Generating and Exploring a Collection of Topological Landscapes for Visualization of Scalar-Valued Functions

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Introduction

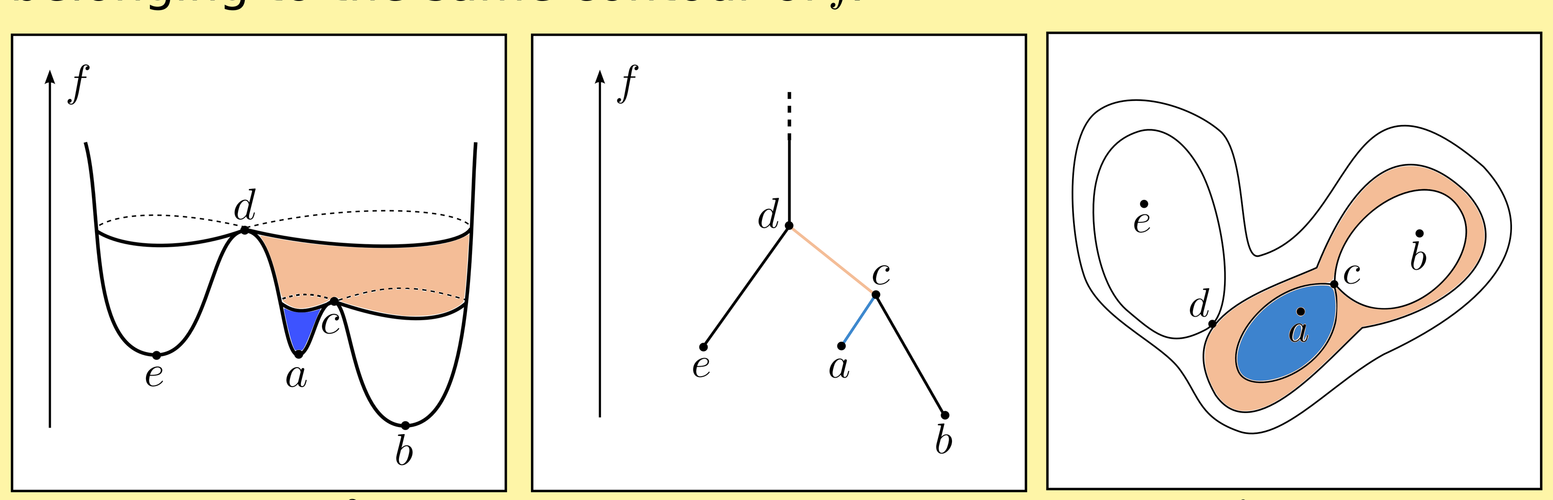
Visualizing scalar functions $f : D \to \mathbb{R}$ is an important aspect of scientific data analysis. Scalar functions are prevalent in a variety of disciplines and sometimes admit simple and natural visualizations when D takes certain forms, especially low-dimensional Euclidean spaces or manifolds.

However, as the dimensionality or complexity of D increases, an effective visualization technique may no longer be obvious. Dimensionality reduction techniques such as PCA, ISOMAP, or Laplacian Eigenmaps focus on preserving metric information, but there is usually no guarantee that the topological structure of f is preserved.

We present a method for visualizing by constructing a family of new scalar fields $g_i : [0,1]^2 \to \mathbb{R}$ whose contour trees and topological persistences are identical to those of f. We call these functions *terrain models*. We also present a method for visually exploring this space of possible terrain models.

The Contour Tree

Let $f : M \to \mathbb{R}$ be a scalar field defined on a simply connected domain M. A contour of f is a set $f^{-1}(\alpha) := \{x \in M \mid f(x) = \alpha\}$ for some value $\alpha \in \mathbb{R}$. As we vary α, the connected components in the level set may appear, disappear, split, and merge. The contour tree of f tracks such changes; it is the quotient space induced by the equivalence relation of points belonging to the same contour of f.



