Unsupervised Learning - Dimensionality reduction.

- A very brief introduction to unsupervised learning
- Dimensionality reduction:
  - Principal Component Analysis (PCA)
  - Kernelizing PCA
  - Other non-linear dimensionality reduction techniques

Unsupervised Learning (cont'd).

- Until now, we focused on supervised learning (e.g. regression and classification):
  - We have access to labeled data: we observe both features for each object $\mathbf{x}_1, \cdots, \mathbf{x}_m$ *and the corresponding target variable* $y_1, \cdots, y_m$. The goal is to *predict the target from the features*.
- In unsupervised learning, we only have access to unlabeled data, i.e. the features $\mathbf{x}_1, \cdots, \mathbf{x}_m$, and we want to *discover interesting things about the data* (i.e. identify the underlying structure of the data).

Unsupervised Learning (cont'd).

- Unsupervised learning is more subjective than supervised learning (no simple goal, such as prediction in supervised learning).
- But of growing importance:
  - Easier to obtain unlabeled data than labeled data.
  - One of the next challenges of ML:
    - Overwhelming amount of unlabeled data available
    - Human don't need so many labeled examples to learn: few labeled examples and large amount of unlabeled data is often enough (semi-supervised learning)...

Unsupervised Learning.

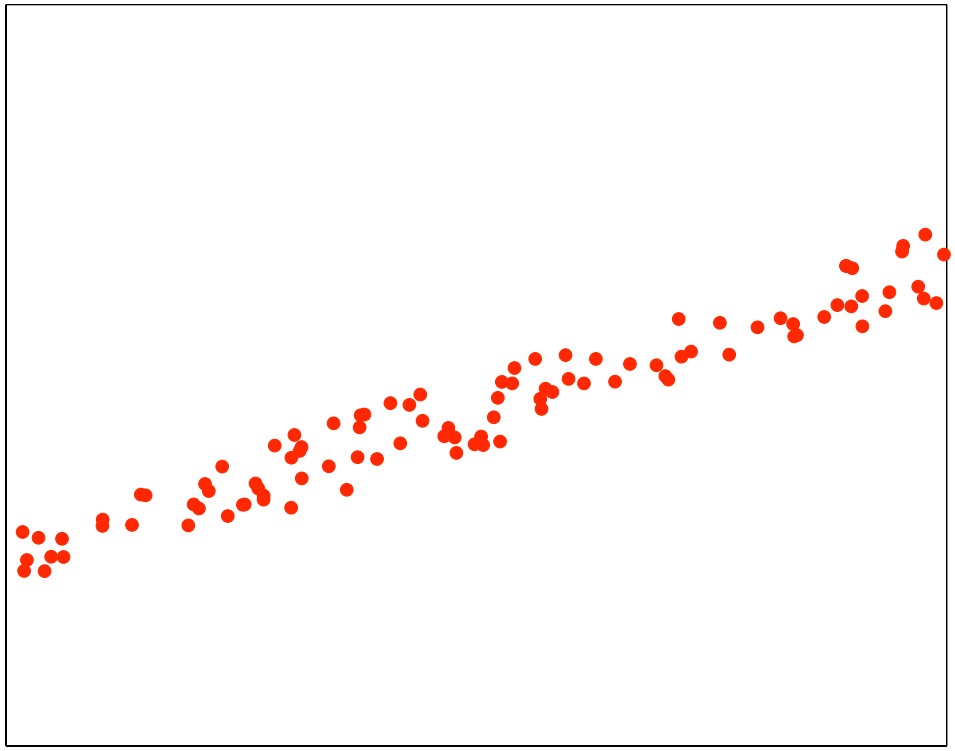
- Examples of unsupervised learning tasks:
  - Density estimation: estimate the distribution of the data (e.g. fit a Gaussian to the data, or a mixture of Gaussians). Closely related to generative models (e.g. GANs)...
  - Clustering: identify groups of similar objects (for e.g. market segmentation, data exploration). For example k-means is a very popular clustering algorithm:.
  - Dimensionality reduction: find a low-dimensional representation of the data (e.g. to reduce the complexity of learning algorithm, data visualization).

$\Rightarrow$ We focus on dimensionality reduction in this lecture.

What is dimensionality reduction?

- Dimensionality reduction (or embedding) techniques:
  - Assign instances to real-valued vectors, in a space that is much smaller-dimensional (even 2D or 3D for visualization).
  - Approximately preserve similarity/distance relationships between instances.
- Some techniques:
  - Linear: Principal components analysis
  - Non-linear
    - Kernel PCA
    - Independent components analysis
    - Self-organizing maps
    - Locally linear embeddings
    - Multi-dimensional scaling
    - Autoencoders
    - ...

What is the true dimensionality of this data?



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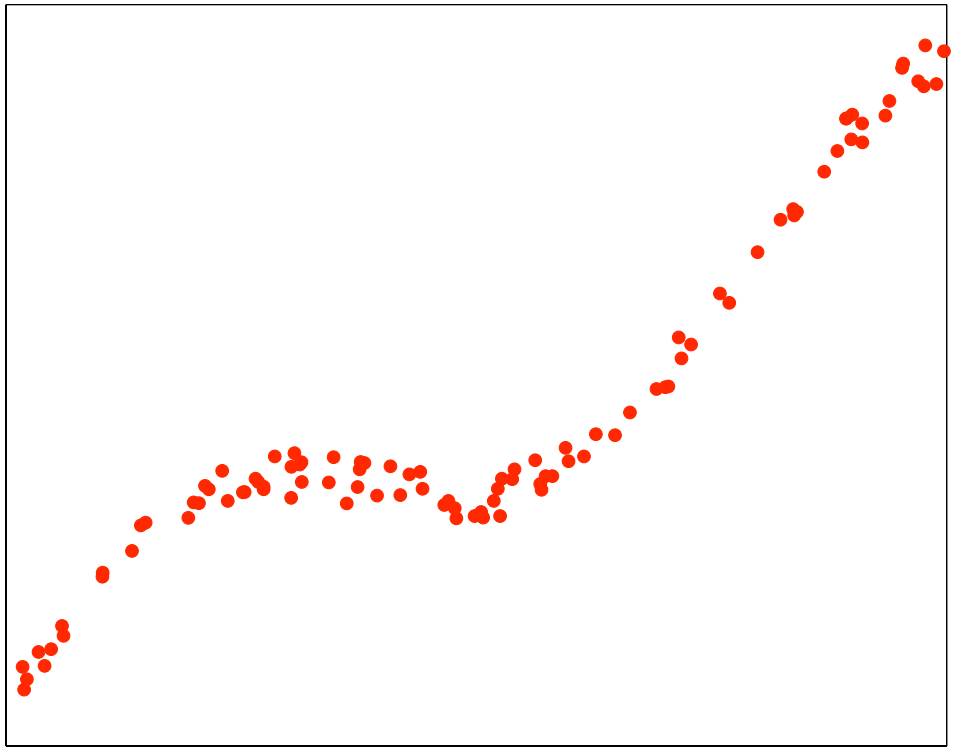

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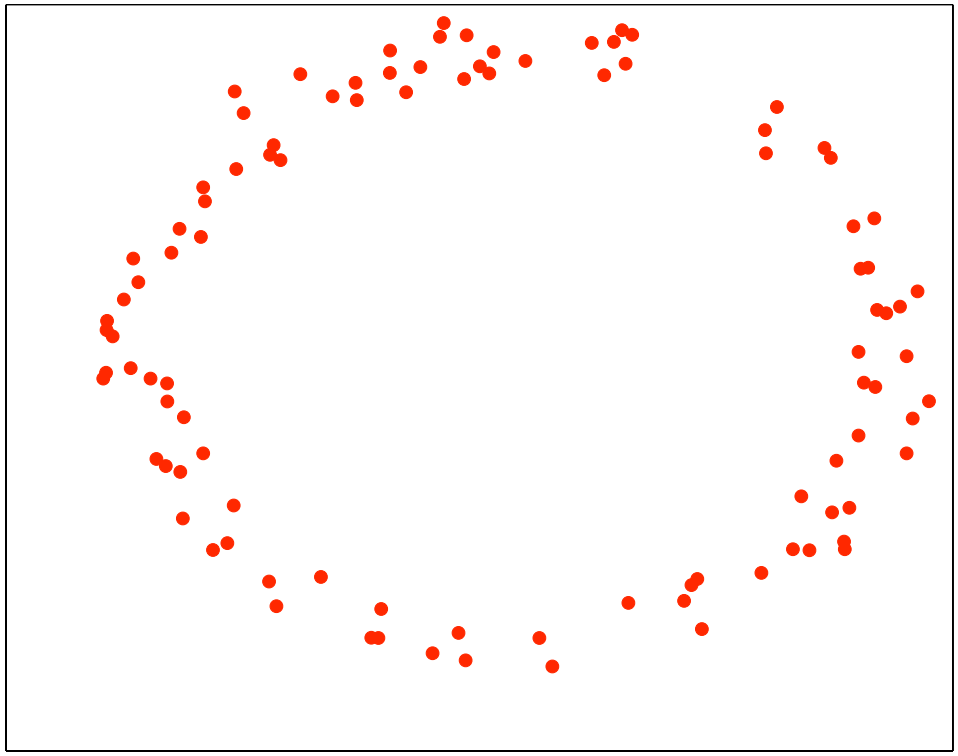

