Dimensionality Reduction

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Why Reduce Dimensionality?

- Reduces time complexity: Less computation
- Reduces space complexity: Less parameters
- Saves the cost of observing the feature
- Simpler models are more robust on small datasets
- More interpretable; simpler explanation
- Data visualization (structure, groups, outliers, etc) if plotted in 2 or 3 dimensions

2

2

Feature Selection vs Extraction

- Feature selection: Choosing $k<d$ important features, ignoring the remaining $d - k$
  Subset selection algorithms
- Feature extraction: Project the
  original x_i , i =1,...,d dimensions to
  new $k<d$ dimensions, z_j , j =1,...,k
  Principal components analysis (PCA), linear discriminant analysis (LDA), factor analysis (FA)

3

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Subset Selection

- There are 2^d subsets of d features
- Forward search: Add the best feature at each step
  - Set of features F initially $\emptyset$.
  - At each iteration, find the best new feature
    $j = \text{argmin}_i\, E(F \cup x_i)$
  - Add x_j to F if $E(F \cup x_j) < E(F)$
- Hill-climbing $O(d^2)$ algorithm
- Backward search: Start with all features and remove one at a time, if possible.
- Floating search (Add k, remove l)

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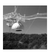
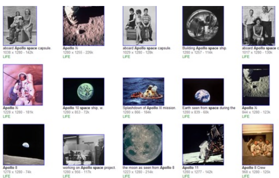
Recall: Representing images





- The most common element in the image: background
  - Or rather large regions of relatively featureless shading
  - Uniform sequences of numbers

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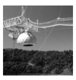
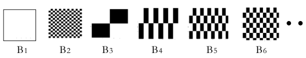
Adding more bases



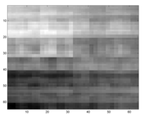


- Checkerboards with different variations

$$\text{Image} \approx w_1 B_1 + w_2 B_2 + w_3 B_3 + \ldots$$

$$W = \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ . \\ . \end{bmatrix} \qquad B = [B_1 \ B_2 \ B_3]$$

$$BW \approx \text{Image}$$
$$W = pinv(B)\,\text{Image}$$
$$PROJECTION = BW$$



Getting closer at 625 bases!

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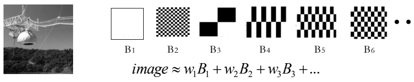
"Bases"



$$image \approx w_1 B_1 + w_2 B_2 + w_3 B_3 + ...$$

- "Bases" are the "standard" units such that all instances can be expressed a weighted combinations of these units
- Ideal requirements: Bases must be orthogonal
- Checkerboards are one choice of bases
  - Orthogonal
  - But not "smooth"
- Other choices of bases: Complex exponentials, Wavelets, etc..

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Data specific bases?

- **Issue**: **The bases we have considered so far are *data agnostic***
  - Checkerboards, Complex exponentials, Wavelets..
  - We use the same bases regardless of the data we analyze
    - Image of face vs. Image of a forest
    - Segment of speech vs. Seismic rumble
- How about data specific bases
  - Bases that consider the underlying data
    - E.g. is there something better than checkerboards to describe faces
    - Something better than complex exponentials to describe music?

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Principal Components Analysis (PCA)

- Find a low-dimensional space such that when $\boldsymbol{x}$ is projected there, information loss is minimized.
- The projection of $\boldsymbol{x}$ on the direction of $\boldsymbol{w}$ is: $z = \boldsymbol{w}^T\boldsymbol{x}$
- Find $\boldsymbol{w}$ such that Var(z) is maximized

$$\begin{aligned}\mathrm{Var}(z) &= \mathrm{Var}(\boldsymbol{w}^T\boldsymbol{x}) = \mathrm{E}[(\boldsymbol{w}^T\boldsymbol{x} - \boldsymbol{w}^T\boldsymbol{\mu})^2] \\ &= \mathrm{E}[(\boldsymbol{w}^T\boldsymbol{x} - \boldsymbol{w}^T\boldsymbol{\mu})(\boldsymbol{w}^T\boldsymbol{x} - \boldsymbol{w}^T\boldsymbol{\mu})] \\ &= \mathrm{E}[\boldsymbol{w}^T(\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^T\boldsymbol{w}] \\ &= \boldsymbol{w}^T\,\mathrm{E}[(\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^T]\boldsymbol{w} = \boldsymbol{w}^T \Sigma \boldsymbol{w}\end{aligned}$$

where $\mathrm{Var}(\boldsymbol{x}) = \mathrm{E}[(\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^T] = \Sigma$

