

MultiLayerMatrix: Visualizing Large Taxonomic Datasets

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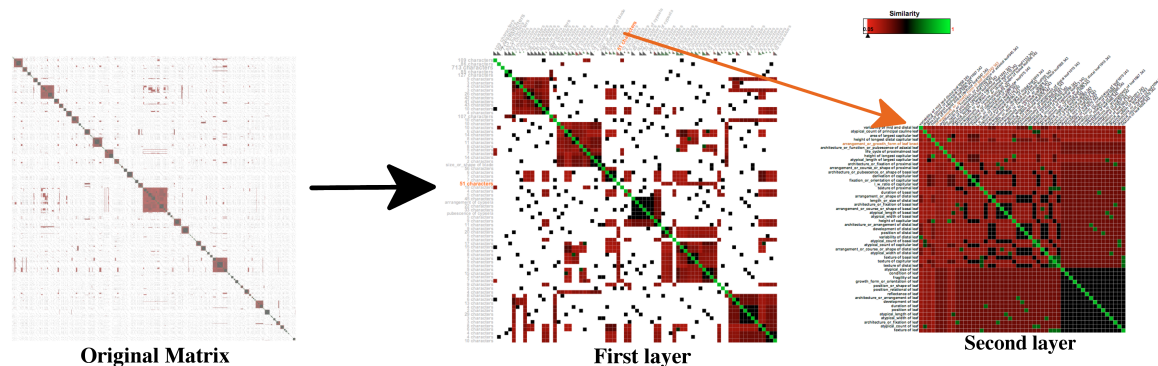


Figure 1: Visualizing 2048 nodes in a regular adjacency matrix (left) and in a MultiLayerMatrix of two layers: The middle panel shows the first layer, and the right panel shows an example of the second layer, which is shown when users select a cluster in the first layer. Green indicates similar characters while red highlights dissimilarity.

Abstract

Adjacency matrices can be a useful way to visualize dense networks. However, they do not scale well as the network size increases due to limited screen space, especially when the number of rows and columns exceeds the pixel height and width of the screen. We introduce a new scalable technique, MultiLayerMatrix, to visualize very large matrices by breaking them into multiple layers. In our technique, the top layer shows the relationships between different groups of clustered data while each sub-layer shows the relationships between nodes in each group as needed. This process can be applied iteratively to create multiple sub-layers for very large datasets. We illustrate the usefulness of MultiLayerMatrix by applying it to a network representing similarity measures between 2,048 characters in the Asteraceae taxonomy, a rich dataset that describes characteristics of species of flowering plants. We also discuss the scalability of our technique by investigating its effectiveness on a large synthetic dataset with 20,000 columns by 20,000 rows.

1. Introduction

Taxon-character matrices are one of the primary tools that biologists use to classify organisms and to study evolution. Although traditionally created by hand, newer software tools [OK11, RCH⁺14] make it possible to create matrices much larger than a manual workflow could support. For example, O’Leary et al. [OBF⁺13] make use of a matrix with 86 rows and 4,541 columns and Dececchi et al. [DBLM15] use a matrix with 1,051 rows and 639 columns. The size of these matrices demands novel visualization techniques that

are scalable and intuitive to support the curation, management, and exploration of large taxon-character matrices and their derivatives (e.g. character-character matrices).

An obvious way to visualize character-by-character similarity is by using an adjacency matrix where the color in each cell encodes the similarity of each pair of characters. An example of this approach is depicted in the left panel of Figure 1. However, this approach does not scale well due to the size constraints of a typical computer screen (i.e., there are not enough pixels to represent thousands of characters on

each side of a matrix). To mitigate this scalability issue, we can provide a high-level abstraction [Zei97] of the original matrix. Rather than drawing every single cell, we can instead apply a smoothing function on the matrix to ease perceptual recognition [LAE*12]. By so doing, we hide certain fine-grained details of the original matrix at higher levels while still enabling a user to interactive view these details on demand.

