Introduction to Principal Component Analysis (PCA)

CS 510

Lecture #09

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Colorado State University

To Start – Correlation Matching

- Assume you have a gallery (database) of images, and a “probe” (test) image.
- The goal is to find the database image that is most similar to the probe image.
- “Similar” defined according to any measure
  - e.g. correlation

Example: Finding Cats

"Probe" image -- image to be matched

Gallery of database images





Registration

- Whole image matching presumes alignment
- Images are points in N-dimensional space
  - Dimensions meaningless unless points correspond
- Comparisons undefined if sizes differ
- The same restrictions as (strict) correlation
- Faces, often eye's map to same positions.
  - Specifies rotation, translation and scale.

Example: Aligned Cats

Probe image, registered to gallery

Registered Gallery of Images





Multiple Images of One Object

- Another reason for matching a probe against a gallery
  - Sample possible object variants, e.g.
  - Object seen from all (standard) viewpoints
  - Object seen from all (standard) illuminations
- Goal: find pose or illumination condition
- Bit brute force,
  - but strong if variants are present.

Alternate Example

Example Probe image

Five of 71 gallery images (COIL)

But Wait, This is Expensive!

- It is very costly to compare whole images.
- How can we save effort …
  - A lot of effort!
- Just how much variation is there in …
  - Faces of cats
- Is there a systematic way to measure
  - … and then work with less data?
- Yes, which takes us next to covariance.

Background Concepts: Variance

- Variance - the central tendency,
  - variance is defined as:

$$\frac{\sum (x_i - \bar{x})^2}{N}$$

- Square root of variance is the standard deviation

Background Concepts: Covariance

- Covariance measures if two signals vary together:

$$\Omega = \frac{\sum_l (x_l - \bar{x})(y_l - \bar{y})}{N}$$

- How does this differ from correlation?
- The range of the covariance of two signals?
- Note the covariance of two signals is a scalar

Covariance Matrices (I)

- Let x and y be sets of vectors…
- What if I want to know the relation between the ith element of x and the jth element of y?

$$\frac{1}{N}\Sigma = \begin{bmatrix} \sigma_{x_1,y_1} & \sigma_{x_1,y_2} & \cdots \\ \sigma_{x_2,y_1} & \sigma_{x_2,y_2} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

$$\sigma_{x_i,y_j} = \sum \left(x_{i,k} - \bar{x}_i\right)\left(y_{j,k} - \bar{y}_j\right)$$

Background Concepts: Outer Products

- Remember outer products :

$$\begin{bmatrix} ad & ae & af \\ bd & be & bf \\ cd & ce & cf \end{bmatrix} = \begin{bmatrix} a \\ b \\ c \end{bmatrix} \begin{bmatrix} d & e & f \end{bmatrix}$$

- Why?
- Because if I have two vectors, their covariance term is their outer product

Covariance Matrices (II)

- The covariance between two vectors isn't too interesting, just a set of scalars, but…
- What if we have two sets of vectors:
  - Let $X = \{(a_1, b_1, c_1), (a_2, b_2, c_2)\}$
  - Let $Y = \{(d_1, e_1, f_1), (d_2, e_2, f_2)\}$
- And assume the vectors are ***<u>centered</u>***
  - Meaning that the average X vector is subtracted from the X set, and the average Y is subtracted from the Y set
- What is the covariance between the sets of vectors?

Covariance Matrices (III)

- The covariance matrix is the outer product:

$$\begin{bmatrix} a_1 & a_2 \\ b_1 & b_2 \\ c_1 & c_2 \end{bmatrix} \begin{bmatrix} d_1 & e_1 & f_1 \\ d_2 & e_2 & f_2 \end{bmatrix} = \begin{bmatrix} a_1 d_1 + a_2 d_2 & a_1 e_1 + a_2 e_2 & a_1 f_1 + a_2 f_2 \\ b_1 d_1 + b_2 d_2 & b_1 e_1 + b_2 e_2 & b_1 f_1 + b_2 f_2 \\ c_1 d_1 + c_2 d_2 & c_1 e_1 + c_2 e_2 & c_1 f_1 + c_2 f_2 \end{bmatrix}$$

- $\Omega_{i,j}$ is the covariance of position i in set X with position j in set Y,
- assumes pair wise matches

Covariance Matrices (IV)

