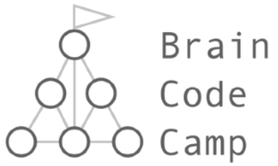

Nonlinear Dimensionality Reduction

Itthi Chatnuntawech

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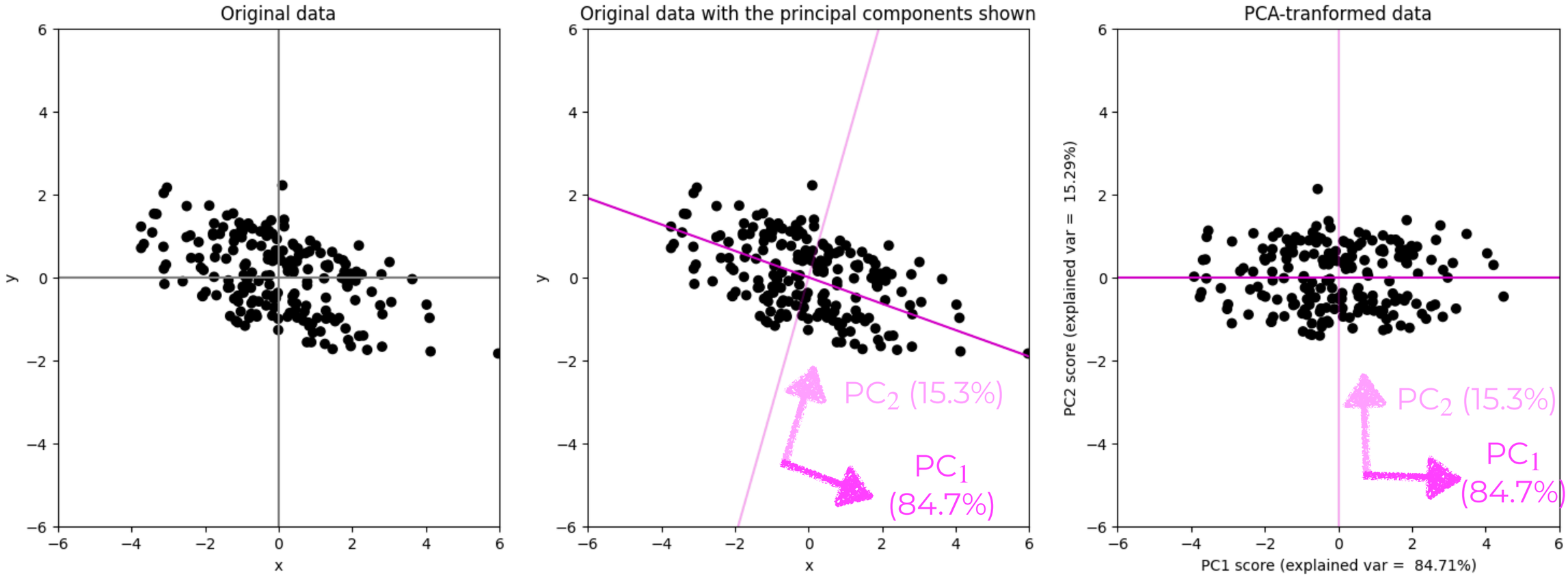
PCA Example



