PCA

PCA is "an orthogonal linear transformation that transfers the data to a new coordinate system such that the greatest variance by any projection of the data comes to lie on the first coordinate (*first principal component*), the second greatest variance lies on the second coordinate (*second principal component*), and so on."

Background for PCA

- Suppose attributes are A_1 and A_2, and we have n training examples. x's denote values of A_1 and y's denote values of A_2 over the training examples.

- Variance of an attribute:

$$\mathrm{var}(A_1) = \frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{(n-1)}$$

- Covariance of two attributes:

$$\operatorname{cov}(A_1, A_2) = \frac{\sum_{i=1}^{n} (x_i - \overline{x})(y_i - \overline{y})}{(n-1)}$$

- If covariance is positive, both dimensions increase together. If negative, as one increases, the other decreases. Zero: independent of each other.

- Covariance matrix
  - Suppose we have n attributes, A_1, ..., A_n.
  - Covariance matrix:

$$C^{n\times n} = (c_{i,j}), \text{ where } c_{i,j} = \operatorname{cov}(A_i, A_j)$$

	Hours(H)	*Mark(M)*
Data	9	39
	15	56
	25	93
	14	61
	10	50
	18	75
	0	32
	16	85
	5	42
	19	70
	16	66
	20	80
Totals	167	749
Averages	13.92	62.42

Covariance:

H	M	$(H_i - H)$	$(M_i - M)$	$(H_i - H)(M_i - M)$
9	39	-4.92	-23.42	115.23
15	56	1.08	-6.42	-6.93
25	93	11.08	30.58	338.83
14	61	0.08	-1.42	-0.11
10	50	-3.92	-12.42	48.69
18	75	4.08	12.58	51.33
0	32	-13.92	-30.42	423.45
16	85	2.08	22.58	46.97
5	42	-8.92	-20.42	182.15
19	70	5.08	7.58	38.51
16	66	2.08	3.58	7.45
20	80	6.08	17.58	106.89
Total				1149.89
Average				104.54

Table 2.2: 2-dimensional data set and covariance calculation

$$\begin{pmatrix} \operatorname{cov}(H,H) & \operatorname{cov}(H,M) \\ \operatorname{cov}(M,H) & \operatorname{cov}(M,M) \end{pmatrix}$$

$$= \begin{pmatrix} \operatorname{var}(H) & 104.5 \\ 104.5 & \operatorname{var}(M) \end{pmatrix}$$

$$= \begin{pmatrix} 47.7 & 104.5 \\ 104.5 & 370 \end{pmatrix}$$

Covariance matrix

- Eigenvectors:
  - Let **M be** an $n \times n$ matrix.
    - **v** is an *eigenvector* of M if M × **v** = λ**v**
    - λ is called the *eigenvalue* associated with **v**
  - For any eigenvector **v** of **M** and scalar *a*,
  - Thus you can always choose eigenvectors of length 1:

$$\mathbf{M} \times a\mathbf{v} = \lambda a\mathbf{v}$$

  - If **M** has any eigenvectors, it has *n* of them, and they are orthogonal to one another.

$$\sqrt{v_1^{\;2} + \ldots + v_n^{\;2}} = 1$$

  - Thus eigenvectors can be used as a new basis for a n-dimensional vector space.

