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Visualizing and Controlling the Optimization Process of Geometric Multidimensional Scaling

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Multidimensional Scaling (MDS) is a special technique for dimensionality reduction and data visualization, aiming to represent high-dimensional data in a low-dimensional Euclidean space. The quality of this representation is typically improved by minimizing a stress function.

However, the stress function is well-known for being non-convex, characterized by a complex surface with numerous local minima. Traditional optimization algorithms, most notably SMACOF (Scaling by Majorizing a Complicated Function), often become trapped in these inferior solutions. Furthermore, these algorithms operate as “black boxes”, providing researchers with little insight into the optimization process and no tools to identify or improve an inferior result. The consistency of the outcome heavily depends on the random initial configuration, making MDS analysis often frustratingly unclear.

This research introduces a paradigm shift by leveraging the Geometric Multidimensional Scaling (GMDS) method to transform this unclear process into one that is transparent, interpretable, and controllable. GMDS is derived from a clear geometric interpretation of the optimization problem, where the iterative step is defined as the centroid of intermediate points representing ideal locations based on individual dissimilarities. Crucially, this geometric step has been proven to correspond exactly to the anti-gradient direction of the local stress function. We utilize this analytical foundation to deconstruct the optimization process.

By employing dynamic visualization tools (Desmos, GeoGebra) and conducting a thorough asymptotic analysis of the GMDS iteration formula, we map the optimization process. The asymptotic analysis reveals that as a point approaches singularities (coinciding points) or diverges to infinity, the subsequent GMDS steps converge to well-defined hyperspheres. These hyperspheres form a “topographical map” of the stress structure, visualizing the basins of attraction.

While this visualization provides profound insight, we found that visual inspection alone is insufficient to consistently differentiate global minima from local ones. This motivated the development of a novel, analytically driven assessment and iterative improvement cycle. This enhanced GMDS framework allows us to analytically determine whether any point in the configuration is trapped in a local minimum. If so, the algorithm systematically relocates the point to a globally superior position and re-optimizes the configuration.

Empirical studies demonstrate that this enhanced GMDS consistently outperforms SMACOF, achieving lower stress values. Additionally, the intrinsic structure of GMDS is highly suitable for parallel computing, allowing for the efficient processing of large datasets. By integrating geometric intuition, visual analysis, and analytical precision, this work not only presents a superior algorithm but also fundamentally changes how researchers can interact with and control dimensionality reduction optimization problems.