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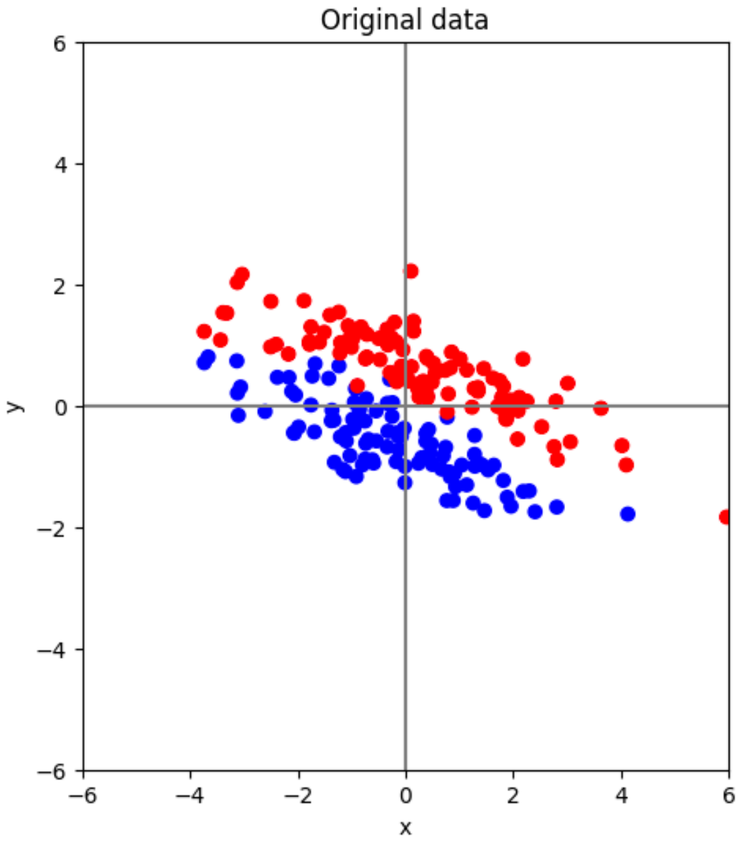
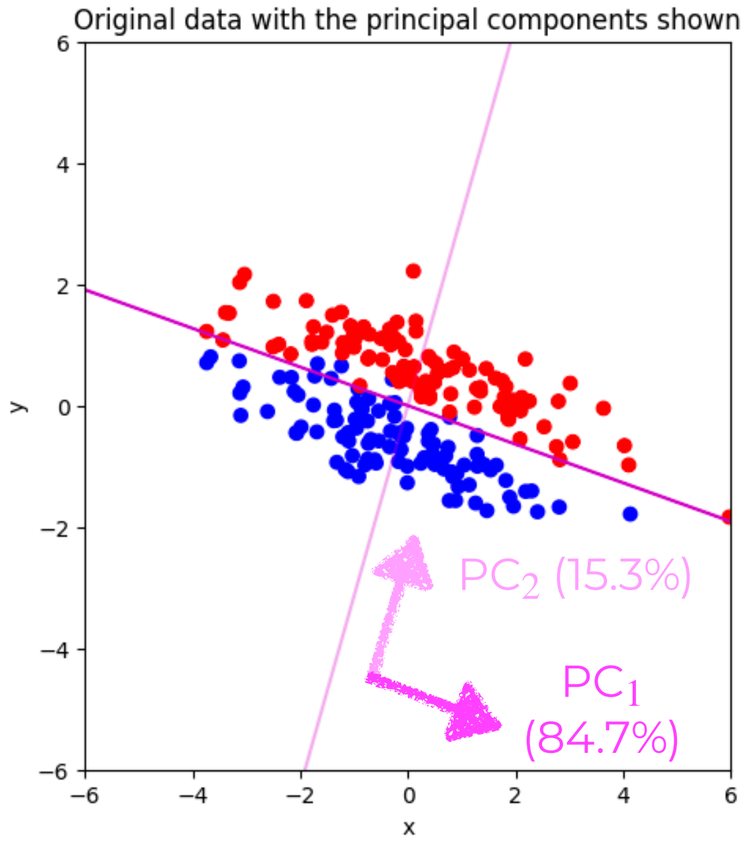
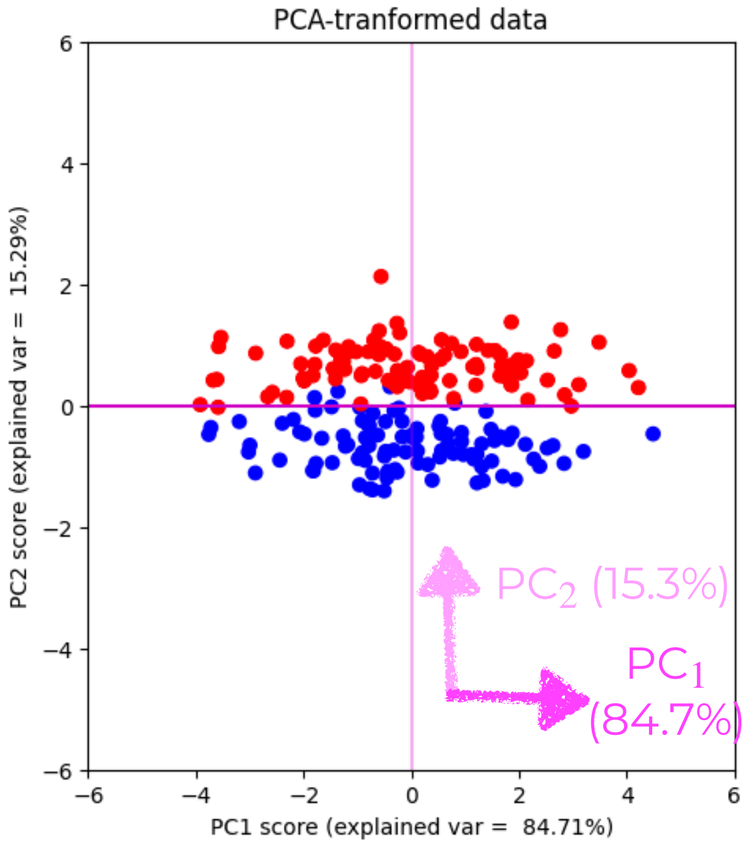
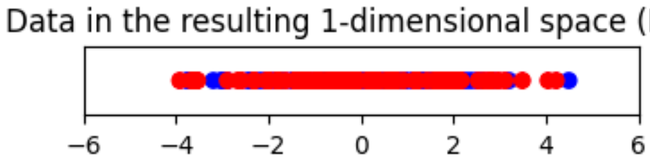
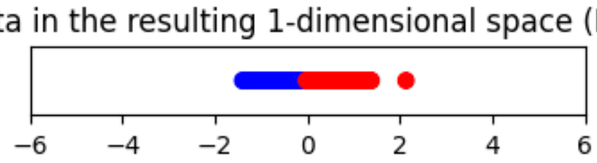
PCA Example











