Machine learning - HT 2016

9. Dimensionality Reduction & Multidimensional Scaling

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Supervised Learning: Summary

- Training data is of the form $\langle(\mathbf{x}_i, y_i)\rangle$ where $\mathbf{x}_i$ are features and y_i is target
- We formulate a probabilistic (or deterministic) model for $y \mid \mathbf{x}, \mathbf{w}$
- Choose a suitable loss function; minimize training loss
- Use regularization or other techniques to reduce overfitting
- Use trained classifier to predict targets/labels on unseen $\mathbf{x}_{\text{new}}$

Unsupervised Learning

- Training data is of the form $\langle (\mathbf{x}_i) \rangle_{i=1}^{m}$
- Infer properties about the data
- Example: Clustering - can the data be grouped into categories?
- Example: Density Estimation
- **Today**: Dimensionality Reduction and Multi-dimensional Scaling (MDS)

Outline

Today, we'll study techniques for dimensionality reduction and multidimensional scaling

- Principal Component Analysis (PCA)
- Kernel PCA
- Multidimensional Scaling: Reconstruct data from similarity or dissimilarity measures

Dimensionality Reduction

Why perform dimensionality reduction?

- Computational Reasons - time/storage efficiency
- Statistical Resaons - better generalization guarantees
- Visualization - helps understand data

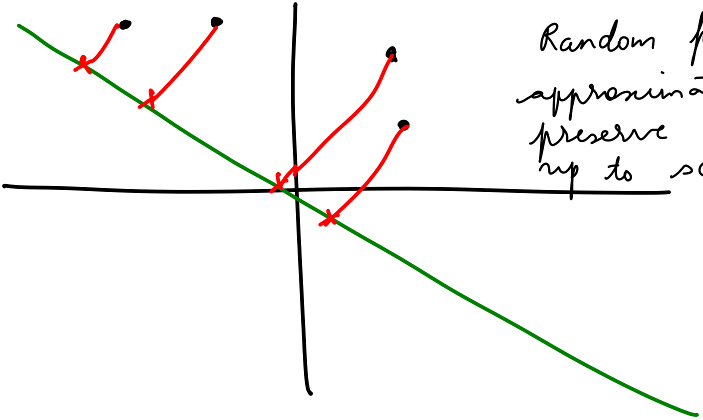
Objective

- Lower dimensional representation that preserves *essential* properties

Johnson-Lindenstrauss Lemma

Project data onto random k dimensional subspace

All pairwise distances are approximately preserved



Random projections approximately preserve distances up to scaling.

Principal Component Analysis (PCA)

PCA is a *linear* dimensionality reduction technique

Find the directions of maximum variance in the data $\langle(\mathbf{x}_i)\rangle_{i=1}^m$

Assume that data is centered, *i.e.*, $\sum_i \mathbf{x}_i = \mathbf{0}$

Find a set of orthogonal vectors $\mathbf{v}_1, \ldots, \mathbf{v}_k$

- The first principal component (PC) $\mathbf{v}_1$ is the direction of largest variance
- The second PC $\mathbf{v}_2$ is the direction of largest variance orthogonal to $\mathbf{v}_1$
- The i^{th} PC $\mathbf{v}_i$ is the direction of largest variance orthogonal to $\mathbf{v}_1, \ldots, \mathbf{v}_{i-1}$

$\mathbf{V}_{n \times k}$ gives projection

$$\mathbf{z}_i = \mathbf{V}^T \mathbf{x}_i$$

PCA: Directions that maximise variance

We are given i.i.d. data $\langle (\mathbf{x}_i) \rangle_{i=1}^{m}$; data matrix $\mathbf{X}$

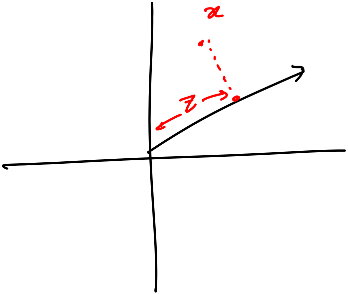
Want to find $\mathbf{v}_1 \in \mathbb{R}^n$, $\|\mathbf{v}_1\| = 1$, that maximizes $\|\mathbf{X}\mathbf{v}_1\|^2$

