Visualizing Multimodality in Combinatorial Search Landscapes

Xavier F. C. Sánchez Díaz   Ole Jakob Mengshoel

Norwegian University of Science and Technology

Abstract

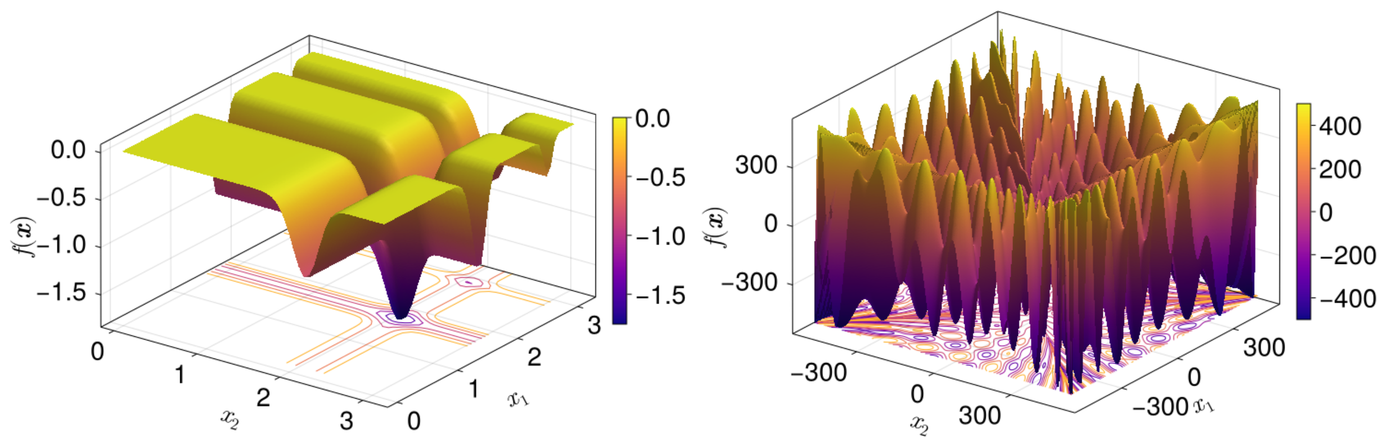
We present different visualization techniques for **combinatorial search landscapes**, focusing on **multimodality** (search spaces with multiple optima). We illustrate some of these techniques and discuss how to combine them via **juxtaposition** and **superimposition** based on their geometric and aesthetic elements according to the Grammar of Graphics, to provide a more comprehensive view of the search space. We use **Feature Selection** under **Regularization** as a study case, where each optimum is a subset of features used to train a Machine Learning (ML) model.

What is a *Search Landscape?*

A *search landscape* is a visual representation of the solution space, as it is navigated by a search method or optimization algorithm. Any search landscape can be represented using a tuple $\mathfrak{L} = (\mathcal{X}, f, \mathcal{N})$, where $\mathcal{X}$ is the search space, f is a *fitness* or objective function, and $\mathcal{N}$ is any neighborhood or notion of accessibility from a given state $\boldsymbol{b} \in \mathcal{X}$.

In our case, $\mathcal{X}$ is set of bitstrings $\boldsymbol{b}$ representing a feature subset used to train an ML model, f is the classification error over a given dataset, and $\mathcal{N}(\boldsymbol{b})$ is the set of all bitstrings at a Hamming distance of 1 from $\boldsymbol{b}$.

We define a local optimum $\boldsymbol{b}^+$ as a solution which is not worse than its neighborhood, and denote the set of all local optima in a landscape with the symbol $\mathcal{L}$. A global optimum is denoted as $\boldsymbol{b}^*$, which is the $\boldsymbol{b}^+ \in \mathcal{L}$ with the lowest fitness value $f(\boldsymbol{b}^+)$.



(a) Michalewicz function   (b) Rana's function

Figure 1. The landscapes of some 2D test functions in the continuous domain [5].

