Principal Component Analysis

Applications of PCA

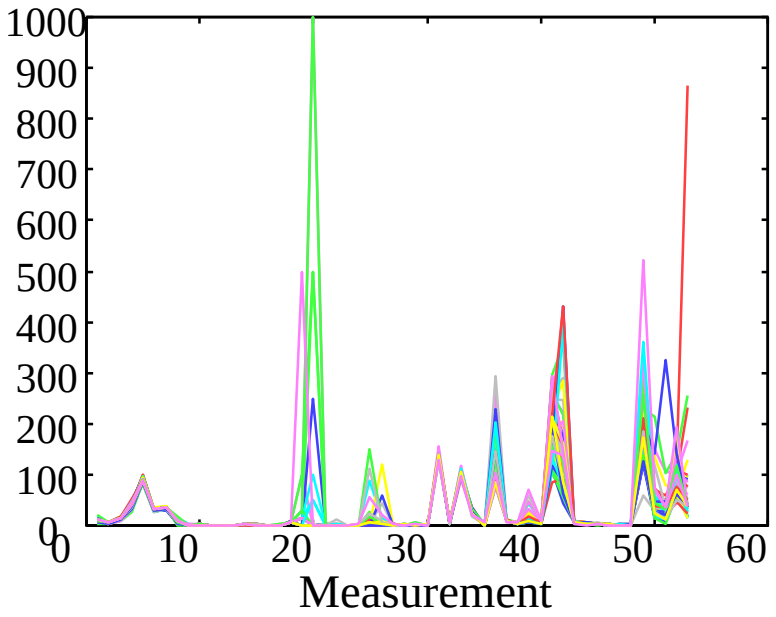
- Data Visualization/Presentation
- Data Compression
- Noise Reduction
- Data Classification
- Trend Analysis
- Factor Analysis

Data Presentation

- Example: 53 Blood and urine measurements (wet chemistry) from 65 people (33 alcoholics, 32 non-alcoholics).
- Matrix Format

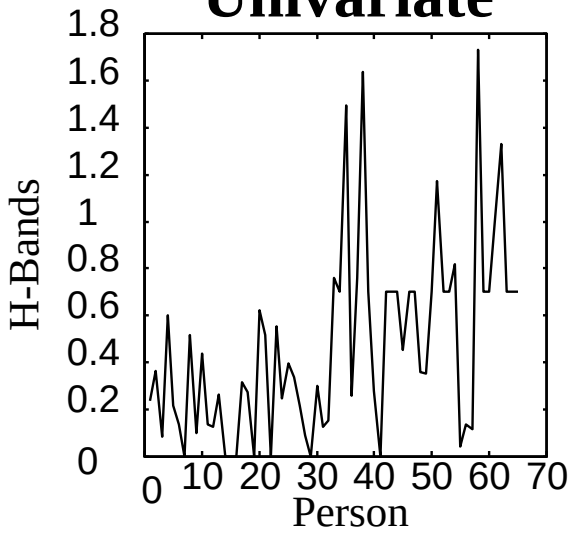
	H-WBC	H-RBC	H-Hgb	H-Hct	H-MCV	H-MCH	H-MCHC
A1	8.0000	4.8200	14.1000	41.0000	85.0000	29.0000	34.0000
A2	7.3000	5.0200	14.7000	43.0000	86.0000	29.0000	34.0000
A3	4.3000	4.4800	14.1000	41.0000	91.0000	32.0000	35.0000
A4	7.5000	4.4700	14.9000	45.0000	101.0000	33.0000	33.0000
A5	7.3000	5.5200	15.4000	46.0000	84.0000	28.0000	33.0000
A6	6.9000	4.8600	16.0000	47.0000	97.0000	33.0000	34.0000
A7	7.8000	4.6800	14.7000	43.0000	92.0000	31.0000	34.0000
A8	8.6000	4.8200	15.8000	42.0000	88.0000	33.0000	37.0000
A9	5.1000	4.7100	14.0000	43.0000	92.0000	30.0000	32.0000

