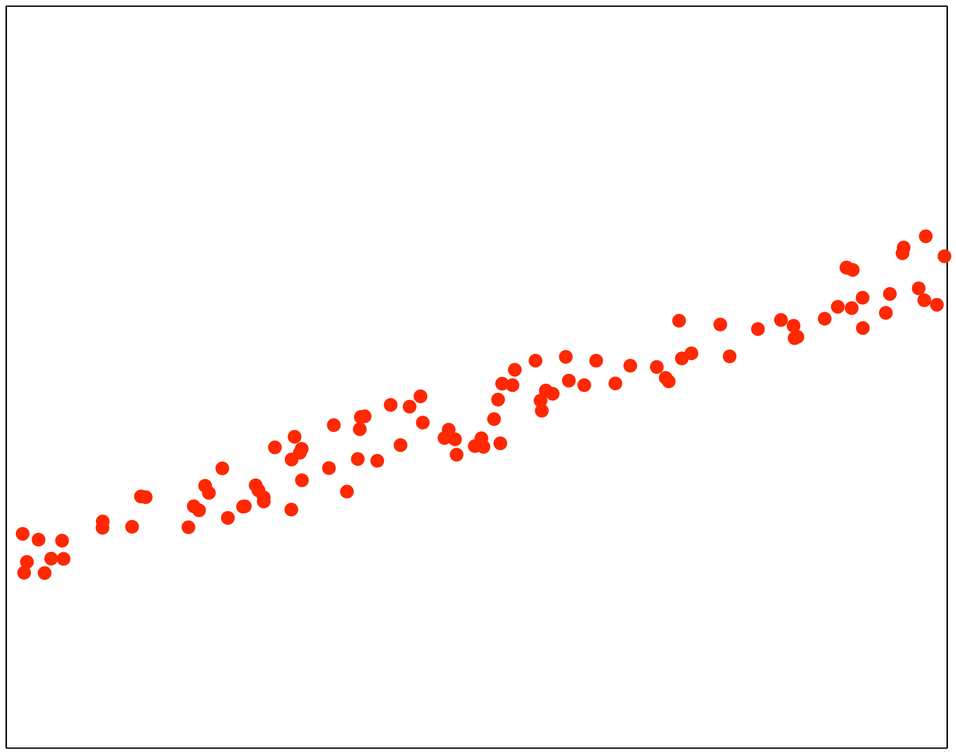
Dimensionality reduction. PCA. Kernel PCA.

- Dimensionality reduction
- Principal Component Analysis (PCA)
- Kernelizing PCA
- If we have time: Autoencoders

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
    - Multi-dimensional scaling
    - Autoencoders

What is the true dimensionality of this data?



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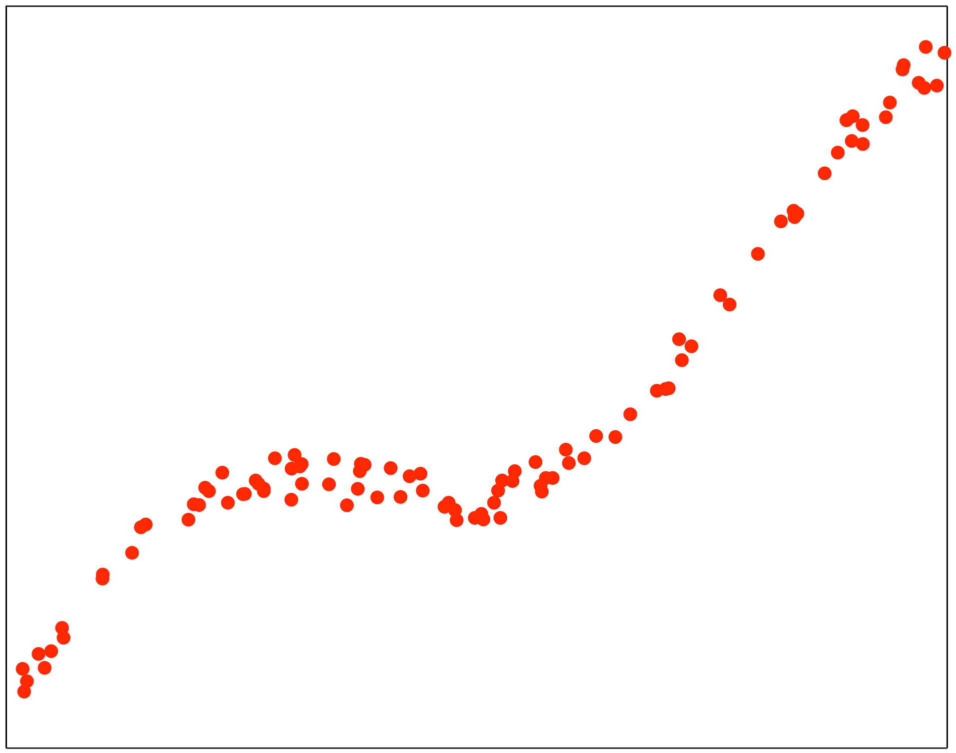

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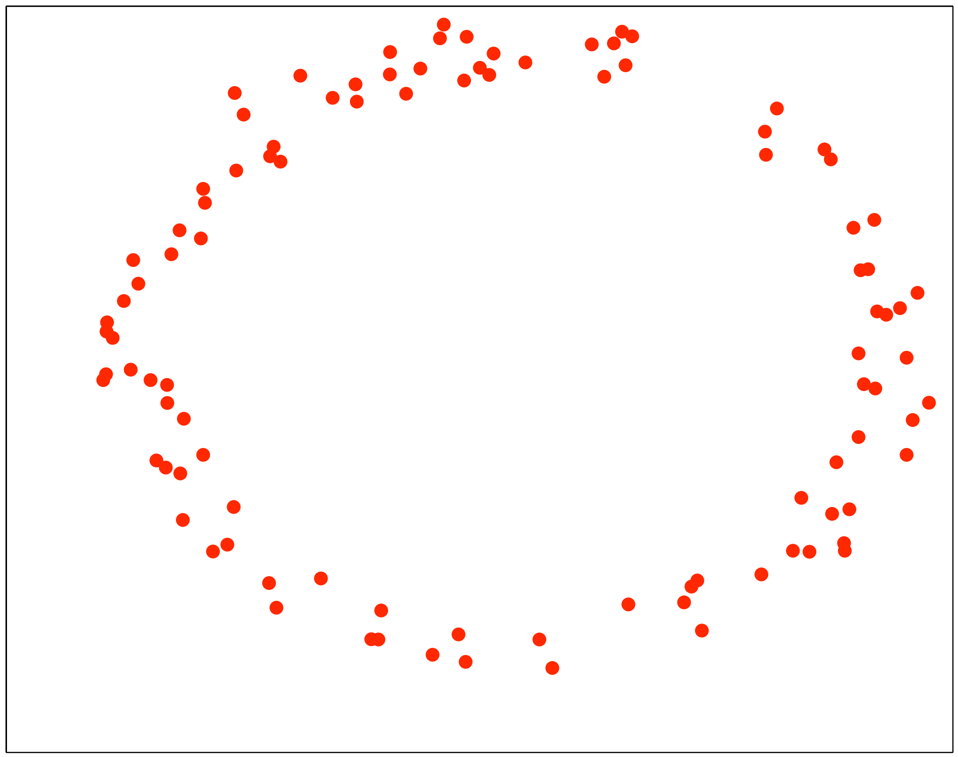

