Comparison of features between SAMMI and other popular graph visualization tools

In this supplemental material we provide a comparison of several features between SAMMI and five other graph visualization tools, three specific to metabolic networks and two general graph visualization tools.

Summary Table:

Feature	SAMMI	Escher	MetExploreViz	MetDraw	Cytscape	Gephi
Force-directed layout	Present	Not present	Present	Present	Present	Present
Tunable automated positioning	Present	Not present	Not present	Not present	Present	Present
Animated, real-time node-positioning	Present	Not present	Present	Not present	Not present	Not present
Node fixing	Present	Not present	Present	Not present	Not present	Not present
Manual node positioning	Present	Present	Present	Not present	Present	Present
Denote nodes as secondary	Present	Present	Present	Present	Not present	Not present
Subgraphing functionality	Present	Limited	Not present	Not present	Not present	Not present
Node duplication/joining	Present	Limited	Limited	Limited	Not present	Not present
Data Mapping	Present	Limited	Limited	Limited	Present	Present
Arrange nodes in shapes (e.g. straight lines)	Present	Present	Present	Not present	Not present	Not present
Node shelving	Present	Limited	Not present	Not present	Not present	Present
Edge curving	Present	Present	Not present	Not present	Present	Limited
Web implementation	Present	Present	Limited	Present	Not present	Not present
Integration with MATLAB or Python	Present	Present	Not present	Present	Not present	Not present
Preserves original layout	Present	Present	Present	Present	Present	Present
Long-term support available	Present	Present	Present	Present	Present	Present
Supports SBML and/or BioPax upload	Present	Limited	Limited	Present	Present	Not present
Modify default node color, shape and size	Present	Not present	Present	Not present	Present	Present
Modify node labels	Present	Limited	Limited	Not present	Present	Present
Import and edit custom node attributes	Present	Not present	Not present	Not present	Present	Present

Legend: Present (green), Limited (yellow), Not present (red)

Detailed Comparison:

Automated node positioning:
All applications included in this comparison with the exception of Escher allow for automated node positioning based on network topology, such as force-directing layout.

Adjustable automated positioning:

MetExploreViz and MetDraw do not allow for modifications to the force-directing algorithm. Gephi and Cytoscape offer different algorithms besides force-directing. While SAMMI does not offer different algorithms, Gephi, Cytoscape and SAMMI allow users to modify parameters of the node-positioning algorithm.

Animated, real-time node-positioning:
SAMMI and MetExploreViz are the only applications that render the graph as animated, constantly updated layouts. This feature allows the graph to update in real time as nodes are repositioned and fixed.

Node fixing:
SAMMI and MetExploreViz allow users to fix the position of selected nodes, allowing the force-directed layout to arrange around these fixed nodes. All other applications that provide automated node positioning apply this feature to all nodes in the graph.

Manual node positioning:
MetDraw is the only application that provides a static image and does not allow for manual node repositioning. All other applications allow users to select and drag nodes to new positions.

Denote nodes as secondary:
The classification of nodes as secondary is a feature specific to the drawing of metabolic networks. Since Gephi and Cytoscape are generalized graph drawing tools they do not possess this embedded functionality. All other application are tailored to metabolic networks and possess this feature.

Subgraphing functionality:
All tools compared here plot a single graph at a time with the exception of Escher and SAMMI. Escher allows for the development of multiple subgraphs for the same model, allowing data to be mapped to multiple subgraphs simultaneously and allowing users to easily switch between subgraphs. Besides these functionalities, SAMMI also offers navigation between subgraphs, searching for similar nodes between them, and allows users to combine subgraphs.

Node duplication/joining:
Making multiple copies or joining similar nodes are also features usually desirable in the context of metabolic networks. Due to this fact, Gephi and Cytosape do not offer node duplication or joining directly from the application, although this task could be accomplished by editing the uploaded network files. MetDraw and MetExploreViz allow for the duplication of secondary nodes making one copy of the metabolite for each reaction it is associated with. Escher adds one node to the map at a time and allows similar nodes to be joined by overlapping them manually. SAMMI provides similar features but also allows metabolite nodes to be split into fewer copies than one per reaction. This feature is usually desirable for metabolites that are represented multiple times but not once per reaction, such as pyruvate or frequently occurring amino acids.