Distance-Fitness Correlation and Number of Optima

A common approach to highlight multimodality in combinatorial search spaces is plotting the correlation between the distance between local optima, against their objective function values—either aggregated into bins or as a scatter plot.

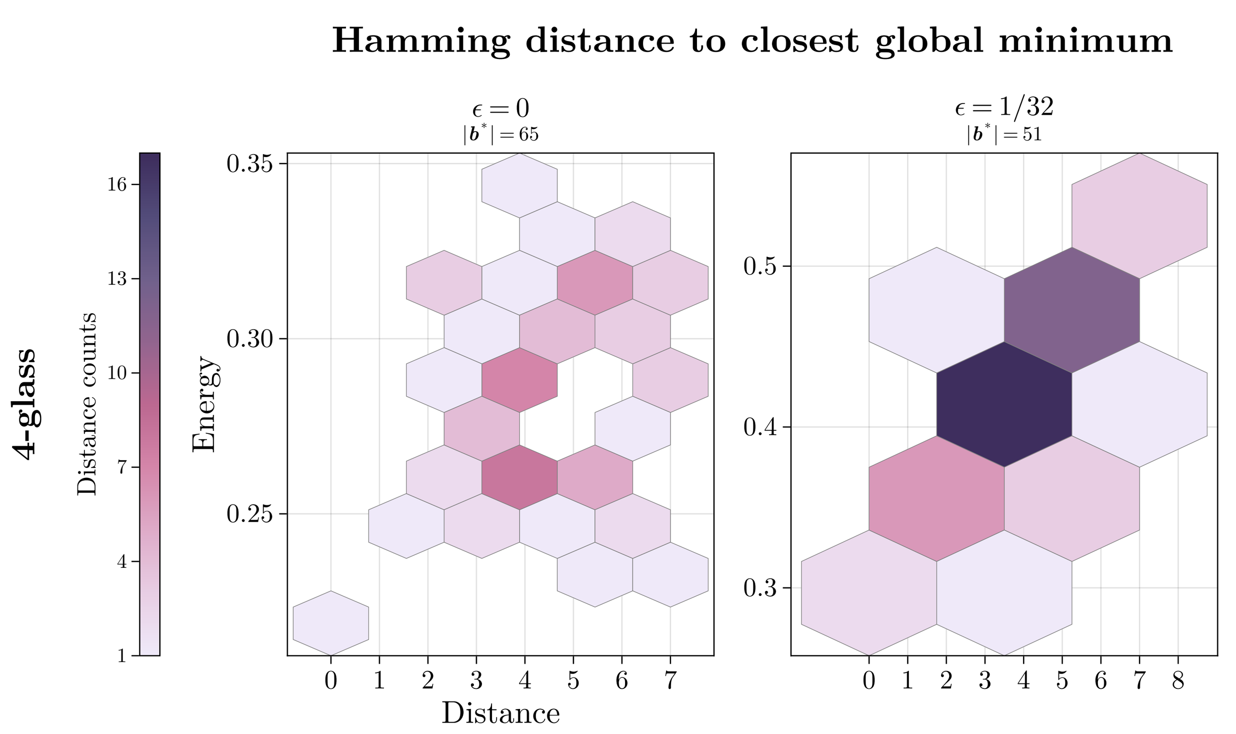
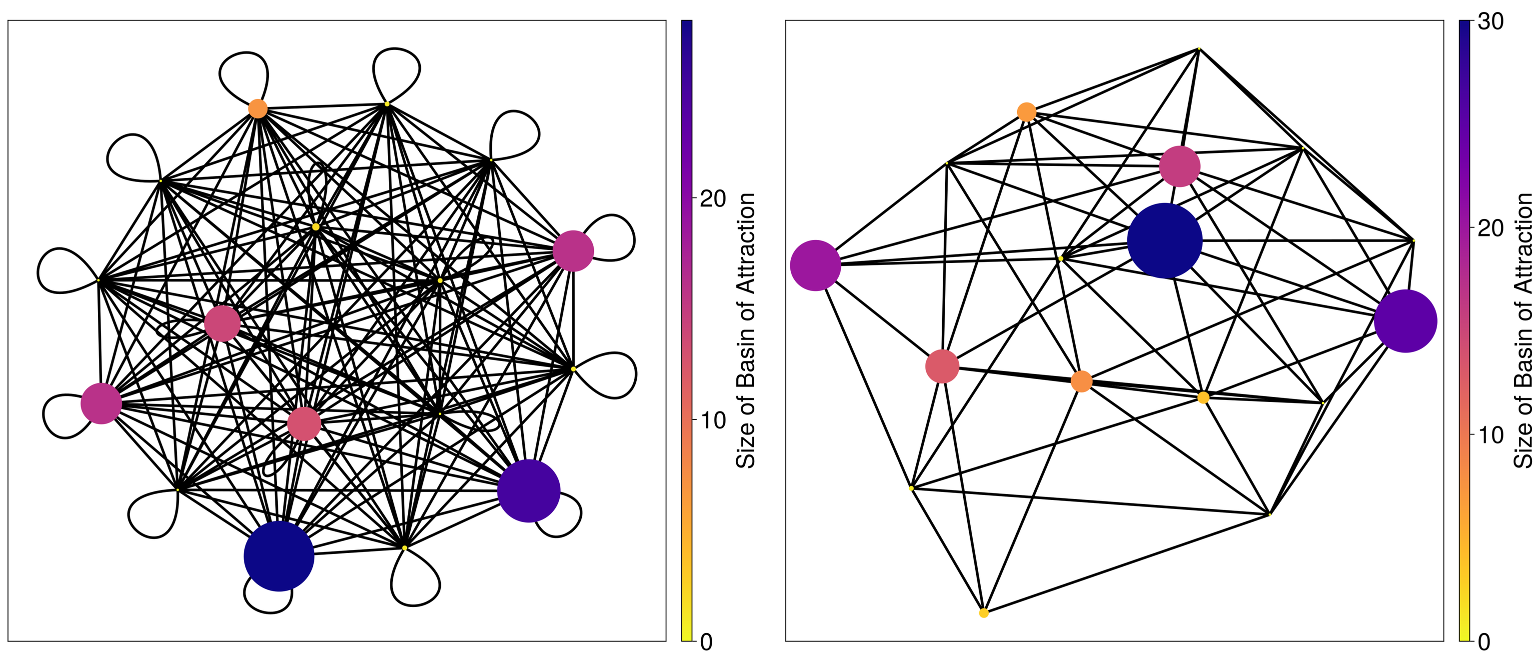