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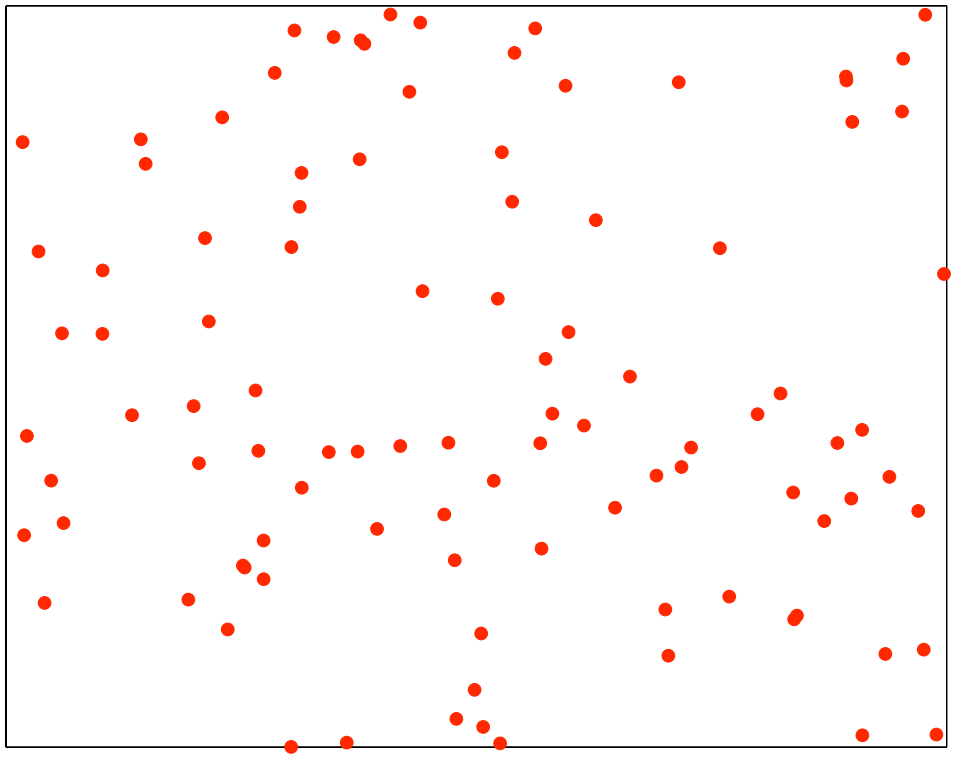
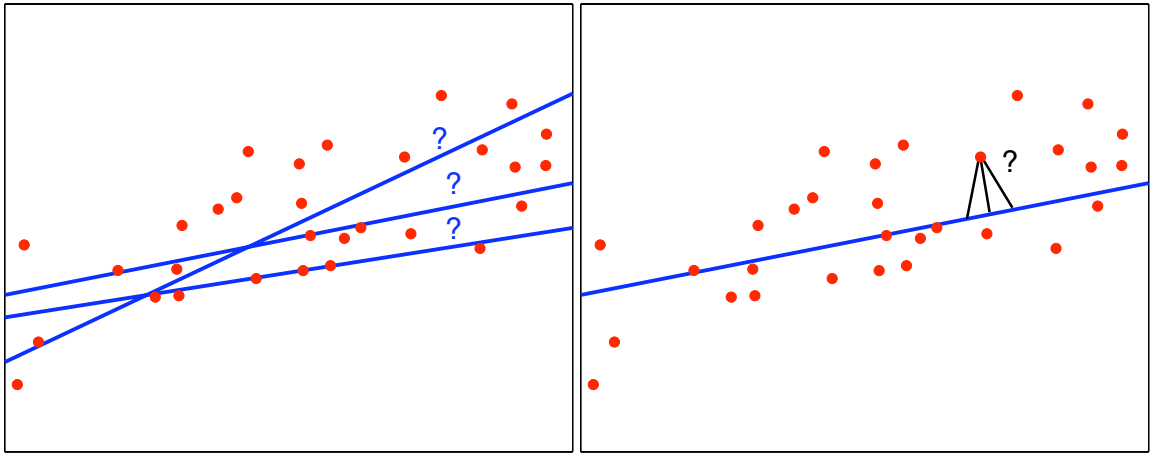


Remarks

- All dimensionality reduction techniques are based on an implicit assumption that the data lies along some *low-dimensional manifold*
- This is the case for the first three examples, which lie along a 1-dimensional manifold despite being plotted in 2D
- In the last example, the data has been generated randomly in 2D, so no dimensionality reduction is possible without losing information
- The first three cases are in increasing order of difficulty, from the point of view of existing techniques.

Simple Principal Component Analysis (PCA)

- Given: m instances, each being a length-n real vector.
- Suppose we want a 1-dimensional representation of that data, instead of n-dimensional.
- Specifically, we will:
  - Choose a line in $\mathbb{R}^n$ that "best represents" the data.
  - Assign each data object to a point along that line.



Reconstruction error

- Let the line be represented as $\mathbf{b} + \alpha\mathbf{v}$ for $\mathbf{b}, \mathbf{v} \in \mathbb{R}^n$, $\alpha \in \mathbb{R}$.
  For convenience assume $\|\mathbf{v}\| = 1$.
- Each instance $\mathbf{x}_i$ is associated with a point on the line $\hat{\mathbf{x}}_i = \mathbf{b} + \alpha_i\mathbf{v}$.
- We want to choose $\mathbf{b}$, $\mathbf{v}$, and the α_i to minimize the total reconstruction error over all data points, measured using Euclidean distance:

$$R = \sum_{i=1}^{m} \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|^2$$

A constrained optimization problem!

$$\begin{array}{rl} \text{min} & \sum_{i=1}^{m} \|\mathbf{x}_i - (\mathbf{b} + \alpha_i \mathbf{v})\|^2 \\ \text{w.r.t.} & \mathbf{b}, \mathbf{v}, \alpha_i, i = 1, \ldots m \\ \text{s.t.} & \|\mathbf{v}\|^2 = 1 \end{array}$$

- This is a quadratic objective with quadratic constraint
- Suppose we fix a $\mathbf{v}$ satisfying the condition, and find the best $\mathbf{b}$ and α_i given this $\mathbf{v}$
- So, we solve:

$$\min R = \min_{\alpha, \mathbf{b}} \sum_{i=1}^{m} \|\mathbf{x}_i - (\mathbf{b} + \alpha_i \mathbf{v})\|^2$$

where R is the *reconstruction error*

Solving the optimization problem (II)

- We write the gradient of R wrt to α_i and set it to 0:

$$\frac{\partial R}{\partial \alpha_i} = 2\|\mathbf{v}\|^2 \alpha_i - 2\mathbf{v}\mathbf{x}_i + 2\mathbf{b}\mathbf{v} = 0 \Rightarrow \alpha_i = \mathbf{v} \cdot (\mathbf{x}_i - \mathbf{b})$$

  where we used $\|\mathbf{v}\|^2 = 1$.

- We write the gradient of R wrt $\mathbf{b}$ and set it to 0:

$$\nabla_{\mathbf{b}} R = 2m\mathbf{b} - 2\sum_{i=1}^{m} \mathbf{x}_i + 2\left(\sum_{i=1}^{m} \alpha_i\right)\mathbf{v} = 0 \Rightarrow m\mathbf{b} = \sum_{i=1}^{m} \mathbf{x}_i - \sum_{i=1}^{m} \alpha_i \mathbf{v}$$

- From above:

$$\sum_{i=1}^{m} \alpha_i \mathbf{v} = \left(\sum_{i=1}^{m} \mathbf{v}^\top (\mathbf{x}_i - \mathbf{b})\right)\mathbf{v} = \mathbf{v}\mathbf{v}^\top \left(\sum_{i=1}^{m} \mathbf{x}_i - m\mathbf{b}\right)$$

Solving the optimization problem (III)

- Combining the previous two equations we get:

$$(\mathbf{I} - \mathbf{v}\mathbf{v}^\top) m\mathbf{b} = (\mathbf{I} - \mathbf{v}\mathbf{v}^\top) \sum_{i=1}^{m} \mathbf{x}_i$$

- This is satisfied when:

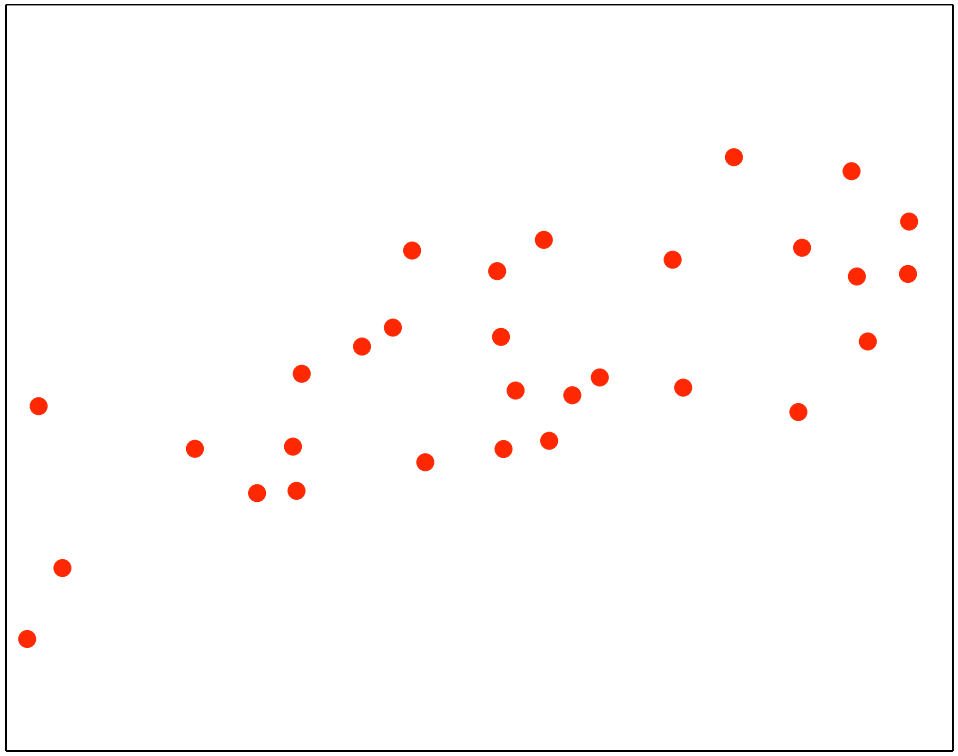
$$\mathbf{b} = \frac{1}{m} \sum_{i=1}^{m} \mathbf{x}_i$$

- This means that the line goes through the mean of the data
- By substituting $\alpha_i = \mathbf{v}^\top (\mathbf{x}_i - \mathbf{b})$, we get:

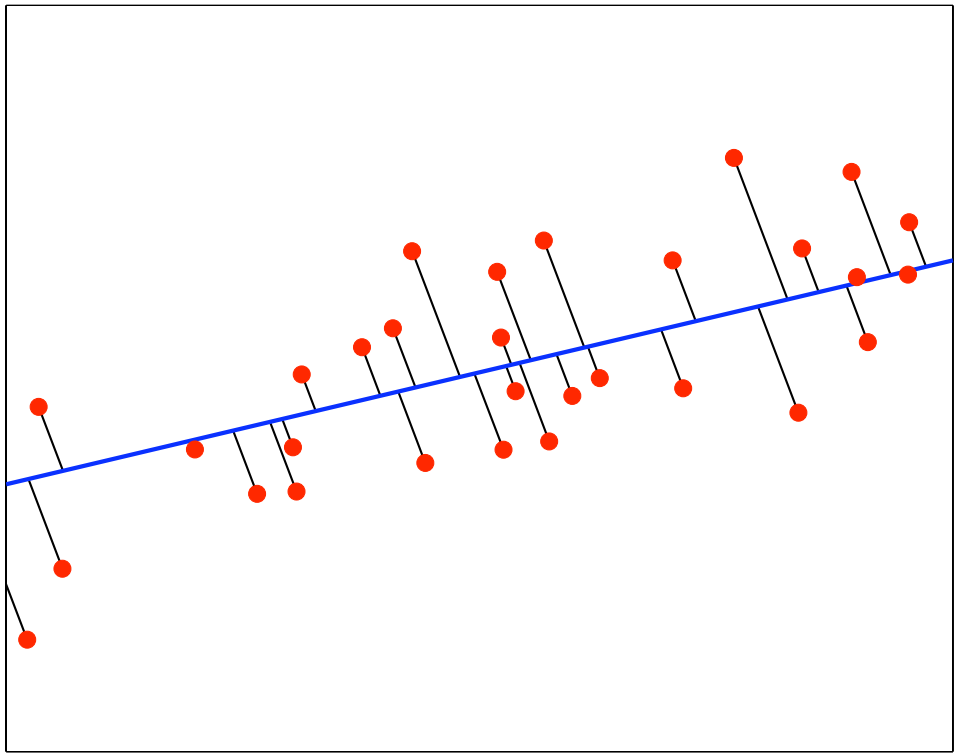
$$\hat{\mathbf{x}}_i = \mathbf{b} + \alpha_i \mathbf{v} = \mathbf{b} + \mathbf{v}\mathbf{v}^\top (\mathbf{x}_i - \mathbf{b})$$

- This means that instances are projected orthogonally on the line to get the associated point.

Example data



Example with $\mathbf{v} \propto (1, 0.3)$



Finding the direction of the line

- Substituting $\hat{\mathbf{x}}_i = \mathbf{b} + \mathbf{v}\mathbf{v}^\top(\mathbf{x}_i - \mathbf{b})$, we want to solve:

$$\min_{\mathbf{v}} \sum_{i=1}^{m} \|(\mathbf{I} - \mathbf{v}\mathbf{v}^\top)(\mathbf{x}_i - \mathbf{b})\|^2 \quad \text{s.t. } \|\mathbf{v}\|^2 = 1$$

- Using the fact that $\|(\mathbf{I} - \mathbf{v}\mathbf{v}^\top)(\mathbf{x}_i - \mathbf{b})\|^2 = \|\mathbf{x}_i - \mathbf{b}\|^2 - \|\mathbf{v}\mathbf{v}^\top(\mathbf{x}_i - \mathbf{b})\|^2$ (since $\|\mathbf{v}\|^2 = 1$) this is equivalent to

$$\max_{\mathbf{v}} \sum_{i=1}^{m} \|\mathbf{v}\mathbf{v}^\top(\mathbf{x}_i - \mathbf{b})\|^2 \quad \text{s.t. } \|\mathbf{v}\|^2 = 1$$

  which (using $\|\mathbf{v}\mathbf{v}^\top(\mathbf{x}_i - \mathbf{b})\|^2 = (\mathbf{v}^\top(\mathbf{x}_i - \mathbf{b}))^2$) can be rewritten into

$$\max_{\mathbf{v}} \sum_{i=1}^{m} \mathbf{v}^\top(\mathbf{x}_i - \mathbf{b})(\mathbf{x}_i - \mathbf{b})^\top\mathbf{v} \quad \text{s.t. } \|\mathbf{v}\|^2 = 1$$

Finding the direction of the line (cont'd)

- We want to solve

$$\max_{\mathbf{v}} \sum_{i=1}^{m} \mathbf{v}^\top (\mathbf{x}_i - \mathbf{b})(\mathbf{x}_i - \mathbf{b})^\top \mathbf{v} \quad \text{s.t. } \|\mathbf{v}\|^2 = 1$$

- The Lagrangian is:

$$L(\mathbf{v}, \lambda) = \mathbf{v}^\top \left(\sum_{i=1}^{m} (\mathbf{x}_i - \mathbf{b})(\mathbf{x}_i - \mathbf{b})^\top \right) \mathbf{v} + \lambda - \lambda \|\mathbf{v}\|^2$$

- Let $\mathbf{S} = \sum_{i=1}^{m} (\mathbf{x}_i - \mathbf{b})(\mathbf{x}_i - \mathbf{b})^\top$ be an n-by-n matrix, which we will call the *scatter matrix*
- Setting $\nabla_{\mathbf{v}} L = 0$, the solution of the problem must satisfy

$$\mathbf{S}\mathbf{v} = \lambda \mathbf{v}$$

Optimal choice of $\mathbf{v}$

- Recall: an *eigenvector* $\mathbf{u}$ of a matrix $\mathbf{A}$ satisfies $\mathbf{Au} = \lambda\mathbf{u}$, where $\lambda \in \mathbb{R}$ is the *eigenvalue*.
- Fact: the scatter matrix, $\mathbf{S}$, has n non-negative eigenvalues and n orthogonal eigenvectors.
- The equation obtained for $\mathbf{v}$ tells us that it should be an eigenvector of $\mathbf{S}$.
- The $\mathbf{v}$ that maximizes $\mathbf{v}^\top\mathbf{Sv}$ is the eigenvector of $\mathbf{S}$ with the largest eigenvalue

What is the scatter matrix

- $\mathbf{S}$ is an $n \times n$ matrix with

$$\mathbf{S}_{k,l} = \sum_{i=1}^{m} (\mathbf{x}_i(k) - \mathbf{b}(k))(\mathbf{x}_i(l) - \mathbf{b}(l))$$

- Hence, $\mathbf{S}_{k,l}$ is proportional to the *estimated covariance* between the kth and lth dimension in the data.

Recall: Covariance

- Covariance quantifies a *linear relationship* (if any) between two random variables X and Y.