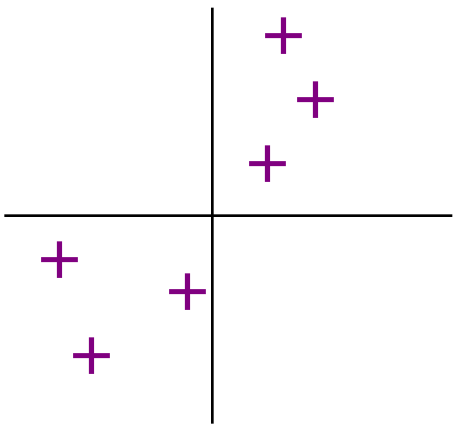
- It is interesting & meaningful to look at the covariance of a set with itself:

$$\begin{bmatrix} a_1 & a_2 \\ b_1 & b_2 \\ c_1 & c_2 \end{bmatrix} \begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \end{bmatrix} = \begin{bmatrix} a_1a_1 + a_2a_2 & a_1b_1 + a_2b_2 & a_1c_1 + a_2c_2 \\ b_1a_1 + b_2a_2 & b_1b_1 + b_2b_2 & b_1c_1 + b_2c_2 \\ c_1a_1 + c_2a_2 & c_1b_1 + c_2b_2 & c_1c_1 + c_2c_2 \end{bmatrix}$$

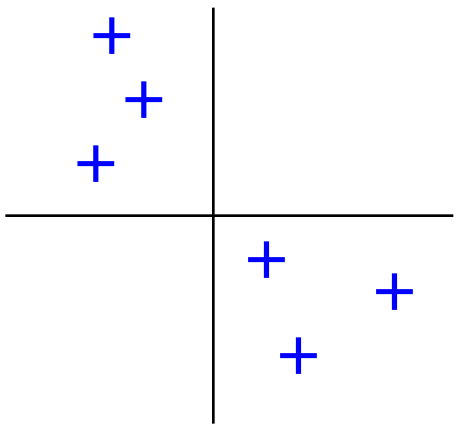
- Now how do you interpret $\Omega_{i,j}$?

Covariance Matrices (V)

Covariance matrices of 2D data sets (easy to draw)



What can you tell me about $\Omega_{x,y}$?



What can you tell me about $\Omega_{x,y}$?

Principal Component Analysis

- PCA $\equiv$ SVD(Cov(X)) = SVD($XX^T/(n-1)$)
- SVD: $XX^T = R\Lambda R^{-1}$
  - R is a rotation matrix (the Eigenvector matrix)
  - Λ is a diagonal matrix (diagonal values are the Eigenvalues)
- The Eigenvalues capture how much the dimensions in X co-vary
- The Eigenvectors show which combinations of dimensions tend to vary together

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PCA (II)

- The Eigenvector with the largest Eigenvalue is the direction of maximum variance
- The Eigenvector with the 2nd largest Eigenvalue is orthogonal to the 1st vector and has the next greatest variance.
- And so on…
- The Eigenvalues describe the amount of variance along the Eigenvectors

We will now motivate and illustrate these ideas using Gaussian Random Variables …

The PCA Cookbook
Step 1: Image as Vector

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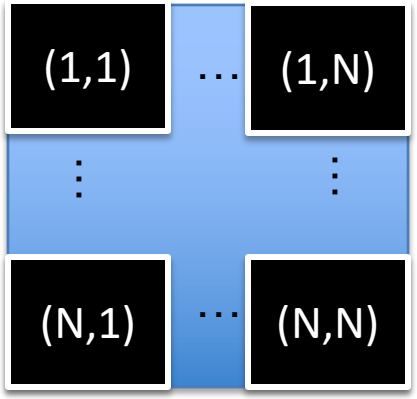


$$\begin{vmatrix} I(1,1) \\ \vdots \\ I(1,N) \\ I(2,1) \\ \vdots \\ I(N,N) \end{vmatrix}$$

Step 2: Normalize

- Normalize each vector:
  - Compute mean value of vector
  - Subtract mean value

$$X = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix}, \overline{X} = \sum_{i=0}^{N} x_i, X - \overline{X} = \begin{bmatrix} x_1 - \overline{x} \\ \vdots \\ x_N - \overline{x} \end{bmatrix}$$

Step 3 (optional) : mean-center data set

- Form data matrix
  - Images (samples) as columns

$$\begin{bmatrix} \vdots & \vdots & \cdots & \vdots \\ I_1 & I_2 & \cdots & I_K \\ \vdots & \vdots & \cdots & \vdots \end{bmatrix}$$