- Spectral Format

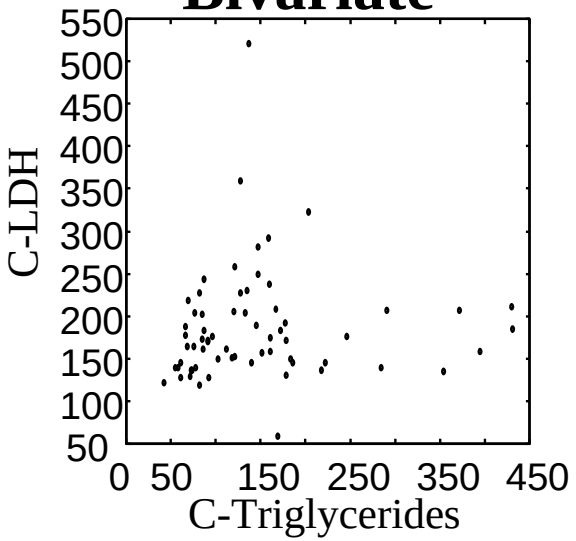


Data Presentation

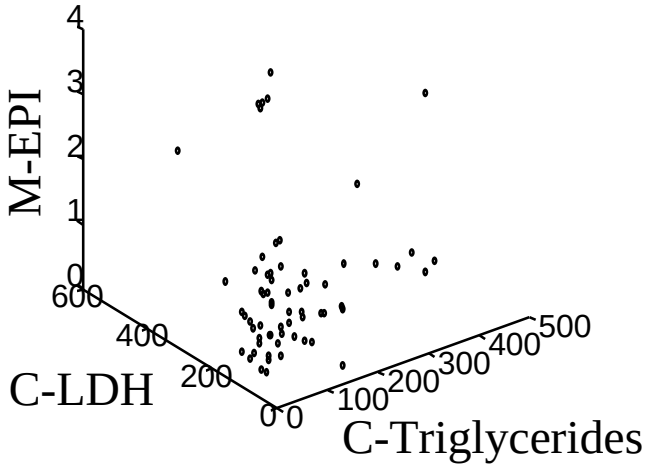
Univariate



Bivariate



Trivariate

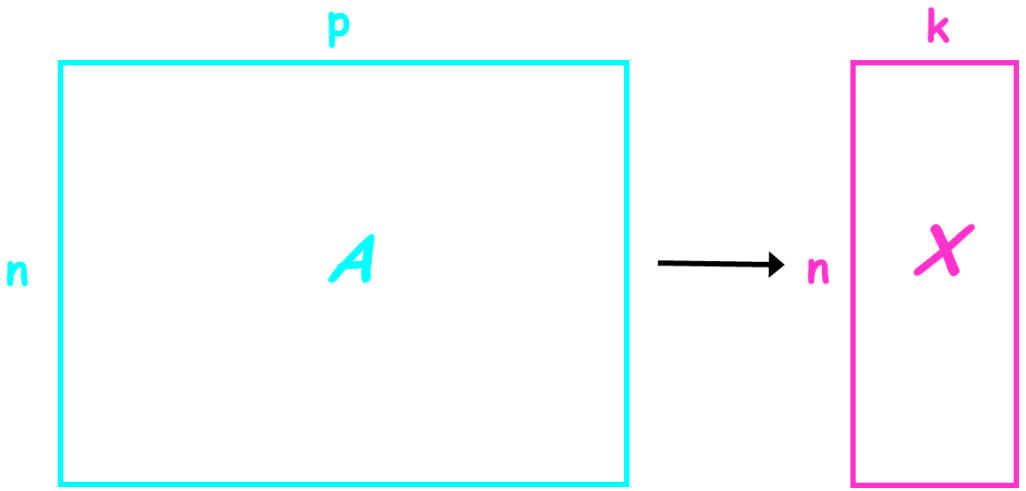


Data Presentation

- Better presentation than ordinate axes?
- Do we need a 53 dimension space to view data?
- How to find the ‘best’ low dimension space that conveys maximum useful information?
- One answer: Find “Principal Components”

Principal Component Analysis (PCA)