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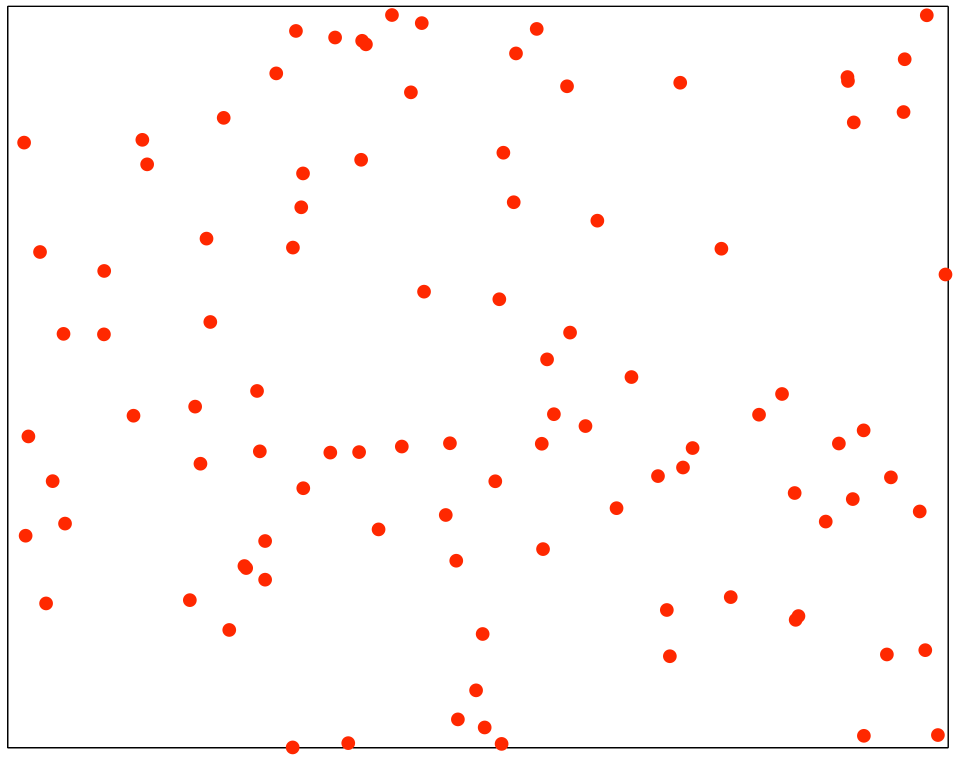
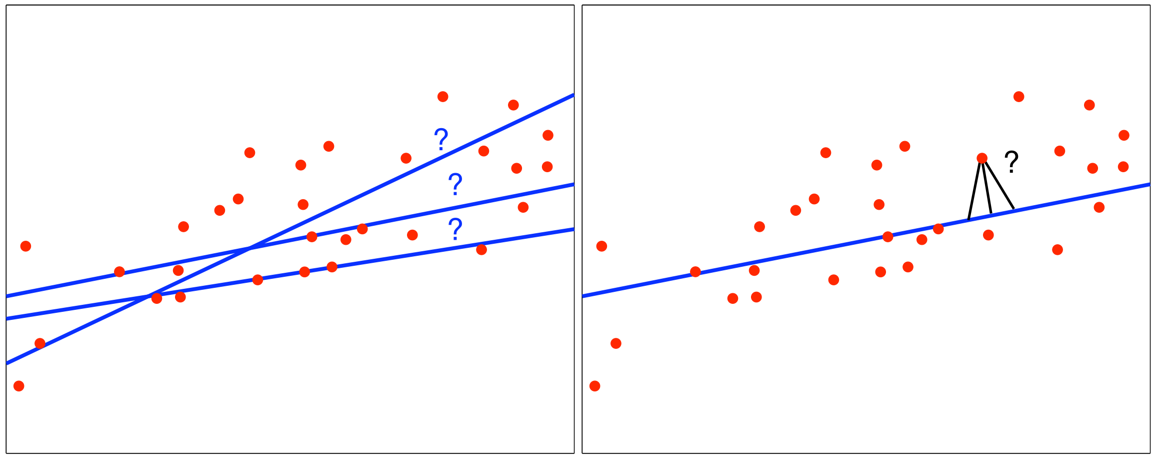


Remarks

- 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 take into account that $\|\mathbf{v}\|^2 = 1$.
- We write the gradient of R wrt $\mathbf{b}$ and set it to 0:

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

- From above:

$$\sum_{i=1}^{m}\alpha_i = \sum_{i=1}^{m}\mathbf{v}^T(\mathbf{x}_i - \mathbf{b}) = \mathbf{v}^T\left(\sum_{i=1}^{m}\mathbf{x}_i - m\mathbf{b}\right) \tag{2}$$

Solving the optimization problem (III)

- By plugging (2) into (1) we get:

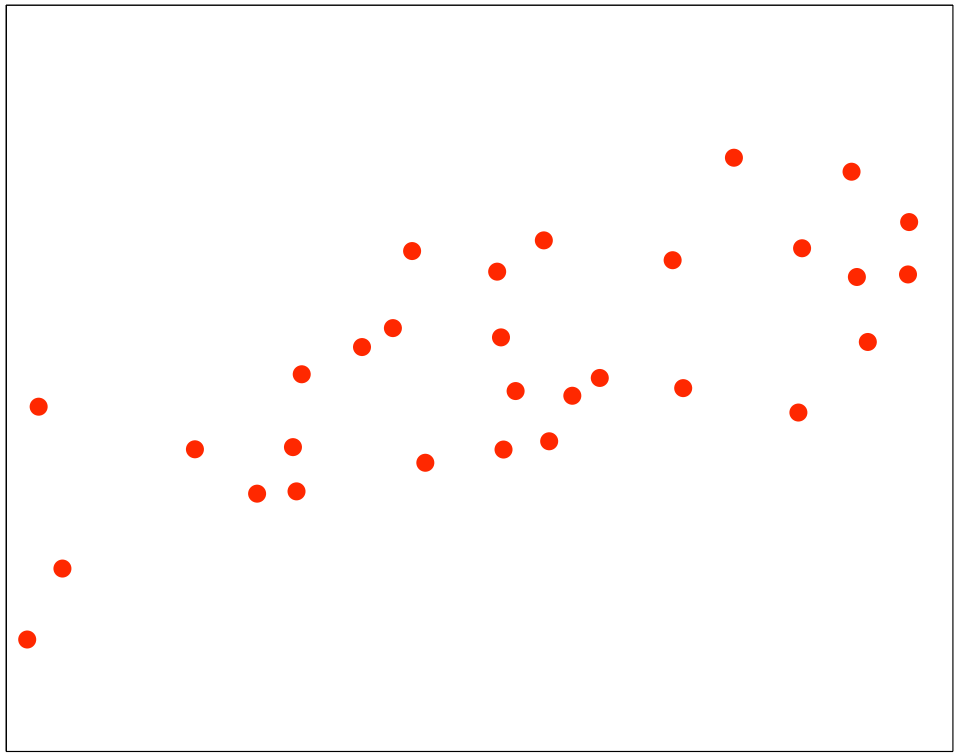
$$\mathbf{v}^T \left(\sum_{i=1}^{m} \mathbf{x}_i - m\mathbf{b} \right) \mathbf{v} = \left(\sum_{i=1}^{m} \mathbf{x}_i - m\mathbf{b} \right)$$

- This is satisfied when:

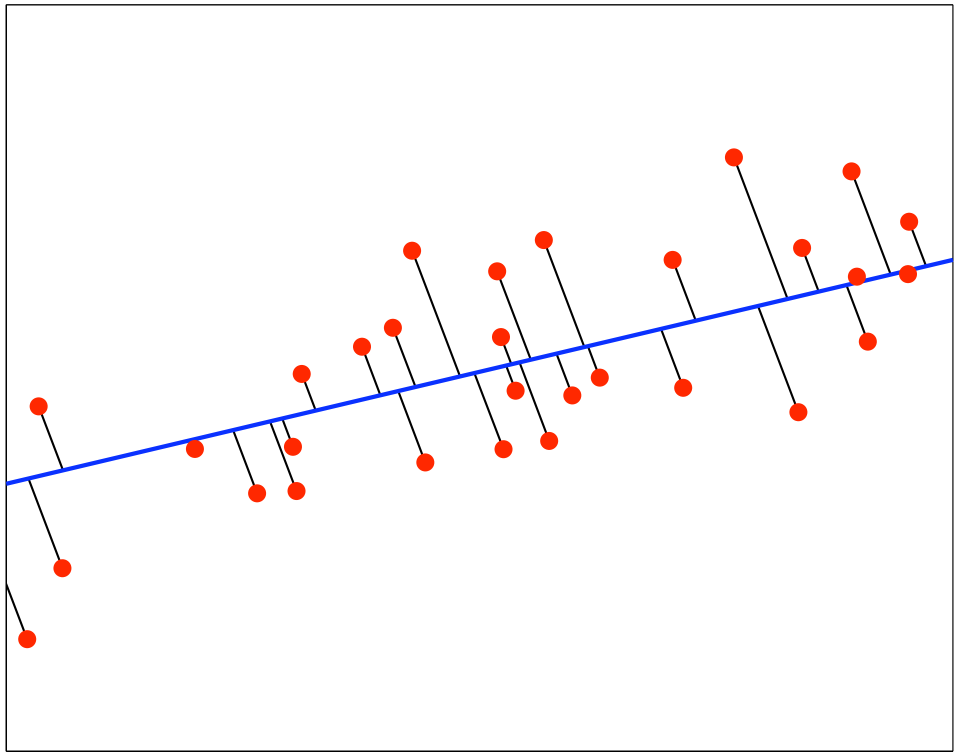
$$\sum_{i=1}^{m} \mathbf{x}_i - m\mathbf{b} = 0 \Rightarrow \mathbf{b} = \frac{1}{m} \sum_{i=1}^{m} \mathbf{x}_i$$