PCA

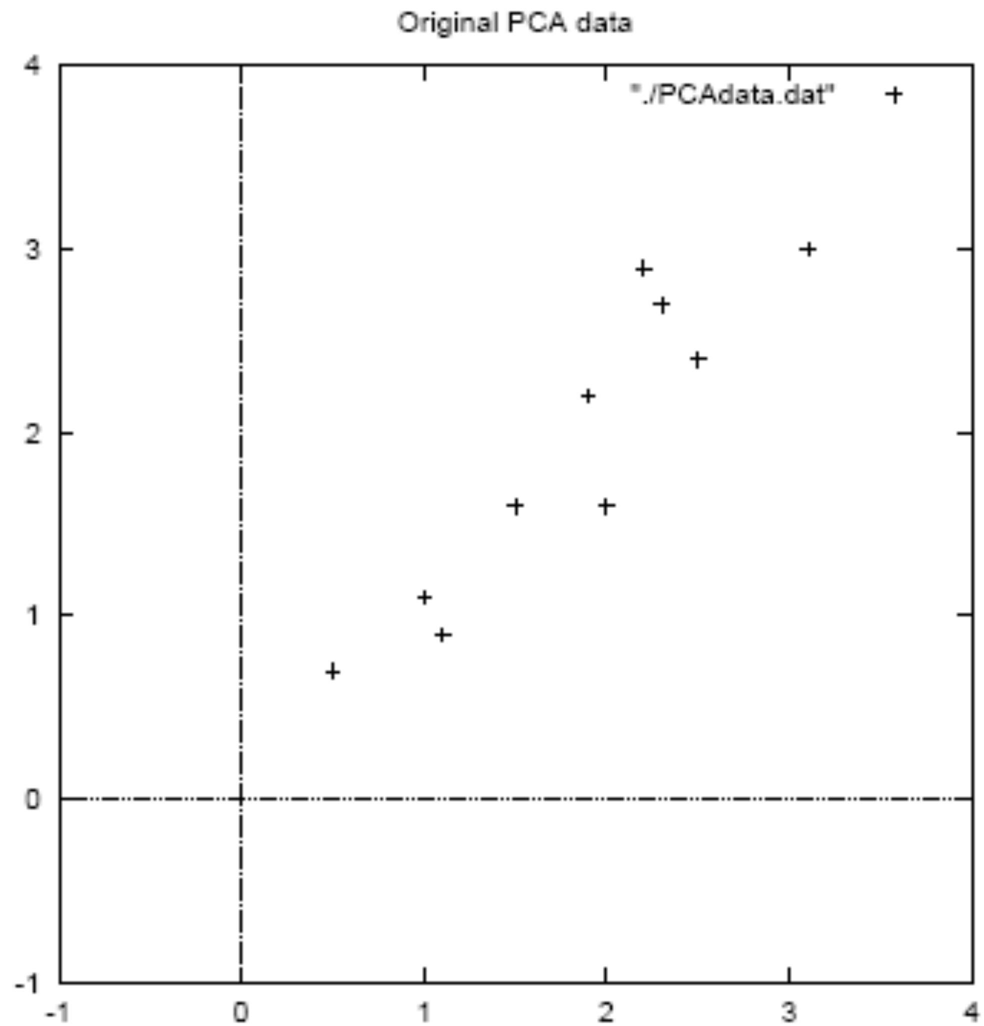
1. Given original data set S = {$\mathbf{x}^1, ..., \mathbf{x}^k$}, produce new set by subtracting the mean of attribute A_i from each x_i.