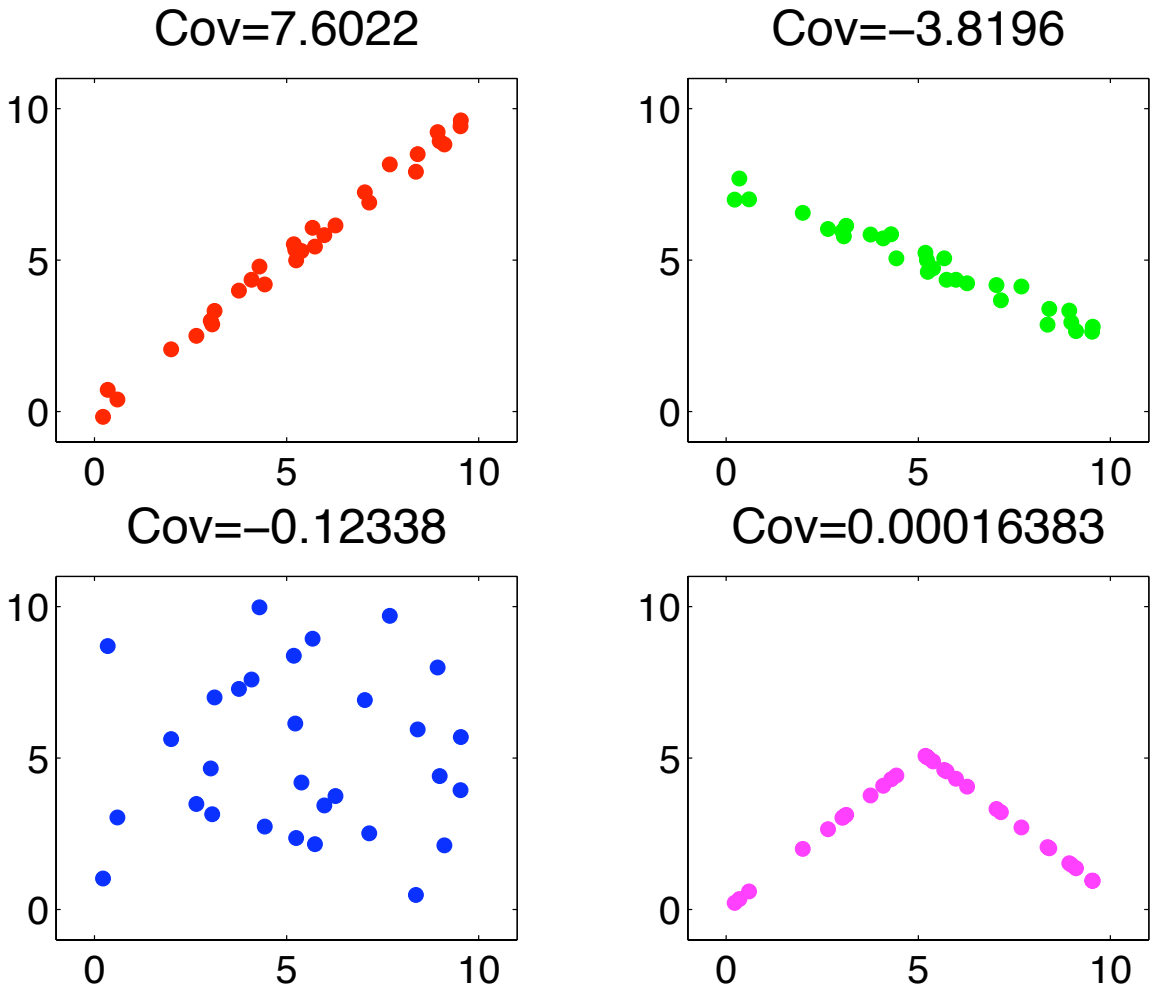
$$Cov(X, Y) = E\{(X - E(X))(Y - E(Y))\}$$

- Given m samples of X and Y, covariance can be estimated as

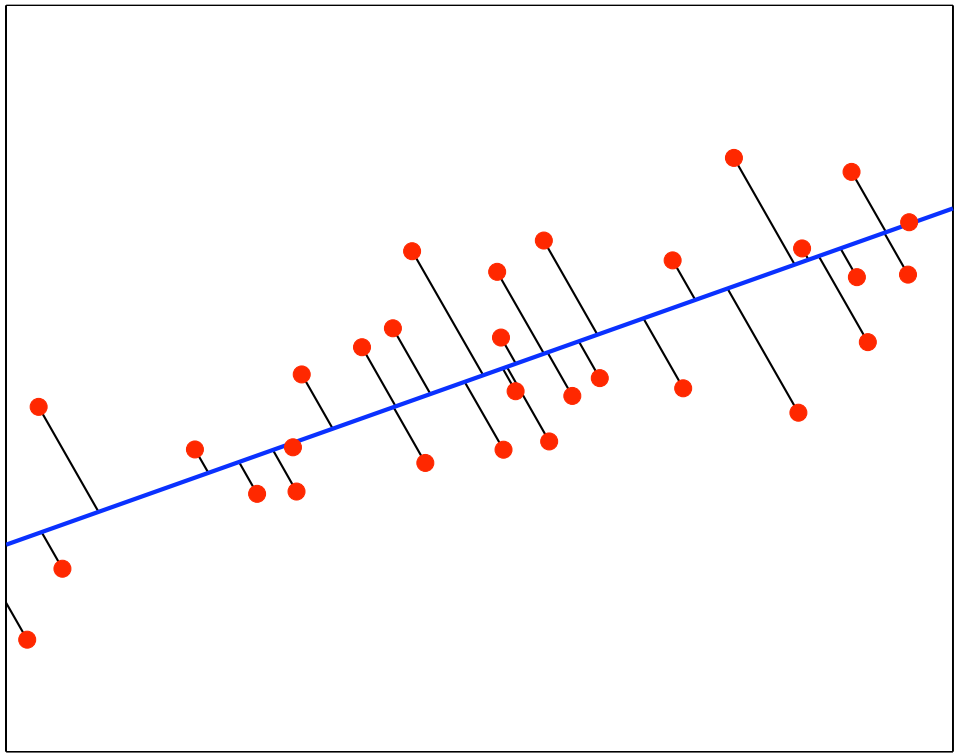
$$\frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_X)(y_i - \mu_Y) \ ,$$

  where $\mu_X = (1/m)\sum_{i=1}^{m} x_i$ and $\mu_Y = (1/m)\sum_{i=1}^{m} y_i$.
- Note: $Cov(X, X) = Var(X)$.

Covariance example



Example with optimal line: $\mathbf{b} = (0.54, 0.52)$, $\mathbf{v} \propto (1, 0.45)$



Remarks

- The line $\mathbf{b} + \alpha\mathbf{v}$ is the *first principal component*.
- The variance of the data along the line $\mathbf{b} + \alpha\mathbf{v}$ is as large as along any other line.
- $\mathbf{b}$, $\mathbf{v}$, and the α_i can be computed easily in polynomial time.

Generalization to d dimensions

- More generally, we can create a d-dimensional representation of our data by projecting the instances onto a hyperplane $\mathbf{b} + \alpha^1 \mathbf{v}_1 + \ldots + \alpha^d \mathbf{v}_d$.
- If we assume the $\mathbf{v}_j$ are of unit length and orthogonal, then the optimal choices are:
  - $\mathbf{b}$ is the mean of the data (as before)
  - The $\mathbf{v}_j$ are orthogonal eigenvectors of $\mathbf{S}$ corresponding to its d largest eigenvalues.
  - Each instance is projected orthogonally on the hyperplane.

PCA: overall algorithm

1. Center the data $\tilde{\mathbf{x}}_i = \mathbf{x}_i - \mathbf{b}$ where $\mathbf{b} = \frac{1}{m}\sum_i \mathbf{x}_i$.
2. (Optional step: normalize the data.)
3. Compute the top d (unit-norm) eigenvectors of $\mathbf{S} = \sum_i \tilde{\mathbf{x}}_i \tilde{\mathbf{x}}_i^\top$.
   (observe that $\mathbf{S} = \tilde{\mathbf{X}}^\top \tilde{\mathbf{X}}$ where $\tilde{\mathbf{X}} \in \mathbb{R}^{m \times n}$ is the centered data matrix)
4. Put these eigenvectors into a matrix $\mathbf{U} \in \mathbb{R}^{n \times d}$.
5. The PCA projection of any point $\mathbf{x}$ is given by
   * $\mathbf{U}^\top(\mathbf{x} - \mathbf{b}) \in \mathbb{R}^d$ in the latent space.
   * $\mathbf{b} + \mathbf{U}\mathbf{U}^\top(\mathbf{x} - \mathbf{b}) \in \mathbb{R}^n$ in the ambient space.

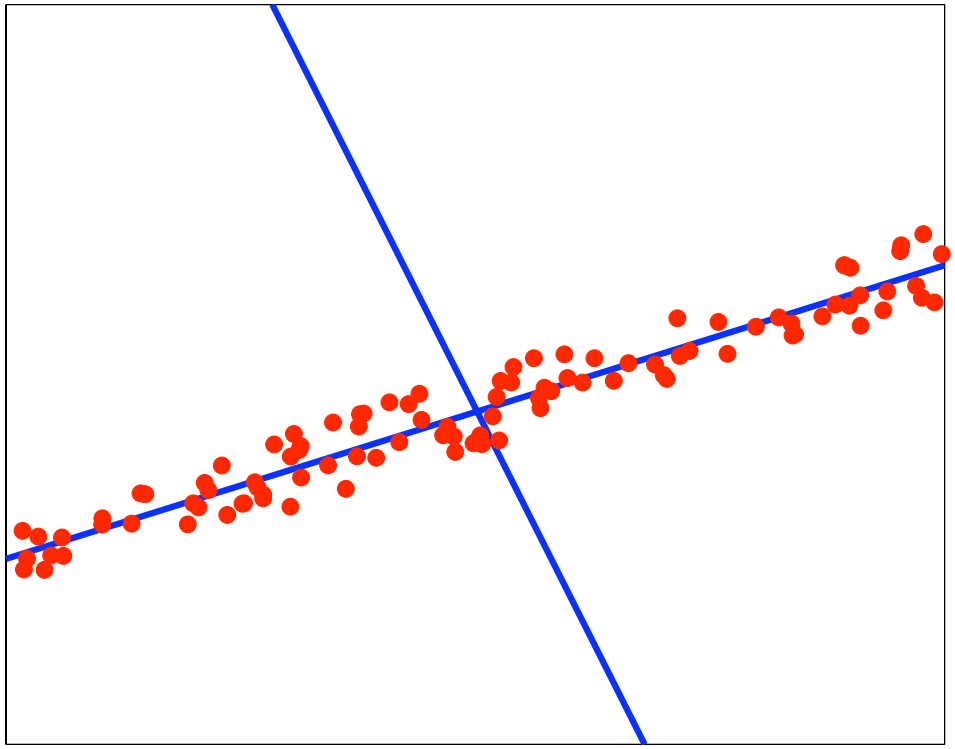
Remarks

- $\mathbf{b}$, the eigenvalues, the $\mathbf{v}_j$, and the projections of the instances can all be computed in polynomial time.
- The magnitude of the j^{th}-largest eigenvalue, λ_j, tells you how much variability in the data is captured by the j^{th} principal component
- So you have feedback on how to choose d!
- When the eigenvalues are sorted in decreasing order, the proportion of the variance captured by the first d components is:

$$\frac{\lambda_1 + \cdots + \lambda_d}{\lambda_1 + \cdots + \lambda_d + \lambda_{d+1} + \cdots + \lambda_n}$$