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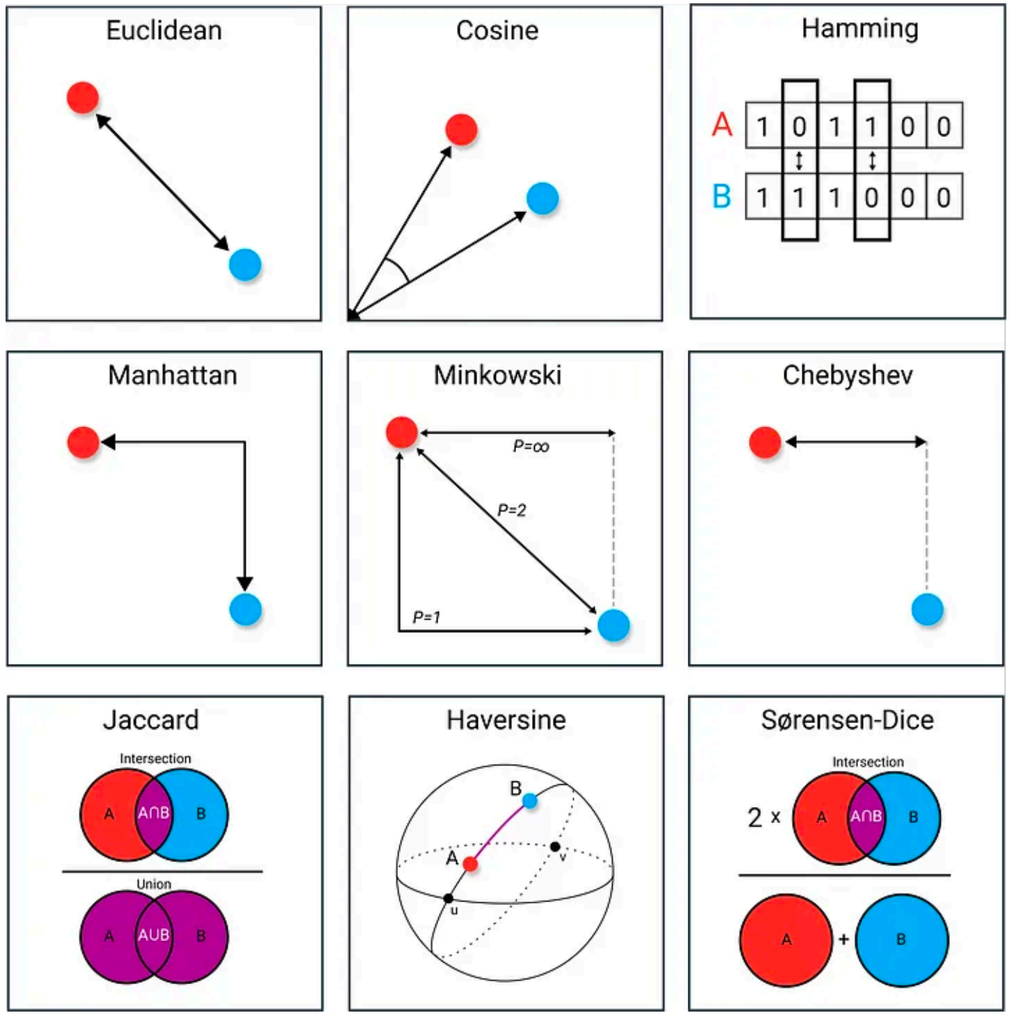