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Principal Components Analysis (PCA)

- Maximize Var(z) subject to $||\mathbf{w}||=1$

$$\max_{\mathbf{w}_1} \mathbf{w}_1^T \Sigma \mathbf{w}_1 - \alpha\left(\mathbf{w}_1^T \mathbf{w}_1 - 1\right)$$

$\Sigma \mathbf{w}_1 = \alpha \mathbf{w}_1$ that is, $\mathbf{w}_1$ is an eigenvector of Σ

Choose the one with the largest eigenvalue for Var(z) to be max

- Second principal component: Max Var(z_2), s.t., $||\mathbf{w}_2||=1$ and orthogonal to $\mathbf{w}_1$

$$\max_{\mathbf{w}_2} \mathbf{w}_2^T \Sigma \mathbf{w}_2 - \alpha\left(\mathbf{w}_2^T \mathbf{w}_2 - 1\right) - \beta\left(\mathbf{w}_2^T \mathbf{w}_1 - 0\right)$$

$\Sigma \mathbf{w}_2 = \alpha\, \mathbf{w}_2$ that is, $\mathbf{w}_2$ is another eigenvector of Σ

and so on.

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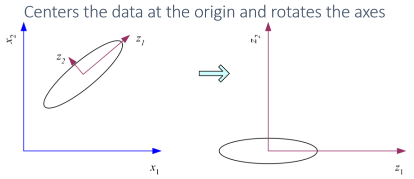
What PCA does

$$z = \mathrm{W}^T(x - m)$$

where the columns of W are the eigenvectors of Σ, and m is sample mean

Centers the data at the origin and rotates the axes



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How to choose k ?

- Proportion of Variance (PoV) explained

$$\frac{\lambda_1 + \lambda_2 + \cdots + \lambda_k}{\lambda_1 + \lambda_2 + \cdots + \lambda_k + \cdots + \lambda_d}$$

when λ_i are sorted in descending order

- Typically, stop at PoV>0.9
- Scree graph plots of PoV vs k, stop at "elbow"

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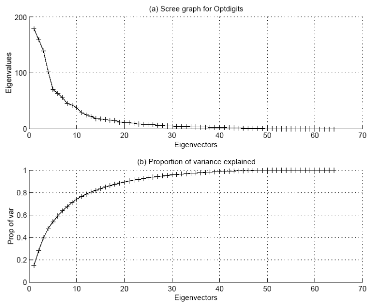
(a) Scree graph for Optdigits
Eigenvalues
Eigenvectors
(b) Proportion of variance explained
Prop of var
Eigenvectors

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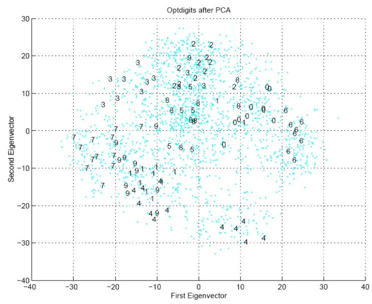
Optdigits after PCA
Second Eigenvector
First Eigenvector

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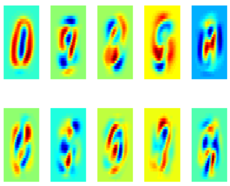
PCA



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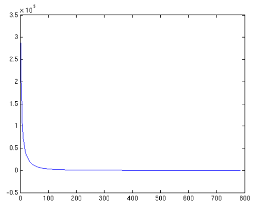
PCA : Eigen Values



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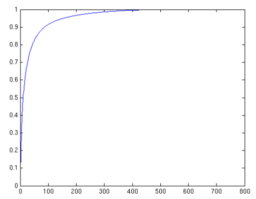
PCA : % information



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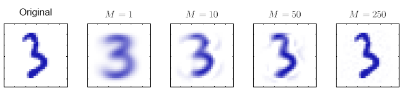
PCA: Reconstruction



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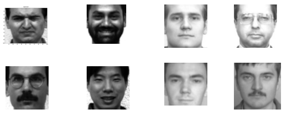
Data-specific description of faces



- A collection of images
  - All normalized to 100x100 pixels
- What is common among all of them?
  - Do we have a common descriptor?

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Eigen Faces!