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
Mean:	1.81	1.91

DataAdjust

	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
Mean:	0	0


Original PCA data
"./PCAdata.dat"
4
3
2
1
0
-1
-1
0
1
2
3
4

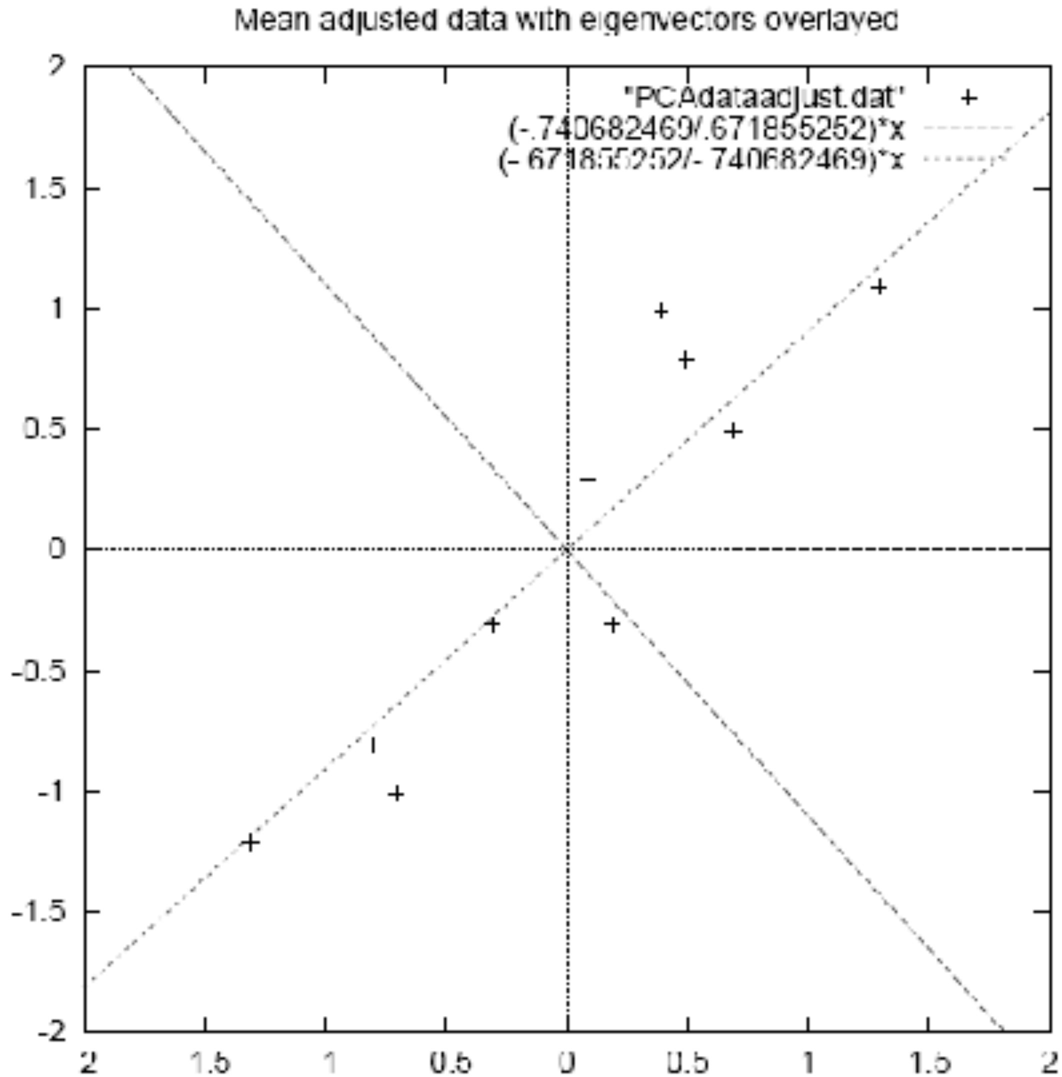
2. Calculate the covariance matrix:

$$cov = \begin{array}{c|c} & \begin{array}{cc} x & y \end{array} \\ \begin{array}{c} x \\ y \end{array} & \begin{pmatrix} .616555556 & .615444444 \\ .615444444 & .716555556 \end{pmatrix} \end{array}$$

3. Calculate the (unit) eigenvectors and eigenvalues of the covariance matrix:

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

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



Eigenvector with largest eigenvalue traces linear pattern in data

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

4. Order eigenvectors by eigenvalue, highest to lowest.

$$\mathbf{v}_1 = \begin{pmatrix} -.677873399 \\ -.735178956 \end{pmatrix} \quad \lambda = 1.28402771$$

$$\mathbf{v}_2 = \begin{pmatrix} -.735178956 \\ .677873399 \end{pmatrix} \quad \lambda = .0490833989$$

In general, you get n components. To reduce dimensionality to p, ignore $n-p$ components at the bottom of the list.

Construct new feature vector.

Feature vector = $(\mathbf{v}_1, \mathbf{v}_2, \ldots \mathbf{v}_p)$

$$FeatureVector1 = \begin{pmatrix} -.677873399 & -.735178956 \\ -.735178956 & .677873399 \end{pmatrix}$$

or reduced dimension feature vector :

$$FeatureVector2 = \begin{pmatrix} -.677873399 \\ -.735178956 \end{pmatrix}$$

5. Derive the new data set.

$$TransformedData = RowFeatureVector \times RowDataAdjust$$

$$RowFeatureVector1 = \begin{pmatrix} -.677873399 & -.735178956 \\ -.735178956 & .677873399 \end{pmatrix}$$

$$RowFeatureVector2 = \begin{pmatrix} -.677873399 & -.735178956 \end{pmatrix}$$

This gives original data in terms of chosen components (eigenvectors)—that is, along these axes.

$$RowDataAdjust = \begin{pmatrix} .69 & -1.31 & .39 & .09 & 1.29 & .49 & .19 & -.81 & -.31 & -.71 \\ .49 & -1.21 & .99 & .29 & 1.09 & .79 & -.31 & -.81 & -.31 & -1.01 \end{pmatrix}$$