$z_i = \langle x_i, v_1 \rangle$

$\sum_i x_i = 0$

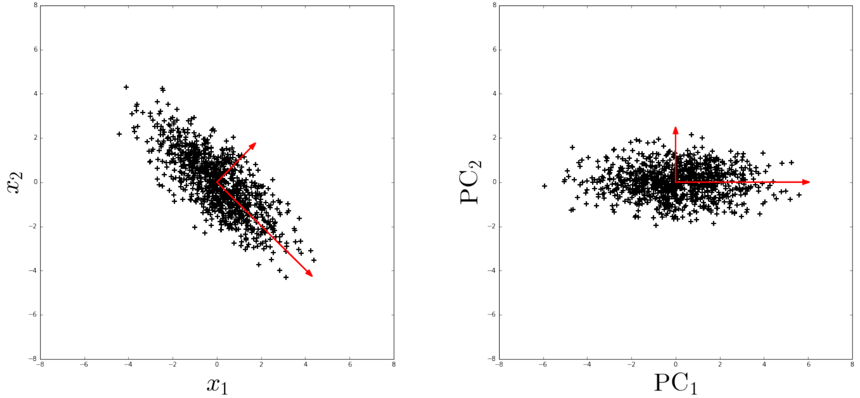
$\sum_i z_i = 0$

Find v_1 that maximises $\sum_i z_i^2$



Find $\mathbf{v}_2, \mathbf{v}_3, \ldots, \mathbf{v}_k$ that are all successively orthogonal to previous directions and maximise (as yet unexplained variance)

Principal Component Analysis (PCA)



PCA: Best Reconstruction

We are given i.i.d. data $\langle (\mathbf{x}_i) \rangle_{i=1}^{m}$; data matrix $\mathbf{X}$

Find a k-dimensional linear projection that best "models" the data

Suppose $\mathbf{V}_k \in \mathbb{R}^{n \times k}$ is such that columns of $\mathbf{V}_k$ are orthogonal

Project data $\mathbf{X}$ on to subspace defined by $\mathbf{V}$

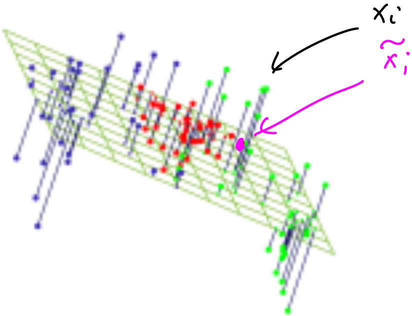
$$\mathbf{Z} = \mathbf{X}\mathbf{V}_k$$

Minimize reconstruction error:

$$\sum_{i=1}^{m} \|\mathbf{x}_i - \mathbf{V}_k \mathbf{V}_k^T \mathbf{x}_i\|^2$$

Principal Component Analysis (PCA)

Minimise: $\sum_i \|x_i - \tilde{x}_i\|^2$



Equivalence between two objectives

Let $\mathbf{v}_1$ be the direction of projection

The point $\mathbf{x}$ is mapped to $\langle \mathbf{v}_1, \mathbf{x} \rangle \mathbf{v}_1$, where $\|\mathbf{v}_1\| = 1$

$z_i = \langle v_1, x_i \rangle$ Find v_1 such that $\sum_i z_i^2 = \sum_i \langle x_i, v_1 \rangle^2$ is maximum

$z_i \in \mathbb{R}$, $v_1 \in \mathbb{R}^n$, $\tilde{x}_i = z_i v_1 \in \mathbb{R}^n$

$$\sum_i \|x_i - \tilde{x}_i\|^2 = \sum_i \left(\|x_i\|^2 - 2 \langle v_1, x_i \rangle^2 + \langle v_1, x_i \rangle^2 \|v_1\|^2 \right)$$

$$= \underbrace{\sum_i \|x_i\|^2}_{\text{constant}} - \underbrace{\sum_i \langle v_1, x_i \rangle^2}_{\text{minimising}}$$

Finding Principal Components: SVD

Let $\mathbf{X}$ be the $m \times n$ data matrix (say $n < m$)

Pair of singular vectors $\mathbf{u} \in \mathbb{R}^m$, $\mathbf{v} \in \mathbb{R}^n$ and singular value $\sigma \in \mathbb{R}^+$ if

$$\sigma \mathbf{u} = \mathbf{X}\mathbf{v} \quad \text{and} \quad \sigma \mathbf{v} = \mathbf{X}^T \mathbf{u}$$

$\mathbf{v}$ is an eigenvector of $\underbrace{\mathbf{X}^T\mathbf{X}}_{n \times n}$ with eigenvalue σ^2

$\mathbf{u}$ is an eigenvector of $\underbrace{\mathbf{X}\mathbf{X}^T}_{m \times m}$ with eigenvalue σ^2