Figure 2. **Juxtaposition** of two Hex-bin plots of the distance-fitness correlation for the Glass Identification dataset [1], using a decision tree classifier under two levels of regularization (ϵ). Each bin aggregates different number of local optima, and a darker shade means a higher concentration of optima.

Connectedness and Local Optima Networks (LONs)

LONs are graphs where vertices represent the local optima, and the edges represent *paths* between them. Size and color are usually employed to represent the size of *basins of attraction*, but can also be used to communicate the fitness of each optimum [4].



(a) A LON with all basin transition edges   (b) A LON with escape edges with $D = 3$

Figure 3. LON-LON: **Juxtaposition** of two LONs, representing the feature selection problem on the E-coli dataset [3], using a decision tree classifier. In 3b, the edges are only kept if the Hamming distance between local optima is less or equal than D.

Hinged-Bitstring Maps (HBMs)

HBMs plot the entire search space. Each solution is split into two halves, and each half is converted to its decimal representation and then mapped to an axis—the first half uses the x-axis, and the second half uses the y-axis. Solutions are plotted using their (x, y) coordinates and colored by their fitness value. Optima are highlighted with a colored outline.

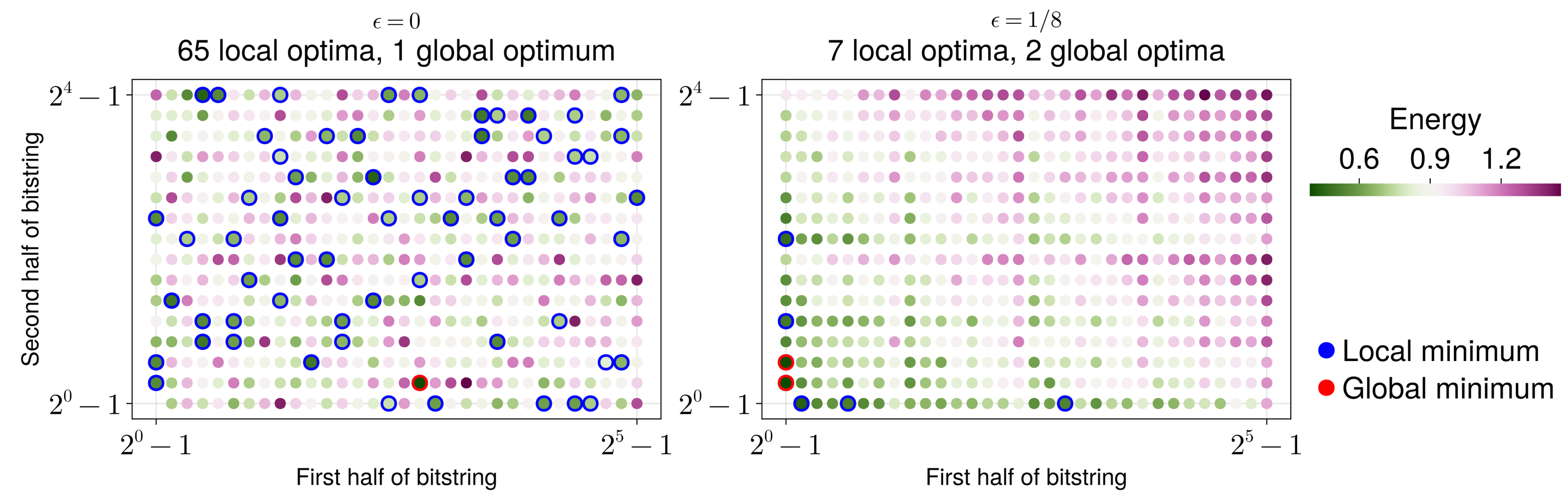


Figure 4. HBM-HBM: **Juxtaposition** of two HBMs for the Glass Identification dataset [1], using a decision tree classifier under two different values of regularization ϵ.

Combining Visualizations

Since different visualizations highlight different aspects of the search space, combining them can provide a more comprehensive view of a combinatorial landscape. In this work, we focus on **juxtaposition** and **superimposition** as bases for combining visualization techniques.