Transformed Data=

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

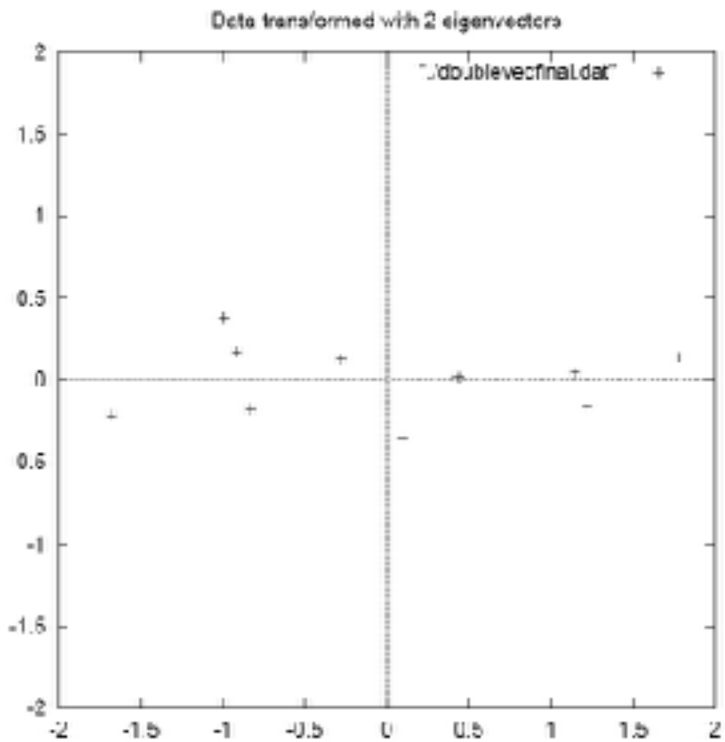
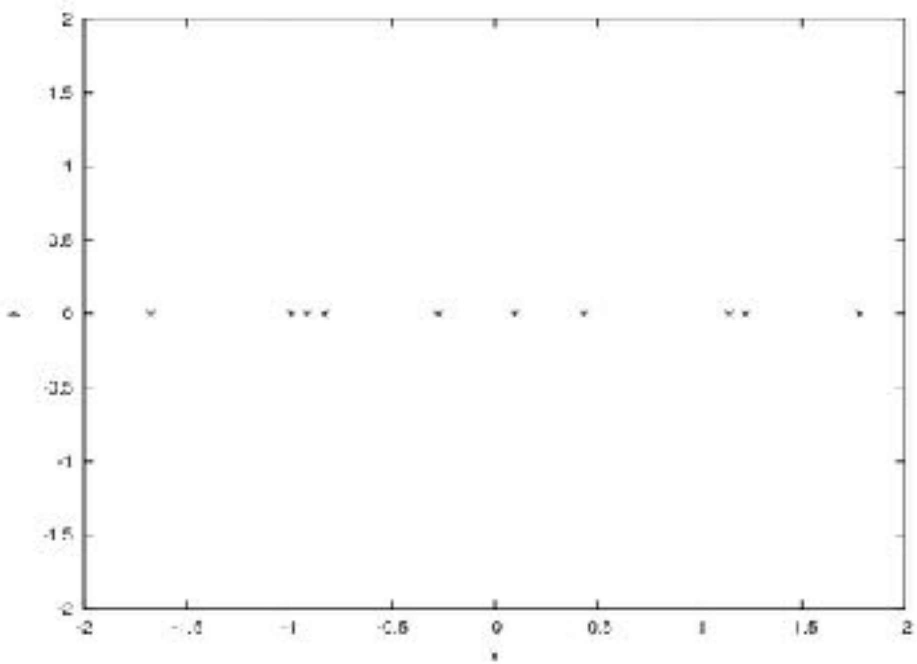


Figure 3.3: The table of data by applying the PCA analysis using both eigenvectors, and a plot of the new data points.