X is a map from $\mathbb{R}^n \to \mathbb{R}^m$

X^T is a map from $\mathbb{R}^m \to \mathbb{R}^n$

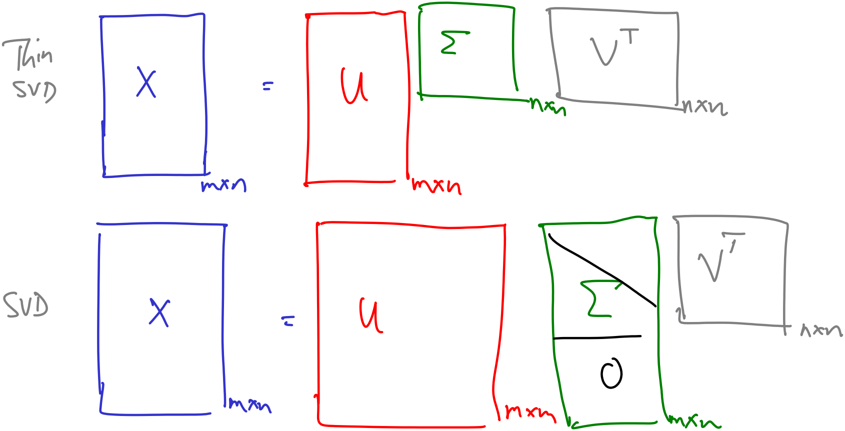
Finding Principal Components: SVD

$\mathbf{X} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$ [$m > n$]

Thin SVD: $\mathbf{U}$ is $m \times n$, $\boldsymbol{\Sigma}$ is $n \times n$, $\mathbf{V}$ is $n \times n$, $\mathbf{U}^T\mathbf{U} = \mathbf{V}^T\mathbf{V} = \mathbf{I}_{n \times n}$

$\boldsymbol{\Sigma}$ is diagonal with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$

The first k principal components are first k columns of $\mathbf{V}$



PCA: Reconstruction Error

We have thin SVD: $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$

Let $\mathbf{V}_k$ be the matrix containing first k columns of $\mathbf{V}$

Projection $\mathbf{Z} = \mathbf{X}\mathbf{V}_k = \mathbf{U}_k\mathbf{\Sigma}_k$

Reconstruction error $= \sum_{i=1}^{m} \|\mathbf{x}_i - \mathbf{V}_k\mathbf{V}_k^T\mathbf{x}_i\|^2 = \sum_{j=k+1}^{n} \sigma_i^2$

We have $\tilde{X} = Z V_k^T = X V_k V_k^T$

$$X = U \Sigma V^T = \sum_{i=1}^{n} \sigma_i u_i v_i^T$$

$$\tilde{X} = U \Sigma V_k^T = \sum_{i=1}^{k} \sigma_i u_i v_i^T$$

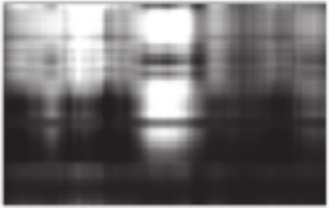
Reconstruction error is the Frobenius norm of

$X - \tilde{X}$

$$X - \tilde{X} = \sum_{i=k+1}^{n} \sigma_i u_i v_i^T$$

$$\|X - \tilde{X}\|_F = \sum_{i=k+1}^{n} \sigma_i^2 \qquad (\text{Since } \|u_i\| = \|v_i\| = 1)$$

(a)

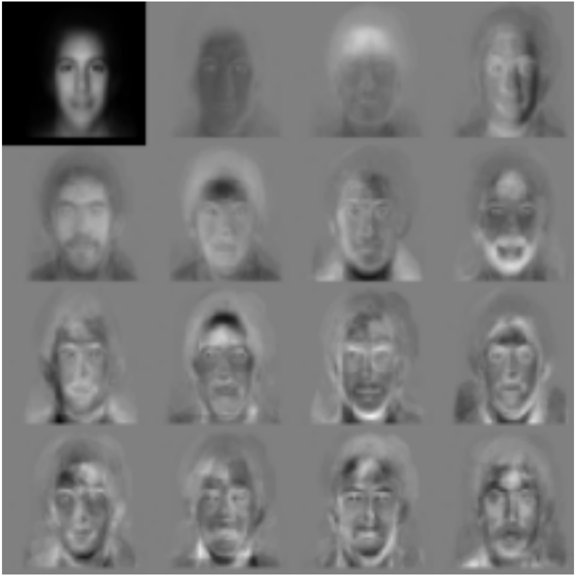


(b)

(c)

(d)

