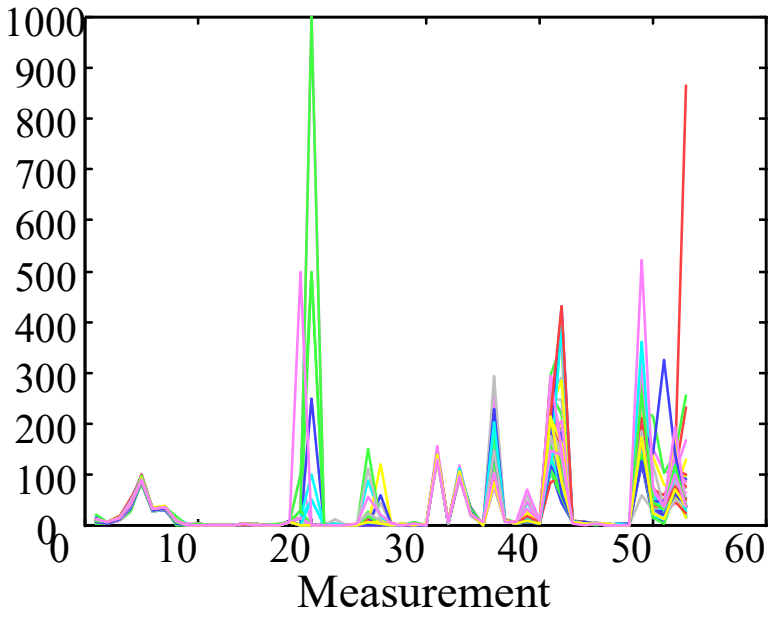
Introduction to Principal Component Analysis/ Dimension Reduction

Data Presentation

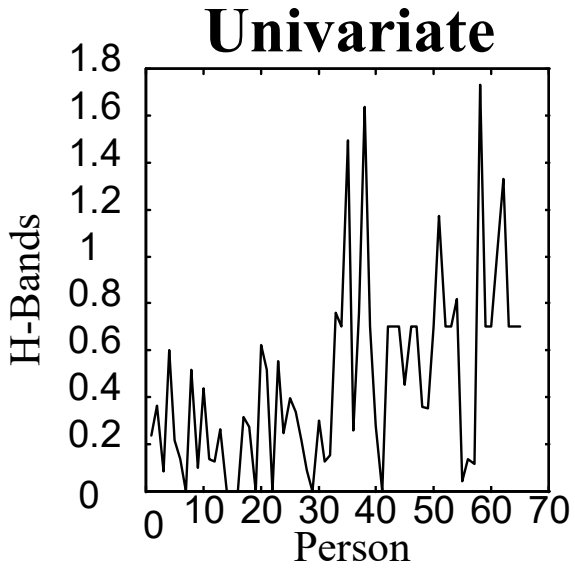
- Example: 53 Blood and urine measurements (wet chemistry) from 65 people (33 alcoholics, 32 non-alcoholics).
- Matrix Format

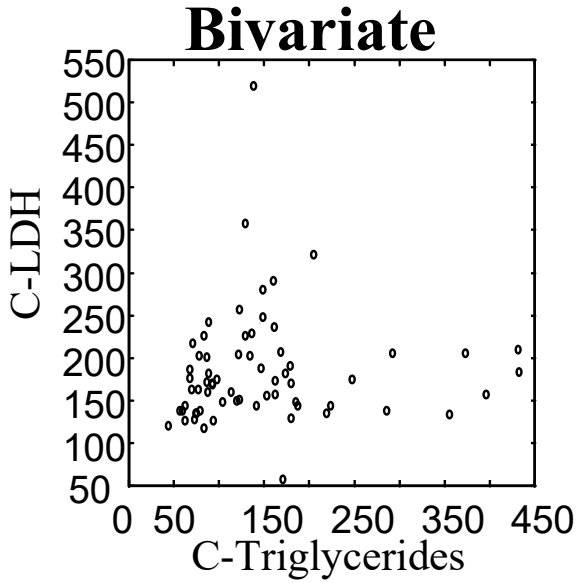
	H-WBC	H-RBC	H-Hgb	H-Hct	H-MCV	H-MCH	H-MCHC
A1	8.0000	4.8200	14.1000	41.0000	85.0000	29.0000	34.0000
A2	7.3000	5.0200	14.7000	43.0000	86.0000	29.0000	34.0000
A3	4.3000	4.4800	14.1000	41.0000	91.0000	32.0000	35.0000
A4	7.5000	4.4700	14.9000	45.0000	101.0000	33.0000	33.0000
A5	7.3000	5.5200	15.4000	46.0000	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