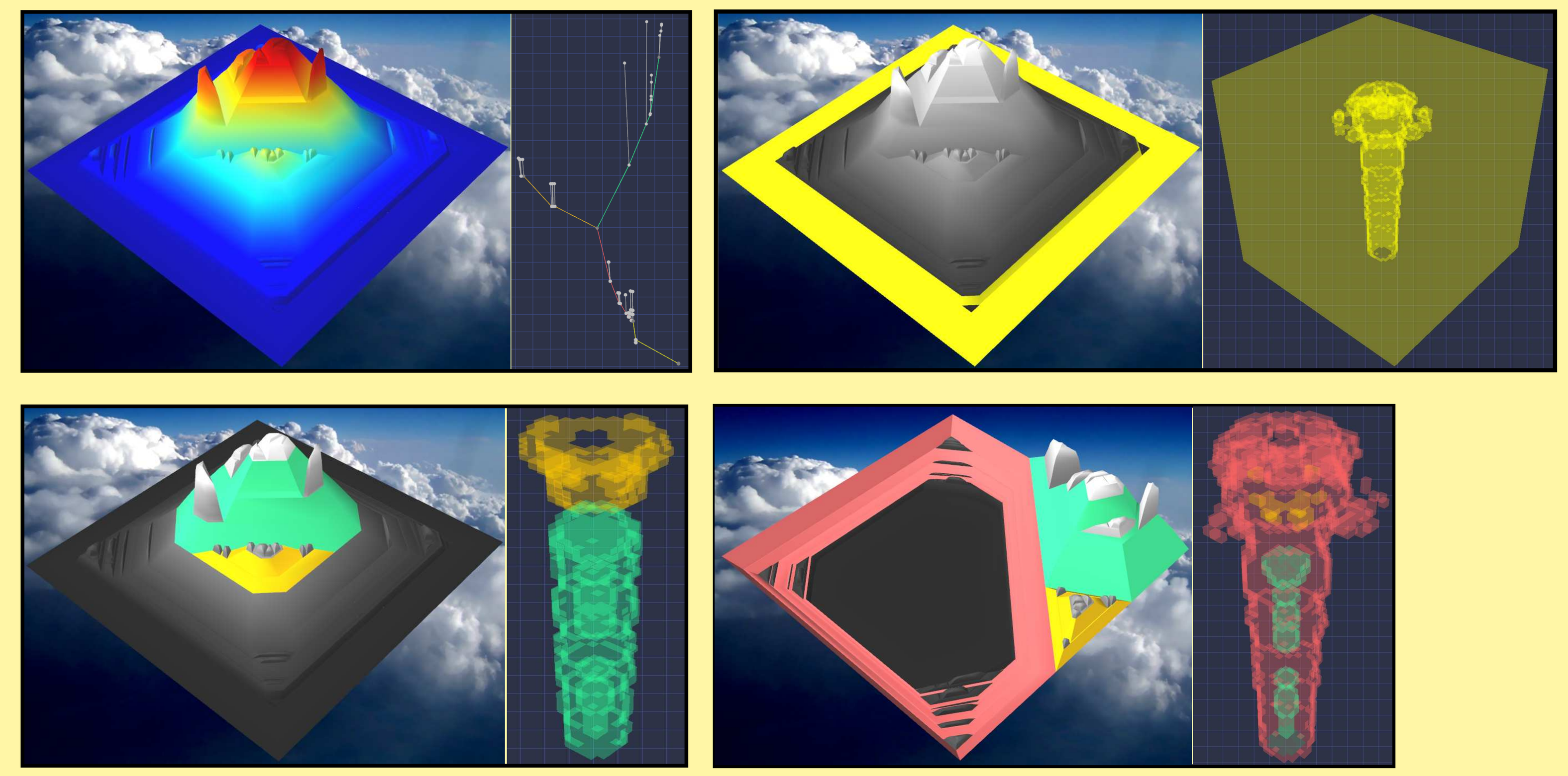
A scalar function $f : \mathbb{R}^2 \to \mathbb{R}$ — The contour tree of f — Contours of f at critical points

