MSPR 4: PCA II

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This lecture is based on presentations made in my course 'Advanced Topics in in Music Technology' at Music Technology Group, Universitat Pompeu Fabra between 2007-2011, Barcelona, especially the ones by Stefan Kersten and Srikanth Cherla, closely following

- *Andrew Moore's machine learning tutorial lectures: Gaussians, Gaussian Mixture Models,* *http://www.autonlab.org/tutorials/*
- *Christopher Bishop: Pattern Recognition and Machine Learning: Chapter 1 (Introduction) 1.2.3 (The Gaussian Distribution) p. 24 - 27, 2.3 (The Gaussian Distribution) p. 78, 84 bottom - 85 top.*

Outline

Eigenvalues and Eigenvectors

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Strang: Chapter 6.1: Introduction to Eigenvalues pp. 283-297

Eigenvalues and Eigenvectors

Generally the vector $\mathbf{x}$ *changes direction* when multiplied by $\mathbf{A}$...

However there are some special vectors $\mathbf{x}$ that are in the same direction as $\mathbf{A}\mathbf{x}$:

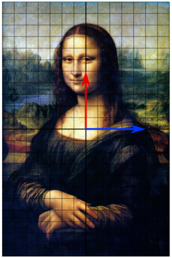
$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$$

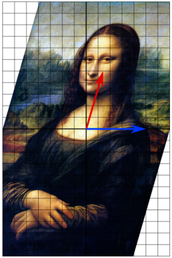
- such a vector $\mathbf{x}$ is an *eigenvector*
- λ is the *eigenvalue* corresponding to $\mathbf{x}$
- λ can is a number, it scales $\mathbf{x}$
- if $\mathbf{A} = \mathbf{I}$, $\mathbf{A}\mathbf{x} = \mathbf{x}$, i.e. all vectors are eigenvectors of $\mathbf{I}$

Example I

- Shearing: $\mathbf{A} = \begin{bmatrix} 1 & 0.25 \\ 0 & 1 \end{bmatrix}$
- $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ is an eigenvector with eigenvalue 1
- $\begin{bmatrix} 0 \\ -1 \end{bmatrix}$ is another eigenvector with eigenvalue 1

http://en.wikipedia.org/wiki/File:Mona_Lisa_eigenvector_grid.png





Example II

Video: `http://en.wikipedia.org/wiki/File:Eigenvectors.gif`

- Transformation matrix
$$\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$
- Example of eigenvectors: $\begin{bmatrix} -1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ with corresponding eigenvalues $1, 3$.

Eigenvalue Decomposition for Symmetric Matrices

Eigenvalue Decomposition for Symmetric Matrices

Strang: Chapter 6.2: Diagonalizing a Matrix pp. 298-311, Chapter 6.4: Symmetric Matrices

Eigenvalue Decomposition for Symmetric Matrices

Definition

An *orthonormal* matrix V is a matrix in which

- all column vectors (row vectors) are orthogonal to each other, i.e. $\mathbf{v} \cdot \mathbf{w} = 0$ for $\mathbf{v} \neq \mathbf{w}$
- all column vectors (row vectors have length 1, i.e. $\|\mathbf{v}\| = 1$
- $\Rightarrow \mathbf{V}^T\mathbf{V} = \mathbf{I} = \mathbf{V}^{-1}\mathbf{V} \Rightarrow \mathbf{V}^{-1} = \mathbf{V}^T$

Theorem

(*Eigenvalue decomposition for symmetric matrices:*) Every symmetric matrix has the matrix decomposition $\mathbf{A} = \mathbf{V\Lambda V}^T$ with real eigenvalues in $\mathbf{\Lambda}$ and orthogonal eigenvectors in $\mathbf{V}$:

$$\mathbf{A} = \mathbf{V\Lambda V}^{-1} = \mathbf{V\Lambda V}^T \qquad \text{with} \qquad \mathbf{V}^{-1} = \mathbf{V}^T (Matlab: [\mathtt{V}\ \Lambda] = \mathtt{eig(A)})$$

Eigenvalue Decomposition for Symmetric Matrices

The *eigenvector matrix* $\mathbf{V}$ has the eigenvectors $\mathbf{v}_1 \ldots \mathbf{v}_n$ as columns.

$$\mathbf{V} = \begin{bmatrix} \mathbf{v}_1 & \ldots & \mathbf{v}_n \end{bmatrix}$$