- This means that the line goes through the mean of the data
- By substituting α_i, we get: $\hat{\mathbf{x}}_i = \mathbf{b} + (\mathbf{v}^T(\mathbf{x}_i - \mathbf{b}))\mathbf{v}$
- 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 $\alpha_i = \mathbf{v}^T(\mathbf{x}_i - \mathbf{b})$ into our optimization problem we obtain a new optimization problem:

$$\begin{array}{rl} \max_{\mathbf{v}} & \sum_{i=1}^{m} \mathbf{v}^T(\mathbf{x}_i - \mathbf{b})(\mathbf{x}_i - \mathbf{b})^T\mathbf{v} \\ \text{s.t.} & \|\mathbf{v}\|^2 = 1 \end{array}$$

- The Lagrangian is:

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

- Let $S = \sum_{i=1}^{m}(\mathbf{x}_i - \mathbf{b})(\mathbf{x}_i - \mathbf{b})^T$ be an n-by-n matrix, which we will call the *scatter matrix*
- The solution to the problem, obtained by setting $\nabla_{\mathbf{v}} L = 0$, is: $S\mathbf{v} = \lambda\mathbf{v}$.

Optimal choice of $\mathbf{v}$

- Recall: an *eigenvector* $\mathbf{u}$ of a matrix A satisfies $A\mathbf{u} = \lambda\mathbf{u}$, where $\lambda \in \mathbb{R}$ is the *eigenvalue*.
- Fact: the scatter matrix, 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 S.
- The $\mathbf{v}$ that maximizes $\mathbf{v}^T S\mathbf{v}$ is the eigenvector of S with the largest eigenvalue

What is the scatter matrix

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

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

- Hence, $S(k,l)$ 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.

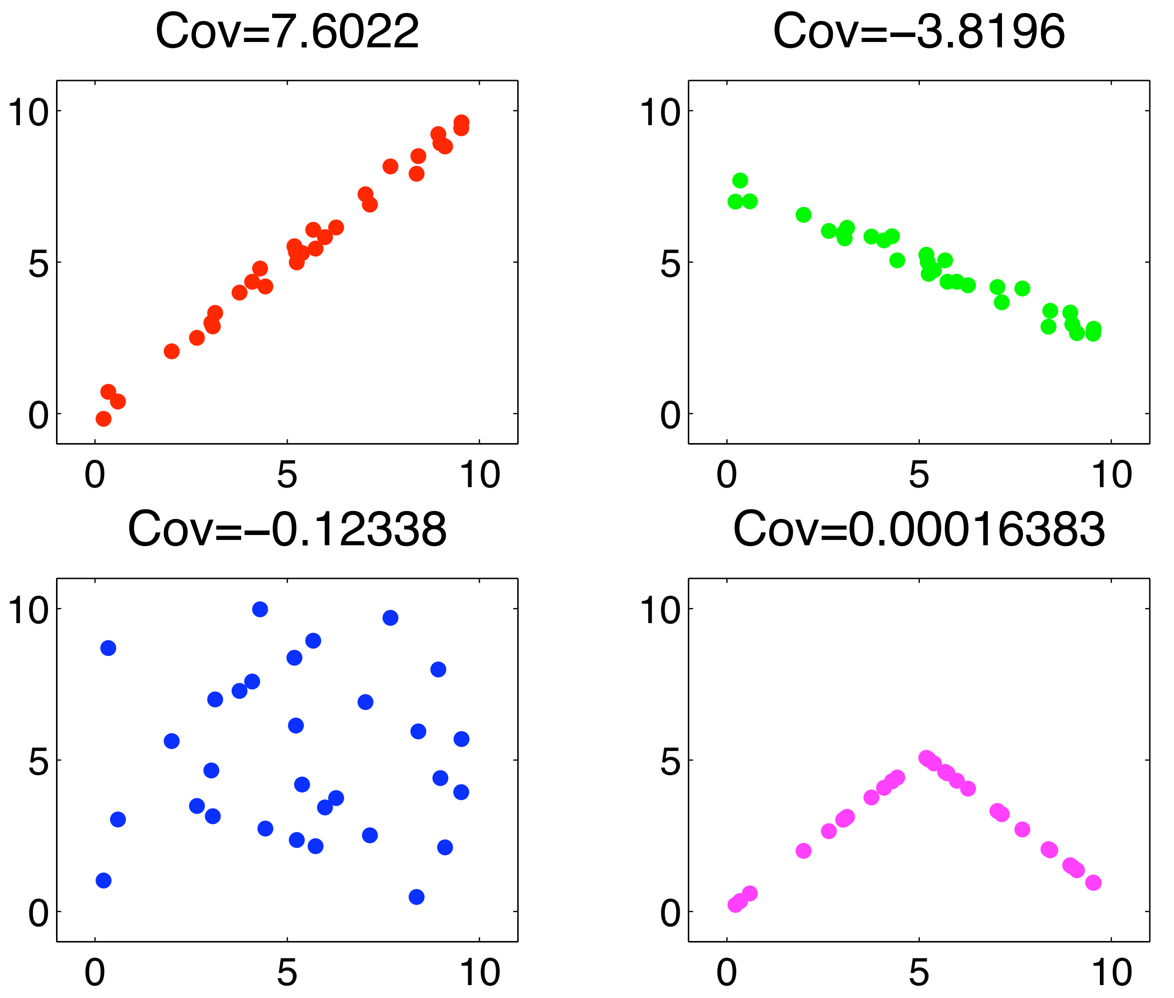
$$Cov(X,Y) = E\{(X - E(X))(Y - E(Y))\}$$

