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 $x_1, \cdots, x_m$ 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 $x_1, \cdots, x_m$, 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).

⇒ 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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What is the true dimensionality of this data?
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 $b + \alpha v$ for $b, v \in \mathbb{R}^n$, $\alpha \in \mathbb{R}$. For convenience assume $\|v\| = 1$.

• Each instance $x_i$ is associated with a point on the line $\hat{x}_i = b + \alpha_i v$.

• We want to choose $b$, $v$, and the $\alpha_i$ to minimize the total reconstruction error over all data points, measured using Euclidean distance:

$$ R = \sum_{i=1}^{m} \| x_i - \hat{x}_i \|^2 $$
A constrained optimization problem!

\[
\begin{align*}
\text{min} & \quad \sum_{i=1}^{m} \| x_i - (b + \alpha_i v) \|^2 \\
\text{w.r.t.} & \quad b, v, \alpha_i, i = 1, \ldots, m \\
\text{s.t.} & \quad \| v \|^2 = 1
\end{align*}
\]

- This is a quadratic objective with quadratic constraint
- Suppose we fix a \( v \) satisfying the condition, and find the best \( b \) and \( \alpha_i \) given this \( v \)
- So, we solve:

\[
\min R = \min_{\alpha, b} \sum_{i=1}^{m} \| x_i - (b + \alpha_i v) \|^2
\]

where \( R \) is the reconstruction error
Solving the optimization problem (II)

• We write the gradient of $R$ wrt to $\alpha_i$ and set it to 0:

$$\frac{\partial R}{\partial \alpha_i} = 2\|v\|^2 \alpha_i - 2vx_i + 2bv = 0 \Rightarrow \alpha_i = v \cdot (x_i - b)$$

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

• We write the gradient of $R$ wrt $b$ and set it to 0:

$$\nabla_b R = 2mb - 2\sum_{i=1}^{m} x_i + 2 \left( \sum_{i=1}^{m} \alpha_i \right) v = 0 \Rightarrow mb = \sum_{i=1}^{m} x_i - \sum_{i=1}^{m} \alpha_i v$$

• From above:

$$\sum_{i=1}^{m} \alpha_i v = \left( \sum_{i=1}^{m} v^\top (x_i - b) \right) v = vv^\top \left( \sum_{i=1}^{m} x_i - mb \right)$$
Solving the optimization problem (III)

• Combining the previous two equations we get:

\[(I - vv^\top)mb = (I - vv^\top) \sum_{i=1}^{m} x_i\]

• This is satisfied when:

\[b = \frac{1}{m} \sum_{i=1}^{m} x_i\]

• This means that the line goes through the mean of the data
• By substituting \(\alpha_i = v^\top (x_i - b)\), we get:

\[\hat{x}_i = b + \alpha_i v = b + vv^\top (x_i - b)\]

• This means that instances are projected orthogonally on the line to get the associated point.
Example with $\mathbf{v} \propto (1, 0.3)$
**Finding the direction of the line**

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

$$\min_v \sum_{i=1}^{m} \|(I - vv^\top)(x_i - b)\|^2 \quad \text{s.t.} \quad \|v\|^2 = 1$$

- Using the fact that $\|(I - vv^\top)(x_i - b)\|^2 = \|x_i - b\|^2 - \|vv^\top(x_i - b)\|^2$ (since $\|v\|^2 = 1$) this is equivalent to

$$\max_v \sum_{i=1}^{m} \|vv^\top(x_i - b)\|^2 \quad \text{s.t.} \quad \|v\|^2 = 1$$

which (using $\|vv^\top(x_i - b)\|^2 = (v^\top(x_i - b))^2$) can be rewritten into

$$\max_v \sum_{i=1}^{m} v^\top(x_i - b)(x_i - b)^\top v \quad \text{s.t.} \quad \|v\|^2 = 1$$
Finding the direction of the line (cont’d)

• We want to solve

\[
\max_v \sum_{i=1}^m v^\top (x_i - b)(x_i - b)^\top v \quad \text{s.t. } \|v\|^2 = 1
\]

• The Lagrangian is:

\[
L(v, \lambda) = v^\top \left( \sum_{i=1}^m (x_i - b)(x_i - b)^\top \right) v + \lambda - \lambda\|v\|^2
\]

• Let \( S = \sum_{i=1}^m (x_i - b)(x_i - b)^\top \) be an \( n \)-by-\( n \) matrix, which we will call the scatter matrix.