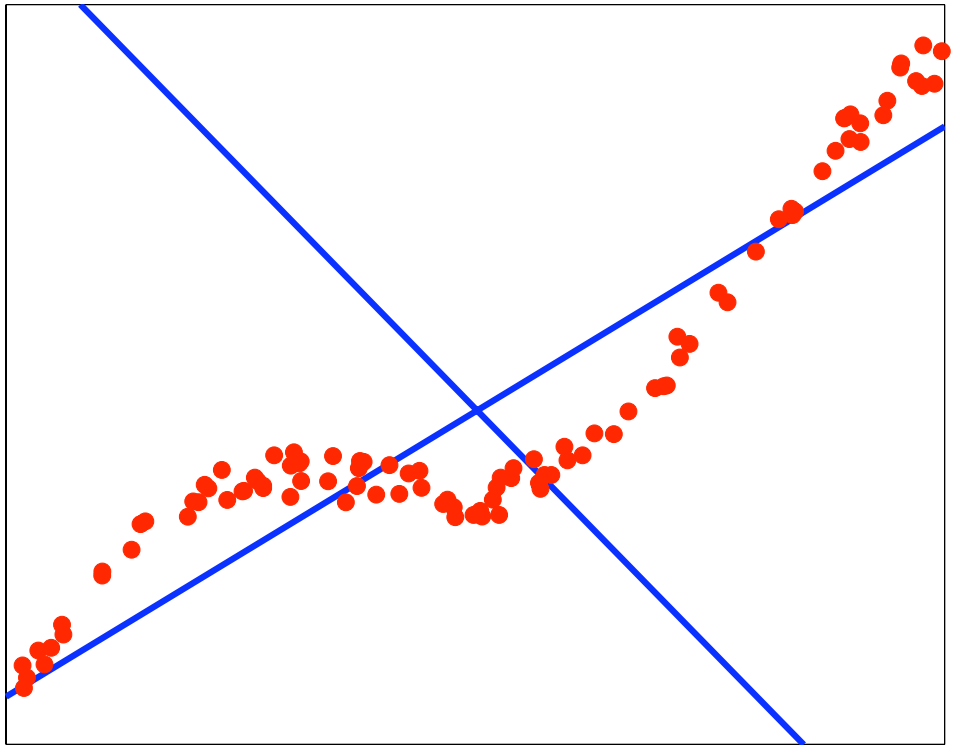
- So if a "big" drop occurs in the eigenvalues at some point, that suggests a good dimension cutoff

Example: $\lambda_1 = 0.0938, \lambda_2 = 0.0007$



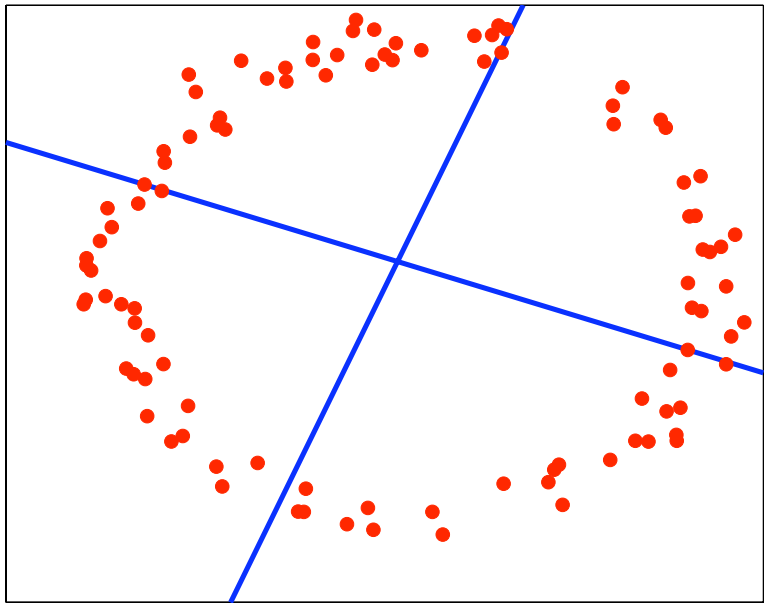
The first eigenvalue accounts for most variance, so the dimensionality is 1

Example: $\lambda_1 = 0.1260, \lambda_2 = 0.0054$



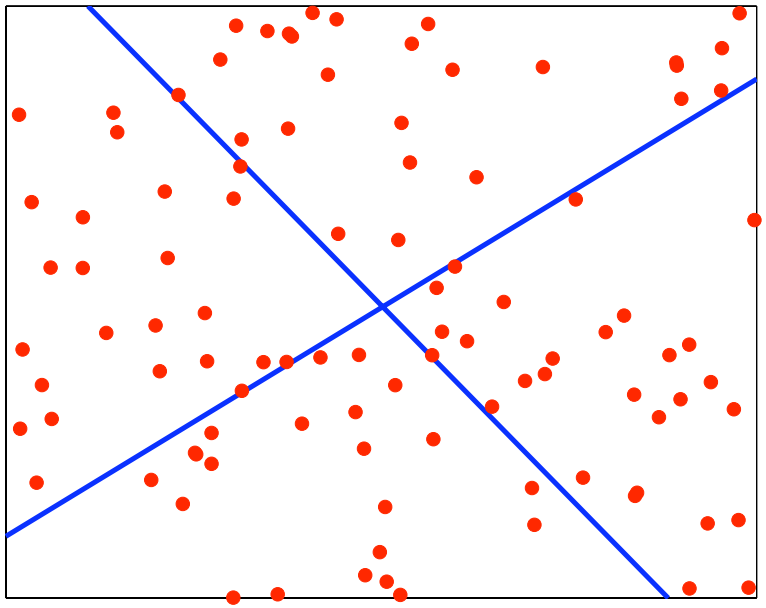
The first eigenvalue accounts for most variance, so the dimensionality is 1 (despite some non-linear structure in the data)

Example: $\lambda_1 = 0.0884, \lambda_2 = 0.0725$



- Each eigenvalue accounts for about half the variance, so the PCA-suggested dimension is 2
- Note that this is the *linear* dimension
- The true "non-linear" dimension of the data is 1 (using polar coordinates)

Example: $\lambda_1 = 0.0881, \lambda_2 = 0.0769$

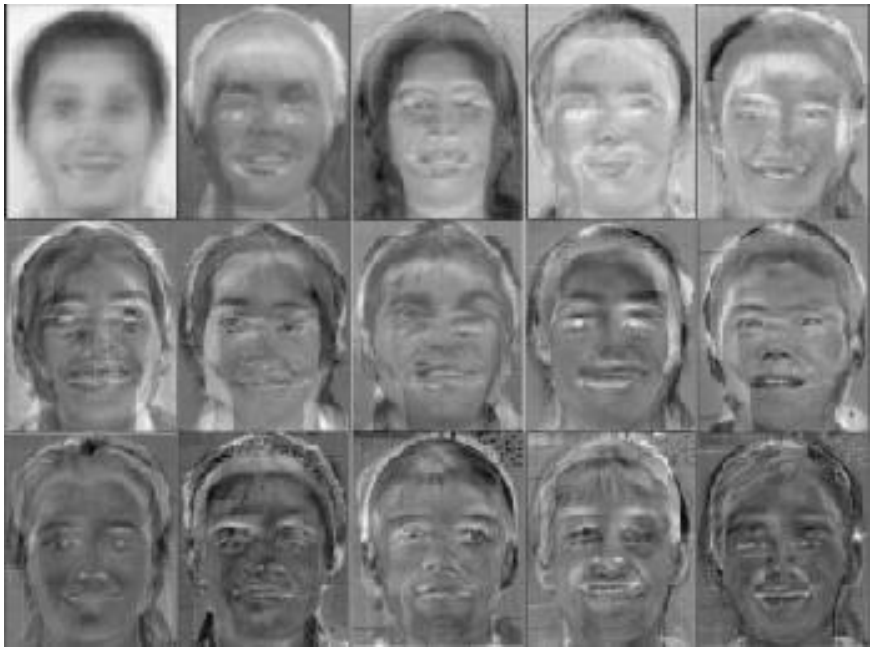


- Each eigenvalue accounts for about half the variance, so the PCA-suggested dimension is 2
- In this case, the non-linear dimension is also 2 (data is fully random)
- Note that *PCA cannot distinguish non-linear structure from no structure*
- This case and the previous one yield a very similar PCA analysis