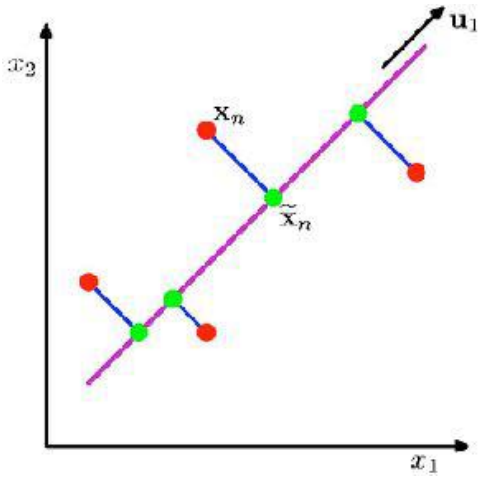
- PCA converts a set of observations of possibly correlated variables into a set of values of linearly uncorrelated variables called **principal components**
- Takes a n X p data matrix of possibly correlated axes and summarizes it by uncorrelated axes.
- The first k components display as much as possible of the variation among objects.



Geometric Rationale of PCA

- objective of PCA is to rigidly rotate the axes of this *p*-dimensional space to new positions (principal axes) that have the following properties:
  - ordered such that principal axis 1 has the highest variance, axis 2 has the next highest variance, ... , and axis *p* has the lowest variance
  - covariance among each pair of the principal axes is zero (the principal axes are uncorrelated).

PCA



- Orthogonal projection of data onto lower-dimension linear space that...
  - maximizes variance of projected data (purple line)
  - minimizes mean squared distance between data point and projections (sum of blue lines)

PCA

Idea:

- Given data points in a d-dimensional space,
- project into lower dimensional space while preserving as much information as possible
  - Eg, find best planar approximation to 3D data
  - Eg, find best 12-D approximation to 104-D data
- In particular, choose projection that minimizes squared error in reconstructing original data

PCA: Algorithm

PCA algorithm($\mathbf{X}$, k): top k eigenvalues/eigenvectors

% $\underline{\mathbf{X}}$ = m × N data matrix,

% … each data point $\mathbf{x}_i$ = row vector, i=1..m

- $\underline{\mathbf{x}} = \frac{1}{m}\sum_{i=1}^{m}\mathbf{x}_i$
- $\mathbf{X}$ ←subtract mean $\underline{\mathbf{x}}$ from each row vector $\mathbf{x}_i$ in $\underline{\mathbf{X}}$
- $\Sigma \leftarrow \mathbf{X}^T\mathbf{X}$ … covariance matrix of $\mathbf{X}$
- $\{\lambda_i, \mathbf{u}_i\}_{i=1..N}$ = eigenvectors/eigenvalues of Σ
  … $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_N$
- Return $\{\lambda_i, \mathbf{u}_i\}_{i=1..k}$
  % top k principle components

PCA Example –STEP 1

- Subtract the mean

  from each of the data dimensions. All the x values have x subtracted and y values have y subtracted from them. This produces a data set whose mean is zero.

  Subtracting the mean makes variance and covariance calculation easier by simplifying their equations. The variance and co-variance values are not affected by the mean value.

PCA Example –STEP 1

http://kybele.psych.cornell.edu/~edelman/Psych-465-Spring-2003/PCA-tutorial.pdf

DATA:

x	y
2.5	2.4
0.5	0.7
2.2	2.9
1.9	2.2
3.1	3.0
2.3	2.7
2	1.6
1	1.1
1.5	1.6
1.1	0.9

ZERO MEAN DATA:

x	y
.69	.49
-1.31	-1.21
.39	.99
.09	.29
1.29	1.09
.49	.79
.19	-.31
-.81	-.81
-.31	-.31
-.71	-1.01