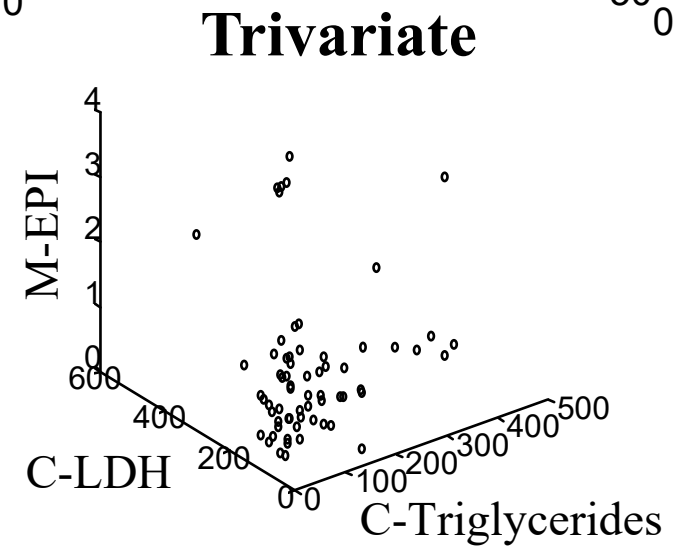
- Spectral Format



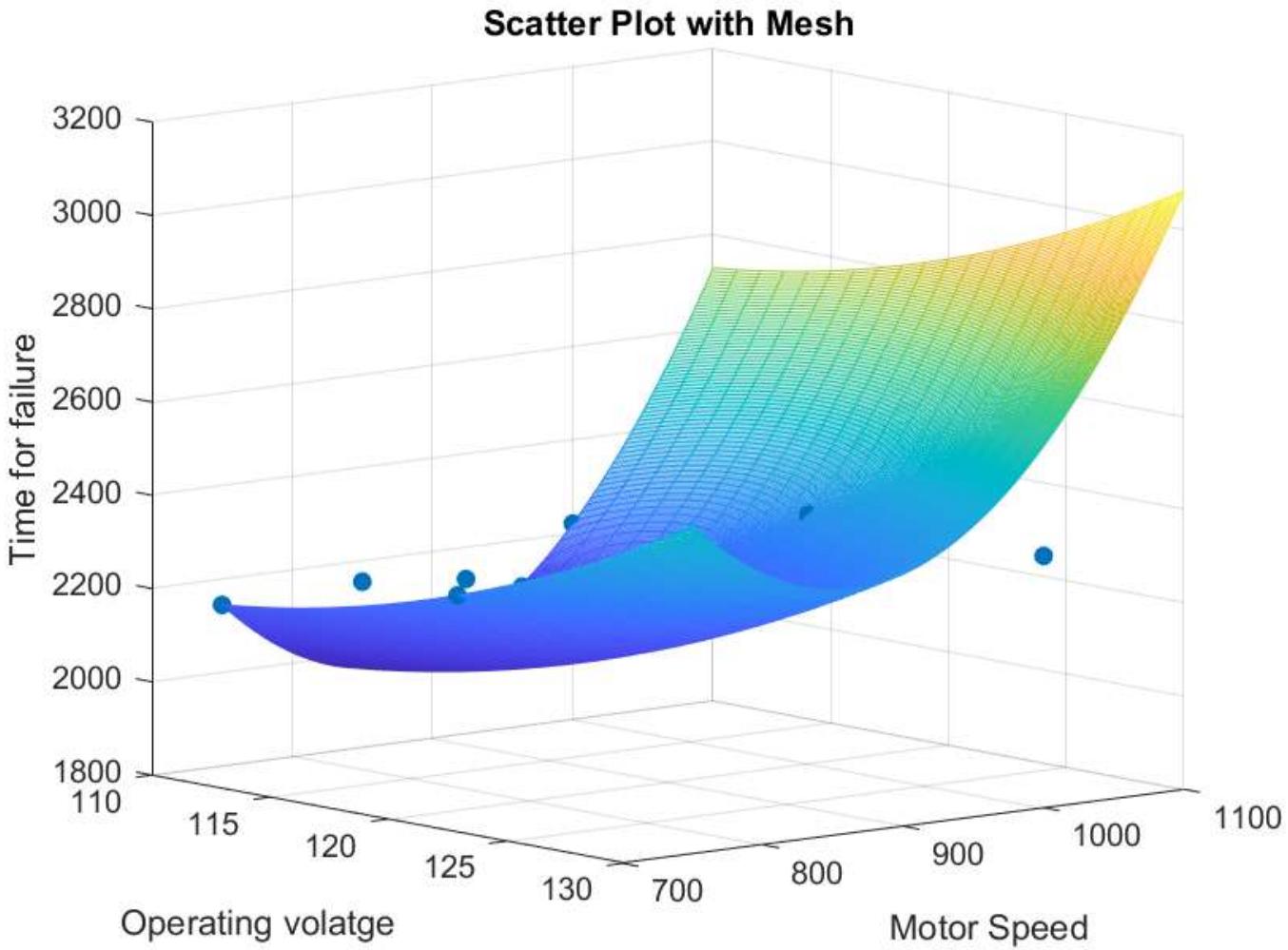