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

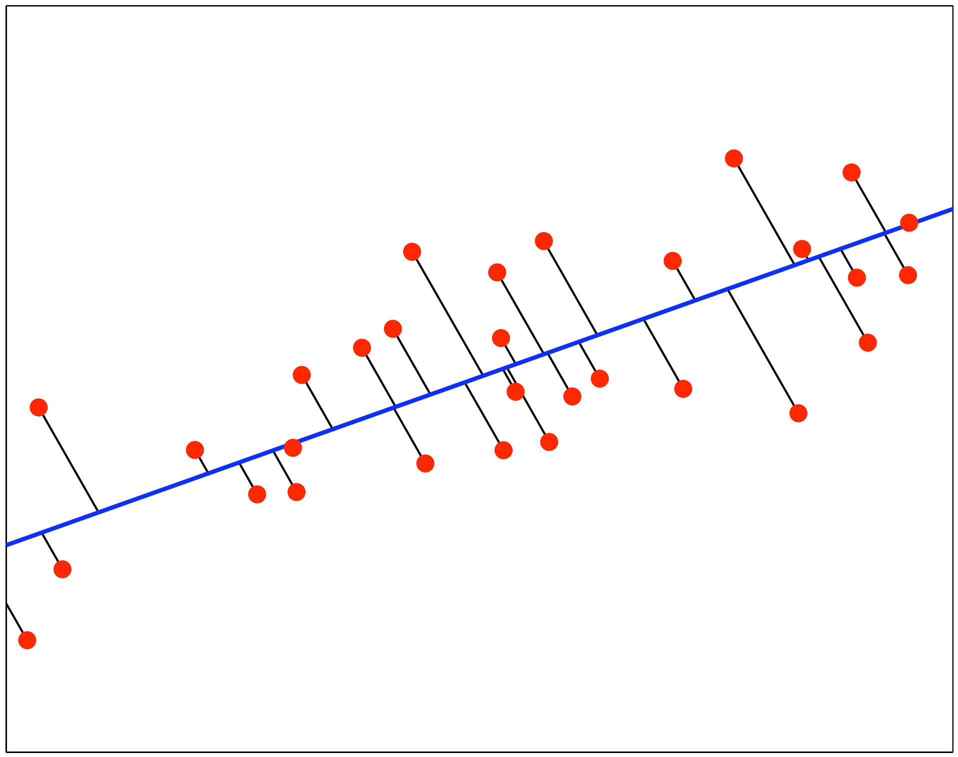
$$\frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_X)(y_i - \mu_Y)\ ,$$

  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.

Reduction 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 S corresponding to its d largest eigenvalues.
  - Each instance is projected orthogonally on the hyperplane.

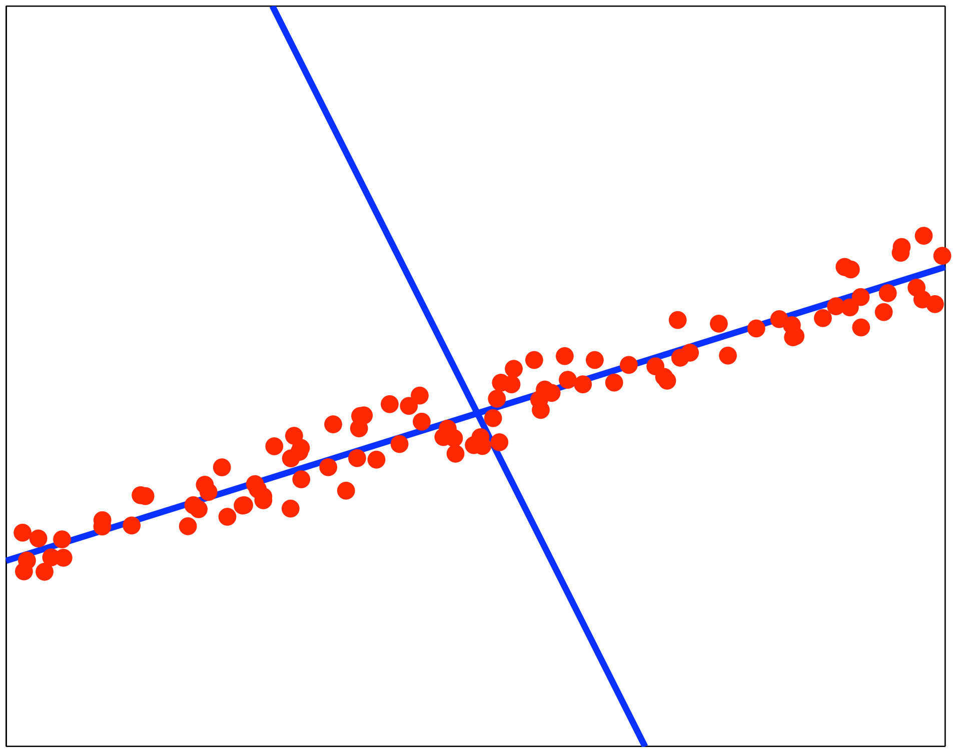
Remarks

- $\mathbf{b}$, the eigenvalues, the $\mathbf{v}_j$, and the projections of the instances can all be computing 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:

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

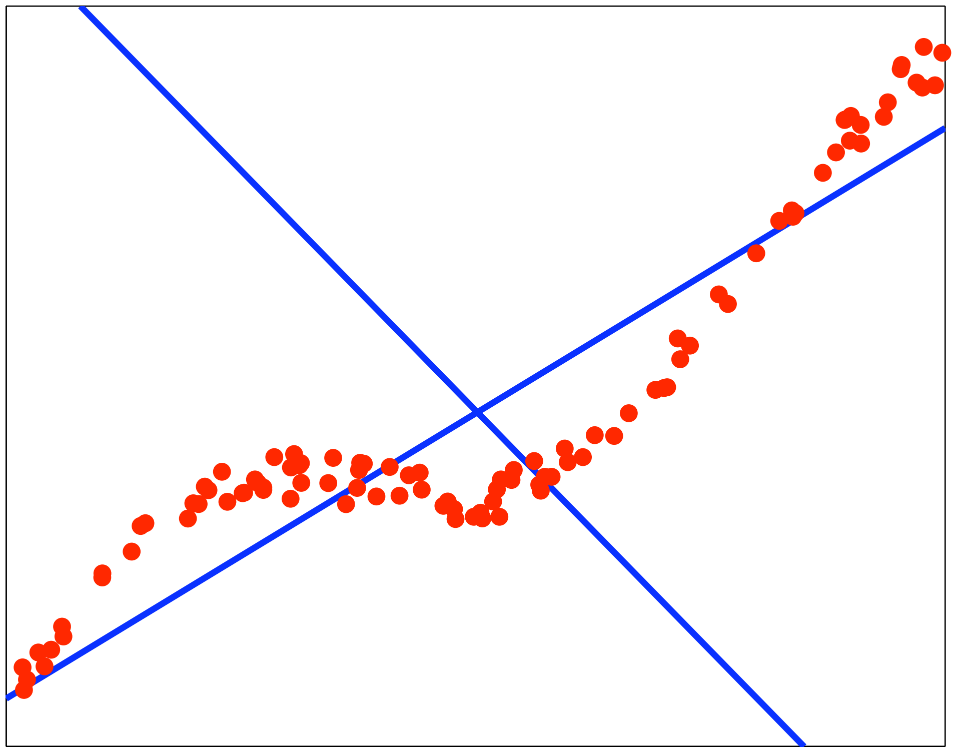
- So if a "big" drop occurs in the eigenvalues at some point, that suggests a good dimension cutoff

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



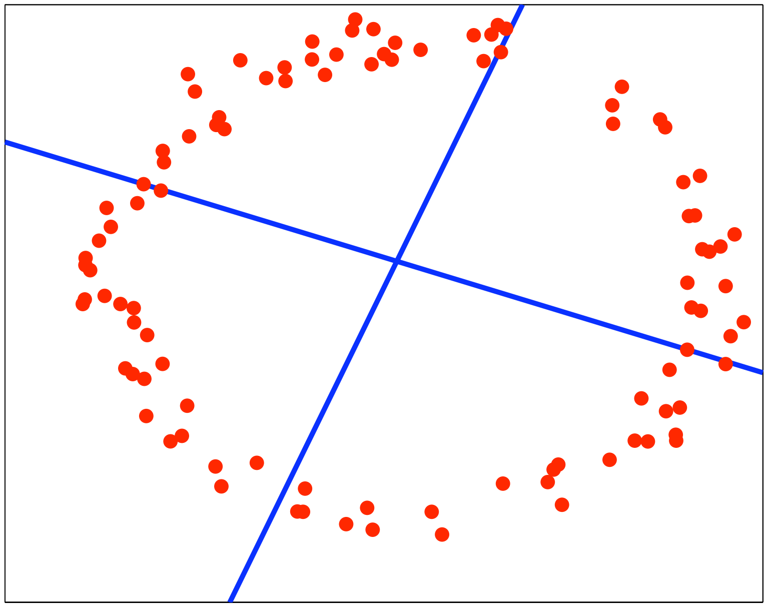
The first eigenvalue accounts for most variance, so the dimensionality is 1