The *eigenvalue matrix* $\mathbf{\Lambda}$ has the eigenvalues as diagonal elements in corresponding order:

$$\mathbf{\Lambda} = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}$$

Eigenvalue Decomposition for Symmetric Matrices

Remark on Diagonalization

- The order of eigenvectors in $\mathbf{V}$ corresponds to the order of eigenvalues in $\mathbf{\Lambda}$ (see proof on diagonalization)

Class Assignment

Find the eigenvectors $\mathbf{v}_1, \mathbf{v}_2$ *and corresponding eigenvalue(s)* λ_1, λ_2 *for*

$$\mathbf{A} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

and sort them according to a descending order of the eigenvalues. Use the following Matlab functions (and others):

- `a=diag(A)` *returns the diagonal of matrix* `A` *as a vector* `a`
- `[x idx]=sort(x,'descend'); A=A(:,idx)` *sorts the elements of* x *in descending order. It also sorts the columns of* A *in descending order of the corresponding elements of* x*.*

Class Assignment

Perform an eigenvalue decomposition of the sample covariance matrix **C***of covariances between the features (sepal length / width, petal length / width). Sort the eigenvalues in descending order, rearrange the eigenvalues and the eigenvectors in that order and plot the eigenvalues. Use the following Matlab functions (and others):*

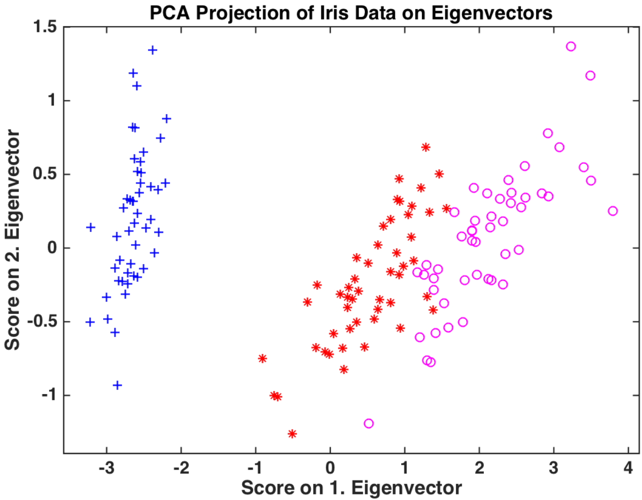
- `a=diag(A)` *returns the diagonal of matrix* `A` *as a vector* `a`
- `[x idx]=sort(x,'descend'); A=A(:,idx)` *sorts the elements of x in descending order. It also sorts the columns of A in descending order of the corresponding elements of x.*

Class Assignment

Display the Eigenvectors over the four features (sepal length / width, petal length / width) using `plot` *and* `hold on` *and explain how they relate to the features.*

Class Assignment

Center the data via: $X_c = X - \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} \bar{\mathbf{x}}$ *where the vertical vector consisting of* I *ones (number of observations/rows in observation matrix* $\mathbf{X}$*) and* $\bar{\mathbf{x}} = (\bar{\mathbf{X}}_{[:,1]}, \bar{\mathbf{X}}_{[:,2]}, \ldots, \bar{\mathbf{X}}_{[:,J]})$ *is the vector of column means of features* $1, 2, \ldots, J$. *Calculate the scores, i.e. the marks on the axes of the new coordinate system (= the eigenvectors) via:* $\mathbf{S} = \mathbf{X}_c \mathbf{V}_{[:,1:2]}$, *where* $\mathbf{V}_{[:,1:2]}$ *is the matrix that consists of just the first two columns (eigenvectors) of eigenvector matrix* $\mathbf{V}$ *of sample covariance matrix* $\mathbf{C}$ *with corresponding 2 highest eigenvectors. Then display the scores of all iris instances. Mark each iris species in a different color. Use the prtools function* `scatterd` *for plotting.*


PCA Projection of Iris Data on Eigenvectors
Score on 2. Eigenvector
Score on 1. Eigenvector
1.5
1
0.5
0
-0.5
-1
-3
-2
-1
0
1
2
3
4

The *Inertia* (average square norm of all points) for set of column-centered points $\mathbf{X}_{c[1,:]}, \mathbf{X}_{c[2,:]}, \ldots, \mathbf{X}_{c[I,:]}$ is a measure for the variance in the data:

$$\frac{1}{I} \sum_{i=1}^{I} \left\| \mathbf{X}_{c[i,:]} \right\|^2 .$$

Consider the scores $\mathbf{S} = \mathbf{X}_c \mathbf{V}_{[:,1:j]}$, where $\mathbf{V}_{[:,1:j]}$ is the matrix that consists of just the j columns (eigenvectors) of eigenvector matrix $\mathbf{V}$ of sample covariance matrix $\mathbf{C}$ that correspond to its j highest eigenvalues. We can measure how much variance of the original data $\mathbf{X}_{[i,:]}$ is kept in the scores $\mathbf{S}_{[i,:]}$ by calculating the *inertia (data variance) quotient*:

$$\tau := \frac{\sum_{i=1}^{I} \|\mathbf{S}_{[i,:]}\|^2}{\sum_{i=1}^{I} \|\mathbf{X}_{[i,:]}\|^2}$$

Principal component analysis (eigenvalue decomposition on the sample covariance matrix of the data) provides the projection with best variance preservation.

