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New Tools for the Visualization of Biological Pathways

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Abstract

This paper presents several geometrically motivated techniques for the visualization of high-dimensional biological data sets. The Grassmann manifold provides a robust framework for measuring data similarity in a subspace context. Sparse radial basis function classification as a visualization technique leverages recent advances in radial basis function learning via convex optimization. In the spirit of deep belief networks, supervised centroid-encoding is proposed as a way to exploit class label information. These methods are compared to linear and nonlinear principal component analysis (autoencoders) in the context of data visualization; these approaches may perform poorly for visualization when the variance of the data is spread across more than three dimensions. In contrast, the proposed methods are shown to capture significant data structure in two or three dimensions, even when the information in the data lives in higher dimensional subspaces. To illustrate these ideas, the visualization techniques are applied to gene expression data sets that capture the host immune system's response to infection by the Ebola virus in non-human primate and collaborative cross mouse.

Keywords: Data visualization, Grassmannian embedding, Autoencoder, Centroid-encoder, Sparse radial basis functions, Ebola virus

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