Data Mapping:
SAMMI, Cytoscape and Gephi allow users to map data using node and link color, node size and edge thickness. Cytoscape and Gephi also allow mapping based on node shape, but this feature is reserved for differentiating between reaction and metabolite nodes in metabolic mapping tools. Escher allows for data mapping using edge color for reactions and node size for metabolites. MetExploreViz allows node coloring for both reactions and metabolites, while MetDraw allows for post-processing edge coloring. For all applications except MetExploreViz full control of color and

size scales, as well as numerical breaks, are available when the data mapping functionality is present. MetExploreViz sets the maximum and minimum scale values to the maximum and minimum of the mapped data and no additional numerical breaks can be added, although the maximum and minimum colors can be changed.

Arrange nodes in shapes (e.g. straight lines):
SAMMI, Escher, MetExploreViz and Cytoscape allow users to arrange nodes in horizontal and vertical lines, with SAMMI and Cytoscape allowing for the scaling of this line size. SAMMI, Escher, Cytoscape and Gephi also allow rotation of selected nodes. SAMMI and Cytoscape allow the arranging into circles and scaling of node position. SAMMI also allows users to arrange the nodes in a rectangular shape. Finally, Gephi allows users to upload node positions directly, but many of the positioning options mentioned here are not directly implemented in the application interface.

Node shelving:
While nearly all applications here provide some functionality to remove nodes, the ability to temporarily remove and subsequently reintroduce nodes is unique to SAMMI. In Escher, removed nodes can be re-introduced by reintroducing the reaction into the map, although this feature is not straightforward.

Edge curving:
SAMMI, Escher and Cytoscape allow full control of edge curving functionality. Gephi allows for predefined edge curving in network preview mode. While MetDraw and MetExploreViz do not currently offer this functionality, MetExploreViz has announced this feature in the version 2.0 yet to be released.

Web implementation:
SAMMI, Escher and MetDraw are readily available online through their respective application webpages. MetExploreViz is a web-based tool, but has to be implemented by a user defined server or accessed through the MetExplore Portal [6]. Cytoscape and Gephi are standalone tools.

Integration with MATLAB or Python:
Escher and MetDraw can be run directly from the Python command line and SAMMI can be run directly from the MATLAB and Python command lines. All other applications require the upload of format specific files for visualization of the data.

Preserves original layout:
All platforms compared here allow users to download maps in the layout they are currently working on, allowing users to return to previously arranged maps.

Long term support:
All platforms offer some sort of support. Gephi and Cytoscape are operated by larger consortia which provide support through each platform's website. SAMMI, Estcher and MetDraw all have GitHub repositories where users can submit bug reports and suggestions. Escher also offers support via Gitter chat room. Finally, the MetExploreViz team can also be contacted via email through the platform's website.

Support SBML and/or BioPAX model upload
SAMMI and MetDraw allow users to upload SBML models directly, while SAMMI also allows BioPAX models. Both formats can also be uploaded into Cytoscape via the cySBML and BioPAX Cytoscape plugins. Gephi does not support the direct upload of either format. While Escher and

MetExploreViz both do not allow for the upload of these formats directly, users can upload SBML models indirectly. SBML models can be uploaded for analysis through the COBRA and COBRApy toolboxes, from which they can then be uploaded to Escher. Similarly, models can be directly uploaded to MetExploreViz through the MetExplore database [6], where a wide number of models are also available in SBML format.

Modify default node color, shape and size
While Escher and MetDraw both allow for users to change node and edge appearance by uploading data onto the visualization, neither platform allows for direct modification of default color and shape. SAMMI, MetExploreViz, Cytoscape and Gephi all allow users to change default color and shape visual aspects.

Modify node labels
SAMMI, Cytoscape and Gephi all allow users to label nodes based on different annotated fields, and also allow users to modify these fields using the tool. While Escher and MetExploreViz also allow users to label nodes based on different annotated properties, users cannot modify these properties from within the platform. MetDraw does not provide functionality for modifying node labels.

Import and edit custom node attributes
SAMMI, Cytoscape and Gephi all allow users to import and edit custom fields for metabolite and reactions nodes, and also allow users to modify these fields from within the tool interface. Escher and MetExploreViz are largely coupled with the BiGG [7] and MetExplore [6] databases, and therefore import all annotated data from these databases not allowing for the import of user-defined fields. MetDraw simply draws the network and does not include annotations beyond node labels.

Bibliography:

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