

Dimensionality reduction

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Concepts and applications in scRNA-seq and DNA microscopy

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Dimensionality reduction is a widely applied set of methods in various data analysis pipelines. It has three main aims:

- *Describe the data manifold*

Parametrise a space that we believe the observed data lives in. This space also serves as generalisation of where we expect future data to show up. Furthermore certain parameterisations - together with information not contained in the dataset - may facilitate interpretation of features.

- *Reduce the observation noise*

We may separate the data variance into "within-manifold" (signal) and "out-of-manifold" (noise).

- *Visualise the concepts discovered in the data*

Most collected data nowadays is very high (100+) dimensional, whereas most humans can only conceptualise a few dimensions at once. We have the responsibility to choose the most effective, yet accurate visualisations of the data to communicate features of the data

These goals are often interspersed, yet both the researcher and their audience should be clear on why a dimensionality reduction method was applied, even when the mathematical methodology to achieve each goal may be the exact same.

- *Manifold learning* (e.g. Isomap)
Estimate within-manifold distances, predict what data is likely in the future, learn about structure embedded within the data

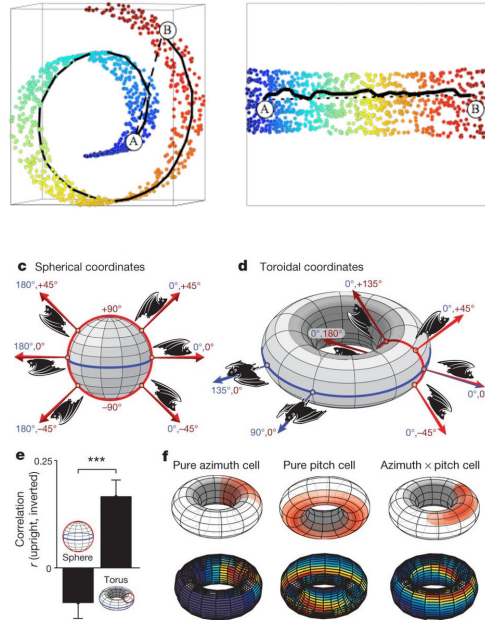


Figure 1: Examples for manifold estimation. (top) Swiss roll artificial dataset shows the concepts of a 2D manifold embedded in 3D (color purely serves as visual aid). (bottom) Comparing different manifold hypotheses (spherical vs toroidal) in behaving bats to explain neural variability (*Finkelstein et al, Nature 2015*)

- *Feature discovery* (e.g. PCA, ICA)
Find a meaningful "basis" for the manifold - a set of features whose combination explains the data well, and
- *Reduce observation noise* (e.g. PCA, pPCA, FA)
TODO
- *Visualise high-D data* (e.g. t-SNE)
TODO