Remarks

- Outliers have a big effect on the covariance matrix, so they can affect the eigenvectors quite a bit
- A simple examination of the pairwise distances between instances can help discard points that are very far away (for the purpose of PCA)
- If the variances in the original dimensions vary considerably, they can "muddle" the true correlations. There are two solutions:
  - Work with the correlation (covariance rescaled to $(-1, 1)$) of the original data, instead of covariance matrix (which provides one type of normalization)
  - Normalize the input dimensions individually (possibly based on domain knowledge) before PCA
- PCA is most often performed using Singular Value Decomposition (SVD)
- In certain cases, the eigenvectors are meaningful; e.g. in vision, they can be displayed as images ("eigenfaces")

Eigenfaces example

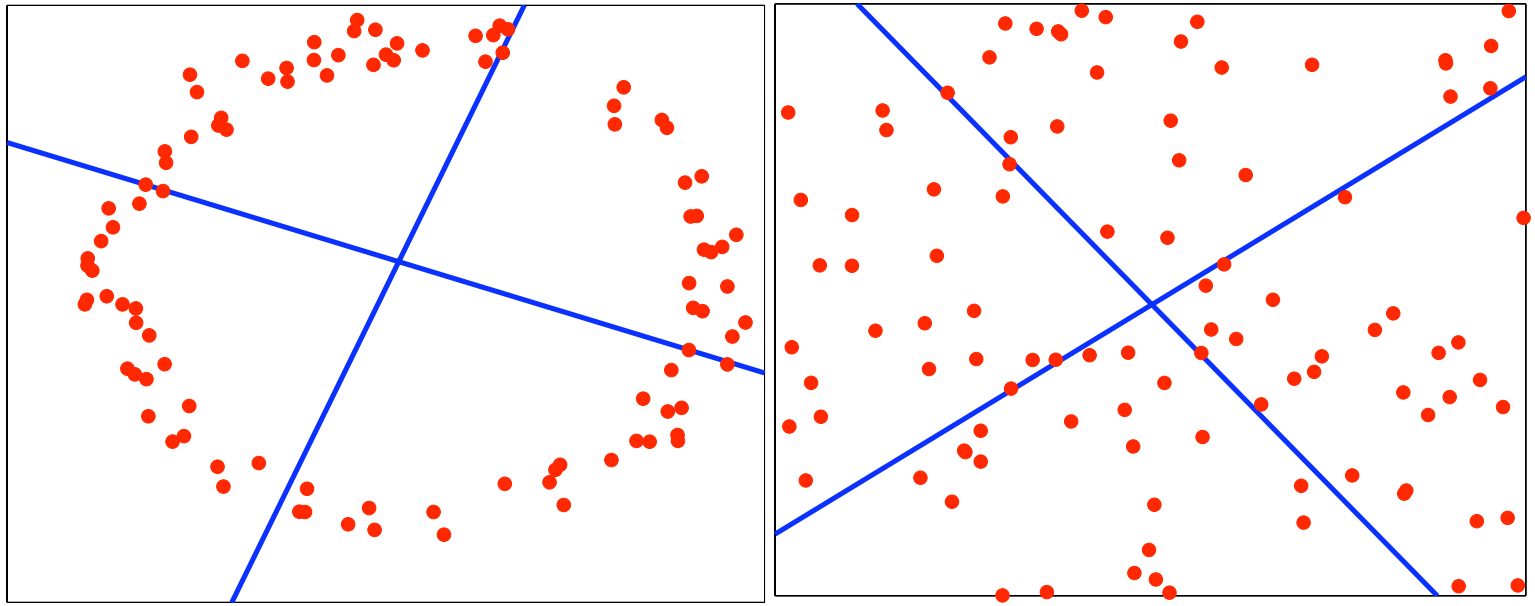


- A set of faces on the left and the corresponding eigenfaces (principal components) on the right
- Note that faces have to be centred and scaled ahead of time
- The components are in the same space as the instances (images) and can be used to reconstruct the images

Uses of PCA

- Pre-processing for a supervised learning algorithm, e.g. for image data, robotic sensor data
- Used with great success in image and speech processing
- Visualization
- Exploratory data analysis
- Removing the linear component of a signal (before fancier non-linear models are applied)

Difficult example



- PCA will make no difference between these examples, because the structure on the left is not linear
- Are there ways to find non-linear, low-dimensional manifolds?

Making PCA non-linear

- Suppose that instead of using the points $\mathbf{x}_i$ as is, we wanted to go to some different *feature space* $\phi(\mathbf{x}_i) \in \mathbb{R}^N$
- E.g. using polar coordinates instead of cartesian coordinates would help us deal with the circle
- In the higher dimensional space, we can then do PCA
- The result will be non-linear in the original data space!
- Similar idea to support vector machines

PCA in feature space (I)

- Suppose for now that the data is centered in feature space, i.e. $\sum_{i=1}^{m} \phi(\mathbf{x}_i) = \mathbf{0}$
- The scatter matrix is:

$$\mathbf{S} = \sum_{i=1}^{m} \phi(\mathbf{x}_i)\phi(\mathbf{x}_i)^\top = \mathbf{\Phi}^\top \mathbf{\Phi} \in \mathbb{R}^{N \times N} \qquad \text{where } \mathbf{\Phi}_{i,:} = \phi(\mathbf{x}_i)^\top$$

- The eigenvectors are:

$$\mathbf{S}\mathbf{v}_j = \lambda_j \mathbf{v}_j, \quad j = 1, \ldots N \quad (N \text{ is the dim. of the feature space})$$

- We want to avoid explicitly going to feature space - instead we want to work with *kernels and the Gram matrix* $\mathbf{K} = \mathbf{\Phi}\mathbf{\Phi}^\top \in \mathbb{R}^{m \times m}$:

$$\mathbf{K}_{i,j} = K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_j)^\top \phi(\mathbf{x}_k)$$

PCA in feature space (II)

- Let $\mathbf{v} \in \mathbb{R}^N$ be any eigenvector of the scatter matrix. We have

$$\lambda \mathbf{v} = \mathbf{S}\mathbf{v} = \mathbf{\Phi}^\top \mathbf{\Phi}\mathbf{v} = \sum_{i=1}^{m} \phi(\mathbf{x}_i)\phi(\mathbf{x}_i)^\top \mathbf{v}$$

$\Rightarrow$ The eigenvectors can be written as a linear combinations of features:

$$\mathbf{v} = \sum_{i=1}^{m} \frac{1}{\lambda}(\phi(\mathbf{x}_i)^\top \mathbf{v})\ \phi(\mathbf{x}_i) = \sum_{i=1}^{m} (\mathbf{a})_i \phi(\mathbf{x}_i) = \mathbf{\Phi}^\top \mathbf{a}$$

- Finding an eigenvector $\mathbf{v}$ of the scatter matrix is equivalent to finding the vector of coefficients $\mathbf{a} \in \mathbb{R}^m$ (since $\mathbf{v} = \mathbf{\Phi}^\top \mathbf{a}$)!

PCA in feature space (III)

- By substituting $\mathbf{v} = \mathbf{\Phi}^\top \mathbf{a}$ back into the eigenvector equation we get:

$$\mathbf{S}\mathbf{v} = \lambda \mathbf{v} \quad \Rightarrow \quad \mathbf{\Phi}^\top \mathbf{\Phi} \mathbf{v} = \mathbf{\Phi}^\top \mathbf{\Phi} \mathbf{\Phi}^\top \mathbf{a} = \lambda \mathbf{\Phi}^\top \mathbf{a} \quad \Rightarrow \quad \mathbf{\Phi}^\top \mathbf{K} \mathbf{a} = \lambda \mathbf{\Phi}^\top \mathbf{a}$$

- A small trick: multiplying by $\mathbf{\Phi}$ to the left gives us

$$\mathbf{\Phi} \mathbf{\Phi}^\top \mathbf{K} \mathbf{a} = \lambda \mathbf{\Phi} \mathbf{\Phi}^\top \mathbf{a} \quad \Rightarrow \quad \mathbf{K}^2 \mathbf{a} = \lambda \mathbf{K} \mathbf{a}$$

- We can remove a factor of $\mathbf{K}$ from both sides of the matrix (this will only affect eigenvectors with eigenvalues 0, which will not be principle components anyway):

$$\mathbf{K}\mathbf{a} = \lambda \mathbf{a}$$

$\Rightarrow$ For any eigenvector $\mathbf{v}$ of the scatter matrix (in feature space), the corresponding vector of coefficients $\mathbf{a}$ is an eigenvector of the Gram matrix (with the same eigenvalue)!

PCA in feature space (IV)

- We know that $\mathbf{a}$ is an eigenvector of $\mathbf{K}$ but we don't know its norm yet...
- Remember that the eigenvector $\mathbf{v}$ of $\mathbf{S}$ must be of norm 1, this implies a dual normalization condition for the vector $\mathbf{a}$:

$$\|\mathbf{v}\|^2 = \mathbf{v}^\top \mathbf{v} = 1 \Rightarrow \mathbf{a}^\top \mathbf{\Phi}\mathbf{\Phi}^\top \mathbf{a} = \mathbf{a}^\top \mathbf{K}\mathbf{a} = 1$$

- Plugging this into $\mathbf{K}\mathbf{a} = \lambda\mathbf{a}$ we get $\|\mathbf{a}\|^2 = \frac{1}{\lambda}$.

