Embedding-Based Methods

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Non-Linear Manifolds

- As we have seen, manifolds are not generally linear
  - E.g., two features can vary together, but not linearly
- Manifolds can also loop back onto themselves
  - E.g., two features that do not have a one-to-one relationship

Non-Linear Manifolds

- PCA: linear manifolds only
  - Construct a global model of the manifold
- Kernel PCA: can express non-linearities
  - Simple case: representation of the manifold is a global model
  - Kernel trick: captures the model in terms of a weighted sum over the training set samples
- Can also take a sample-based approach in the original space!

Locally Linear Embedding

Training set in N-dimensional feature space

1. Measure distance between each pair of training set samples
   - For each sample, identify the closest neighbors
   - Create a local linear model for just that point
2. Place corresponding points in a new M-dimensional space:
   - Select these points, so that the local linear models are still respected

Phase 1: Build Local Models

- Use Euclidean distance metric to identify the k nearest neighbors for each point
  - Generally, these nearest neighbors define a local manifold
  - The dimensionality of this local neighborhood is at most k-1
- For each point, identify a weighted sum of the neighbors that predicts the location of that point

Locally Linear Embedding: Embedding

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LLE: Embedding Phase

- Each Xi has a corresponding Zi in an M-dimensional space
- Pick the location of the Zi's that respect the neighborhood models that we learned in the previous step
  - These are the weights that we have already determined

LLE Query

- Given: a new query point, Xq
- Determine the neighborhood (Nq)
- Compute weights that reconstruct Xq from the Nq points
- Compute Zq

Example: Locally Linear Embedding

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Multidimensional Scaling

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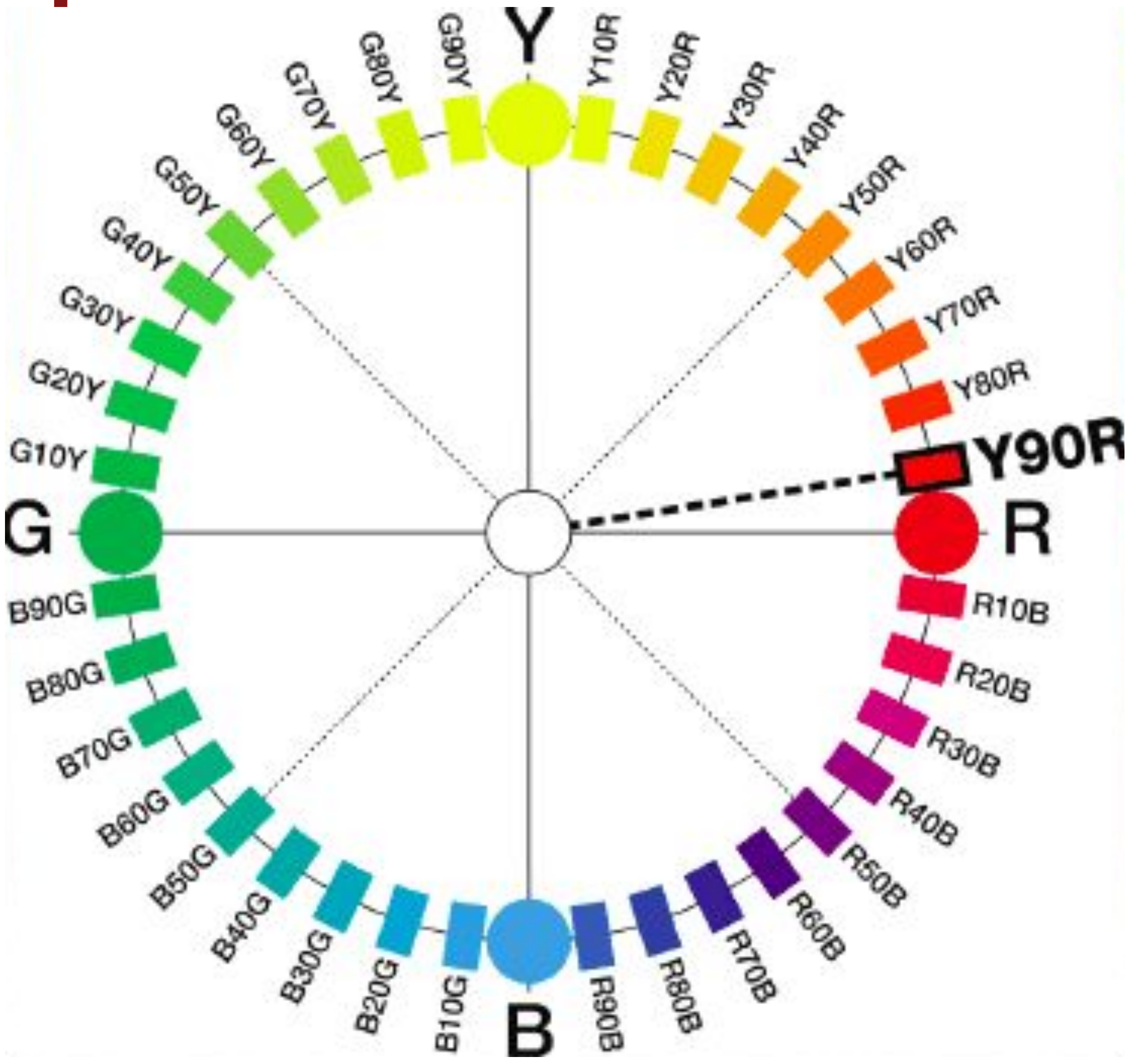
Euclidean Distance Metric