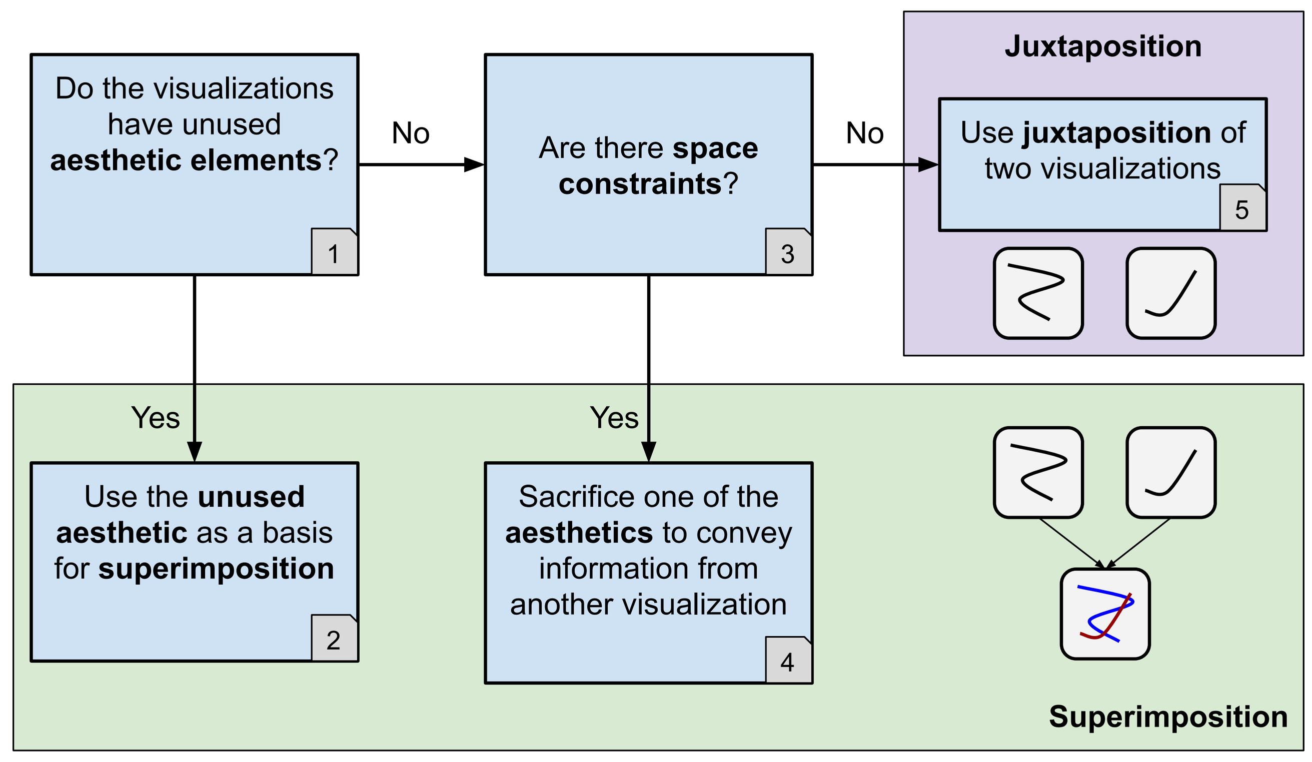


Figure 5. A simple process for combining visualizations. **Superimposition** may require some data transformations, while **juxtaposition** demands more space.

Figures 1, 2, 3 and 4 are examples of the **juxtaposition** of two visualizations. Below, we combine a LON and an HBM via **superimposition**.