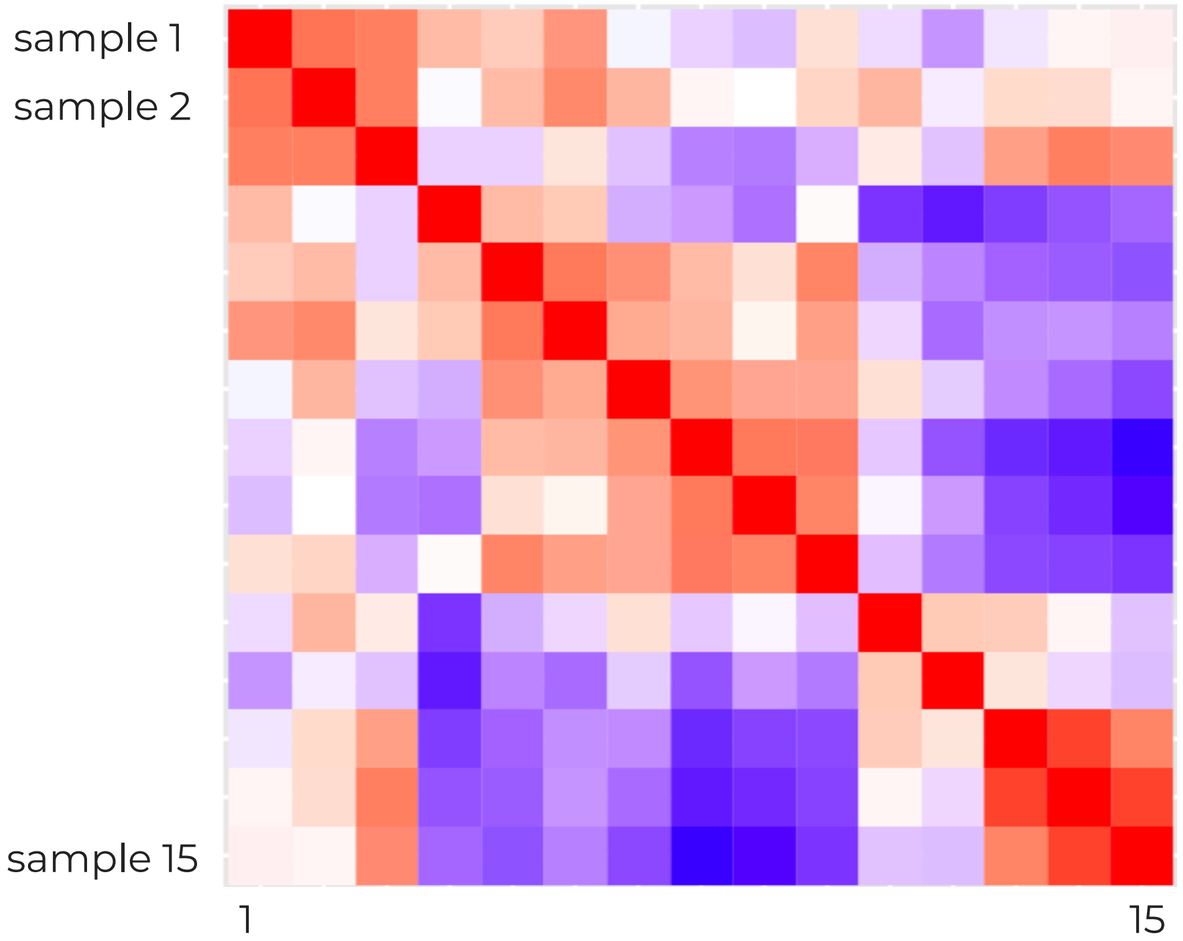
Distance Measures