- Arrange your input data into a matrix $\mathbf{X}$
- Compute the correlation $\mathbf{R} = \mathbf{X}\mathbf{X}^T$
- Solve the Eigen decomposition: $\mathbf{R}\mathbf{V} = \Lambda\mathbf{V}$
- The Eigen vectors corresponding to the K largest eigen values are our optimal bases
- We will refer to these as *eigen faces*.

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Class specificity

- Eigen bases are class specific

- Composing a fishbowl from Eigenfaces

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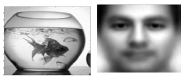
Class specificity

- Eigen bases are class specific



- Composing a fishbowl from Eigenfaces
- With 1 basis

$$f = w_1 \mathbf{v}_1$$

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Class specificity

- Eigen bases are class specific

- Composing a fishbowl from Eigenfaces
- With 10 bases

$$f = w_1 \mathbf{v}_1 + w_2 \mathbf{v}_2 + \ldots + w_{10} \mathbf{v}_{10}$$

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Class specificity

- Eigen bases are class specific

- Composing a fishbowl from Eigenfaces
- With 30 bases

$$f = w_1 \mathbf{v}_1 + w_2 \mathbf{v}_2 + \ldots + w_{10} \mathbf{v}_{10} + \ldots + w_{30} \mathbf{v}_{30}$$

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Class specificity

- Eigen bases are class specific

- Composing a fishbowl from Eigenfaces
- With 100 bases

$$f = w_1\mathbf{v}_1 + w_2\mathbf{v}_2 + \ldots + w_{10}\mathbf{v}_{10} + \ldots + w_{30}\mathbf{v}_{30} + \ldots + w_{100}\mathbf{v}_{100}$$

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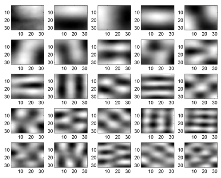
Universal bases

- Universal bases..



- End up looking a lot like *discrete cosine transforms!!!!*
- *DCTs are the best "universal" bases*
  - *If you don't know what your data are, use the DCT*

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Factor Analysis

- Find a small number of factors $\boldsymbol{z}$, which when combined generate $\boldsymbol{x}$:

  $x_i - \mu_i = v_{i1}z_1 + v_{i2}z_2 + \ldots + v_{ik}z_k + \varepsilon_i$

  where z_j, $j = 1,\ldots,k$ are the latent factors with

  $E[z_j]=0$, $Var(z_j)=1$, $Cov(z_i, z_j)=0$, $i \neq j$,

  ε_i are the noise sources

  $E[\varepsilon_i] = \psi_i$, $Cov(\varepsilon_i, \varepsilon_j) = 0$, $i \neq j$, $Cov(\varepsilon_i, z_j) = 0$,

  and v_{ij} are the factor loadings

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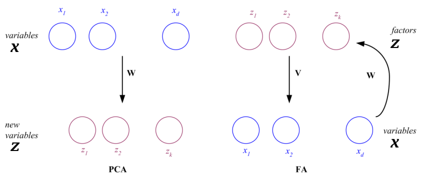
PCA vs FA

- PCA From $\boldsymbol{x}$ to $\boldsymbol{z}$ $\quad\boldsymbol{z} = \mathbf{W}^T(\boldsymbol{x} - \boldsymbol{\mu})$
- FA $\quad$ From $\boldsymbol{z}$ to $\boldsymbol{x}$ $\quad\boldsymbol{x} - \boldsymbol{\mu} = \mathbf{V}\boldsymbol{z} + \boldsymbol{\varepsilon}$



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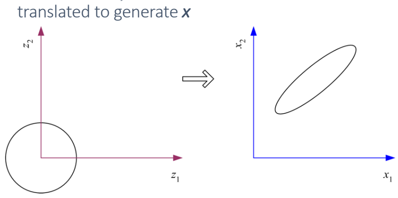
Factor Analysis

- In FA, factors z_j are stretched, rotated and translated to generate $\boldsymbol{x}$



