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
- Measure distance between each pair of training set samples
  - For each sample, identify the closest neighbors
  - The closest neighbors give us a sense of the shape of the local neighborhood
- Place corresponding points in a new M-dimensional space:
  - Select these points, so that the distances to the neighbors are preserved
Locally Linear Embedding

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Locally Linear Embedding (LLE)

- Phase 1: Build local models
- Phase 2: Embedded corresponding points into a lower-dimensional space
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 the 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
Locally Linear Embedding: Query

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LLE Query

• Given: a new query point, $X_q$
• Determine the neighborhood ($N_q$)
• Compute weights that reconstruct $X_q$ from the $N_q$ points
• Compute $Z_q$
Example: Locally Linear Embedding

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Live demo
Example 2: Locally Linear Embedding

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Example 2: Locally Linear Embedding

New data set:
• Original space: 3D
• Varying density
  – 1D manifold mixed with 2D manifolds
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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

• Compute or measure all pair-wise distances between samples (these may be given)
• 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)
Example: Multidimensional Scaling

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Multidimensional Scaling

Both data sets:
• Swiss roll
• Arrow
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
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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 Z_i’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
Example: T-SNE

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Live demo
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