Dimensionality Reduction

CS/DSA 5970: Machine Learning Practice

Challenges

Most data that we wish to analyze live in high-dimensional spaces

- Potentially need ***really*** large data sets to achieve a reasonable representation of the sample distribution
- Our intuition can go out the door quickly
- Some of our math breaks
- Computational tools may not scale to high dimensions well

Challenges

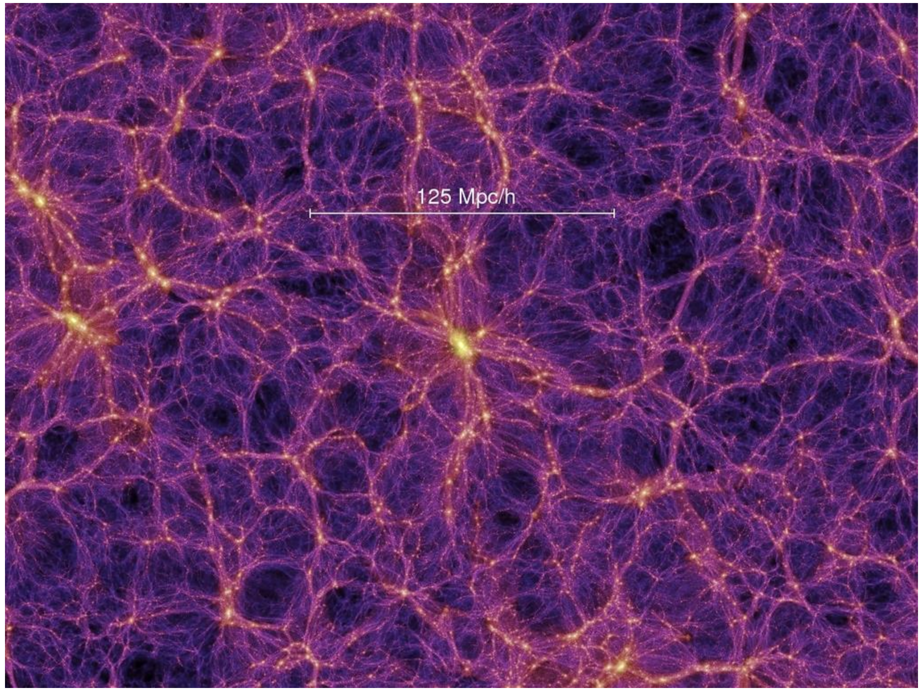
Random points selected uniformly from a unit N-cube:

- Distances become really large
- Distribution of distances becomes very narrow
  - By N=30, all uniformly selected point pairs have <u>very</u> similar distances
  - This suggests that the Euclidean distance metric may not have much meaning

Sample Distribution

For many data sets, samples are not drawn uniformly from the feature space

- 0 D: clusters
- 1 D: line segments / curves
- 2 D: planes / surfaces
- :



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Use the term ***manifold*** to describe a group of samples that locally vary in some dimensions, but not in others

Dimensionality Reduction

- Goal:
  - Given a set of samples from some N-dimensional feature space
  - Re-encode the samples into a smaller M-dimensional space

- Challenge:
  - No labels

Projection Approaches

Projection: linear transformation of a point in N space onto a nearby M-dimensional manifold (where $M \ll N$)

- Projection into linear subspaces
- Warping space, followed by projection

Embedding Approaches

- Identify samples that are "near" one-another in the N-dimensional feature space
- Find a way to embed corresponding points into an M-dimensional space that respects this "nearness"
- Again: M << N

Benefits of Reducing the Dimensionality of a Feature Set

- Make explicit the primary variance in the samples
  - While: removing only small variance
- Through visualization of the reduced-dimensionality data:
  - Possible to reclaim some of our intuition about the data
  - Or even discover new, interesting relationships

Benefits of Reducing the Dimensionality of a Feature Set

Can use as a means of preprocessing our data before applying other learning techniques. Smaller dimensionality implies:

- Subsequent models have fewer parameters
- Reduced potential for overfitting
- Training times can be much faster

Principal Component Analysis

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Principal Component Analysis

Incremental process:

- Identify the one axis in a feature space along which we have the highest variance
- Subtract all variance along this axis
- Repeat

Drawing…

Example: Principal Component Analysis

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Live demo

Example: PCA with Kinematics

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Live demo

Kernel PCA and Kinematics

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Kernel PCA

- PCA involves only linear transformations
  - This could be a problem for feature spaces that contain non-linear manifolds
- As with linear regression and SVMs:
  - We can add a set of non-linear transformations on the features
  - Then, we can perform PCA on the expanded feature vectors
  - The Kernel Trick works here, too!

Live demo