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Multidimensional Scaling

- Given pairwise distances between N points,
  d_{ij}, $i,j = 1,\dots,N$
  place on a low-dim map s.t. distances are preserved.
- $\boldsymbol{z} = \boldsymbol{g}(\boldsymbol{x} \mid \vartheta)$ $\quad$ Find ϑ that min Sammon stress

$$E(\theta \mid \mathcal{X}) = \sum_{r,s} \frac{\left(\|\mathbf{z}^r - \mathbf{z}^s\| - \|\mathbf{x}^r - \mathbf{x}^s\|\right)^2}{\|\mathbf{x}^r - \mathbf{x}^s\|^2}$$

$$= \sum_{r,s} \frac{\left(\|\mathbf{g}(\mathbf{x}^r \mid \theta) - \mathbf{g}(\mathbf{x}^s \mid \theta)\| - \|\mathbf{x}^r - \mathbf{x}^s\|\right)^2}{\|\mathbf{x}^r - \mathbf{x}^s\|^2}$$

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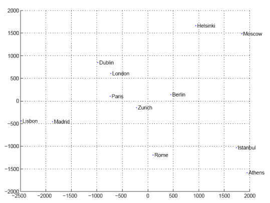
Map of Europe by MDS



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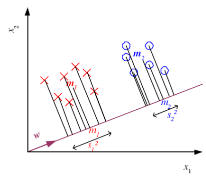
Linear Discriminant Analysis

- Find a low-dimensional space such that when $\boldsymbol{x}$ is projected, classes are well-separated.
- Find $\boldsymbol{w}$ that maximizes

$$J(\mathbf{w})=\frac{(m_1-m_2)^2}{s_1^2+s_2^2}$$

$$m_1=\frac{\sum_t \mathbf{w}^T\mathbf{x}^t r^t}{\sum_t r^t} \qquad s_1^2=\sum_t\left(\mathbf{w}^T\mathbf{x}^t-m_1\right)^2 r^t$$



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Linear Discriminant Analysis

- Between-class scatter:

$$(m_1-m_2)^2=\left(\mathbf{w}^T\mathbf{m}_1-\mathbf{w}^T\mathbf{m}_2\right)^2$$
$$=\mathbf{w}^T(\mathbf{m}_1-\mathbf{m}_2)(\mathbf{m}_1-\mathbf{m}_2)^T\mathbf{w}$$
$$=\mathbf{w}^T\mathbf{S}_B\mathbf{w} \text{ where } \mathbf{S}_B=(\mathbf{m}_1-\mathbf{m}_2)(\mathbf{m}_1-\mathbf{m}_2)^T$$

- Within-class scatter:

$$s_1^2=\sum_t\left(\mathbf{w}^T\mathbf{x}^t-m_1\right)^2 r^t$$
$$=\sum_t \mathbf{w}^T\left(\mathbf{x}^t-\mathbf{m}_1\right)\left(\mathbf{x}^t-\mathbf{m}_1\right)^T\mathbf{w}r^t=\mathbf{w}^T\mathbf{S}_1\mathbf{w}$$
$$\text{where } \mathbf{S}_1=\sum_t\left(\mathbf{x}^t-\mathbf{m}_1\right)\left(\mathbf{x}^t-\mathbf{m}_1\right)^T r^t$$
$$s_1^2+s_1^2=\mathbf{w}^T\mathbf{S}_W\mathbf{w} \text{ where } \mathbf{S}_W=\mathbf{S}_1+\mathbf{S}_2$$

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Fisher's Linear Discriminant

- Find $\mathbf{w}$ that max

$$J(\mathbf{w}) = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}} = \frac{\left|\mathbf{w}^T(\mathbf{m}_1 - \mathbf{m}_2)\right|^2}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

- LDA soln:

$$\mathbf{w} = c \cdot \mathbf{S}_W^{-1}(\mathbf{m}_1 - \mathbf{m}_2)$$

- Parametric soln:

$$\mathbf{w} = \Sigma^{-1}(\mu_1 - \mu_2)$$

when $p(\mathbf{x} \mid C_i) \sim \mathcal{N}(\mu_i, \Sigma)$

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K>2 Classes

- Within-class scatter:

$$\mathbf{S}_W = \sum_{i=1}^{K} \mathbf{S}_i \qquad \mathbf{S}_i = \sum_t r_i^t (\mathbf{x}^t - \mathbf{m}_i)(\mathbf{x}^t - \mathbf{m}_i)^T$$

- Between-class scatter:

$$\mathbf{S}_B = \sum_{i=1}^{K} N_i (\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^T \qquad \mathbf{m} = \frac{1}{K}\sum_{i=1}^{K} \mathbf{m}_i$$