Transformed Data (Single eigenvector)

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



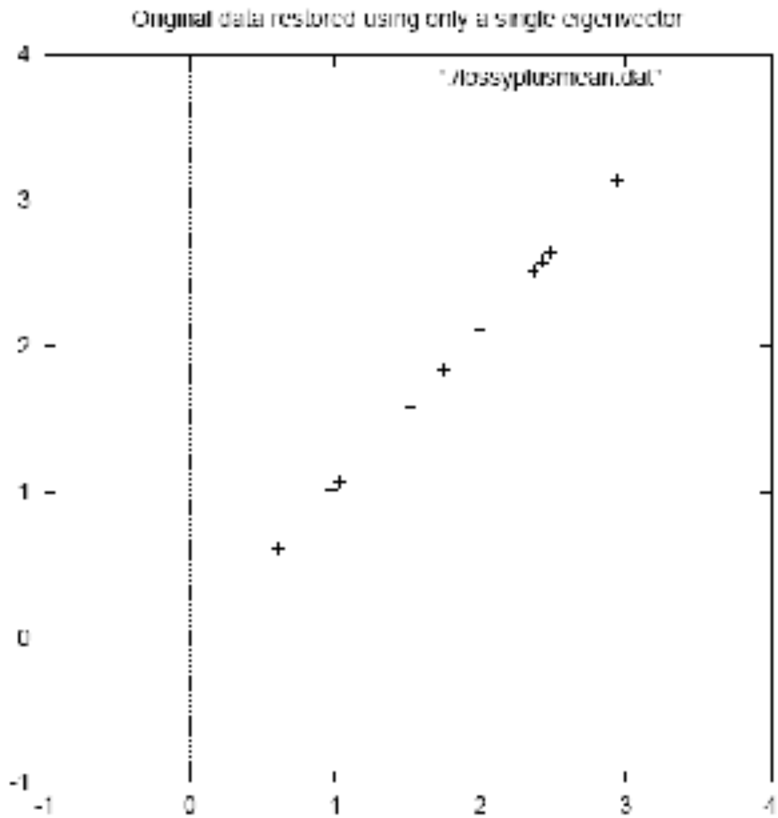
Reconstructing the original data

We did:
$$TransformedData = RowFeatureVector \times RowDataAdjust$$

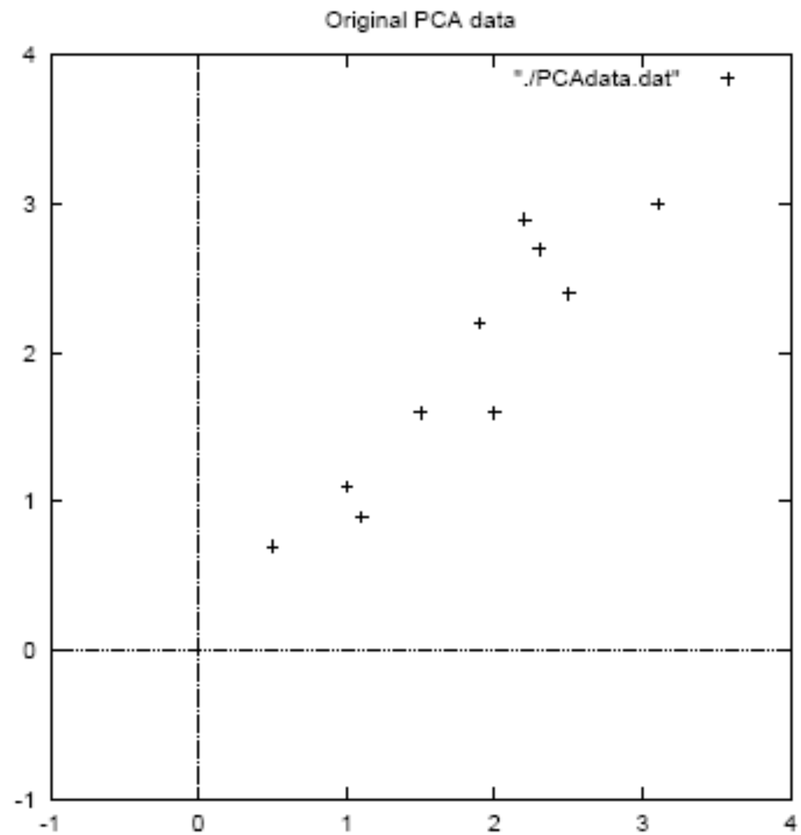
so we can do
$$RowDataAdjust = RowFeatureVector^{-1} \times TransformedData$$

$$= RowFeatureVector^{T} \times TransformedData$$

and
$$RowDataOriginal = RowDataAdjust + OriginalMean$$



Original data restored using only a single eigenvector
"./lossyplusmean.dat"



Original PCA data
"./PCAdata.dat"