  $\rightarrow$ We can rescale a unit-norm eigenvector $\mathbf{z}$ of $\mathbf{K}$ to obtain $\mathbf{a} = \frac{1}{\sqrt{\lambda}}\mathbf{z}$.
- As before, for a new point $\mathbf{x}$, let $\mathbf{k_x} \in \mathbb{R}^m$ be defined by $(\mathbf{k_x})_i = K(\mathbf{x}, \mathbf{x}_i)$. The projection of $\mathbf{x}$ onto the jth principal components is:

$$\phi(\mathbf{x})^\top \mathbf{v}_j = \phi(\mathbf{x})^\top \mathbf{\Phi}^\top \mathbf{a}_j = \mathbf{k}_\mathbf{x}^\top \mathbf{a}_j$$

  where $\mathbf{v}_j$ is the jth eigenvector of $\mathbf{S}$ and $\mathbf{a}_j$ is the scaled jth eigenvector of $\mathbf{K}$!

Normalizing the feature space

- In general, the features $\phi(\mathbf{x}_i)$ may not have mean 0
- We want to work with $\tilde{\phi}(\mathbf{x}_i) = \phi(\mathbf{x}_i) - \frac{1}{m}\sum_{k=1}^{m}\phi(\mathbf{x}_k)$
- The corresponding kernel matrix entries are given by:

$$\tilde{\mathbf{K}}_{i,j} = \tilde{K}(\mathbf{x}_i, \mathbf{x}_j) = \tilde{\phi}(\mathbf{x}_i)^\top \tilde{\phi}(\mathbf{x}_j)$$

- After some algebra, we get:

$$\tilde{\mathbf{K}} = \mathbf{K} - \mathbf{O}_{1/m}\mathbf{K} - \mathbf{K}\mathbf{O}_{1/m} + \mathbf{O}_{1/m}\mathbf{K}\mathbf{O}_{1/m}$$

and

$$\tilde{\mathbf{k}}_{\mathbf{x}} = \mathbf{k}_{\mathbf{x}} - \mathbf{O}_{1/m}\mathbf{k}_{\mathbf{x}} - \mathbf{K}\mathbf{1}_{1/m} + \mathbf{O}_{1/m}\mathbf{K}\mathbf{1}_{1/m}$$

where $\mathbf{O}_{1/m}$ (resp. $\mathbf{1}_{1/m}$) is the matrix (resp. vector) with all elements equal to $1/m$.

Kernel PCA: overall algorithm

1. Pick a kernel and build the Gram matrix $\mathbf{K} \in \mathbb{R}^{m \times m}$.
2. Compute the Gram matrix of the centered the data in the feature space:

$$\tilde{\mathbf{K}} = \mathbf{K} - \mathbf{O}_{1/m}\mathbf{K} - \mathbf{K}\mathbf{O}_{1/m} + \mathbf{O}_{1/m}\mathbf{K}\mathbf{O}_{1/m}$$

3. Compute the top d eigenvalues and (unit-norm) eigenvectors of $\tilde{\mathbf{K}}$.
4. Put the eigenvectors into a matrix $\mathbf{U} \in \mathbb{R}^{n \times d}$ and the corresponding eigenvalues in a diagonal matrix $\mathbf{D} \in \mathbb{R}^{d \times d}$.
5. The PCA projection of any point $\mathbf{x}$ is given by

$$\hat{\mathbf{x}} = \mathbf{D}^{-1/2}\mathbf{U}^\top \tilde{\mathbf{k}}_{\mathbf{x}}$$

where $\tilde{\mathbf{k}}_{\mathbf{x}}$ is defined as in the previous slide.
(Note that multiplying by $\mathbf{D}^{-1/2}$ corresponds to rescaling the unit-norm eigenvectors of $\tilde{\mathbf{K}}$ to get the vectors of coefficients $\mathbf{a}_j$).

Representation obtained by kernel PCA

- Each $y_j = \phi(\mathbf{x})^\top \mathbf{v}_j = \mathbf{a}_j^\top \mathbf{k}_\mathbf{x}$ is the coordinate of $\phi(\mathbf{x})$ along one of the feature space axis $\mathbf{v}_j$
- Since the $\mathbf{v}_j$'s are orthogonal, the projection of $\phi(\mathbf{x})$ onto the space spanned by the top d eigenvectors is:

$$\Pi\phi(\mathbf{x}) = \sum_{j=1}^{d} y_j \mathbf{v}_j = \sum_{j=1}^{d} (\mathbf{a}_j^\top \mathbf{k}_\mathbf{x}) \mathbf{\Phi}^\top \mathbf{a}_j$$

- The *reconstruction error in feature space* can be evaluated as:

$$\|\phi(\mathbf{x}) - \Pi\phi(\mathbf{x})\|^2$$

This can be re-written by expanding the norm; we obtain dot-products which can all be replaced by kernels

- Note that the error will be 0 on the training data if enough $\mathbf{v}_j$ are retained

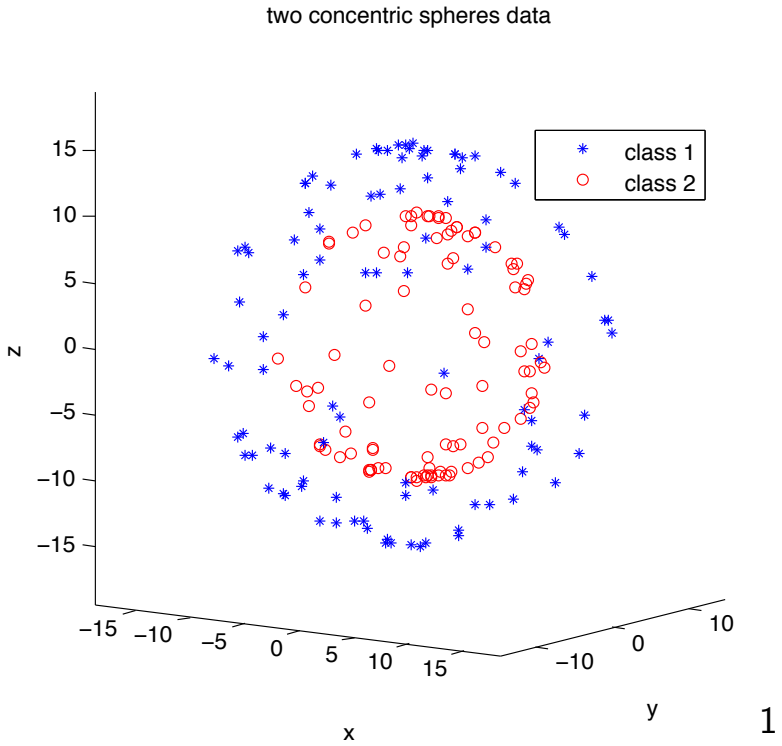
Alternative reconstruction error measures

- An alternative way of measuring performance is by looking at how well kernel PCA preserves distances between data points
- In this case, the Euclidian distance in kernel space between points $\phi(\mathbf{x}_i)$ and $\phi(\mathbf{x}_j)$, d_{ij}, is:

$$\|\phi(\mathbf{x}_i) - \phi(\mathbf{x}_j)\|^2 = K(\mathbf{x}_i, \mathbf{x}_i) + K(\mathbf{x}_j, \mathbf{x}_j) - 2K(\mathbf{x}_i, \mathbf{x}_j)$$

- The distance $\hat{d}_{ij}$ between the projected points in kernel space is defined as above, but with $\phi(\mathbf{x}_i)$ replaced by $\Pi\phi(\mathbf{x}_i)$.
- The average of $d_{ij} - \hat{d}_{ij}$ over all pairs of points is a measure of reconstruction error
- Note that reconstruction error in the original space of the $\mathbf{x}_i$ is very difficult to compute, because it requires taking $\Pi\phi(\mathbf{x})$ and finding its pre-image in the original feature space, which is not always feasible (though approximations exist)

Example: Two concentric spheres

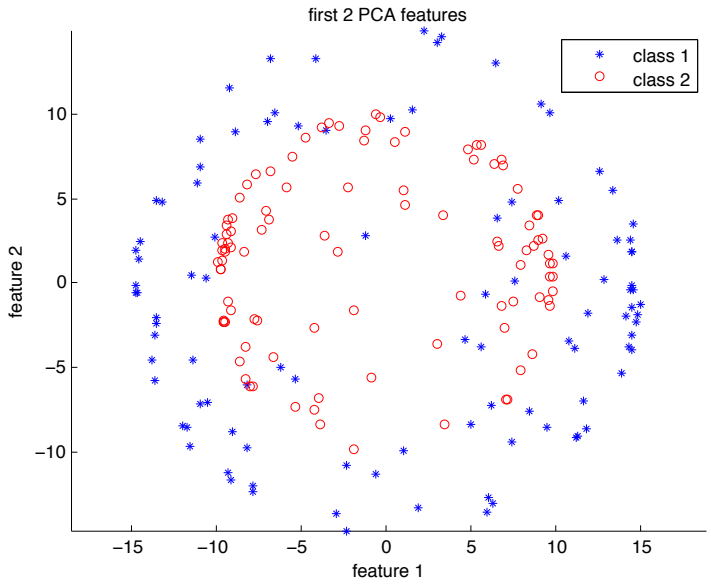


1

- Colours are used for clarity in the picture, but the data is presented unlabelled
- We want to project form 3D to 2D