Data Presentation







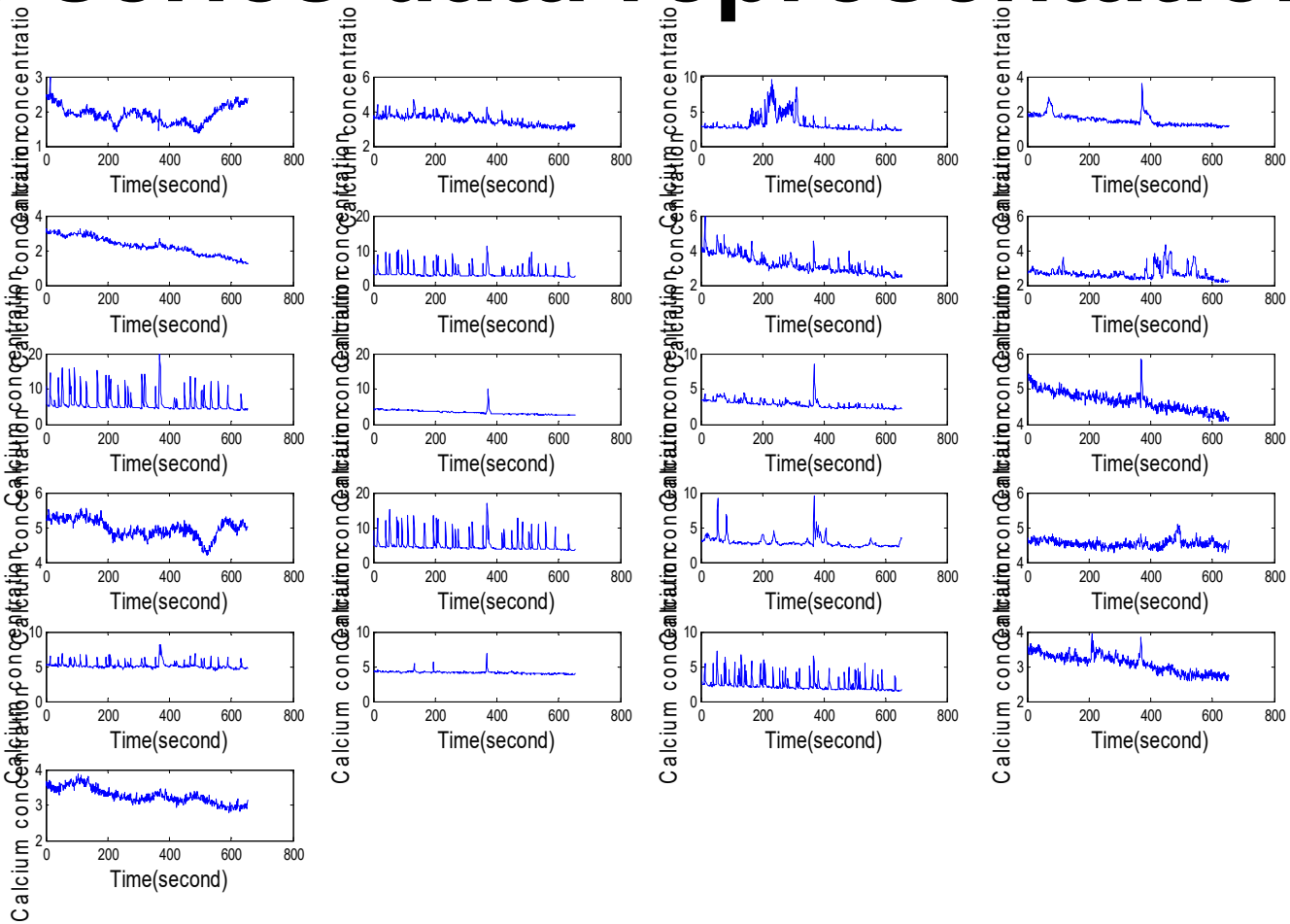
Data presentation- 3D