https://towardsdatascience.com/9-distance-measures-in-data-science-918109d069fa

Pairwise Distance Matrix



The element at row i and column j represents the distance between sample i and sample j

$$D_{ij} = D_{ji}$$

$$D_{ii} = 0$$

Modified from https://www.datanovia.com/en/lessons/clustering-distance-measures/

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Generalized Multi-Dimensional Scaling (MDS)

High-dimensional feature space

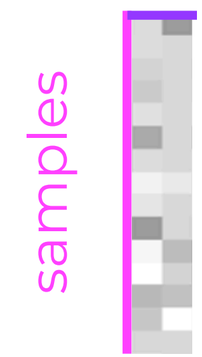
features

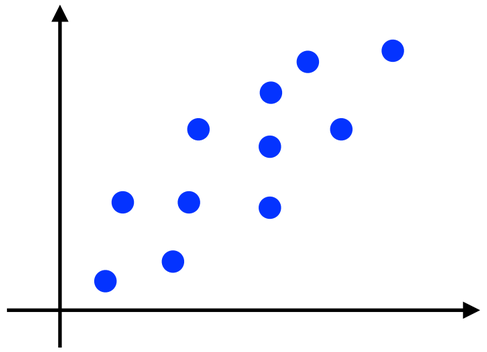
samples

Low-dimensional space

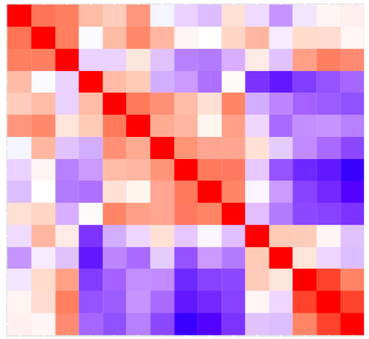
new features

samples





pairwise distance matrix created using any types of distance



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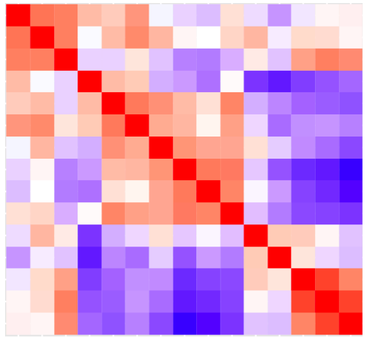