PCA Example –STEP 1

http://kybele.psych.cornell.edu/~edelman/Psych-465-Spring-2003/PCA-tutorial.pdf

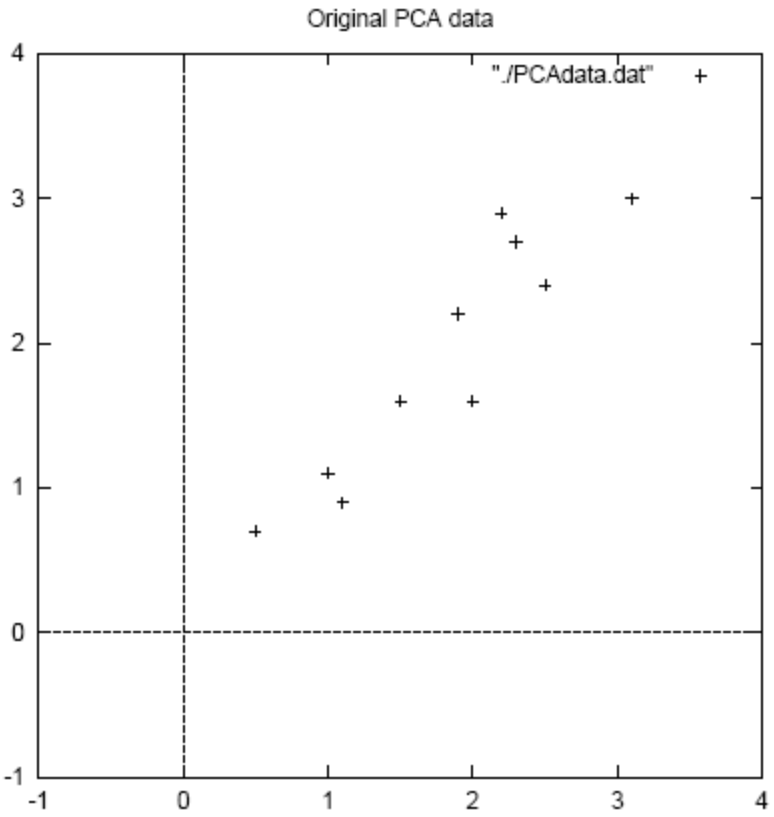


Figure 3.1: PCA example data, original data on the left, data with the means subtracted on the right, and a plot of the data

PCA Example –STEP 2

- Calculate the covariance matrix

$$cov = \begin{pmatrix} .616555556 & .615444444 \\ .615444444 & .716555556 \end{pmatrix}$$

- Since the non-diagonal elements in this covariance matrix are positive, we should expect that both the x and y variable increase together.

PCA Example –STEP 3

- Calculate the eigenvectors and eigenvalues of the covariance matrix

$$\text{eigenvalues} = \begin{pmatrix} .0490833989 \\ 1.28402771 \end{pmatrix}$$

$$\text{eigenvectors} = \begin{pmatrix} -.735178656 & -.677873399 \\ .677873399 & -.735178656 \end{pmatrix}$$