Terrain Model Configuration

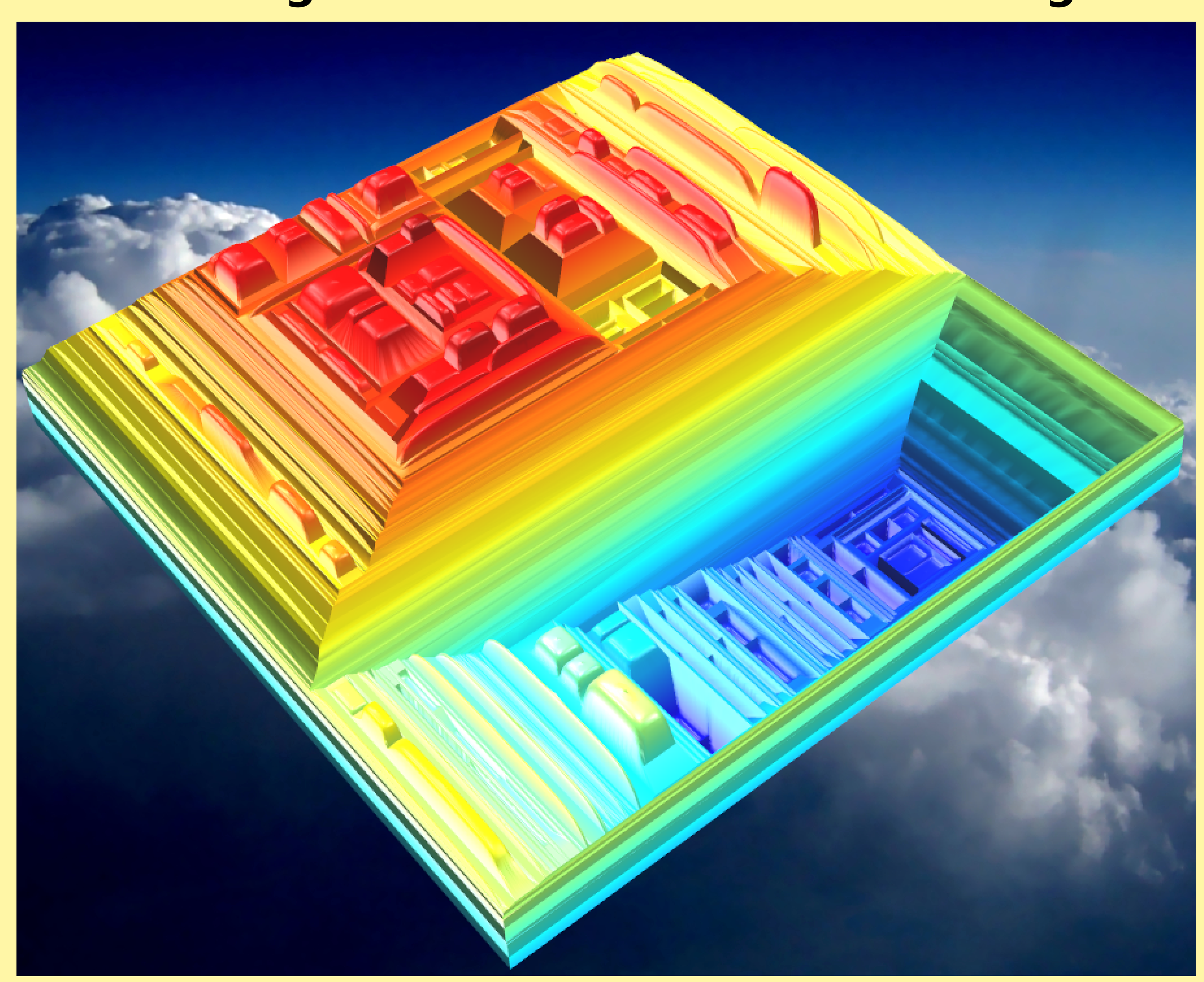
Choosing a point at infinity z induces a partial ordering on the points $x \in \mathcal{T}(h_z)$ indicating the nesting relationships of their corresponding contours in h_z. This induces an arborescence $\mathcal{A}^z_{\mathcal{T}}(f)$ whose edge directions indicate contour inclusion relationships. We call the arrangement of the contours of h_z in the plane a *terrain model configuration.*