- Find $\mathbf{W}$ that max

$$J(\mathbf{W}) = \frac{\left|\mathbf{W}^T \mathbf{S}_B \mathbf{W}\right|}{\left|\mathbf{W}^T \mathbf{S}_W \mathbf{W}\right|}$$

The largest eigenvectors of $\mathbf{S}_W^{-1}\mathbf{S}_B$
Maximum rank of K-1

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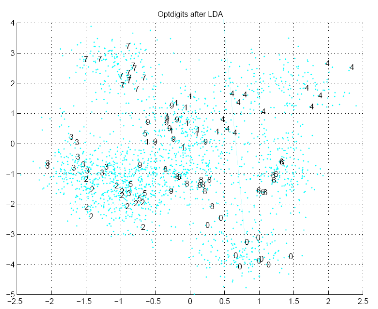

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Neighborhood Components Analysis

- NCA learns a Mahalanobis distance metric for the KNN classifier by maximizing the leave-one-out cross validation.
  - Let p_{ij} be the probability that point x_j is selected as point x_i's neighbour.
  - The probability that points are correctly classified when x_i is used as the reference is:

$$P_i = \sum_{j \in C_i} p_{ij}$$
$$C_i = \{x_j | \text{class}(x_j) = \text{class}(x_i)\}$$

  - p_{ij} is related to the distance between x_i and x_j

$$p_{ij} = \frac{e^{-d_{ij}}}{\sum_{k \neq i} e^{-d_{ik}}}, \, p_{ii} = 0$$

  - The expected number of correctly classification points:

$$f(A) = \sum_i P_i$$

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Neighborhood Components Analysis

- How do we define d_{ij}?
- Limit the distance measure within Mahalanobis (quadratic) distance:

$$d(x, y) = (x - y)^T Q (x - y)$$
$$Q = A^T A$$
$$d(x, y) = (Ax - Ay)^T (Ax - Ay)$$

- That is to say, we project the original feature vectors x into another vector space with transformation matrix A.

Distance Learning ⇔ Finding the Best matrix A

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Neighborhood Components Analysis

- Subtitute d_{ij} in p_{ij}

$$p_{ij} = \frac{\exp\left(-\|Ax_i - Ax_j\|^2\right)}{\sum_{k \neq i} \exp(-\|Ax_i - Ax_k\|^2)}$$

- The **objective function**:

$$f(A) = \sum_i P_i = \sum_i \sum_{j \in C_i} p_{ij}$$

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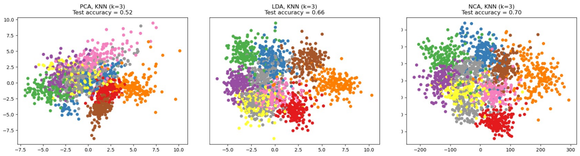
Neighborhood Components Analysis



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t-SNE

- SNE - Stochastic Neighbor Embedding
- t-SNE
- KL divergence

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Local Embedding

- t-SNE is an alternative dimensionality reduction algorithm.
- PCA tries to find a **global** structure
  - Low dimensional subspace
  - Can lead to local inconsistencies
    - Far away point can become nearest neighbors
- t-SNE tries to preserve **local** structure
  - Low dimensional neighborhood should be the same as original neighborhood.
- Unlike PCA almost only used for visualization
  - No easy way to embed new points

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Stochastic Neighbor Embedding (SNE)

- ”Encode” high dimensional neighborhood information as a distribution
- Intuition: Random walk between data points.
  - High probability to jump to a close point
- Find low dimensional points such that their neighborhood distribution is similar
- How do you measure distance between distributions?
  - Most common measure: KL divergence

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Neighborhood Distributions

- Consider the neighborhood around an input data point $x_i \in \mathbb{R}^d$
- Imagine that we have a Gaussian distribution centered around x_i
- Then the probability that x_i chooses some other datapoint x_j as its neighbor is in proportion with the density under this Gaussian
- A point closer to x_i will be more likely than one further away
- $P_{j|i}$ probability (similar to NCA), is the probability that point x_i chooses x_j as its neighbor:

$$P_{j|i} = \frac{\exp\left(-\left\|x_i - x_j\right\|^2 / 2\sigma_i^2\right)}{\sum_{k \neq i} \exp\left(-\|x_i - x_k\|^2 / 2\sigma_i^2\right)}$$