[1] Wang, 2012

Example: Two concentric spheres - PCA

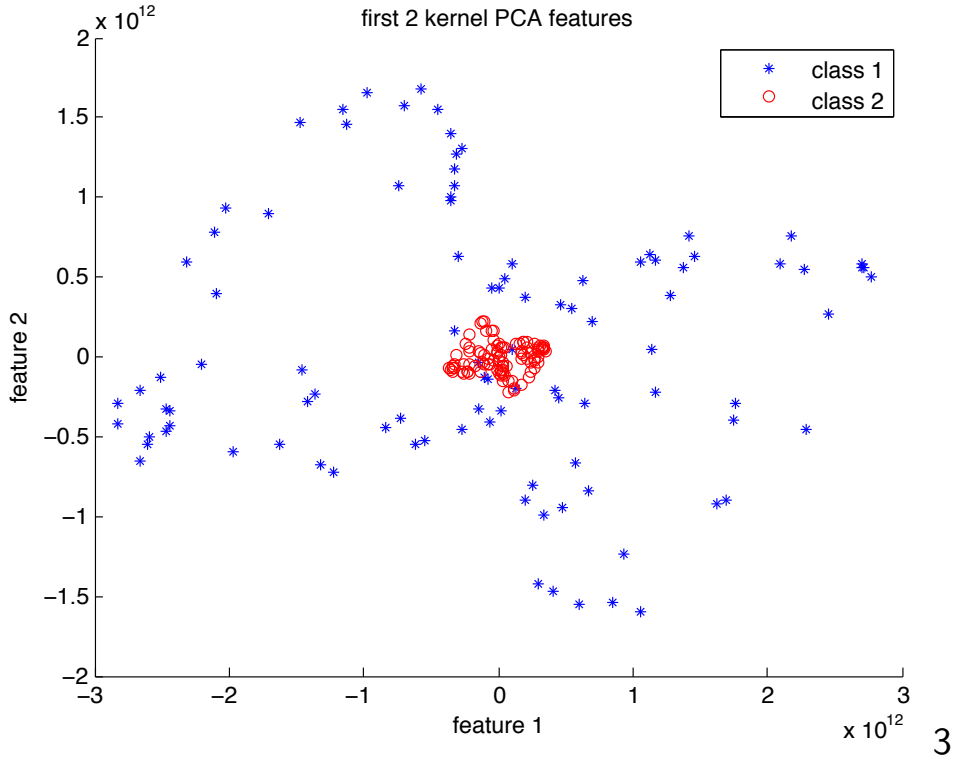


[2]

Note that PCA is unable to separate the points from the two spheres

[2] Wang, 2012

Example: Kernel PCA with Polynomial Kernel ($d = 5$)

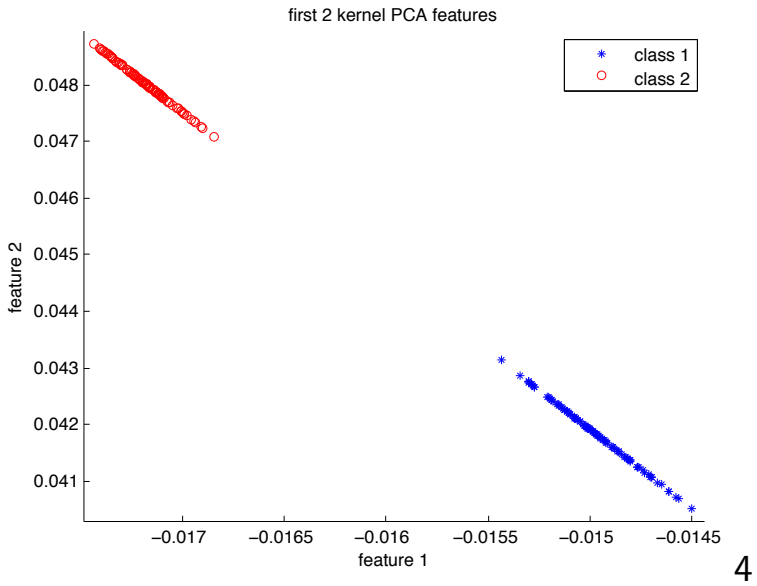


[3]

- Points from one sphere are much closer together, the others are scattered
- The projected data is not linearly separable

[3] Wang, 2012

Example: Kernel PCA with Gaussian Kernel ($\sigma = 20$)



[4]

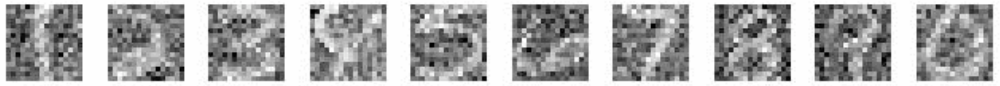
- Points from the two spheres are really well separated
- Note that the choice of parameter for the kernel matters!
- Validation can be used to determine good kernel parameter values

[4] Wang, 2012

Example: De-noising images

Original data

Data corrupted with Gaussian noise



Result after linear PCA

Result after kernel PCA, Gaussian kernel

PCA vs Kernel PCA

- Kernel PCA can give a good re-encoding of the data when it lies along a non-linear manifold
- The kernel matrix is $m \times m$, so kernel PCA will have difficulties if we have lots of data points
- In this case, we may need to use dictionary methods to pick a subset of the data
- For general kernels, we may not be able to easily visualize the image of a point in the input space, though visualization still works for simple kernels

Locally Linear Embedding

- $\mathbf{x}_1, \cdots, \mathbf{x}_m \in \mathbb{R}^n$ lies on a k-dimensional manifold.

$\Rightarrow$ Each point and its neighbors lie close to a *locally linear* patch of the manifold.

- We try to reconstruct each point from its neighbors:

$$\min_{\mathbf{W}} \sum_i \|\mathbf{x}_i - \sum_j \mathbf{W}_{i,j}\mathbf{x}_j\|^2$$

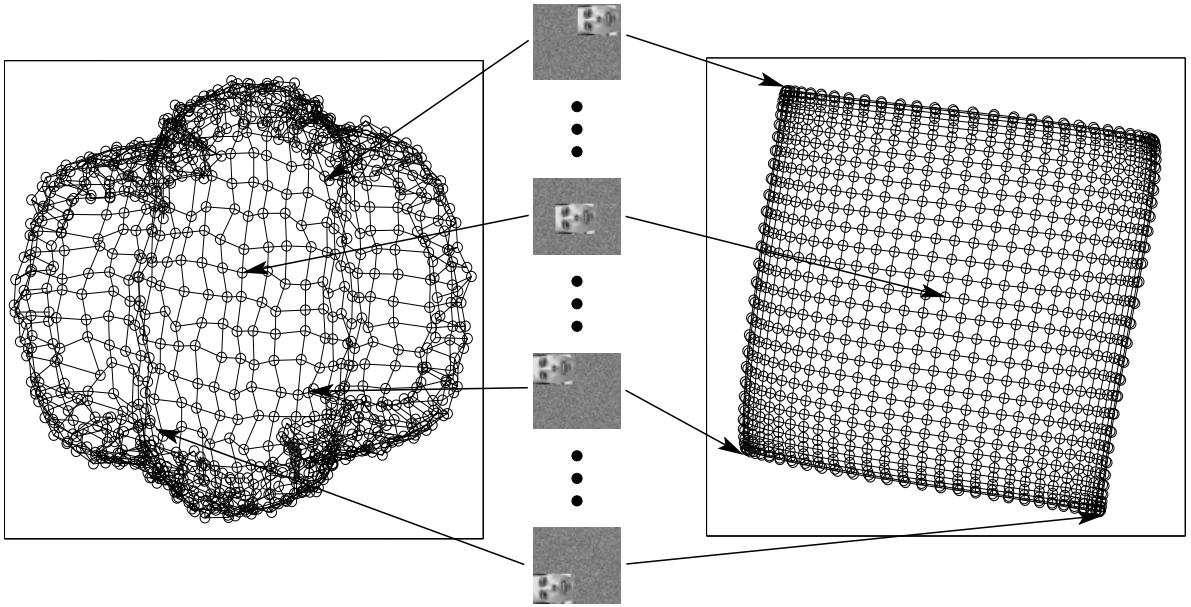
s.t. $\mathbf{W1} = \mathbf{1}$ and $\mathbf{W}_{i,j} = 0$ if $\mathbf{x}_j \notin neighbors(\mathbf{x}_i)$

$\Rightarrow$ For each point the weights are invariant to rotation, scaling and translations: the weights $\mathbf{W}_{i,j}$ capture intrinsic geometric properties of each neighborhood.

- These local properties of each neighborhood should be preserved by the embedding:

$$\min_{\mathbf{z}_1,\ldots,\mathbf{z}_m \in \mathbb{R}^k} \sum_i \|\mathbf{z}_i - \sum_j \mathbf{W}_{i,j}\mathbf{z}_j\|^2$$

PCA vs Locally Linear Embedding



[Saul, L. K., & Roweis, S. T. (2000). An introduction to locally linear embedding.]