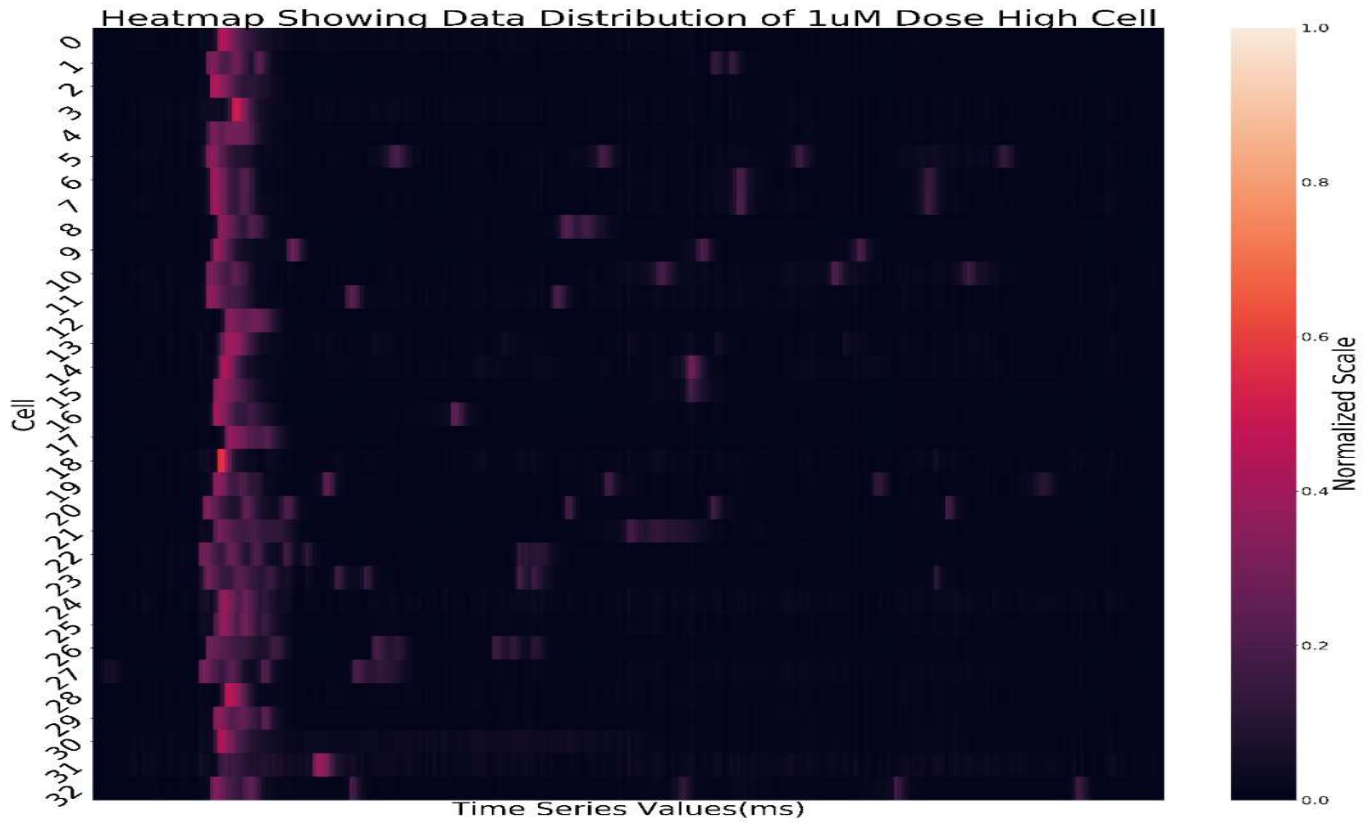
Data Presentation

- 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”