Class Assignment

1. *Calculate the inertia quotient τ between the scores and the column centered iris data.*
2. *Calculate the cumulative sum of eigenvalue percentage for the two ($k = 2$) highest eigenvalues λ_1, λ_2 according to: $c_k = \frac{\sum_{j=1}^{k} \lambda_j}{\sum_{j=1}^{J} \lambda_j}$ and compare it with the inertia quotient calculated before.*
3. *Calculate and plot the cumulative sum of eigenvalue percentage c_k for the $k = 1, 2, 3, 4$ highest eigenvalues using Matlab function* `cumsum` *for calculating cumulative sums.*

Class Assignment

(Principal Component Analysis for Compression and Reconstruction) *Reconstruct the original Iris data, using the following reconstruction equation for scores* $\mathbf{S}$ *and* $\mathbf{V}'_{[:,1:j]}$ *whos columns are are the* j *eigenvectors corresponding to the highest* j *eigenvalues of the sample covariance matrix of the data:*

$$\mathbf{X}_r = \mathbf{S}\mathbf{V}'_{[:,1:j]} + \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} \bar{\mathbf{x}}$$

where the vertical vector consisting of I *ones (number of observations/rows in observation matrix* $\mathbf{X}$*) and* $\bar{\mathbf{x}} = (\bar{\mathbf{X}}_{[:,1]}, \bar{\mathbf{X}}_{[:,2]}, \ldots, \bar{\mathbf{X}}_{[:,J]})$ *is the vector of column means of features* $1, 2, \ldots, J$*.*

Principal Component Analysis Cookbook I

1. *Data matrix*: I observations of J features:

$$\mathbf{X} := \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1j} & \cdots & x_{1J} \\ x_{21} & x_{22} & \cdots & x_{2j} & \cdots & x_{2J} \\ x_{31} & x_{32} & \cdots & x_{3j} & \cdots & x_{3J} \\ \vdots & \vdots & \ldots & \vdots & \ldots & \vdots \\ x_{i1} & x_{i2} & \cdots & x_{ij} & \cdots & x_{iJ} \\ & & \cdots & & \cdots & \\ x_{I1} & x_{I2} & \cdots & x_{Ij} & \cdots & x_{IJ} \end{pmatrix}$$

2. Calculate: *sample mean vector* $\bar{\mathbf{x}}$ (Matlab: `mean(X)`):

$$\bar{\mathbf{x}} = \frac{1}{I} \underbrace{(1, 1 \ldots, 1)}_{I\times} \mathbf{X}$$

3. *Centerize data* column/featurewise via: $X_c = X - \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} \bar{\mathbf{x}}$

Principal Component Analysis Cookbook II

1. Calculate *sample covariance*:

$$\mathbf{C} = \frac{1}{l-1}\mathbf{X}_c^T\mathbf{X}_c$$

   Matlab: `C=cov(X)`

2. *Eigenvalue decomposition for symmetric matrices*: $\mathbf{C}$ is symmetric: $\mathbf{C} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$ with eigenvectors as the columns of $\mathbf{V}$ and the corresponding eigenvectors in the same order on the diagonal of $\mathbf{\Lambda}$
   Matlab: `[V   D]=eig(C)`

3. Pick eigenvalues from diagonal of $\mathbf{\Lambda}$ and form a vector λ:
   Matlab: `eigval=diag(D);`

Principal Component Analysis Cookbook III

1. *Sort eigenvectors* and eigenvalues in descending order: Matlab: `[eigval idx]=sort(eigval,'descend'); V=V(:,idx);`
2. *[Plot eigenvectors]* and interpret them in terms of the original features, they are a linear combination of. Matlab: `plot (V(: , j ) )`
3. Calculate and plot the *cumulative sum of eigenvalue percentage* :
   $c_k = \frac{\sum_{j=1}^{k} \lambda_j}{\sum_{j=1}^{J} \lambda_j}$

```
cs=cumsum(eigval)/sum(eigval); plot(cs)
```

The eigenvector corresponding to the highest eigenvalue points in the direction of maximal variance. Check the graph for a 'knee' to decide how many dimensions k to keep.