Eigenfaces



Source: http://vismod.media.mit.edu/vismod/demos/facerec/basic.html

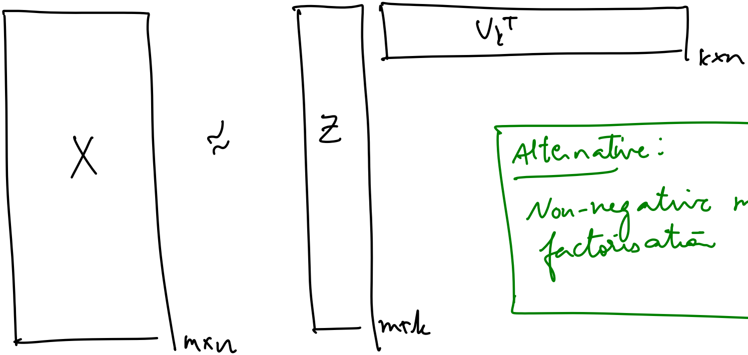
Latent Semantic Analysis

$\mathbf{X}$ is an $m \times n$, n is the size of dictionary

$\mathbf{x}_i$ is a vector of word counts (bag of words)

Reconstruction using k eigenvectors $\mathbf{X} \approx \mathbf{Z}\mathbf{V}_k^T$, where $\mathbf{Z} = \mathbf{X}\mathbf{V}_k$

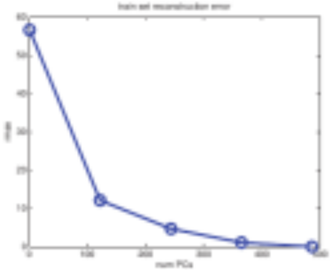
$\langle \mathbf{z}_i, \mathbf{z}_j \rangle$ is probably a better notion of similarity than $\langle \mathbf{x}_i, \mathbf{x}_j \rangle$

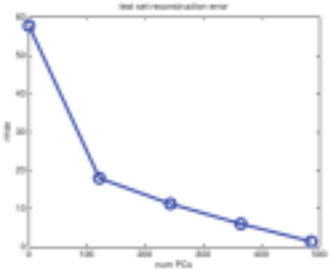


Alternative:

Non-negative matrix factorisation

How many principal components to pick?





PCA Summary

Algorithm: We've expressed PCA as SVD of data matrix $\mathbf{X}$

Equivalently, we can use eigendecomposition of co-variance matrix $\mathbf{X}^T\mathbf{X}$

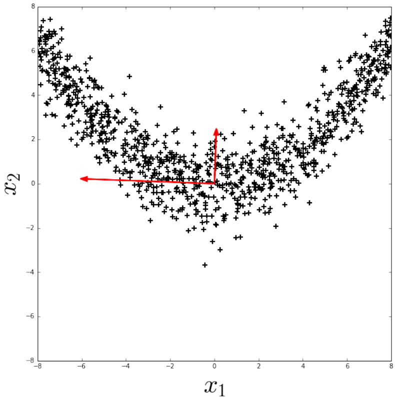
Running Time: $O(mnk)$ to compute k principal components (avoid computing covariance matrix)

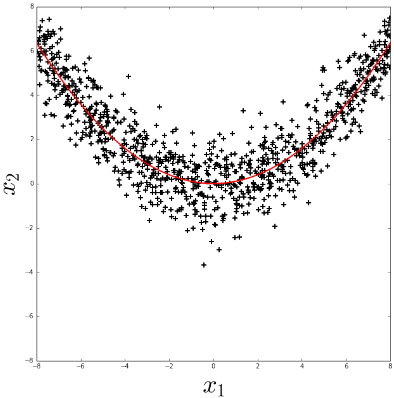
PCs are uncorrelated, but there may be non-linear (higher-order) effects

PCA depends on scale or units of measurement; it may be a good idea to standardize data

PCA is sensitive to outliers

PCA: Going beyond linearity





We can perform basis expansion $\phi(\mathbf{x}) = (x_1, x_1^2, x_1 x_2, \ldots,)^T$

Kernel PCA

Representation:

PCs can be expressed in terms of the datapoints $\mathbf{x}_i$. Why?