In this paper we introduce *MultiLayerMatrix*, a new technique for visualizing large matrices with thousands of items. Our technique “breaks” the original matrix into multiple layers by using the leader algorithm [Har75]. The top layer shows the similarity between clusters represented by the leaders. The additional layers shows similarity between characters in each cluster and sub-cluster. Our technique aims to achieve the following goals related to the analysis of taxonomies:

- **Pattern discovery and hypothesis generation:** An effective visualization should be able to support the discovery of interesting patterns in existing data which could lead to the generation of novel hypotheses. For example, taxonomists, ecologists, and phylogeneticists would like to identify unusual distribution patterns of characters across taxa such as when taxa share the same characters but are located far apart in a phylogenetic tree.
- **Curation and management of existing taxon-by-character data:** Analysts who regularly interact with taxonomies and ontologies have a common need to perform curation and editing tasks for existing datasets, such as merging sets of characters and removing characters that are unnecessary or redundant.

These high-level design goals are supported through enabling the specific tasks described in Section 3.

2. Related Work

In general, node-link diagrams and most varieties of adjacency matrices, such as *NodeTrix* [HFM07], *Compressed Adjacency Matrices* [DWvW12], *BioFabric* [Lon12], *GeneaQuilts* [BDF*10], and *DAGView* [KT13], are not suitable for visualizing very dense networks where the degree of nodes is consistently high. To mitigate difficulties in representing dense networks, *ZAME* [EDG*08] visualizes large graphs by aggregating information. Aggregates are arranged into a pyramid hierarchy that allows for on-demand paging to GPU programs to support smooth multiscale browsing. In particular, every level of detail has half the number of nodes as the level below it. Consequently, each cell in a higher level is the summary of four cells at the level below it. Similarly, *Net-Ray* [KLKF14] projects a large matrix onto a smaller one, where an element of the small matrix is set to the number of non-zero elements in the corresponding submatrix of the big matrix. However, this leads to another challenge: the small matrix is almost full in most cases. *Net-Ray* handles

this problem by reordering nodes in the matrix before projecting and by scaling the x and y axes and the numerical value of each submatrix.

A main difference between *ZAME*, *Net-Ray*, and our technique, *MultiLayerMatrix* is the way in which aggregations are computed and represented. *ZAME* simply groups two neighboring nodes into one element in subsequent abstraction levels. *Net-Ray* projects large matrices into a predefined resolution and each cell in the target matrix is given a color based on the average value, which can present a false impression about the data in the original matrix. *MultiLayerMatrix* uses the leader algorithm to cluster similar nodes. In particular, two nodes are considered to be similar if they have similar connections to other nodes. For example, in social networks, two people are considered to be similar if they have similar sets of friends. Nodes in a cluster can thus be drawn from different spatial locations and cluster sizes can vary. This algorithm has been successfully used in clustering similar scatterplots [DW14b], images [DW14a], and proteins with similar biochemical interactions [DMF15].

Existing work that takes advantage of the hierarchical structure to collapse or expand groups for large adjacency matrix visualization is described in a recent state-of-the-art report by Vehlow et al. [VBW15]. In contrast, *MultiLayerMatrix* collapses the characters (nodes) based on the data available directly within the raw adjacency matrix, that is, without requiring a specified hierarchical structure. Inspired by previous work [AvH04, AK02, DFLF15, PF15, vH03], our technique also enables the interactive navigation of the matrix layout, as discussed below.

3. Overview of Visualization Tasks

Taxonomists, ecologists, and phylogeneticists regularly need interact with biological taxonomies in order to make sense of data for a range of scientific tasks. They have a common need to cluster related characters and to manage and to edit taxonomic data. To this end, an effective visualization tool should enable a user to:

- **T1:** Automatically cluster related characters and provide a high level overview of the large character-by-character table.
- **T2:** Merge sets of characters that are determined by the analyst to be identical for the current analysis.
- **T3:** Separate a selected set of characters from a group that is determined by the analyst to be irrelevant. Moreover, the analyst should be able to remove characters that are unnecessary or redundant.

The input data in a typical taxonomic analysis contains both a character-by-character similarity table and a taxon-by-character table, and it is often interesting (albeit challenging) to link both tables in order to visualize interesting patterns. This could lead to the generation of novel hypotheses.

characters in the cluster. The supplementary video shows examples of these cluster curations in action. (The video is also available via our project repository at <https://github.com/CreativeCodingLab/MultiLayerMatrix>).