pairwise distance matrix created using any types of distance

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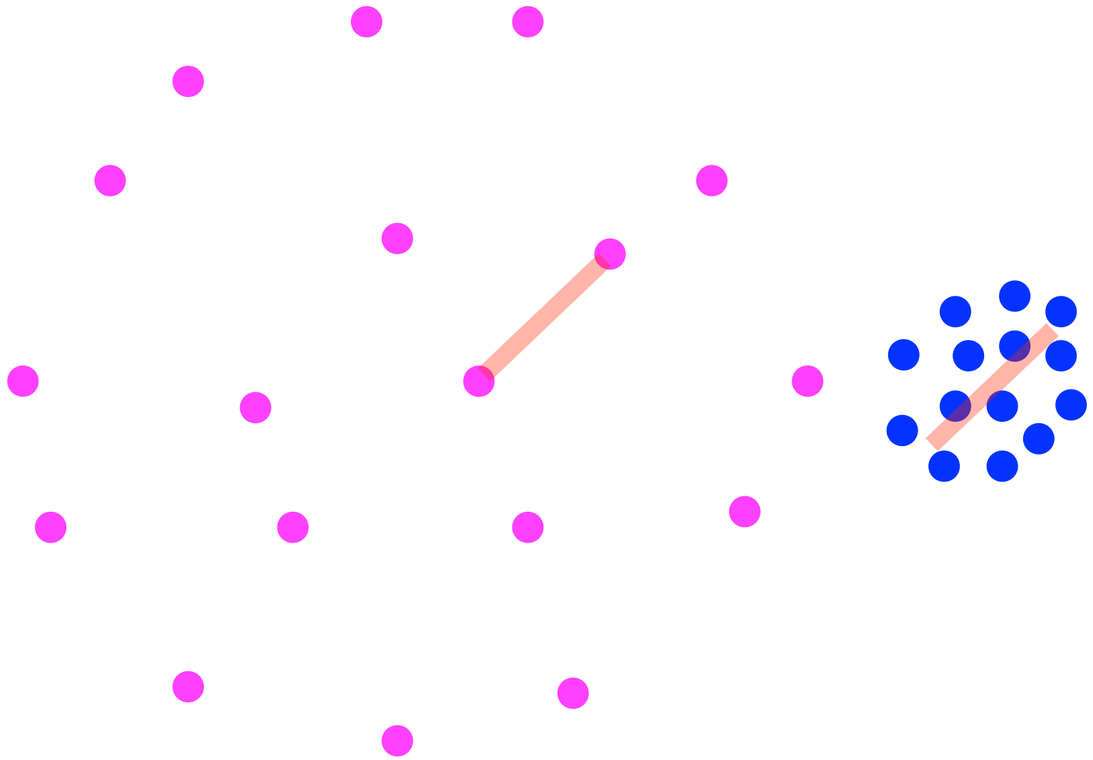
Beyond MDS



Should we use distance metrics that take into account data density?

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Popular Nonlinear Dimensionality Reduction Methods

t-distributed Stochastic Neighbor Embedding (t-SNE)

sklearn.manifold.TSNE

class `sklearn.manifold.TSNE`(*n_components=2, *, perplexity=30.0, early_exaggeration=12.0, learning_rate='auto', n_iter=1000, n_iter_without_progress=300, min_grad_norm=1e-07, metric='euclidean', metric_params=None, init='pca', verbose=0, random_state=None, method='barnes_hut', angle=0.5, n_jobs=None*) [source]

Uniform Manifold Approximation and Projection (UMAP)

class **umap.umap_.UMAP**(*n_neighbors=15, n_components=2, metric='euclidean', metric_kwds=None, output_metric='euclidean', output_metric_kwds=None, n_epochs=None, learning_rate=1.0, init='spectral', min_dist=0.1, spread=1.0, low_memory=True, n_jobs=-1, set_op_mix_ratio=1.0, local_connectivity=1.0, repulsion_strength=1.0, negative_sample_rate=5, transform_queue_size=4.0, a=None, b=None, random_state=None, angular_rp_forest=False, target_n_neighbors=-1, target_metric='categorical', target_metric_kwds=None, target_weight=0.5, transform_seed=42, transform_mode='embedding', force_approximation_algorithm=False, verbose=False, unique=False, densmap=False, dens_lambda=2.0, dens_frac=0.3, dens_var_shift=0.1, output_dens=False, disconnection_distance=None*) [source]