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Neighborhood Distributions

- $P_{j|i}$ probability (similar to NCA), is the probability that point x_i chooses x_j as its neighbor:

$$P_{j|i} = \frac{\exp\left(-\left\|x_i - x_j\right\|^2 / 2\sigma_i^2\right)}{\sum_{k \neq i} \exp\left(-\|x_i - x_k\|^2 / 2\sigma_i^2\right)}$$

With $P_{i|i} = 0$

- The parameter σ_i sets the size of the neighborhood
  - Very low σ_i: all the probability is in the nearest neighbor.
  - Very high σ_i: Uniform weights.
- We set σ_i differently for each data point
- Results depend heavily on σ_i:
  - it defines the neighborhoods we are trying to preserve.
- Final distribution over pairs is symmetrized: $P_{ij} = \frac{1}{2N}\left(P_{i|j} + P_{j|i}\right)$
- Random Walk:
  - Pick i uniformly and then ”jump” to j according to $P_{j|i}$

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SNE objective

- Given $x_1, x_2, \dots, x_N \in \mathbb{R}^d$, we define the distribution P_{ij}
- Goal: Find good embedding $y_1, y_2, \dots, y_N \in \mathbb{R}^p$ for some $p \ll d$ (normally 2 or 3 for visualization)
- How do we measure an embedding quality?
- For points $y_1, y_2, \dots, y_N \in \mathbb{R}^p$, we can define distribution Q similarly the same (notice no σ_i^2 and not symmetric)

$$Q_{ij} = \frac{\exp\left(-\|y_i - y_j\|^2\right)}{\sum_{k \neq i} \exp(-\|y_i - y_k\|^2)}$$

- Optimize Q to be close to P
  - Minimize KL-divergence
- The embeddings $y_1, y_2, \dots, y_N \in \mathbb{R}^p$ are the parameters we are optimizing.
  - How do you embed a new point? No embedding function!

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SNE objective

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- The embeddings $y_1, y_2, \dots, y_N \in \mathbb{R}^p$ are the parameters we are optimizing.
  - How do you embed a new point? No embedding function!

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SNE algorithm

- We have P, and are looking for $y_1, y_2, \dots, y_N \in \mathbb{R}^p$ such that the distribution Q we infer will minimize $\mathbb{C}(Q) = \mathrm{KL}(P\|Q)$(notice Q on right)

$$\mathrm{KL}(P\|Q) = \sum_{ij} P_{ij} \log\left(\frac{P_{ij}}{Q_{ij}}\right) = -\sum_{ij} P_{ij} \log(Q_{ij}) + const$$

- Not a convex problem! can use multiple restarts.
- Main issue: crowding problem

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Crowding Problem: Neighborhood

- In high dimension we have more room, points can have a lot of different neighbors
- In 2D a point can have a few neighbors at distance one all far from each other
  - what happens when we embed in 1D?
- Crowding problem:
  - We don't have enough room to accommodate all neighbors.
  - One of the biggest problems with SNE.
- t-SNE solution: Change the Gaussian in Q to a heavy tailed distribution.
- if Q changes slower, we have more wiggle room to place points at.

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T-SNE: t-Distributed Stochastic Neighbor Embedding

- Student-t Probability density $p(x) \propto \left(1 + \frac{x^2}{v}\right)^{-\frac{v+1}{2}}$
  - For $v = 1$ we get $p(x) \propto \frac{1}{1+x^2}$
- Probability goes to zero much slower than a Gaussian
- We can now redefine Q_{ij} as

$$Q_{ij} = \frac{\left(1 + \|y_i - y_j\|^2\right)^{-1}}{\sum_k \sum_{l \neq k} (1 + \|y_k - y_l\|^2)^{-1}}$$

- We leave P_{ij} as is

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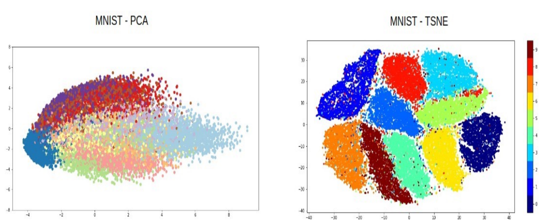
PCA vs t-SNE



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Conclusions

- A lot of tools can be used for dimensionality reduction linear and not linear.
- Helpful for visualization
- Helps to understand ”black-box” algorithms
- t-SNE is a great way to visualize data

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