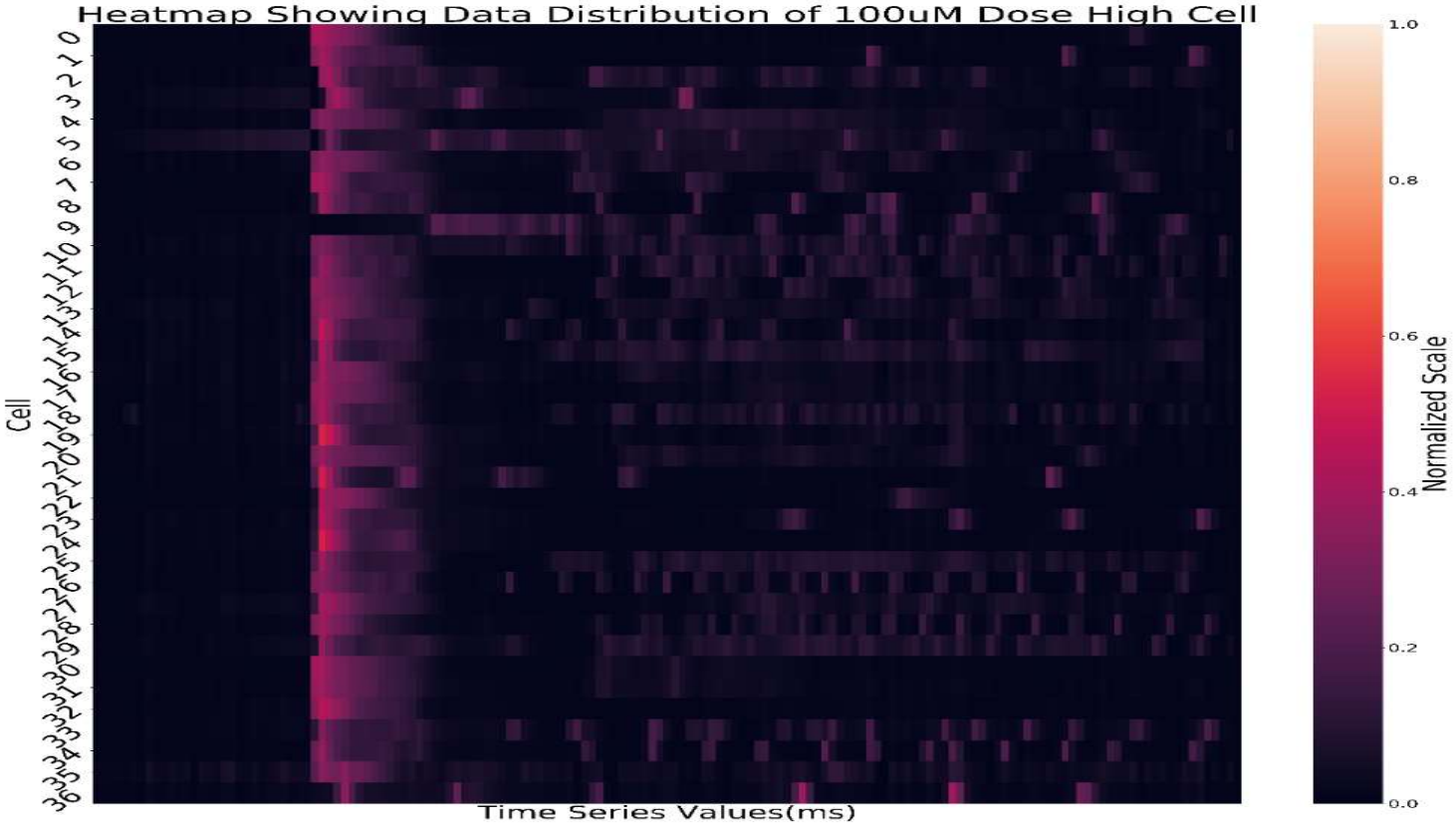
Time series data representation



Time series data representation

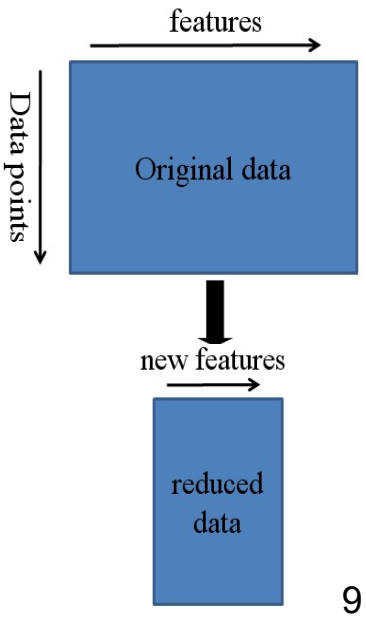


