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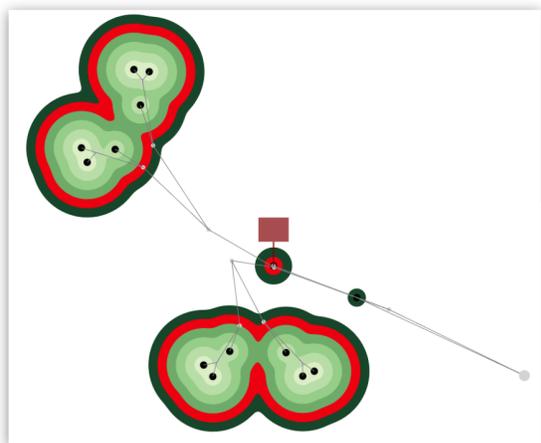
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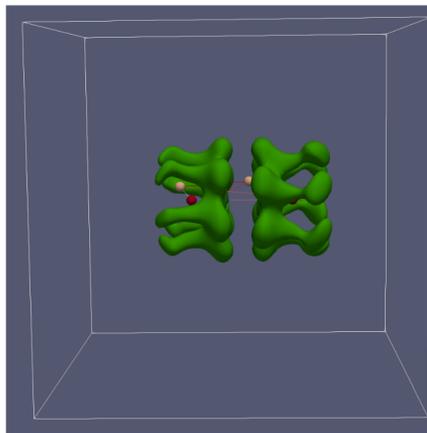
Understanding Merge Trees with Force-Directed Landscapes

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(a) EMD-1134. The merge tree contains 27 nodes after persistence-driven simplification using a 5% threshold.



(b) EMD-1654. The merge tree contains 41 nodes after persistence-driven simplification using a 3% threshold.

Figure 1: Mergescapes for exploring 3D cryo-EM data of proteins and their symmetric regions. Multiscale symmetry in the protein structure is directly perceived from the mergescape shown on the left. A user may selected regions on the layout (red). Corresponding subvolumes are shown in the right.

ABSTRACT

Topological abstractions such as merge trees play an important role in scalar field analysis. However, such abstractions are difficult to interpret and time-consuming. To bridge this gap, we propose *mergescapes*, a force directed landscape for understanding merge trees. We illustrate the usefulness of this design using an application to the study of protein structures.

Keywords: topological data analysis, merge trees, landscape

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1 INTRODUCTION

Topological methods for data analysis have proven to be useful in multiple contexts ranging from exploring molecular surfaces to understanding cyclones. While abstract topological representations are powerful, they are still yet to gain widespread popularity, because their interpretation requires background in algebraic topology and Morse theory. To this extent, multiple attempts have been made to provide user interfaces that convey topological information in an intuitive manner. In this work, we aim at improving the understanding of a topological abstraction called merge tree.

2 MERGE TREES

Consider a scalar function $f: D \rightarrow \mathbb{R}$ defined on a manifold domain D . A value c in the range of f is called an *isovalue*. Given an isovalue, an *isocontour* or *level set* is defined as the collection of

all points $x \in D$ such that $f(x) = c$. A merge tree captures the connectivity of sub-level sets $f^{-1}(-\infty, c]$ (*join tree*) or super-level sets $f^{-1}[c, \infty)$ (*split tree*) of f . The split tree consists of maxima $M = \{M_i\}$, split saddles $S = \{s_j\}$, and the global minimum. The join tree consists of minima $m = \{m_i\}$, join saddles $S = \{s_k\}$, and the global maximum. Figure 2 shows the merge trees for the height function defined on a horse model.

3 METHOD

Mergescape is a force-directed landscape that is constructed directly from a merge tree as opposed to the branch decomposition. It is an intuitive display of the hierarchical structure of the tree and enables comparisons between subtrees at different levels of the hierarchy. Current variants of topological landscapes [1, 2, 7] require a mesh to render a 3D terrain. In contrast, *mergescape* is a planar layout.

The algorithm for constructing *mergescape* follows from Topo-phylogeny [6], a tool for visualizing phylogenetic trees. We adapt the algorithm for merge trees.

Given an input merge tree with weights associated with each node, we first compute a radial layout. The length of the arc subtended at a node with respect to its parent is proportional to the weight of the node. Next, a disk is drawn corresponding to each node. The disk is centered at the node, its radius and color determined by the node’s weight and depth in the tree, respectively. Finally, a force directed layout is computed for the tree nodes and the associated disks. All disks associated with nodes from a common level are blended together when they are rendered on the plane, creating the perception of a single shape. All nodes are attracted to their siblings and relatives, internal nodes are attracted to their children and initial positions, and leaf nodes repel each other based on the cumulative weight of their parents.

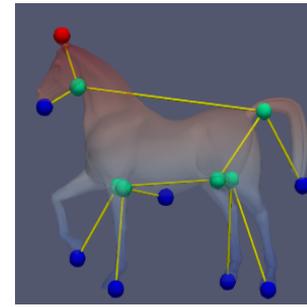
For a split tree, the root corresponds to minima, the saddles to interior nodes and the maxima to leaves. Here, the weights are naturally distributed such that the heaviest nodes are present as leaves, the interior nodes have lower weights, and the root has the lowest weight. This results in a landscape layout, where the nodes organically attract and repel each other, allowing for easy topological exploration. Conversely, for a join tree, the interior nodes are heavier compared to leaf nodes. Then, the input nodes to the landscape should be inversely weighted.

4 EXAMPLES

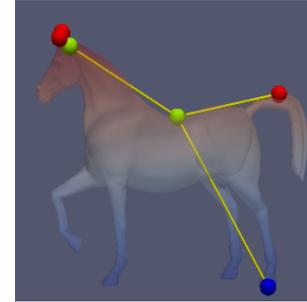
Understanding symmetry in scalar fields using merge trees has been well studied [4, 5]. Current approaches focus on automated symmetry detection. Instead, we propose to use *mergescapes* for perceptually understanding multiscale symmetry.

We discuss how *mergescapes* help a user identify symmetry in cryo-electron microscopy images of two proteins: EMD-1134 and EMD-1654 [3]. Figure 1 shows the *mergescape* for the two datasets. In both cases, we construct the merge tree on the maxima. The weight associated with a node is equal to the volume corresponding to the subtree above the node in the merge tree. The user interacts with the *mergescape* to browse through different scales, select subtrees to view the corresponding subvolumes, and identify different relationships.

The multiscale symmetry is easily perceived in these datasets. In EMD-1134, we identify and select two symmetric structures from the *mergescape* and in the case of EMD-1654, we identify and select four such structures. Based on our experience with exploring cryo-EM data using *mergescapes*, we recommend their use after a noise removal stage that removes small sized features. The user is less likely to identify interesting structures directly from large trees without noise removal. Further, the force directed layout converges slowly for large trees.



(a) Join Tree



(b) Split Tree

Figure 2: Merge trees for a horse model on the height field rendered using a blue-red colormap (blue to red). Maxima are shown in red, join saddles in dark cyan, split saddles in light green, and minima in blue.

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