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



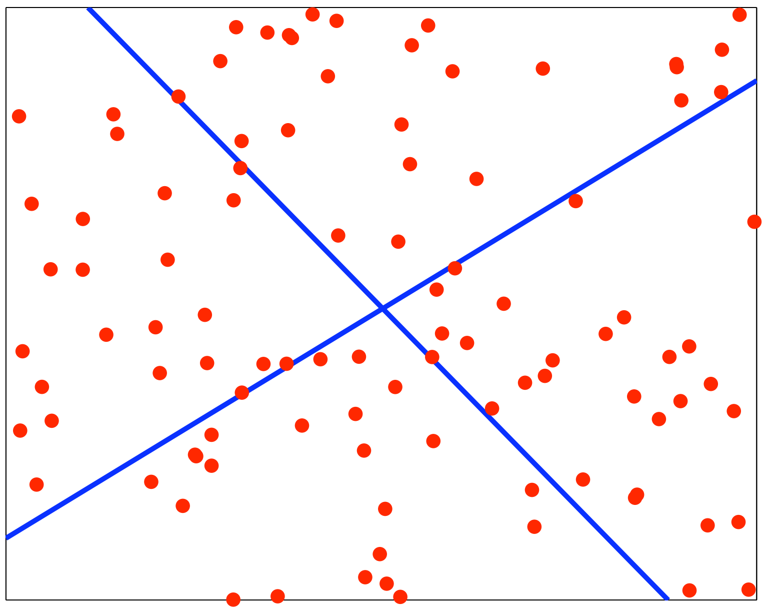
The first eigenvalue accounts for most variance, so the dimensionality is 1 (despite some non-linear structure in the data)

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

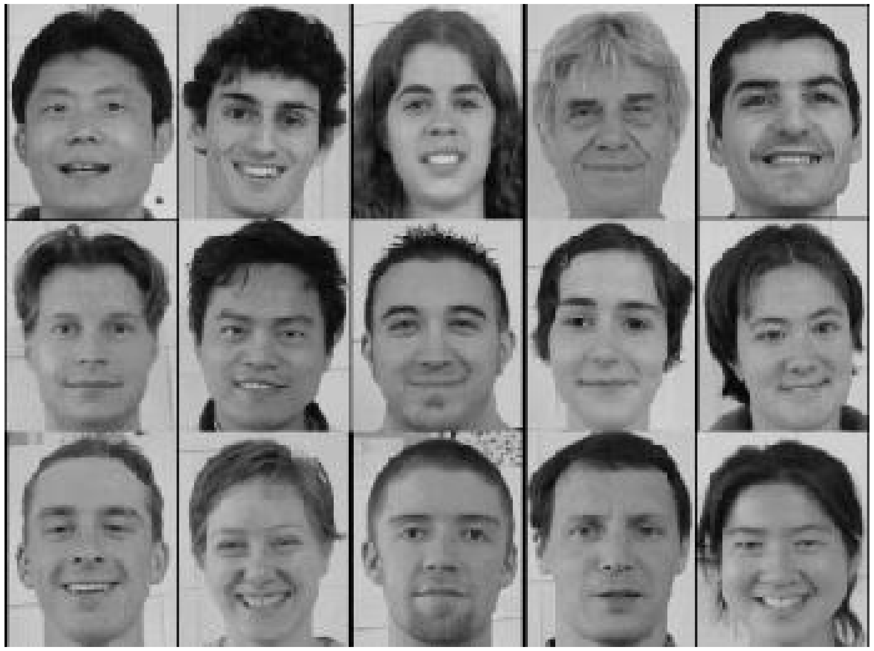


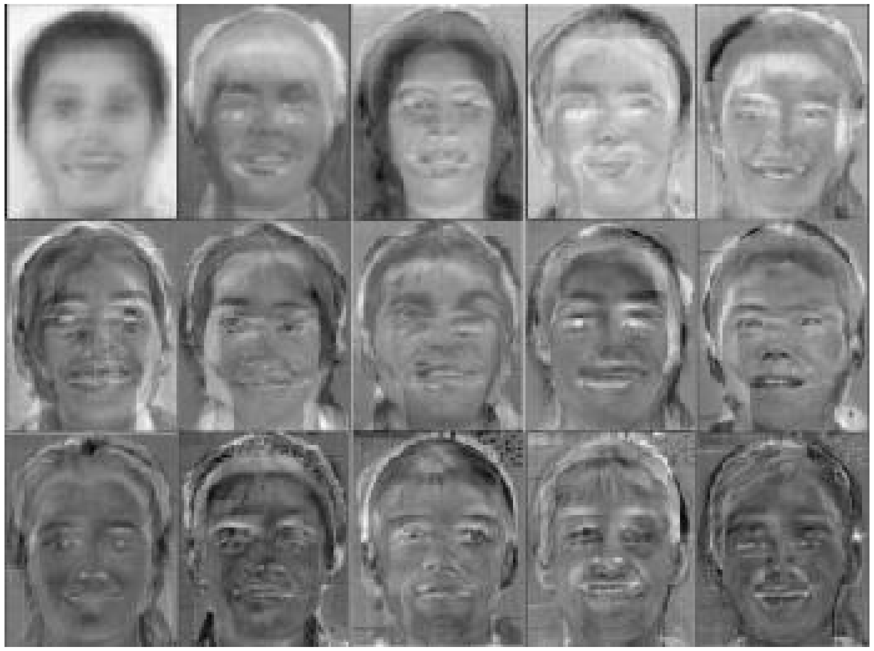
- Each eigenvalue accounts for about half the variance, so the PCA-suggested dimension is 2
- In this case, the non-linear dimension is also 2 (data is fully random)
- Note that *PCA cannot distinguish non-linear structure from no structure*
- This case and the previous one yield a very similar PCA analysis

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 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



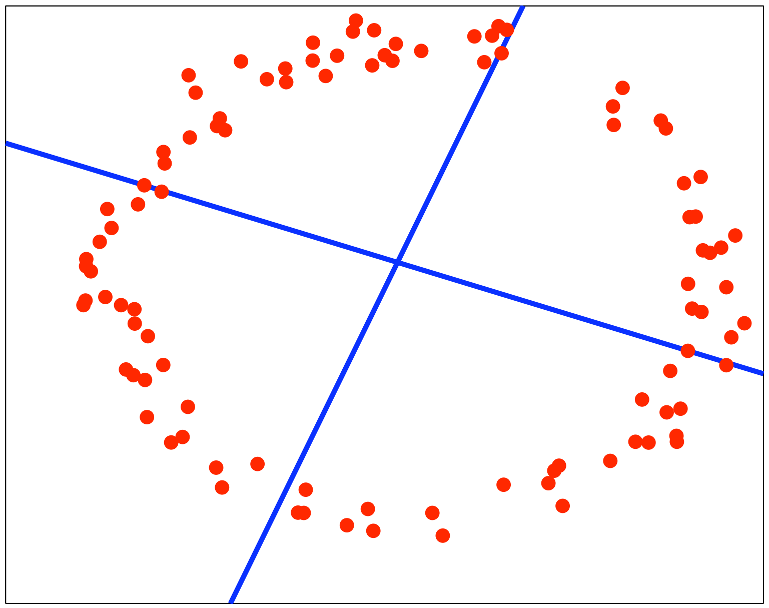


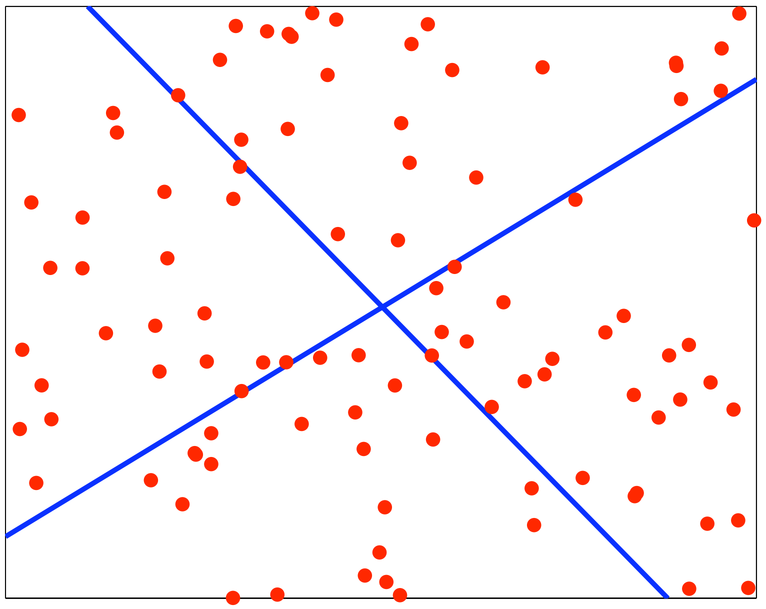
- A set of faces on the left and the corresponding eigenfaces (principal components) on the right
- Note that faces have to be centred and scaled ahead of time
- The components are in the same space as the instances (images) and can be used to reconstruct the images