  - Subtract mean image from all columns

Step 4: Covariance of a Data Set

$$\text{Cov} = XX^T$$

$$\begin{bmatrix} \omega_{1,1} & \cdots & \omega_{1,N} \\ \vdots & \vdots & \vdots \\ \omega_{N,1} & \cdots & \omega_{N,N} \end{bmatrix} = \begin{bmatrix} \vdots & \vdots & \cdots & \vdots \\ I_1 & I_2 & \cdots & I_K \\ \vdots & \vdots & \cdots & \vdots \end{bmatrix} \begin{bmatrix} \cdots & I_1 & \cdots \\ \cdots & I_2 & \cdots \\ \vdots & \vdots & \vdots \\ \cdots & I_K & \cdots \end{bmatrix}$$

$$\omega_{i,j} = \sum_{k}^{K} \left(x^k{}_i - \bar{x}^k \right) \left(x^k{}_j - \bar{x}^k \right)$$

Step 5: PCA

- Let $I_1, \ldots, I_N$ be normalized images

$$X \equiv \begin{bmatrix} \vdots & \cdots & \vdots \\ I_1 & \cdots & I_N \\ \vdots & \cdots & \vdots \end{bmatrix}$$

$$Cov(X) = XX^T$$

$$PCA(X) = SVD\left(XX^T\right) = R^T \Lambda R$$

PCA: where are we?

- Done
  - Mechanics & algorithms
  - Motivation as maximizing variance
- To do
  - Motivation as Gaussian Random Process
  - Image space interpretation

Multivariate Normal Random Variables

- The equation of a 1D Gaussian

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

  – μ is the mean and σ is the standard deviation
- Covariance generalizes variance to n-dimensions.
- The N-dimensional Gaussian is defined as

$$f(\vec{x}) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} e^{\frac{-1}{2}(\vec{x}-\mu)\Sigma^{-1}(\vec{x}-\mu)}$$

Multivariate Normal (II)

- Consider the case of a 2D Gaussian.

$$f(x,y) = \frac{1}{2\pi \left\| \begin{vmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{xy} & \sigma_{yy} \end{vmatrix} \right\|^{1/2}} e^{-\frac{1}{2} \begin{vmatrix} x-\mu_x \\ y-\mu_y \end{vmatrix}^T \begin{vmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{xy} & \sigma_{yy} \end{vmatrix}^{-1} \begin{vmatrix} x-\mu_x \\ y-\mu_y \end{vmatrix}}$$

Covariance Matrix

Special Case: Axis Aligned

$$\sigma_{xx} = \sigma_x^{\ 2} \quad \sigma_{yy} = \sigma_y^{\ 2} \quad \sigma_{xy} = 0$$

$$f(\vec{x}) = \frac{1}{2\pi\left(\sigma_x^{\ 2}\sigma_y^{\ 2}\right)^{1/2}} \exp\left[-\frac{1}{2}\begin{vmatrix} x-\mu_x \\ y-\mu_y \end{vmatrix}^T \begin{vmatrix} \frac{1}{\sigma_x^{\ 2}} & 0 \\ 0 & \frac{1}{\sigma_y^{\ 2}} \end{vmatrix} \begin{vmatrix} x-\mu_x \\ y-\mu_y \end{vmatrix}\right]$$

$$= \frac{1}{2\pi\left(\sigma_x\sigma_y\right)} \exp\left[-\frac{1}{2}\left(\frac{\left(x-\mu_x\right)^2}{\sigma_x^{\ 2}} + \frac{\left(y-\mu_y\right)^2}{\sigma_y^{\ 2}}\right)\right]$$

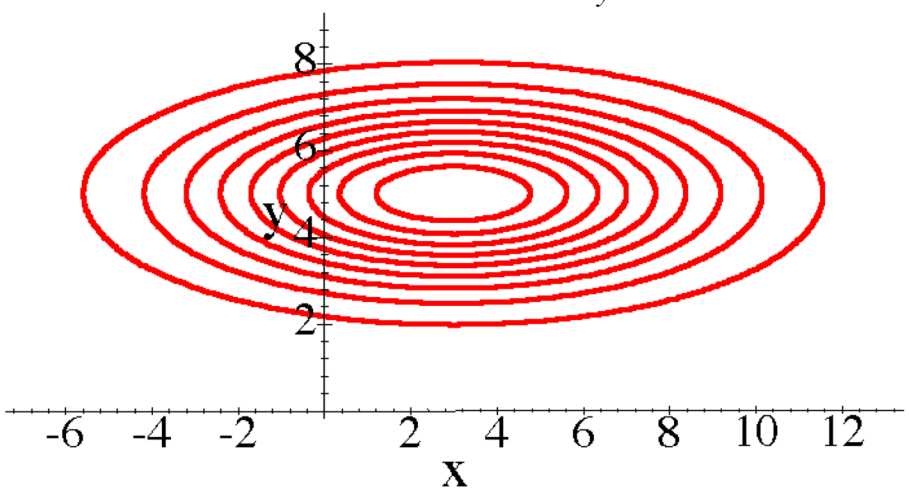
$$= \left(\frac{1}{\sqrt{2\pi}\sigma_x} \exp\left[-\frac{1}{2}\frac{\left(x-\mu_x\right)^2}{\sigma_x^{\ 2}}\right]\right)\left(\frac{1}{\sqrt{2\pi}\sigma_y} \exp\left[-\frac{1}{2}\frac{\left(y-\mu_y\right)^2}{\sigma_y^{\ 2}}\right]\right)$$

