

ML2 Sheet 1

Lecture:

Dimensionality reduction - why?

- fewer parameters to describe data
- visualization in 2D or 3D
- compress data and ~~reduce space~~ ~~speed up algorithm~~
- less overfitting
- speed up algorithm

Why not use PCA always?

→ only works if data lays on ~~non~~ linear manifold

Nonlinear dimension reduction:

- kernel PCA
- tSNE
- Local linear embedding (LLE)
- ...

LLE Algorithm:

1. assign K nearest neighbors to each datapoint \vec{x}_i

2. calc weights w_{ij} that best linearly reconstruct \vec{x}_i

from its neighbors by solving n datapoints $N_i = k$ neighbors

$$R(w) = \sum_{i=1}^n \|\vec{x}_i - \sum_{j \in N_i} w_{ij} \vec{x}_j\|^2 \text{ with the constraint } \sum_{j \in N_i} w_{ij} = 1$$

3. calc low-dim embedding vector \vec{y}_i by minimizing $\phi(y) = \sum_{i=1}^n \|\vec{y}_i - \sum_{j \in N_i} w_{ij} \vec{y}_j\|^2$



Limitations of LLE:

- sensitive to noise
- sensitive to non-uniform sampling of the manifold
- does not provide a mapping
- quadratic complexity on training set size
- no info about intrinsic dimensionality (unlike ISOMAP)
- no good method to define hyperparameters of k neighbors

t-SNE

p : discrete input space

q : embedding space

~~same as~~ Kullback-Leibler divergence:

\rightarrow measure of how much two probability distributions vary from each other

t-SNE: minimizes KL-divergence between q and p