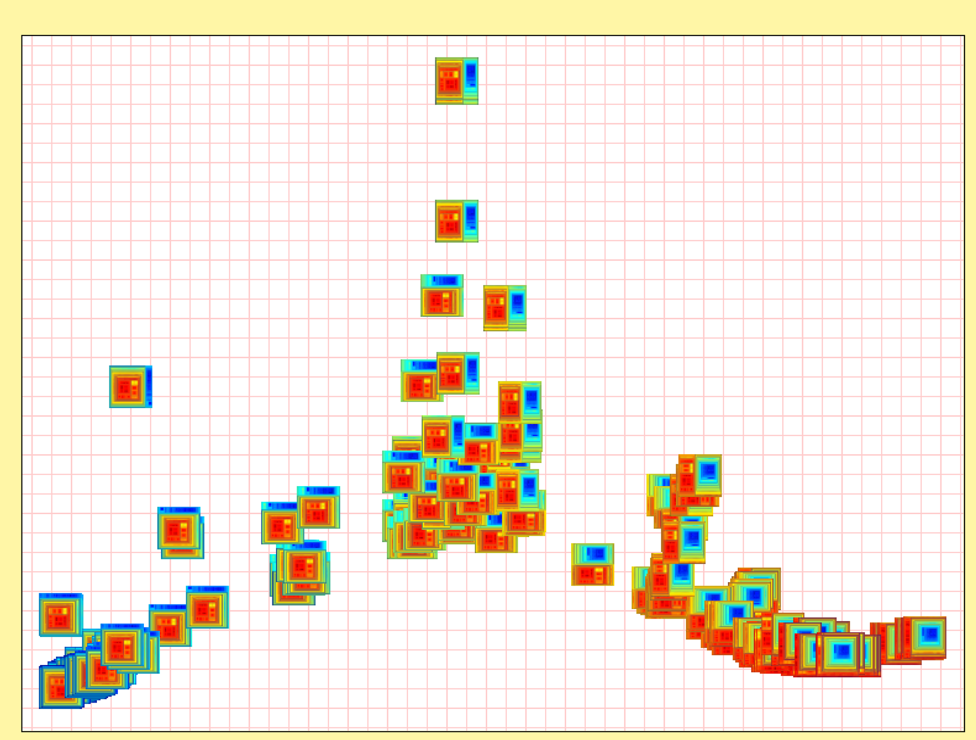
Any treemap algorithm can be used to translate $\mathcal{A}^z_{\mathcal{T}}(f)$ into a configuration, guaranteeing that the areas of the topological components of the configuration exactly match the (scaled) volumes of their high-dimensional counterparts. Function values between adjacent contours are interpolated using a standard Gaussian-weighted Laplacian.

Results: Volumetric Data

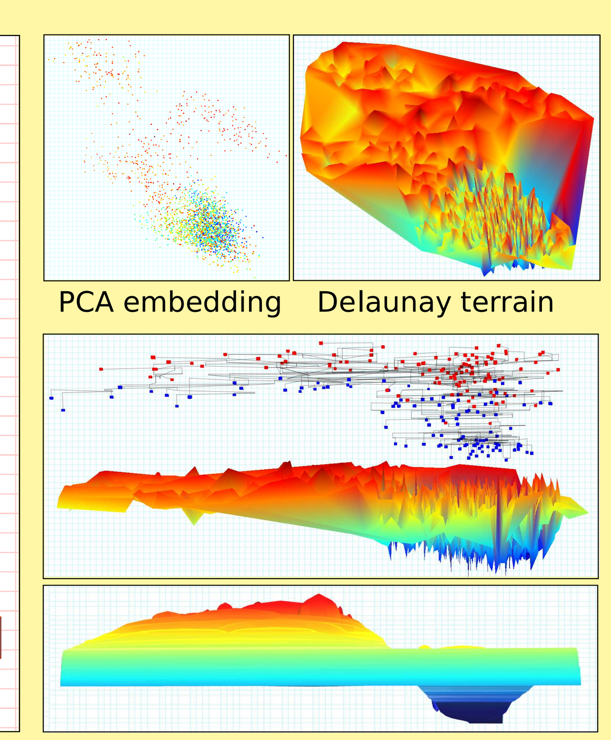


Results: High-Dimensional Protein Folding Data





ISOMAP visualization of the space of possible terrain models



PCA embedding — Delaunay terrain

PCA (above) and our result (below)