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 the moment that the mean of the data in feature space is 0, so: $\sum_{i=1}^{m} \phi(\mathbf{x}_i) = 0$
- The covariance matrix is:

$$\mathbf{C} = \frac{1}{m} \sum_{i=1}^{m} \phi(\mathbf{x}_i)\phi(\mathbf{x}_i)^T$$

- The eigenvectors are:

$$\mathbf{C}\mathbf{v}_j = \lambda_j \mathbf{v}_j, j = 1, \ldots N$$

- We want to avoid explicitly going to feature space - instead we want to work with *kernels*:

$$K(\mathbf{x}_i, \mathbf{x}_k) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_k)$$

PCA in feature space (II)

- Re-write the PCA equation:

$$\frac{1}{m}\sum_{i=1}^{m}\phi(\mathbf{x}_i)\phi(\mathbf{x}_i)^T\mathbf{v}_j = \lambda_j\mathbf{v}_j, j = 1, \dots N$$

- So the eigenvectors can be written as a linear combination for features:

$$\mathbf{v}_j = \sum_{i=1}^{m} a_{ji}\phi(\mathbf{x}_i)$$

- Finding the eigenvectors is equivalent to finding the coefficients $a_{ji}, j = 1, \dots N, i = 1, \dots m$

PCA in feature space (III)

- By substituting this back into the equation we get:

$$\frac{1}{m}\sum_{i=1}^{m}\phi(\mathbf{x}_i)\phi(\mathbf{x}_i)^T\left(\sum_{l=1}^{m}a_{jl}\phi(\mathbf{x}_l)\right)=\lambda_j\sum_{l=1}^{m}a_{jl}\phi(\mathbf{x}_l)$$

- We can re-write this as:

$$\frac{1}{m}\sum_{i=1}^{m}\phi(\mathbf{x}_i)\left(\sum_{l=1}^{m}a_{jl}K(\mathbf{x}_i,\mathbf{x}_l)\right)=\lambda_j\sum_{l=1}^{m}a_{jl}\phi(\mathbf{x}_l)$$

- A small trick: multiply this by $\phi(\mathbf{x}_k)^T$ to the left:

$$\frac{1}{m}\sum_{i=1}^{m}\phi(\mathbf{x}_k)^T\phi(\mathbf{x}_i)\left(\sum_{l=1}^{m}a_{jl}K(\mathbf{x}_i,\mathbf{x}_l)\right)=\lambda_j\sum_{l=1}^{m}a_{jl}\phi(\mathbf{x}_k)^T\phi(\mathbf{x}_l)$$

PCA in feature space (IV)

- We plug in the kernel again:

$$\frac{1}{m}\sum_{i=1}^{m} K(\mathbf{x}_k,\mathbf{x}_i)\left(\sum_{l=1}^{m} a_{jl}K(\mathbf{x}_i,\mathbf{x}_l)\right) = \lambda_j \sum_{l=1}^{m} a_{jl}K(\mathbf{x}_k,\mathbf{x}_l), \forall j,k$$

- By rearranging we get: $\mathbf{K}^2\mathbf{a}_j = m\lambda_j\mathbf{K}\mathbf{a}_j$
- 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):

$$\mathbf{K}\mathbf{a}_j = m\lambda_j\mathbf{a}_j$$

PCA in feature space (V)

- We have a normalization condition for the $\mathbf{a}_j$ vectors:

$$\mathbf{v}_j^T\mathbf{v}_j = 1 \Rightarrow \sum_{k=1}^{m}\sum_{l=1}^{m} a_{jl}a_{jk}\phi(\mathbf{x}_l)^T\phi(\mathbf{x}_k) = 1 \Rightarrow \mathbf{a}_j^T\mathbf{K}\mathbf{a}_j = 1$$

- Plugging this into:

$$\mathbf{K}\mathbf{a}_j = m\lambda_j\mathbf{a}_j$$

  we get: $\lambda_j m\mathbf{a}_j^T\mathbf{a}_j = 1, \forall j$

- For a new point $\mathbf{x}$, its projection onto the principal components is:

$$\phi(\mathbf{x})^T\mathbf{v}_j = \sum_{i=1}^{m} a_{ji}\phi(\mathbf{x})^T\phi(\mathbf{x}_i) = \sum_{i=1}^{m} a_{ji}K(\mathbf{x}, \mathbf{x}_i)$$

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:

$$\tilde{K}(\mathbf{x}_k, \mathbf{x}_l) = \tilde{\phi}(\mathbf{x}_l)^T\tilde{\phi}(\mathbf{x}_j)$$

- After some algebra, we get:

$$\tilde{\mathbf{K}} = \mathbf{K} - 2\mathbf{1}_{1/m}\mathbf{K} + \mathbf{1}_{1/m}\mathbf{K}\mathbf{1}_{1/m}$$

where $\mathbf{1}_{1/m}$ is the matrix with all elements equal to $1/m$

Summary of kernel PCA

1. Pick a kernel
2. Construct the normalized kernel matrix $\tilde{\mathbf{K}}$ of the data (this will be of dimension $m \times m$)
3. Find the eigenvalues and eigenvectors of this matrix λ_j, $\mathbf{a}_j$
4. For any data point (new or old), we can represent it as the following set of features:
$$y_j = \sum_{i=1}^{m} a_{ji} K(\mathbf{x}, \mathbf{x}_i), j = 1, \ldots m$$
5. We can limit the number of components to $k < m$ for a more compact representation (by picking the $\mathbf{a}$'s corresponding to the highest eigenvalues)

Representation obtained by kernel PCA

- Each y_j is the coordinate of $\phi(\mathbf{x})$ along one of the feature space axes $\mathbf{v}_j$
- Remember that $\mathbf{v}_j = \sum_{i=1}^{m} a_{ji}\phi(\mathbf{x}_i)$ (the sum goes to k if $k < m$)
- Since $\mathbf{v}_j$ are orthogonal, the projection of $\phi(\mathbf{x})$ onto the space spanned by them is:

$$\Pi\phi(\mathbf{x}) = \sum_{j=1}^{m} y_j \mathbf{v}_j = \sum_{j=1}^{m} y_j \sum_{i=1}^{m} a_{ji}\phi(\mathbf{x}_i)$$

  (again, sums go to k if $k < m$)
- 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

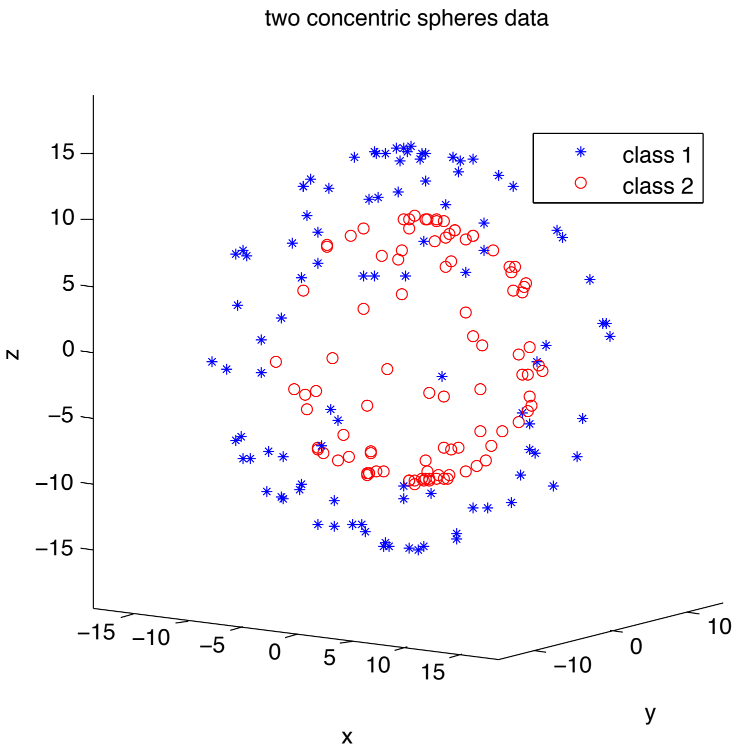
Alternative reconstruction error measures