• Setting \( \nabla_v L = 0 \), the solution of the problem must satisfy

\[
Sv = \lambda v
\]
Optimal choice of $\mathbf{v}$

- Recall: an *eigenvector* $\mathbf{u}$ of a matrix $\mathbf{A}$ satisfies $\mathbf{A}\mathbf{u} = \lambda \mathbf{u}$, 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 $\mathbf{v}^\top \mathbf{S} \mathbf{v}$ is the eigenvector of $\mathbf{S}$ with the largest eigenvalue.
What is the scatter matrix

- $S$ is an $n \times n$ matrix with

$$S_{k,l} = \sum_{i=1}^{m} (x_i(k) - b(k))(x_i(l) - b(l))$$

- Hence, $S_{k,l}$ is proportional to the estimated covariance between the $k$th and $l$th 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

Cov = 7.6022

Cov = -3.8196

Cov = -0.12338

Cov = 0.00016383
Example with optimal line: $b = (0.54, 0.52), \ v \propto (1, 0.45)$
Remarks

- The line $\mathbf{b} + \alpha \mathbf{v}$ is the \textit{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 $\alpha_i$ 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 $b + \alpha^1v_1 + \ldots + \alpha^dv_d$.
- If we assume the $v_j$ are of unit length and orthogonal, then the optimal choices are:
  - $b$ is the mean of the data (as before)
  - The $v_j$ are orthogonal eigenvectors of $S$ corresponding to its $d$ largest eigenvalues.
  - Each instance is projected orthogonally on the hyperplane.
PCA: overall algorithm

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

• b, the eigenvalues, the v_j, and the projections of the instances can all be computed in polynomial time.

• The magnitude of the j^{th}-largest eigenvalue, \lambda_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)
• 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 $x_i$ as is, we wanted to go to some different feature space $\phi(x_i) \in \mathbb{R}^N$

• 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.
  \[ \sum_{i=1}^{m} \phi(x_i) = 0 \]

• The scatter matrix is:
  \[ S = \sum_{i=1}^{m} \phi(x_i)\phi(x_i)^\top = \Phi^\top \Phi \in \mathbb{R}^{N \times N} \]
  where \( \Phi_{i,:} = \phi(x_i)^\top \)

• The eigenvectors are:
  \[ Sv_j = \lambda_j v_j, \quad j = 1, \ldots, N \quad (N \text{ is the dim. of the feature space}) \]

• We want to avoid explicitly going to feature space - instead we want to work with kernels and the Gram matrix \( K = \Phi \Phi^\top \in \mathbb{R}^{m \times m} \):
  \[ K_{i,j} = K(x_i, x_j) = \phi(x_j)^\top \phi(x_k) \]
Let \( \mathbf{v} \in \mathbb{R}^N \) be any eigenvector of the scatter matrix. We have

\[
\lambda \mathbf{v} = S \mathbf{v} = \Phi^\top \Phi \mathbf{v} = \sum_{i=1}^{m} \phi(x_i) \phi(x_i)^\top \mathbf{v}
\]

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

\[
\mathbf{v} = \sum_{i=1}^{m} \frac{1}{\lambda} (\phi(x_i)^\top \mathbf{v}) \phi(x_i) = \sum_{i=1}^{m} (a_i) \phi(x_i) = \Phi^\top \mathbf{a}
\]

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

• By substituting $v = \Phi^T a$ back into the eigenvector equation we get:

$$Sv = \lambda v \Rightarrow \Phi^T \Phi v = \Phi^T \Phi \Phi^T a = \lambda \Phi^T a \Rightarrow \Phi^T Ka = \lambda \Phi^T a$$

