Lecture 19: Kernel PCA, Random projections, tSNE, Isomaps

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- Let $C = \sum_{i=1}^{m} x_i x_i^\top = X^\top X$ be the data correlation matrix, neglecting the $1/m$ factor.
- C is symmetric and positive semi-definite, $C = V \Lambda V^\top$.
- Theorem PCA: among linear hypothesis classes, $E^* = V^\top$, $D^* = V$, where V is the matrix of eigenvectors of $C = X^\top X$.

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- $\nabla r(x) = \frac{2}{x^\top x}(Ax - r(x)x)$.

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- Computational complexity: $O(\min(m^2 d, md^2))$.

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- Separates dissimilar points

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- For some PD kernel, if $K_{ij} = k(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle = (XX^\top)_{ij}$, can compute K only using kernel evaluations.

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- Graph laplacian: $L = D - W$.
- Detects local structure / clusters in data.

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- L is positive semi-definite.

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- Another interpretation: top n eigenvectors of $L^\dagger$. $L^\dagger_{ij}$ represents expected time for random walk $i \to j \to i$.
- Kernel PCA with $K = L^\dagger$ is equivalent to Laplacian eigenmaps.

Stochastic neighbor embedding [Hinton and Roweis 2002]

- Stochastic neighbor embedding(SNE): conditional probability that x_i would pick x_j as its neighbor, given by

$$p(x_j|x_i) = \frac{\exp(-\|x_i - x_j\|^2/2\sigma_i^2)}{\sum_{k\neq i}\exp(-\|x_i - x_k\|^2/2\sigma_i^2)}.$$

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- SNE minimizes $\sum_{i=1}^{m} D_{\mathrm{KL}}(p_i\|q_i)$, where p_i and q_i are the conditional probabilities of x_i and y_i respectively.
- Penalizes large distances between x_i and x_j but also preserves local structure.

tSNE [Van der Maaten and Hinton 2008]

- tSNE cost function is $D_{\mathrm{KL}}(p \| q) = \sum_{i=1}^{m} \sum_{j \neq i} p_{ij} \log \frac{p_{ij}}{q_{ij}}$, where $p_i j$ and q_{ij} are the joint probabilities of (x_i, x_j) and (y_i, y_j) respectively.
- Changes joint distribution to a heavy-tailed distribution, $q(y_j, y_i) = \frac{(1+\|y_i - y_j\|^2)^{-1}}{\sum_{k \neq i}(1+\|y_i - y_k\|^2)^{-1}}$.

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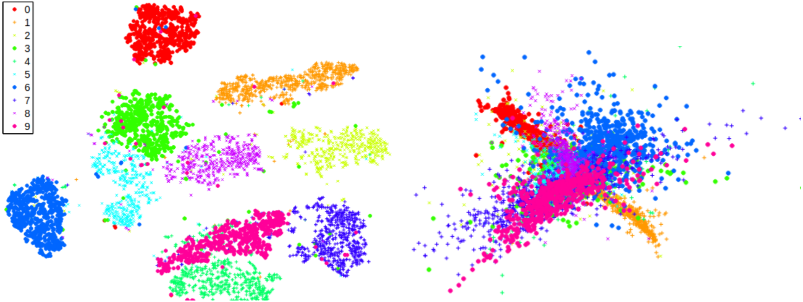
- approaches inverse square law on embedded space.

tSNE visualization



From Van der Maaten and Hinton 2008. tSNE (left) and LLE (right) on MNIST dataset.

Convolutional Neural Networks (source: cs231n.stanford.edu)

- Suitable for image recognition. Won the 2012 ImageNet competition and subsequent ones.
- Three types of layers: convolutional, FC, pooling
- Convolutional layer: accepts a volume of size $W_1 \times H_1 \times D_1$ and outputs a volume of size $W_2 \times H_2 \times D_2$ where $W_2 = (W_1 - F + 2P)/S + 1$ and $H_2 = (H_1 - F + 2P)/S + 1$ and $D_2 = K$.
- K is number of filters, F is filter size, S is stride, P is padding.
- Pooling layer: downsamples along width and height, and optionally along depth.
- FC layer: computes class scores, resulting in volume of size $1 \times 1 \times K$.