- Easy to compute
- In many data sets, it is not trivial or appropriate to compare samples in this way:
  - Different features have different units and different scales
  - For some representations, we can't simply take a difference between two values (e.g., angles)

Color Perception

How well does a human distinguish colors?

- Are two colors different?
- If so, by how much?



Tseghai et al.; researchgate.net

Multidimensional Scaling

Useful for situations where:

- We want to use different (non-Euclidean) distance metrics
- We can't measure the features, but can measure the distances
- We only have a vague sense of similarity or dissimilarity (but not a metric one)

Multidimensional Scaling

Algorithm outline

- Given: all pair-wise distances between samples
- Embed a set of points into M dimensions that respect these differences

Multidimensional Scaling

Notes

- The MDS cost function is a global metric
- All pair-wise distances must be respected (not just the nearest neighbors)
  - However, there are forms of MDS that can deal with not having all pair-wise distances

Geodesic Distance

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Geodesic Distance

- Euclidean distance: not always meaningful in high-dimensional spaces
- Here, assume that Euclidean distance is only meaningful for short distances
- Use this neighborhood relation to define a weighted graph structure among the k-nearest neighbors
- Geodesic distance between all pairs of points: shortest distance in this graph

ISOmap

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ISOmap

- Compute geodesic distance for each pair of points in the training set
- Use multi-dimensional scaling to embed corresponding points into a new space
- Advantage over Euclidean distance: points that are somewhat near in Euclidean space, but are far away in geodesic distance are considered far away from one-another

t-Stochastic Neighbor Embedding

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t-Stochastic Neighbor Embedding

Similarity metric in the original space:

- For a given sample: the probability of selecting one of the other samples from the training set to be its neighbor
- Gaussian distribution: highest similarity when the two samples are the same & drops off as they move apart

Embedded space:

- Select Zi's so that the probability distributions are the same across the two spaces

t-SNE

- Use of the probability distribution emphasizes nearest points and treats all far points the same
- PDs really emphasize clusters of points
- Perplexity hyper-parameter:
  - Higher values: include more neighbors in the computation
  - Gives us smoother functions
- No good way to query after the fact:
  - Hence, this is often used for visualization of the given data set

Uniform Manifold Approximation and Projection (UMAP)

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Dimensionality Reduction: Final Thoughts

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Dimensionality Reduction Methods

- Global methods: PCA and (sort of) Kernel PCA
- Local models: LLE, MDS, ISOmap, tSNE
  - And, with the kernel trick, Kernel PCA

Dimensionality Reduction Methods

- PCA: first thing to try
- LLE:
  - Capture local manifold, but ignore larger structure
- MDS:
  - Allows us to use any distance metric that we want
  - We don’t even need to have a feature-based representation of the samples

Embedding Methods

- ISOmap:
  - Very curved manifolds, especially those that loop back onto themselves
- t-SNE:
  - Looking for pockets (clusters) of samples
  - Most often used for visualization purposes

Dimensionality Reduction Uses

- Visualization: give domain experts and data analysis practitioners a better understanding of the geometry of the feature space
- Preprocessing for other methods
  - By unwarping curved manifolds, linear models potentially become viable again
  - By reducing dimensionality, we have less of an opportunity to overfit the data