Principal Component Analysis Cookbook IV

1. *Reduction to k dimensions:* Calculate the scores via: $\mathbf{S} = \mathbf{X}_c \mathbf{V}_{[:,1:k]}$, where $\mathbf{V}_{[:,1:k]}$ is the matrix that consists of just the first k columns (eigenvectors) of eigenvector matrix $\mathbf{V}$ of sample covariance matrix C with corresponding k highest eigenvalues. Matlab:

```
scores=Xc*V(: ,1:k)
```

2. *Visualize scores* (2d for the 2 highest eigenvalues) Matlab (if the data have labels):

```
z=prdataset(scores , labels); scatterd(z)
```

Principal Component Analysis Cookbook V

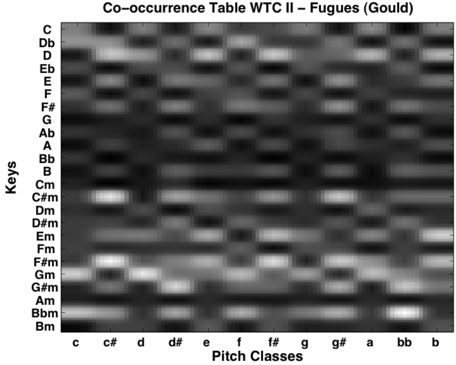
1. *[Reconstruct data]* from the compressed representation:

$$\mathbf{X}_r = \mathbf{S}\mathbf{V}'_{[:,1:k]} + \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} \bar{\mathbf{x}}$$

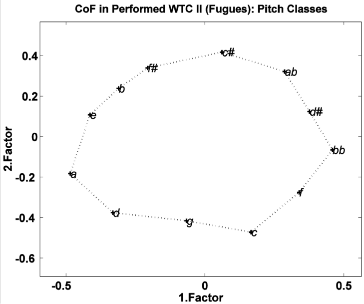
```
Xr=scores*V(:,1:k) +ones(I,1)*mean(X);
```

Relations between Pitch Classes in Bachs Wohltemperiertes Klavier II

- Bach: Wohltemperiertes Klavier, Part II (Fugen), Glenn Gould (Audio) Greyscale matrix: estimated strength of 12 pitch clases in all 24 keys (CQ-Profile, Purwins et al. 2000) Pitch classes: 24-dimensional frequency vector in each key
- Dimension reduction (correspondence analysis: Greenacre, 1984) maps 24 dimensions to 2 dimensions, to preserve structural relationships between keys.



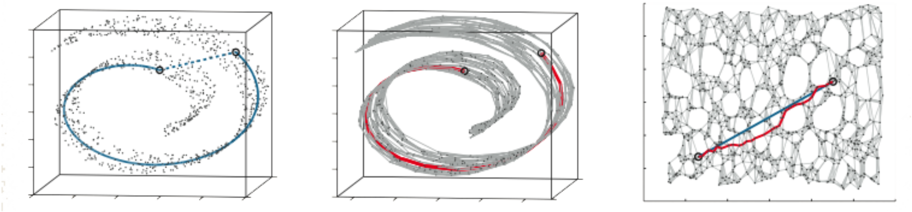
Visualisation of Pitch Classes in Bach's WT II, Fugues, recording Glenn Gould



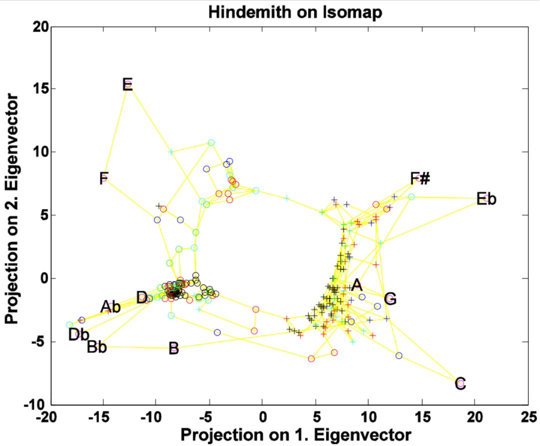
Circle of fifths emerges! Check out Matlab dimension reduction toolbox:
`http://lvdmaaten.github.io/drtoolbox/`

Isomap

Non-linear Mapping: Geodesic distance + PCA



Musical Style Visualization



'Landscapes' of all pieces: Bach (black), Chopin (red), Alkan (cyan), Scriabin (green), Shostakovich (blue), Hindemith (magenta, outlier) marked, 'o'/'+:Major/minor (Purwins et al. 2004)