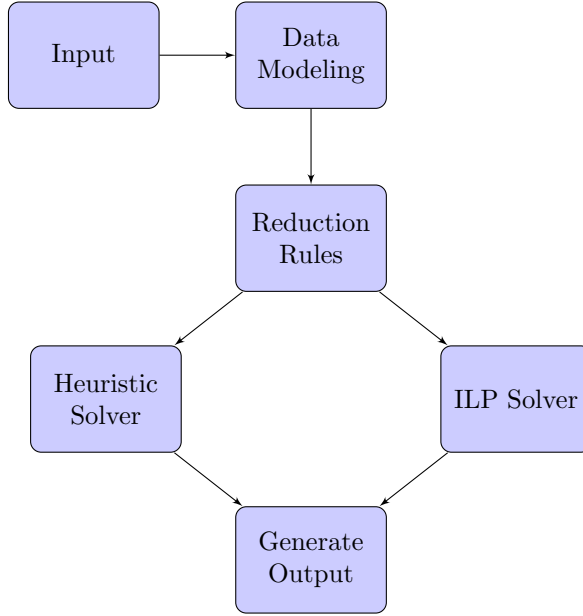
2.1 Technical Details

2.2 Algorithm

Figure 1: Overview of the Yoshiko Algorithm

2.2.1 Data Modeling

Theory The Yoshiko algorithm models the data as a complete graph $G = (V, E)$ with an associated edge-cost function $C : E \rightarrow \mathbb{R} \cup \{-\infty\} \cup \{\infty\}$. As many input instances do not describe a full graph, missing edges and costs need to be modeled. This is achieved by using default values for insertion or deletion. A default insertion cost $C_I \in [-\infty, 0]$ is used as $C(e)$ whenever the input instance does not contain an edge e. A default deletion cost $C_D \in [0, \infty]$ is used as $C(e)$ whenever the input instance does contain an edge e that has no cost associated yet.

Implementation The Yoshiko Wrapper provides a clean and simple interface to generate the model.

    Mapping edge costs The user has the possibility to use a numeric Cytoscape column of the node table as a source for the edge-cost function C.

Insertion and deletion cost   The default values C_I and C_D can be set by the user and default to $C_I = -1$ and $C_D = 1$. It should be noted, that the insertion cost value is not normalized or in any way adjusted when a mapping is used. This means that the user needs to adjust this value wisely to fit the data. As an example the user might have mapped the edge costs to a column containing values in the range of $10^6 - 10^7$. The default insertion cost of -1 will be irrelevant in comparison and the algorithm will most likely insert all missing edges and generate one big cluster as a solution. Overall the ratio $R = \frac{|C_I|}{C_D}$ should give you a rough idea how the algorithm will operate.

$R > 1$ means, that the algorithm is more likely to delete edges to generate cliques, a value of $R < 1$ means insertions are more likely.

Mapping permanent or forbidden edges   The Yoshiko app has additional convenience functions: The user can map edges to a boolean Cytoscape column to mark them as either **forbidden** (meaning that those edges will never be part of the solution) or **permanent** (meaning that those edges will always be part of the solution). Marking an edge e as forbidden is equivalent to $C(e) = -\infty$, marking an edge e as permanent is equivalent to $C(e) = \infty$. This way the user is able to apply expert knowledge about the input instance to increase the quality of the solution.