• A small trick: multiplying by $\Phi$ to the left gives us

$$\Phi \Phi^T Ka = \lambda \Phi \Phi^T a \Rightarrow K^2 a = \lambda Ka$$

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

$$Ka = \lambda a$$

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

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

$$\|v\|^2 = v^T v = 1 \Rightarrow a^T \Phi \Phi^T a = a^T K a = 1$$

• Plugging this into $K a = \lambda a$ we get $\|a\|^2 = \frac{1}{\lambda}$.
  $\rightarrow$ We can rescale a unit-norm eigenvector $z$ of $K$ to obtain $a = \frac{1}{\sqrt{\lambda}} z$.
• As before, for a new point $x$, let $k_x \in \mathbb{R}^m$ be defined by $(k_x)_i = K(x, x_i)$. The projection of $x$ onto the $j$th principal components is:

$$\phi(x)^T v_j = \phi(x)^T \Phi^T a_j = k_x^T a_j$$

where $v_j$ is the $j$th eigenvector of $S$ and $a_j$ is the scaled $j$th eigenvector of $K$!
Normalizing the feature space

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

$$\tilde{K}_{i,j} = \tilde{K}(x_i, x_j) = \tilde{\phi}(x_i)^\top \tilde{\phi}(x_j)$$

• After some algebra, we get:

$$\tilde{K} = K - \frac{1}{m} K - K \frac{1}{m} + \frac{1}{m} K \frac{1}{m}$$

and

$$\tilde{k}_x = k_x - \frac{1}{m} k_x - K \frac{1}{m} + \frac{1}{m} K \frac{1}{m}$$

where $\frac{1}{m} K \frac{1}{m}$ (resp. $1 \frac{1}{m}$) 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 $K \in \mathbb{R}^{m \times m}$.
2. Compute the Gram matrix of the centered the data in the feature space:

$$\tilde{K} = K - O_{1/m}K - KO_{1/m} + O_{1/m}KO_{1/m}$$

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

$$\hat{x} = D^{-1/2}U^T\tilde{k}_x$$

where $\tilde{k}_x$ is defined as in the previous slide.
(Note that multiplying by $D^{-1/2}$ corresponds to rescaling the unit-norm eigenvectors of $\tilde{K}$ to get the vectors of coefficients $a_j$).
Representation obtained by kernel PCA

• Each $y_j = \phi(x)^\top v_j = a_j^\top k_x$ is the coordinate of $\phi(x)$ along one of the feature space axis $v_j$.

• Since the $v_j$’s are orthogonal, the projection of $\phi(x)$ onto the space spanned by the top $d$ eigenvectors is:

$$\Pi \phi(x) = \sum_{j=1}^{d} y_j v_j = \sum_{j=1}^{d} (a_j^\top k_x) \Phi^\top a_j$$

• The reconstruction error in feature space can be evaluated as:

$$\|\phi(x) - \Pi \phi(x)\|^2$$

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 $v_j$ 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 $\phi(x_i)$ and $\phi(x_j)$, $d_{ij}$, is:

$$\|\phi(x_i) - \phi(x_j)\|^2 = K(x_i, x_i) + K(x_j, x_j) - 2K(x_i, x_j)$$

- The distance $\hat{d}_{ij}$ between the projected points in kernel space is defined as above, but with $\phi(x_i)$ replaced by $\Pi\phi(x_i)$.
- 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 $x_i$ is very difficult to compute, because it requires taking $\Pi\phi(x)$ and finding its pre-image in the original feature space, which is not always feasible (though approximations exist).
Example: Two concentric spheres

Before we work on real data, we would like to generate some synthetic datasets and test our algorithm on them. In this paper, we use the two-concentric-spheres data.