- 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:

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

- The distance $\hat{d}_i j$ 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

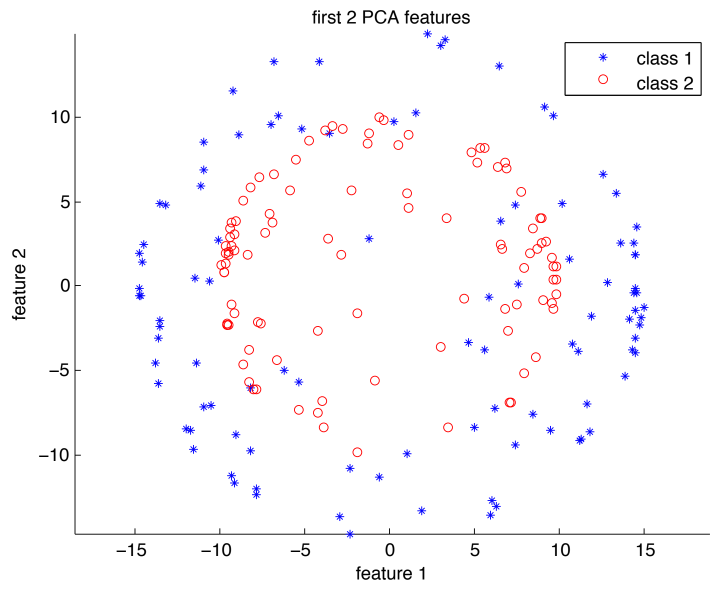


[1]

- 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

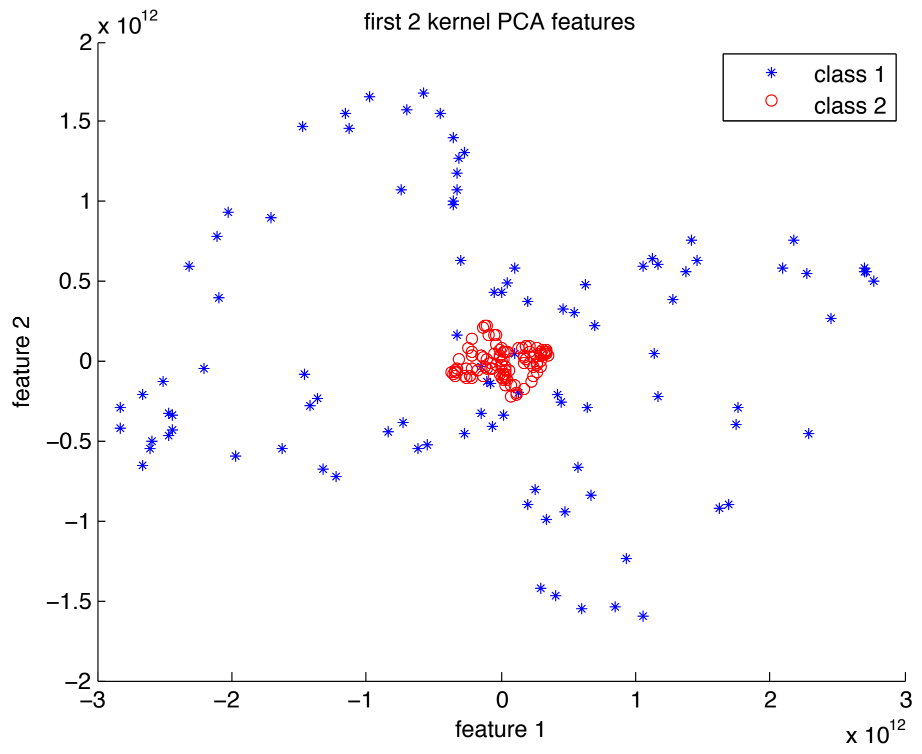


[2]

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

[2]Wang, 2012

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

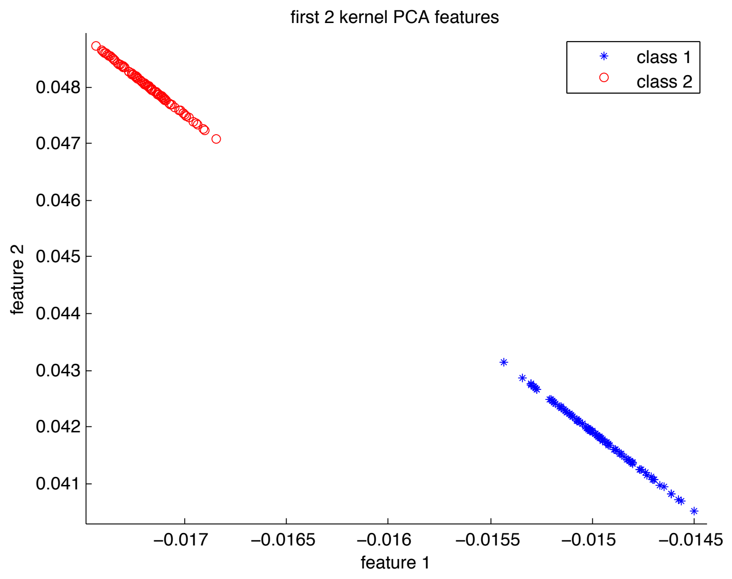


[3]

- 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 ($\sigma = 20$)



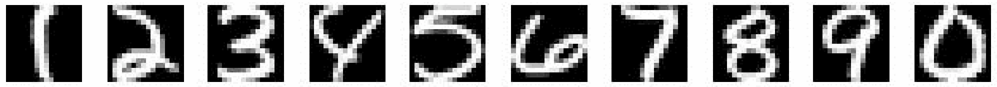
[4]

- 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

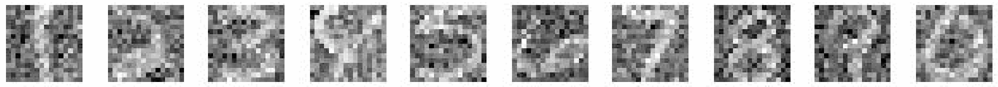
[4]Wang, 2012

Example: De-noising images

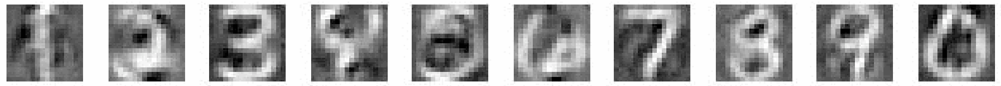
Original data



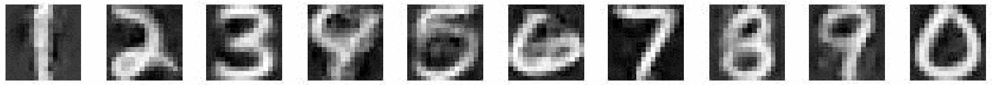
Data corrupted with Gaussian noise



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 visualizethe 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:

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

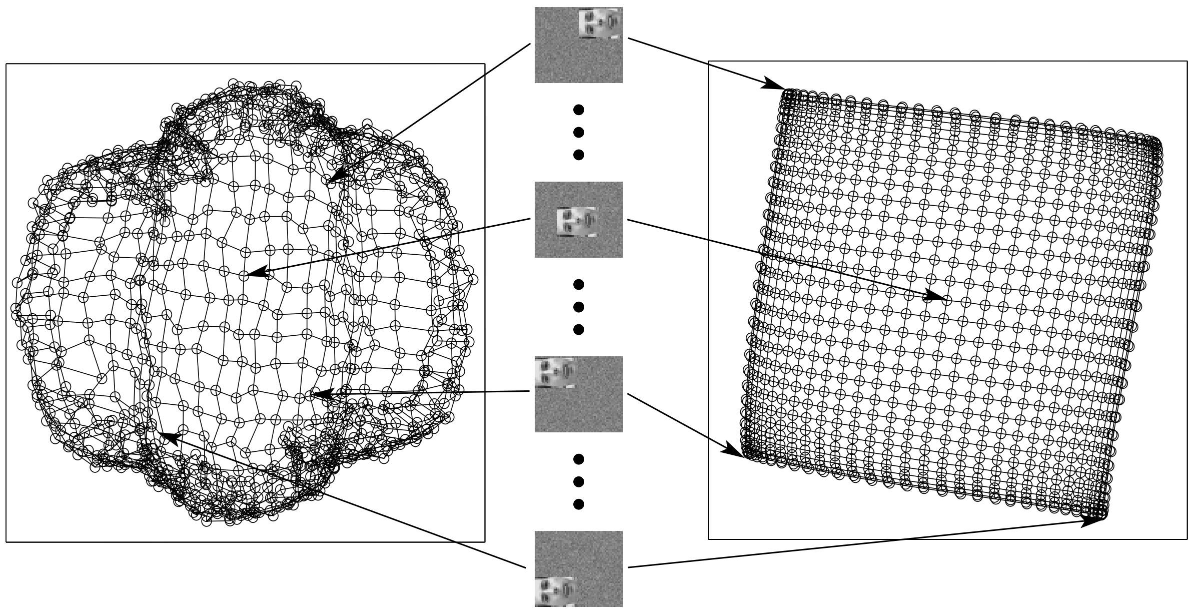
s.t. $\mathbf{W}\mathbf{1} = \mathbf{1}$ and $\mathbf{W}_{i,j} = 0$ if $\mathbf{x}_j \notin neighbors(\mathbf{x}_i)$

$\Rightarrow$ 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:

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

PCA vs Locally Linear Embedding



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

Multi-dimensional scaling

- Input:
  - An $m \times m$ dissimilarity matrix d, where $d(i,j)$ is the distance between instances $\mathbf{x}_i$ and $\mathbf{x}_j$
  - Desired dimension k of the embedding.
- Output:
  - Coordinates $\mathbf{z}_i \in \mathbb{R}^k$ for each instance i that minimize a "stress" function quantifying the mismatch between distances as given by d and distances of the data representation in $\mathbb{R}^k$.

Stress functions

- Common stress functions include:
  - The least-squares or Kruskal-Shephard criterion:

$$\sum_{i=1}^{m} \sum_{j \neq i} (d(i,j) - \|\mathbf{z}_i - \mathbf{z}_j\|)^2$$

  - The Sammon mapping:

$$\sum_{i=1}^{m} \sum_{j \neq i} \frac{(d(i,j) - \|\mathbf{z}_i - \mathbf{z}_j\|)^2}{d(i,j)} \ ,$$

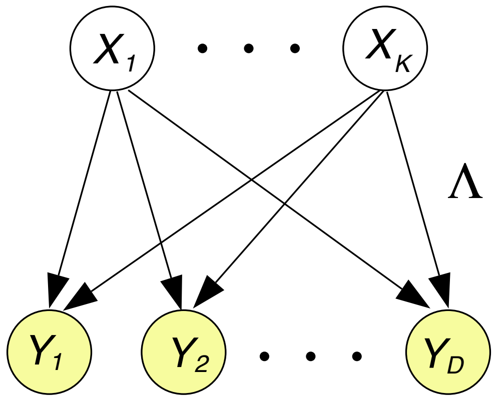
    which emphasizes getting small distances correct.

- Gradient-based optimization is usually used to find $\mathbf{z}_i$

Other dimensionality reduction methods

- Independent component analysis (ICA)
- More generally: factor analysis
- Local linear embeddings (LLE)
- Neighborhood component analysis (NCA)
- ...
- Some methods do dimensionality reduction jointly with a supervised learning task, or a set of such tasks

A generalizing perspective

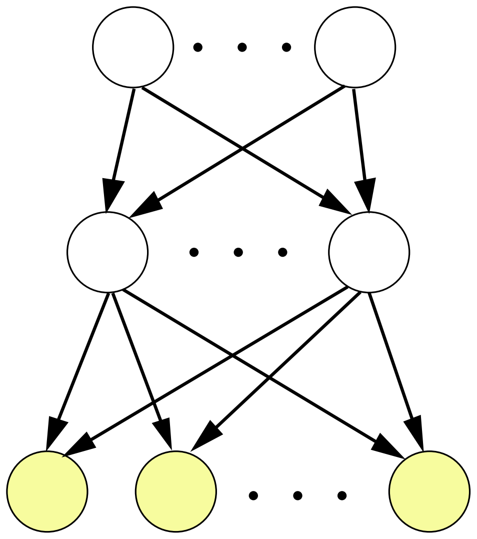


[5]

- Let Y be observed data and X be *hidden (latent) variables* or *factors* that generate the data
- The goal is to find how many such variables there are, and the model through which they generate the data
- E.g. Mixture models: K hidden variables, Gaussian conditional distributions
- E.g. PCA: K hidden variables, Gaussian models
- E.g. ICA: K hidden variables, non-Gaussian models

[5] Roweis and Gharamani, 1999

Graphical models

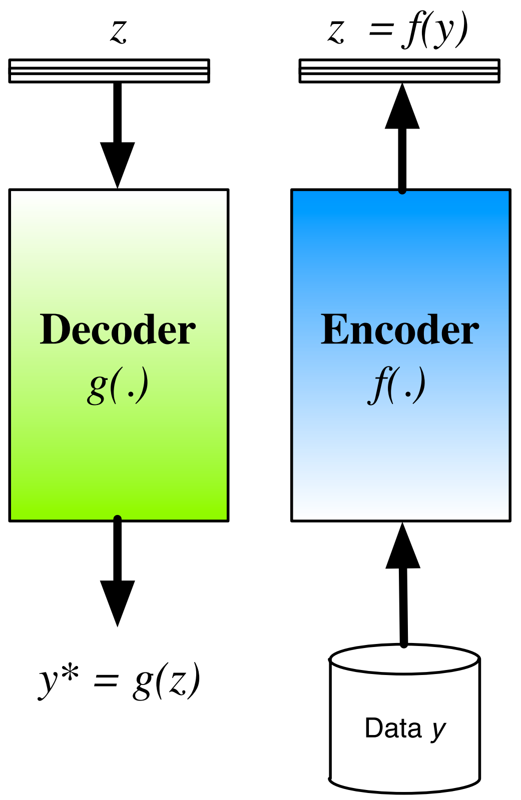


- More generally, the data (yellow circles) can be generated by a more complex structure.
- We can model all variables and their interactions using a graph structure
- Local probabilistic models describe how neighbours influence each other
- The overall model represents a joint probability distribution over all variables (observed and latent)

More generally: Autoencoders

- We have some data and try to learn a latent variable space that explains it
- The goal is to minimize reconstruction error
- In PCA, we used squared loss - this indicates an implicit Gaussian assumption
- More generally, from data bfy we obtain a mapping $\mathbf{z}$, then we can use an *inverse mapping* g to go back from $\mathbf{z}$ to $\mathbf{y}$
- We want to maximize the likelihood of the data

More generally: Autoencoders



$$\mathcal{L} = -\log p(y|g(z))$$
$$\mathcal{L} = \|y - g(f(y))\|_2^2$$

Two views of auto encoders

- We just implement functions for f, g (e.g. lots of sigmoids in layers) - this gives rise to deep auto encoders, trained by gradient descent
- We commit to full-blow probabilistic models, treating z as probabilistic random variable - this gives rise to variational auto encoders