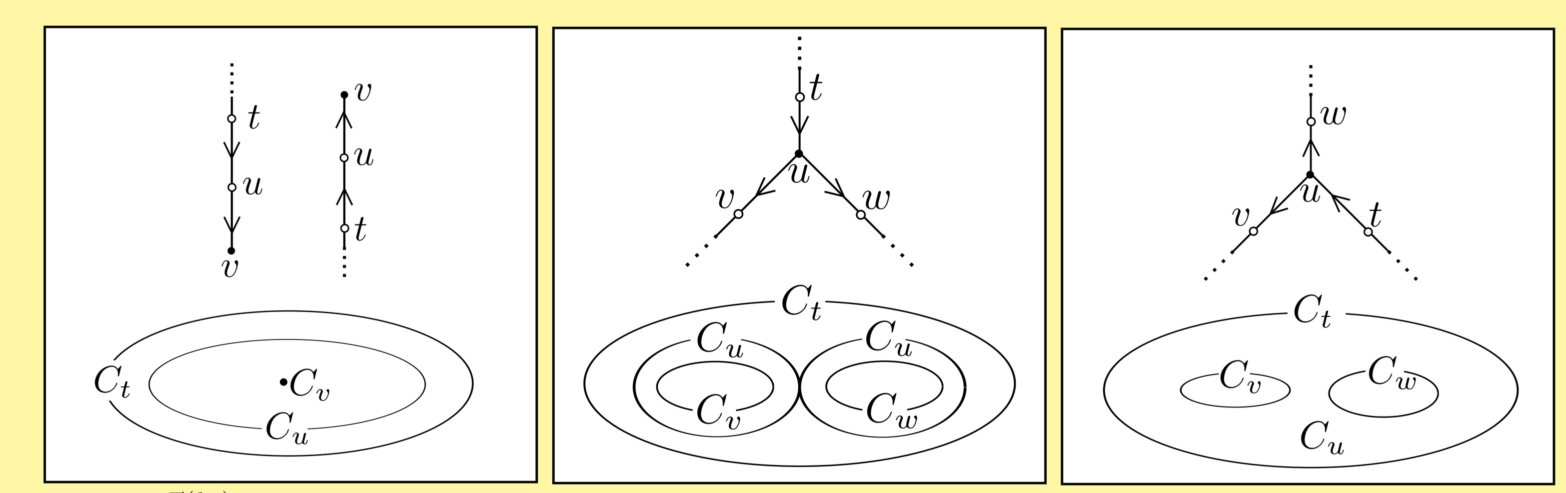
An Ensemble of Equivalent Functions

Let $\mathcal{T}(f)$ be the contour tree of f. There exists a unique function $g : S^2 \to \mathbb{R}$ on the two-sphere with an identical contour tree. A compactification of S^2 (via identifying a point at infinity z) yields a homeomorphism Φ_z between the open set and $\mathbb{R}^2$. Φ_z maps the function $S^2_z := S^2 \setminus \{z\}$ on S^2 to a planar terrain $F_z : \mathbb{R}^2 \to \mathbb{R}$ defined as $F_z := h \circ \Phi_z$.

The interior of the unit square $[0,1]^2$ is homeomorphic to $\mathbb{R}^2$, ergo we can construct functions $h_z : [0,1]^2 \to \mathbb{R}$ such that $\mathcal{T}(f) = \mathcal{T}(h_i)$. We call the resulting functions h_z *terrain models* and the equivalence class $[h] = \{h \in \mathbb{R}^{[0,1]^2} | \mathcal{T}(h) = \mathcal{T}(f)\}$ an *ensemble of terrain models*.

Exploring the Space of Visualizations

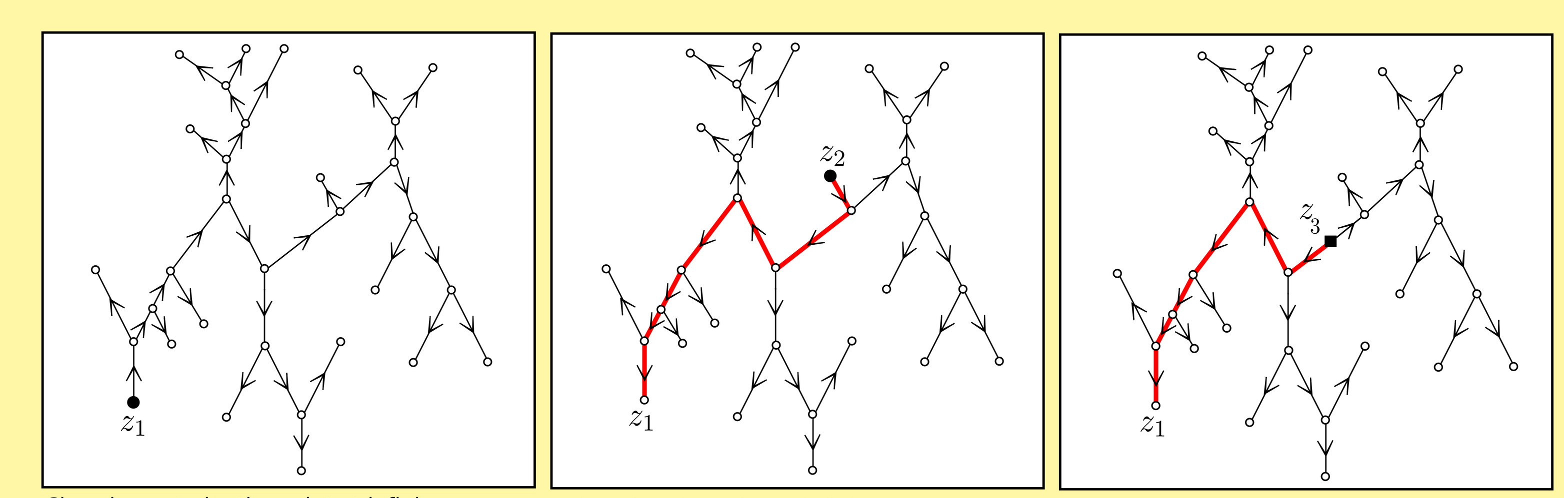
By using the (scaled) volumes of the topological components of as weights on their corresponding edges in $\mathcal{T}(f)$, we derive an earth mover's distance between two terrain models z_i and z_j giving the total weight of the unique path connecting them in $\mathcal{T}(f)$. We use this metric to compute an ISOMAP embedding of the possible terrain models and provide a user interface which enables real time exploration of the data.