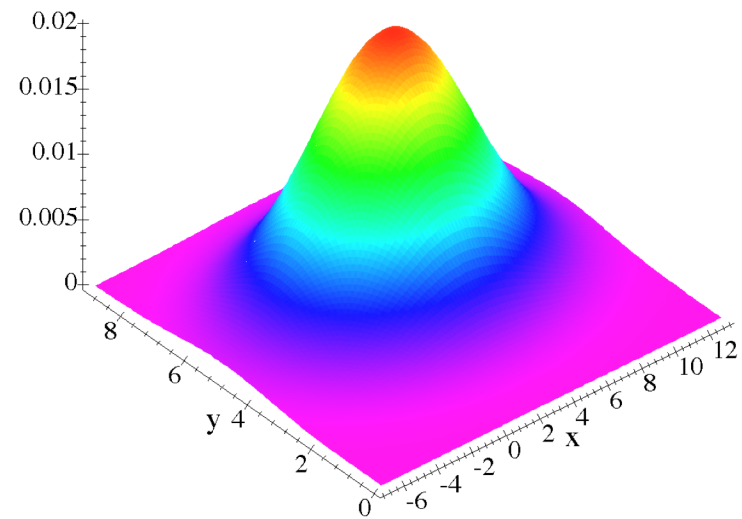
Probability Level Curves

- Consider the following axis-aligned Gaussian:

$$f(x,y) = \frac{1}{2\pi(\sigma_x \sigma_y)} \exp\left[-\frac{1}{2}\left(\frac{(x-\mu_x)^2}{\sigma_x^{\,2}} + \frac{(y-\mu_y)^2}{\sigma_y^{\,2}}\right)\right]$$

$$\sigma_x = 4, \quad \sigma_y = 2, \quad \mu_x = 3, \quad \mu_y = 5$$





Quadratic Forms

- Look at the exponent of the centered (μ=0) 2D Gaussian, it has the form:

$$f(x,y) = V^T M V = \begin{vmatrix} x & y \end{vmatrix} \begin{vmatrix} a & b \\ b & c \end{vmatrix} \begin{vmatrix} x \\ y \end{vmatrix}$$
$$= ax^2 + 2bxy + cy^2$$

- Singular value decomposition tells us that:

$$M = R \Delta R^{-1}$$
$$= \begin{vmatrix} r_{11} & r_{12} \\ r_{21} & r_{22} \end{vmatrix} \begin{vmatrix} \lambda_1 & 0 \\ 0 & \lambda_1 \end{vmatrix} \begin{vmatrix} r_{11} & r_{21} \\ r_{12} & r_{22} \end{vmatrix}$$

- R rotates coordinates so M is diagonal.

Quadratic Forms Rotated

We may specify any quadratic form as being rotated from an axis aligned equivalent.

$$f(u,v) = V^T D V \qquad f(u,v) = [u \quad v]\begin{bmatrix} 8 & 0 \\ 0 & 2 \end{bmatrix}\begin{bmatrix} u \\ v \end{bmatrix}$$

$$V = R X \qquad \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix}$$

$$V^T = (R X)^T \qquad [u \quad v] = [x \quad y]\begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix}$$

$$f(x,y) = X^T R^T D R X = X^T M X$$

Rotated Example

$$R\left(\frac{1}{6}\pi\right) = \begin{bmatrix} .865 & -.500 \\ .500 & .865 \end{bmatrix}$$

$$f_1(u, v) = 8\,x^2 + 2\,y^2 \qquad f_2(x, y) = 6.49\,x^2 - 5.20\,x\,y + 3.50\,y^2$$