Time series data representation



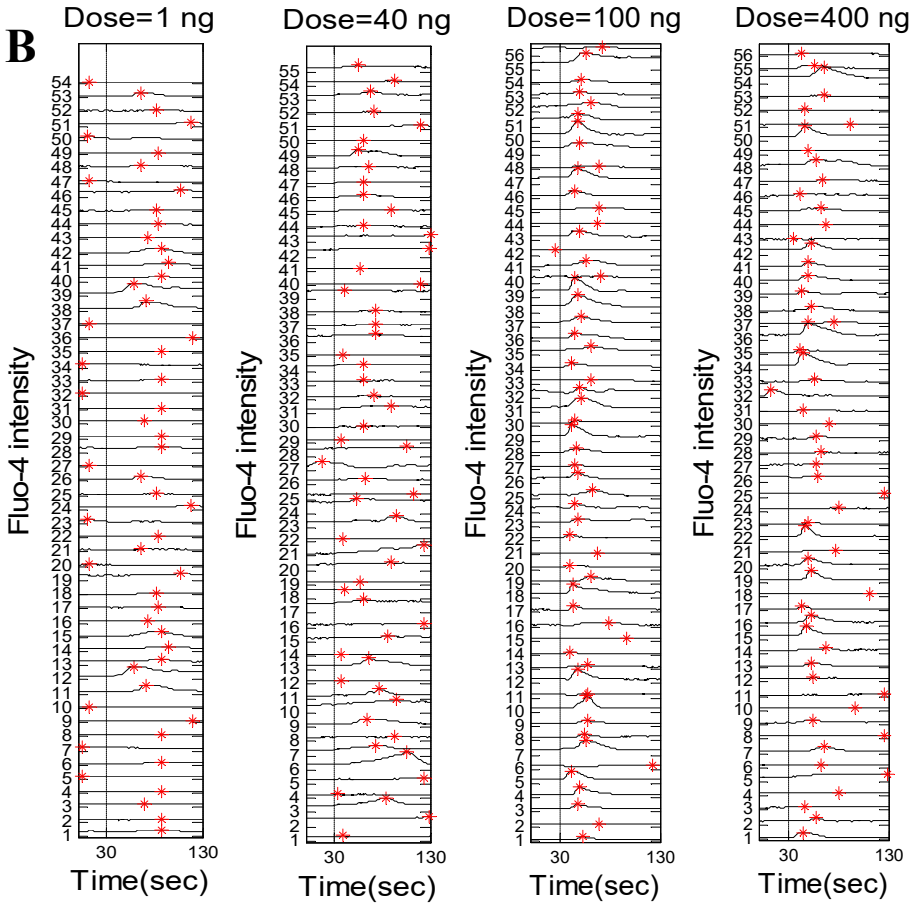
Feature extraction from data

- A group of methods that create new features (predictor variables).