4.4. Pattern Discovery and Hypothesis Generation

Given a taxonomy with associated characters, analysts would like to zoom into or highlight the branches with certain characters. This feature is interesting to educators and can be used in museums or classrooms as a teaching tool. *MultiLayerMatrix* allows users to select a particular branch in the taxonomy and display related characters (T5). The related characters are defined as the characters that contain some data in the taxon-by-character table within the selected branch, such as a tribe, a genus, or a species. Figure 3 uses the Asteraceae family data. This family contains 10 tribes (in the first column), 137 genera (in the second column), and 537 species (in the third column). The links in this taxonomy are color-encoded by tribe. Ten colors (for the ten tribes) were selected from ColorBrewer [HB03]. The thickness of the links are relative to the number of taxa belonging to these branches. Genera (second column) and species (last column) are ordered based on the tribes that they belong to.

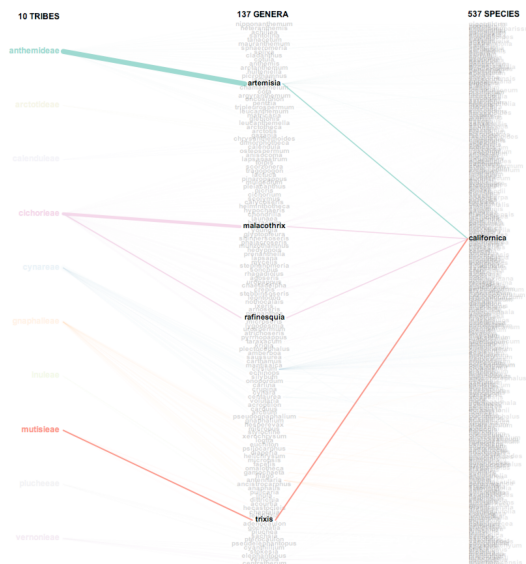


Figure 3: Visualizing the Asteraceae family which contains 10 tribes (color-encoded), 137 genera, and 537 species: Selecting the Californica species in the last column.

Figure 3 shows an example where a particular species, Californica, is selected. As depicted, the Californica species belongs to 4 different genera (Artemisia, Malacothrix, Rafinesquia, and Trixis) which come from 3 different tribes (Anthemideae, Cichorieae, and Mutisiae). Taxonomic names in biology can be complex. At some ranks (for example, family) one word name is sufficient. However, at

sub-ranks, such as tribe or species (sub-species, variety etc.), a binomial naming system is used. For example, a species name has two parts: its genus and its specific epithet (that is, its common name). It is not unusual for a specific epithet to be shared by many genera. The naming system's complexity is reflected by the crossing edges between the second and the last column of Figure 3(a). Related characters of the selected species in Figure 3(b) can be displayed (in the form of a smaller similarity matrix) on demand.

T6 requires exploring the distributions of characters within the input taxonomy. In particular, analysts would like to view character distribution patterns across taxa in order to identify unusual patterns, such as taxa sharing the same characters that are located far apart in a tree. Analysts can choose a group of characters by selecting characters from a cluster or by using the rectangular selection mode to highlight particular characters of interest.

Our technique effectively scales to synthetic datasets with over 20,000 elements. This is ten times larger than the number of characters in the example Asteraceae data, so the adjacency matrix size is 100 times larger. This 20,000 x 20,000 matrix requires nearly all of the memory of our testing computer, a 2.5 GHz Intel Core i7 with 16 GB RAM. The total running time of the leader algorithm on this synthetic dataset is close to 16 seconds on average, generating 50 clusters in the first layer (where each cluster contains roughly 400 elements).

5. Conclusion

In this paper, we presented a novel technique for visualizing and interacting with large matrices by breaking them into multiple layers using the leader algorithm described in Section 4.2. The leader algorithm is roughly linear, making it more scalable than other techniques when working with large networks. We presented this technique using an example dataset which contains a 2,048 x 2,048 character similarity table and a 978 x 2,048 taxon-by-character table. We also ran tests on a 20,000 x 20,000 synthetic character dataset. Future work will explore optimizing our technique (which is completely parallelizable) for even larger datasets. The number of characters can be divided evenly to make use of the available processes and each process will then generate a set of clusters (and leaders) by running the leader algorithm. The results of all processes can then be combined by running the leader algorithm on all leaders (instead of characters) provided by each machine, significantly reducing the running time.

Acknowledgments

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