PCA Example –STEP 3

http://kybele.psych.cornell.edu/~edelman/Psych-465-Spring-2003/PCA-tutorial.pdf

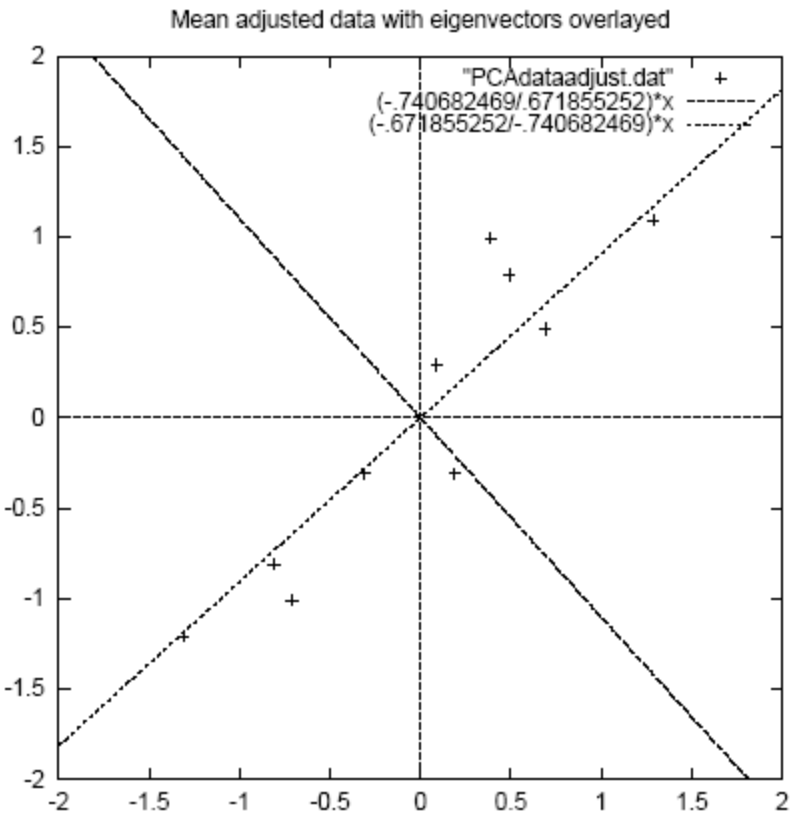


Figure 3.2: A plot of the normalised data (mean subtracted) with the eigenvectors of the covariance matrix overlayed on top.

- eigenvectors are plotted as diagonal dotted lines on the plot.
- Note they are perpendicular to each other.
- Note one of the eigenvectors goes through the middle of the points, like drawing a line of best fit.
- The second eigenvector gives us the other, less important, pattern in the data, that all the points follow the main line, but are off to the side of the main line by some amount.

PCA Example –STEP 4

- Reduce dimensionality and form *feature vector*

  the eigenvector with the *highest* eigenvalue is the *principle component* of the data set.

  In our example, the eigenvector with the larges eigenvalue was the one that pointed down the middle of the data.

  Once eigenvectors are found from the covariance matrix, the next step is to order them by eigenvalue, highest to lowest. This gives you the components in order of significance.

PCA Example –STEP 4

Now, if you like, you can decide to *ignore* the components of lesser significance.

You do lose some information, but if the eigenvalues are small, you don't lose much

- p dimensions in your data
- calculate p eigenvectors and eigenvalues
- choose only the first k eigenvectors
- final data set has only k dimensions.

PCA Example –STEP 4

- Feature Vector

  $$\text{FeatureVector} = (\text{eig}_1\ \text{eig}_2\ \text{eig}_3\ \ldots\ \text{eig}_n)$$

  We can either form a feature vector with both of the eigenvectors:

  $$\begin{pmatrix} -.677873399 & -.735178656 \\ -.735178656 & .677873399 \end{pmatrix}$$

  or, we can choose to leave out the smaller, less significant component and only have a single column:

  $$\begin{pmatrix} -.677873399 \\ -.735178656 \end{pmatrix}$$

PCA Example –STEP 5

- Deriving the new data

  FinalData = RowFeatureVector x RowZeroMeanData

  RowFeatureVector is the matrix with the eigenvectors in the columns *transposed* so that the eigenvectors are now in the rows, with the most significant eigenvector at the top

  RowZeroMeanData is the mean-adjusted data *transposed*, ie. the data items are in each column, with each row holding a separate dimension.

PCA Example –STEP 5

FinalData transpose: dimensions along columns

x	y
-.827970186	-.175115307
1.77758033	.142857227
-.992197494	.384374989
-.274210416	.130417207
-1.67580142	-.209498461
-.912949103	.175282444
.0991094375	-.349824698
1.14457216	.0464172582
.438046137	.0177646297
1.22382056	-.162675287