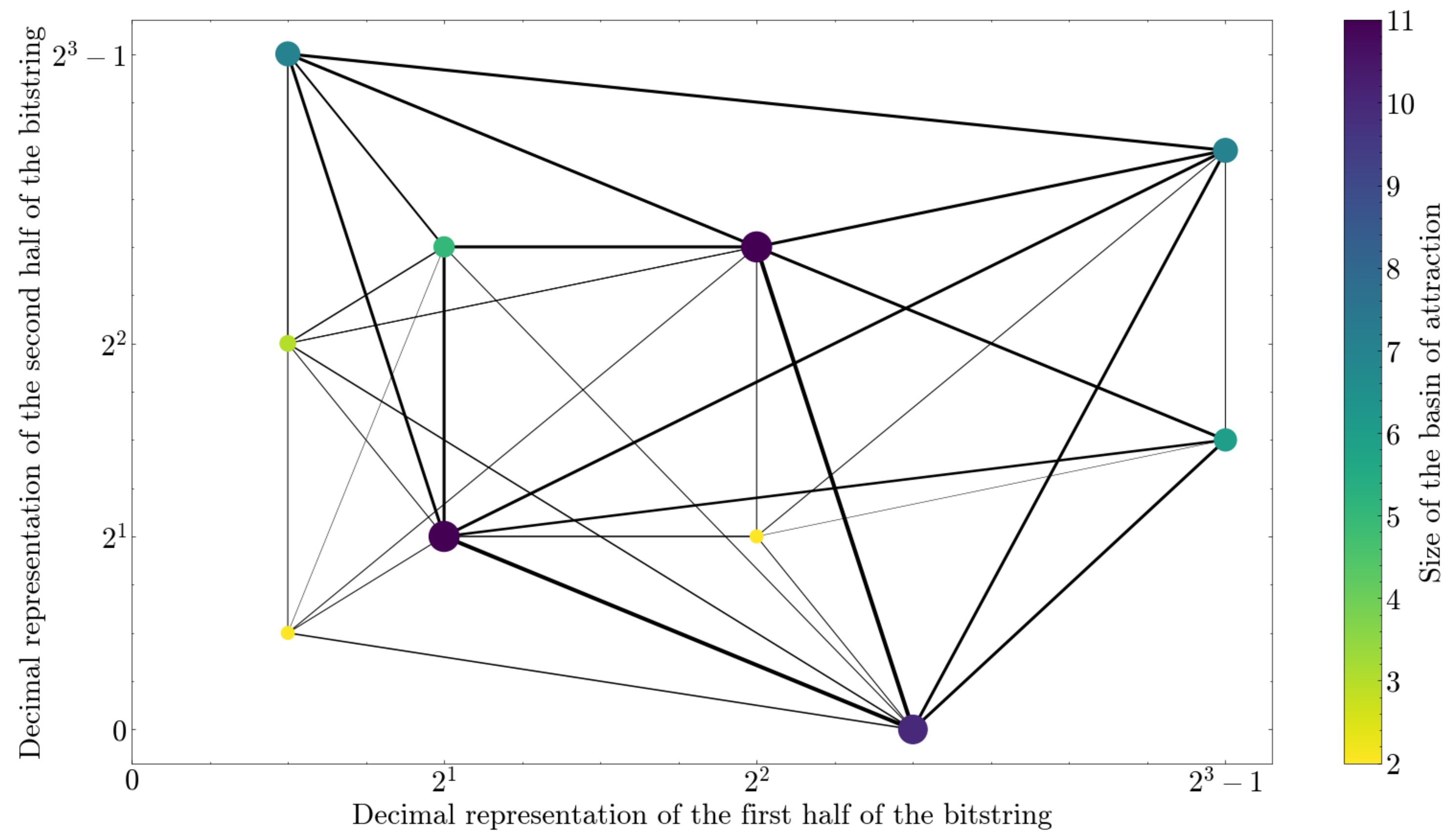


Figure 6. LON+HBM: **Superimposition** of a LON on the HBM coordinate system to visualize a toy problem: $f(\boldsymbol{b}) = \sin(2\,\mathrm{Dec}(\boldsymbol{b}))$, $\forall \boldsymbol{b} \in \mathbb{B}^6$. Color and size are used to represent the size of the basin of attraction [2].

Aesthetic and Geometric Properties of Combined Plots

Table 1. Aesthetic and geometric elements used by LONs and HBMs. Some attributes are not used in the visualization and can therefore be used as a basis for **superimposition**.

Plot type	Geoms		Aesthetics			
	Primary	Secondary	Color	Size	Position	Visibility
LON	Circle	Lines	Basin of attraction	Basin of attraction	N/A	$\mathcal{L} \subset \mathcal{X}$
HBM	Circle	Rings	Fitness	N/A	$\boldsymbol{b}$	$\mathcal{X}$
Combined visualizations						
LON-LON	Circle	Lines	Basin of attraction	Basin of attraction	N/A	$\mathcal{L} \subset \mathcal{X}$
HBM-HBM	Circle	Rings	Fitness	N/A	$\boldsymbol{b}$	$f \circ \mathcal{X}, f' \circ \mathcal{X}$
LON+HBM	Circle	Lines	Basin of attraction	Basin of attraction	$\boldsymbol{b}$	$\mathcal{X}$

Further Reading

More visualization methods, in-depth explanations and references can be consulted in the full report: `https://s.ntnu.no/visual-landscape`.