When $v \in \mathcal{T}(h_z)$ is a lower leaf or an upper leaf, the contours (C_t, C_u, C_v) corresponding to (t, u, v) are nested as shown.

Here, u is a saddle point. Its corresponding contour C_u resembles a lemniscate curve.

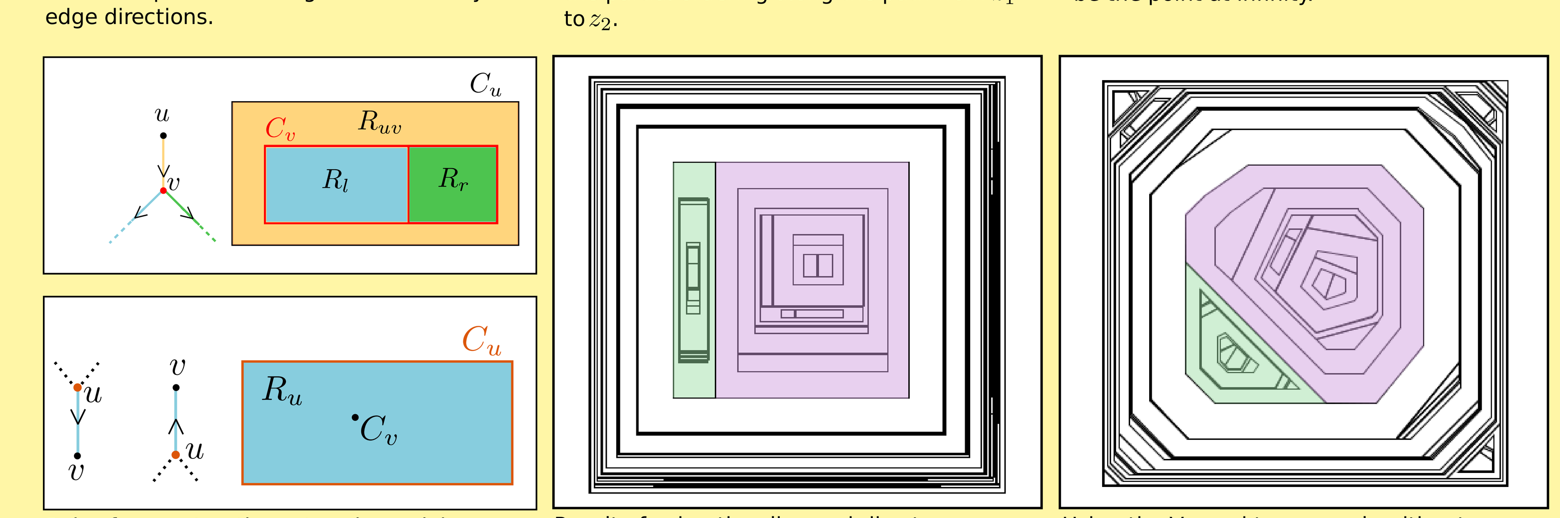
In this case, u is a saddle point, but a different point at infinity is used, resulting in a slightly more complicated nesting of the contours.



Choosing z_1 to be the point at infinity induces a partial ordering as indicated by the edge directions.

Changing the point at infinity to z_2 reverses the partial ordering along the path from z_1 to z_2.

An example of using a noncritical point z_3 to be the point at infinity.



Rules for constructing a terrain model configuration. Top: The configuration of a saddle point. Bottom: The configuration of a local extremum. Any treemap algorithm can be used; simple slice-and-dice is used here.

Result of using the slice-and-dice treemap algorithm to produce a terrain model configuration.

Using the Voronoi treemap algorithm to produce a terrain model configuration.