PCA Example –STEP 5

http://kybele.psych.cornell.edu/~edelman/Psych-465-Spring-2003/PCA-tutorial.pdf

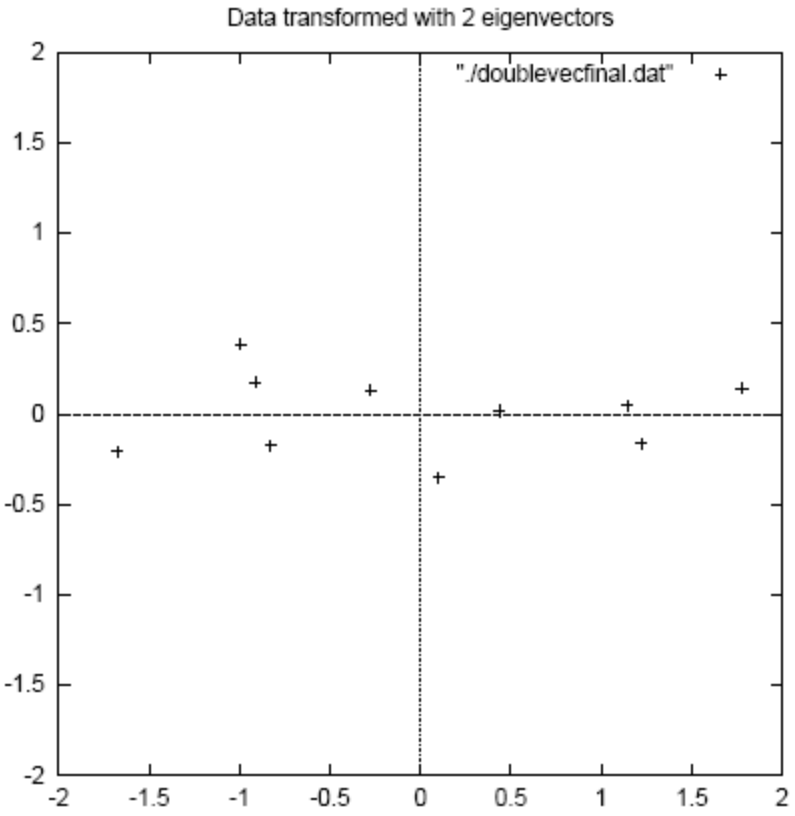


Figure 3.3: The table of data by applying the PCA analysis using both eigenvectors, and a plot of the new data points.

Reconstruction of original Data

- If we reduced the dimensionality, obviously, when reconstructing the data we would lose those dimensions we chose to discard. In our example let us assume that we considered only the x dimension…

Reconstruction of original Data

http://kybele.psych.cornell.edu/~edelman/Psych-465-Spring-2003/PCA-tutorial.pdf

x
-.827970186
1.77758033
-.992197494
-.274210416
-1.67580142
-.912949103
.0991094375
1.14457216
.438046137
1.22382056

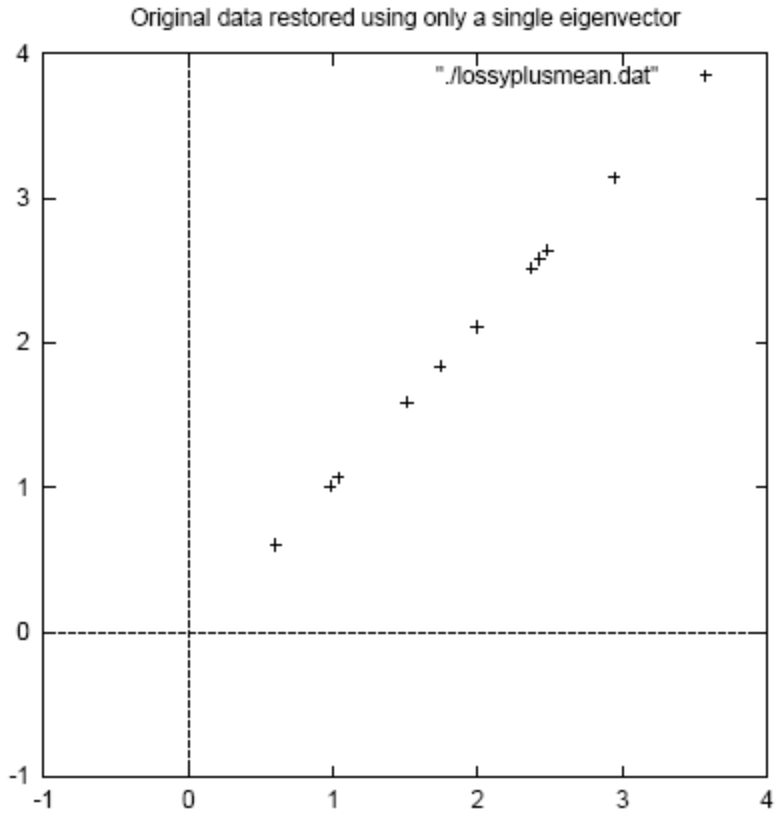


Figure 3.5: The reconstruction from the data that was derived using only a single eigenvector

References and useful links

- http://www.iro.umontreal.ca/~pift6080/H09/documents/papers/pca_tutorial.pdf
- https://www.cs.cmu.edu/~elaw/papers/pca.pdf
- https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues