Coral: a suite of visualizations for comparing clusterings

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Multiple clusterings

Clustering has become a standard analysis for many types of biological data: interaction networks, gene expression, metagenomic abundance, genomic sequences. However, it is possible to obtain a large number of contradictory clusterings of the same data by:

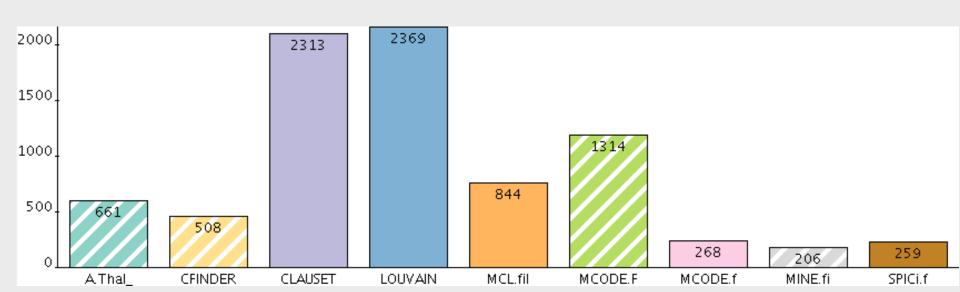
- using different clustering algorithms [1-5]
- tuning algorithm parameters
- exploring optimal and near-optimal solutions [6, 7]
- clustering time-varying data

Visual comparison

Visualization mantra: overview, zoom and filter, details on demand. Users can move from comparing all pairs of clusterings to examining individual item coclustering patterns.

Coordinated displays: selecting an item in one view selects the corresponding items in other views.

Dataset statistics: gain a quick overview of the data by looking at a collection of bar charts for the number of modules, average module size, the number of data items covered by a clustering, or the percentage of elements in the overlapping modules.



Global similarity: explore clustering similarity using the ladder widget. White and pale blue cells represents pairs of disagreeing clusterings while bright blue cells highlight similarity.

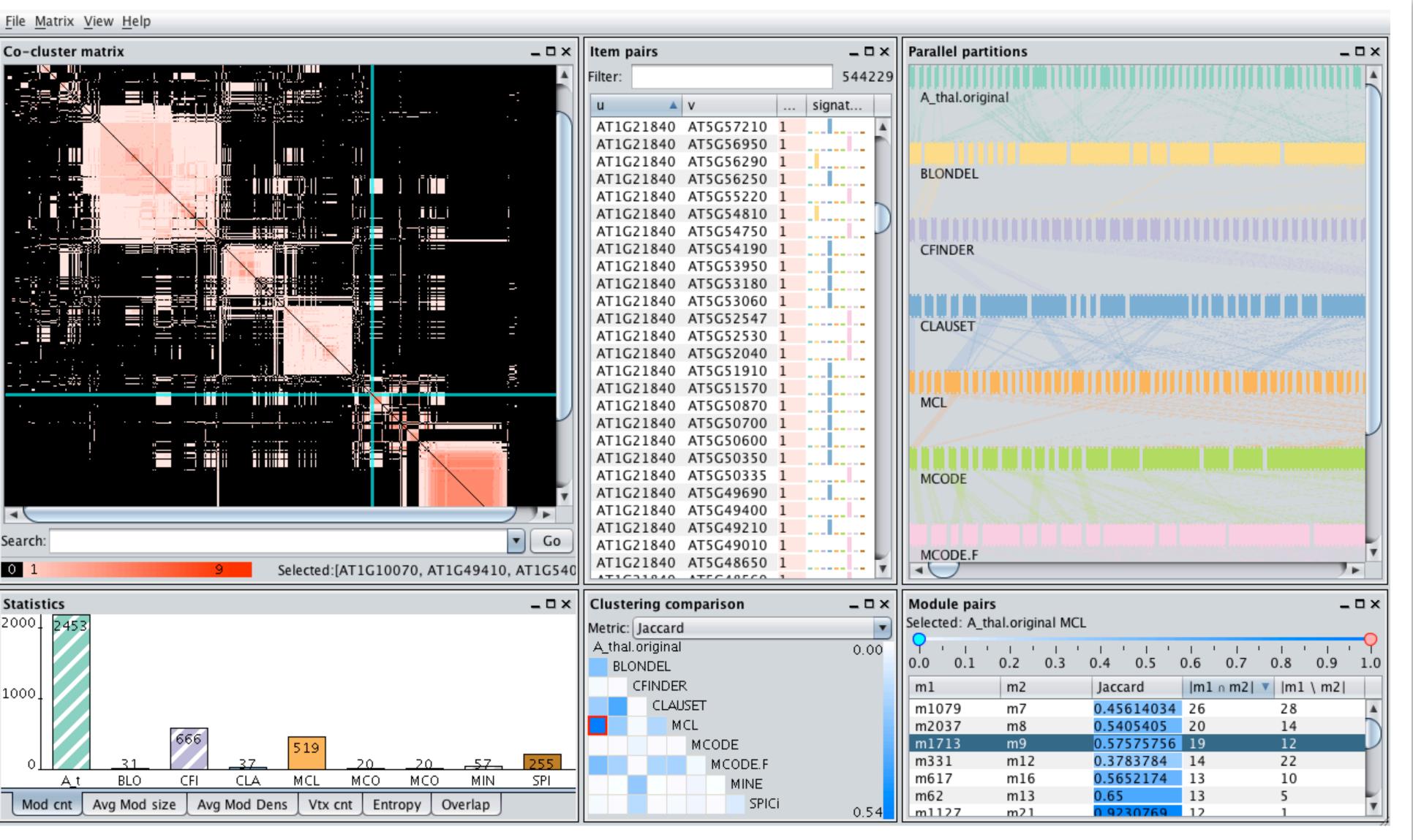
Module comparison: narrow down the exploration to two clusterings and compare their modules. Users can filter the modules by Jaccard similarity and sort the table based on the size of the modules or their intersections and set differences.

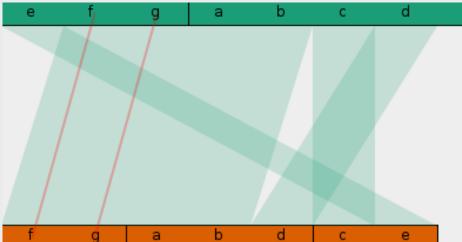
Parallel partitions plot: track individual items and

CLA MCL MCO MCO MIN Mod cnt Avg Mod size Avg Mod Dens Vtx cnt Entropy Overlap whole modules across multiple clusterings at a high levels. The bands of the plot are reordered to match the ordering of columns in the co-cluster matrix and to minimize the number of crossings. **Item pairs**: a table visually encodes in which clusterings the two data items have been placed in a module together. Users can sort the columns to group pair with similar co-cluster patterns or search for patterns using the filter box.

Co-cluster matrix: records which items were placed in the same module in a given clustering K. Matrix

Coral



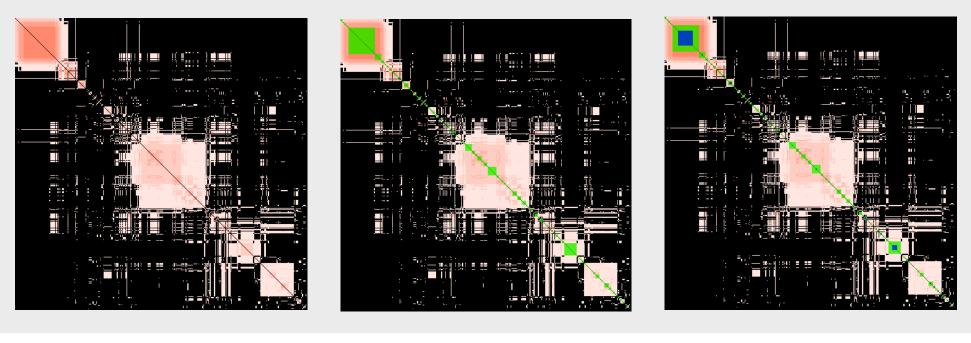


AT1G04100 AT1G50900 1 AT1G04100 AT1G51950 8

elements are defined as:

$$a_{ij}^K = \begin{cases} 0\\1 \end{cases}$$

We search for dense areas in the matrix using a dynamic programming approach. We call such dense areas *cores* (highlighted in green). If the original data was a network, we show the core's *cohesion* — a measure of separation of a core from the rest of the network (highlighted in blue).



Download at: <u>www.cbcb.umd.edu/kingsford-group/coral</u>

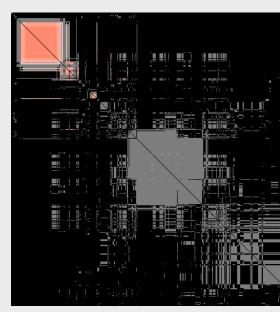
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 v_i and v_j are in different modules in K v_i and v_j are in the same module in K.

Example: A. thaliana PPI network

We applied 9 different clustering algorithms to a recent A. thaliana protein-protein interaction network [7]. Modules of size < 6 and with *partition density* < 0 were removed from the clusterings (as described in [7]). Most cells in the ladder widget (left) are pale blue or white indicating that clusterings **mostly disagreed**. The jaccard similarity for the MCL [4] and link clustering [3] pair can be explained via the module-to-module table: both clusterings identified a large module of 288 proteins and had exact matches among several smaller modules. 65.25% of all items in the co-cluster matrix have the value of 1, and only 6.34% of the matrix' cells have the value of 5 or greater. The DP identified 249 cores, most of them with a low cohesion, i.e. proteins in the cores shared many edges with proteins outside of the core (see left column, bottom). Setting the link clustering [3] as a



References

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base reveals that link clustering recovered only a fraction of modules found by other algorithms, but did include the largest module.