### 3.1. Pattern Classification for Synthetic Data

#### 3.1.1. Data Description

We assume that we have an equal number of data points uniformly distributed on two concentric sphere surfaces. If \( N \) is the total number of all data points, then we have \( \frac{N}{2} \) class 1 points on a sphere of radius \( r_1 \), and \( \frac{N}{2} \) class 2 points on a sphere of radius \( r_2 \). In the spherical coordinate system, the inclination (polar angle) \( \theta \) is uniformly distributed in \([0, \pi]\) and the azimuth (azimuthal angle) \( \phi \) is uniformly distributed in \([0, 2\pi]\) for both classes. Our observations of the data points are the \((x, y, z)\) coordinates in the Cartesian coordinate system, and all the three coordinates are perturbed by a Gaussian noise of standard deviation \( \sigma_{\text{noise}} \). We set \( N = 200 \), \( r_1 = 10 \), \( r_2 = 15 \), \( \sigma_{\text{noise}} = 0.1 \), and give a 3D plot of the data in Figure 1.

#### 3.1.2. PCA and Kernel PCA Results

To visualize our results, we project the original 3-dimensional data into a 2-dimensional feature space by using traditional PCA and kernel PCA respectively. For kernel PCA, we use a polynomial kernel with \( d = 5 \) and a Gaussian kernel with \( \sigma = 20 \). The results of traditional PCA, polynomial kernel PCA and Gaussian kernel PCA are given in Figure 2, Figure 3, and Figure 4 respectively.

\[\text{Figure 1.} \text{ 3D plot of the two-concentric-spheres synthetic data.}\]

\[\text{Figure 2.} \text{ Traditional PCA results for the two-concentric-spheres synthetic data.}\]

\[\text{Figure 3.} \text{ Polynomial kernel PCA results for the two-concentric-spheres synthetic data with} \ d = 5.\]

\[\text{Figure 4.} \text{ Gaussian kernel PCA results for the two-concentric-spheres synthetic data.}\]

We note that here though we mark points in different classes with different colors, we are actually doing unsupervised learning. Neither PCA nor kernel PCA takes the class labels as their input.

In the results we can see that, traditional PCA does not reveal any structural information of the original data.

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\(^1\text{Wang, 2012}\)
Example: Two concentric spheres - PCA

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

\[^2\text{Wang, 2012}\]
Example: Kernel PCA with Polynomial Kernel \((d = 5)\)

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

\(^3\text{Wang, 2012}\)
Example: Kernel PCA with Gaussian Kernel ($\sigma = 20$)

- 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

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4Wang, 2012
Example: De-noising images

Original data

[Original image of hand-written numbers]

Data corrupted with Gaussian noise

[Corrupted image of hand-written numbers]

Result after linear PCA

[Result image after linear PCA]

Result after kernel PCA, Gaussian kernel

[Result image after kernel PCA]
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

• Suppose \( x_1, \ldots, x_m \in \mathbb{R}^n \) lies on a \( k \)-dimensional manifold.

\[ \Rightarrow \text{Each point and its neighbors lie close to a } \text{locally linear} \text{ patch of the manifold.} \]

• After fixing some integer \( \ell \), we try to reconstruct each point from its \( \ell \) closest neighbors:

\[
\min_{W \in \mathbb{R}^{m \times m}} \sum_{i=1}^{m} \left\| x_i - \sum_{j=1}^{m} W_{i,j} x_j \right\|^2
\]

s.t. \( W1 = 1 \) and \( W_{i,j} = 0 \) if \( x_j \not\in \text{neighbors}(x_i) \) (where \( \text{neighbors}(x_i) \) is the set of \( \ell \) closest neighbors of \( x_i \)).

\[ \Rightarrow \text{For each point the weights are invariant to rotation, scaling and translations: the weights } W_{i,j} \text{ capture intrinsic geometric properties of each neighborhood.} \]
• These local properties of each neighborhood should be preserved by the embedding. We thus seek to find points $z_1, \ldots, z_m$ lying in a space of smaller dimension $k$ that satisfies these local properties:

$$\min_{z_1, \ldots, z_m \in \mathbb{R}^k} \sum_{i=1}^{m} \left\| z_i - \sum_{j=1}^{m} W_{i,j} z_j \right\|^2$$
PCA vs Locally Linear Embedding