Suppose $\mathbf{v}_1 = \mathbf{X}^T\boldsymbol{\alpha}$, *i.e.*,$\mathbf{v}_1 = \sum_{i=1}^{m} \alpha_i \mathbf{x}_i$

Objective

$$\max_{\|\mathbf{v}_1\|=1} \mathbf{v}_1^T\mathbf{X}^T\mathbf{X}\mathbf{v}_1 = \max_{\|\boldsymbol{\alpha}^T\mathbf{X}\mathbf{X}^T\boldsymbol{\alpha}\|=1} \boldsymbol{\alpha}^T(\mathbf{X}\mathbf{X}^T)^2\boldsymbol{\alpha}$$

We only need $\mathbf{K} = \mathbf{X}\mathbf{X}^T$ to compute $\boldsymbol{\alpha}$

Kernel PCA

Objective

$$\max_{\|\boldsymbol{\alpha}^T \mathbf{K} \boldsymbol{\alpha}\|=1} \boldsymbol{\alpha}^T \mathbf{K}^2 \boldsymbol{\alpha},$$

where $\mathbf{K} = \mathbf{X}\mathbf{X}^T$. What is the solution $\boldsymbol{\alpha}$?

$\alpha = \frac{u_1}{\sigma}$, where u_1 is the first column of U if the SVD of $X = U \Sigma V^T$. Note that

$u_1^T K u_1 = (u_1^T X)(X^T u_1) = \sigma_1^2 v_1^T v_1$ (where v_1 is the first PC)

Note: If U_k are the first k columns of U, they are the projection of the data X onto the first k columns of V, V_k, i.e. the first k PCs

Kernel PCA

As in the case of SVM, we can use many different types of kernels $\kappa(\mathbf{x}, \mathbf{x}')$

Examples

- Linear kernel: $\kappa(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T \mathbf{x}'$
- Polynomial kernel: $\kappa(\mathbf{x}, \mathbf{x}') = (1 + \mathbf{x}^T \mathbf{x}')^d$
- Gaussian (RBF) kernel: $\kappa(\mathbf{x}, \mathbf{x}') = \exp(\|\mathbf{x}^T - \mathbf{x}'\|^2)$
- Kernels useful for combinatorial objects: cosine, string kernel, etc.

Mercer's Theorem

As long as κ always results in a positive definite Gram matrix, there exists a high-dimensional feature space ϕ, such that $\kappa(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^T \phi(\mathbf{x})$

Multidimensional Scaling

Suppose for some m points in $\mathbb{R}^n$ we are given all pairwise distances in a matrix $\mathbf{D}$

Can we reconstruct $\mathbf{x}_1, \ldots, \mathbf{x}_m$, i.e., all of $\mathbf{X}$?

Multidimensional Scaling

Distances are preserved under translation, rotation, reflection, etc.

We cannot recover $\mathbf{X}$ exactly; we can determine $\mathbf{X}$ up to these transformations

If D_{ij} is the distance between points $\mathbf{x}_i$ and $\mathbf{x}_j$, then

$$
\begin{aligned}
D_{ij}^2 &= \|\mathbf{x}_i - \mathbf{x}_j\|^2 \\
&= \mathbf{x}_i^T \mathbf{x}_i - 2\mathbf{x}_i^T \mathbf{x}_j + \mathbf{x}_j^T \mathbf{x}_j \\
&= M_{ii} - 2M_{ij} + M_{jj}
\end{aligned}
$$

Here $\mathbf{M} = \mathbf{X}\mathbf{X}^T$ is the $m \times m$ matrix of dot products

Exercise: Show that assuming $\sum_i \mathbf{x}_i = \mathbf{0}$, $\mathbf{M}$ can be recovered from $\mathbf{D}$

Multidimensional Scaling

Consider the (non-thin) SVD: $\mathbf{X} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$

We can write $\mathbf{M}$ as

$$\mathbf{M} = \mathbf{X}\mathbf{X}^T = \mathbf{U}\boldsymbol{\Sigma}\boldsymbol{\Sigma}^T\mathbf{U}^T$$

To reconstruct $\tilde{\mathbf{X}}$, consider the eigendecomposition of $\mathbf{M}$

$$\mathbf{M} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^T$$

Because, $\mathbf{M}$ is symmetric and positive semi-definite, $\mathbf{U}^T = \mathbf{U}^{-1}$ and all entries of (diagonal matrix) $\boldsymbol{\Lambda}$ are non-negative

Let $\tilde{\mathbf{X}} = \mathbf{U}\boldsymbol{\Lambda}^{1/2}(= \mathbf{U}\boldsymbol{\Sigma}$ *[after truncation]*)

If we are satisfied with approximate reconstruction, we can use truncated eigendecomposition

Multidimensional Scaling: Comments

If the similarity matrix $\mathbf{M}$ is not positive semi-definite, cannot necessarily find a Euclidean embeddding

Minimize stress function: Find $\mathbf{z}_1, \ldots, \mathbf{z}_m$ that minimizes

$$S(\mathbf{Z}) = \sum_{i \neq j} (D_{ij} - \|\mathbf{z}_i - \mathbf{z}_j\|)^2$$

Many other types of stress functions