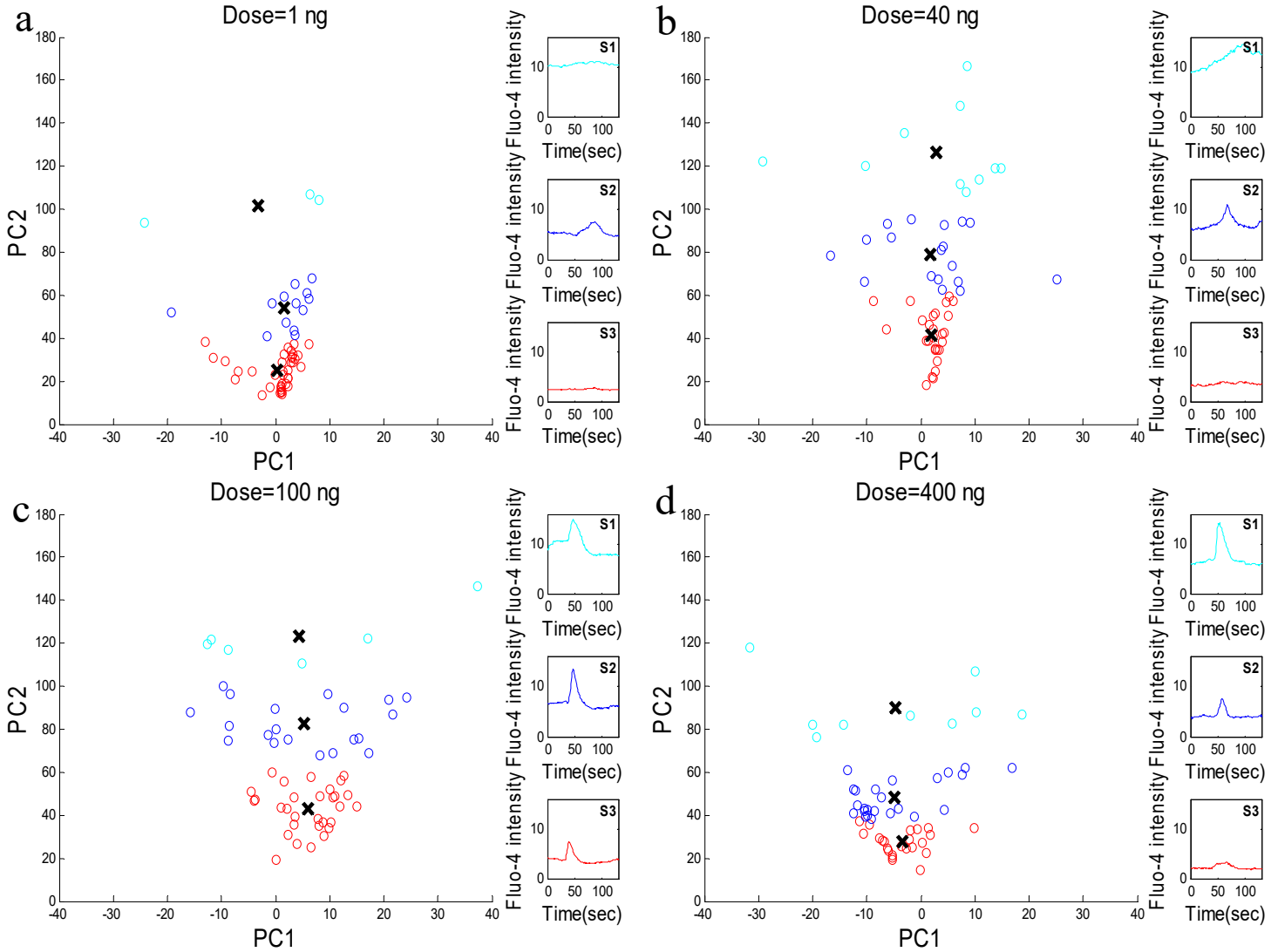
  - **Principal component analysis(PCA)**

Time series data



- At lower drug dose, cells are not responding appropriate (up 40 ng).
- At increased dose (100 and 400 ng) cells are responding

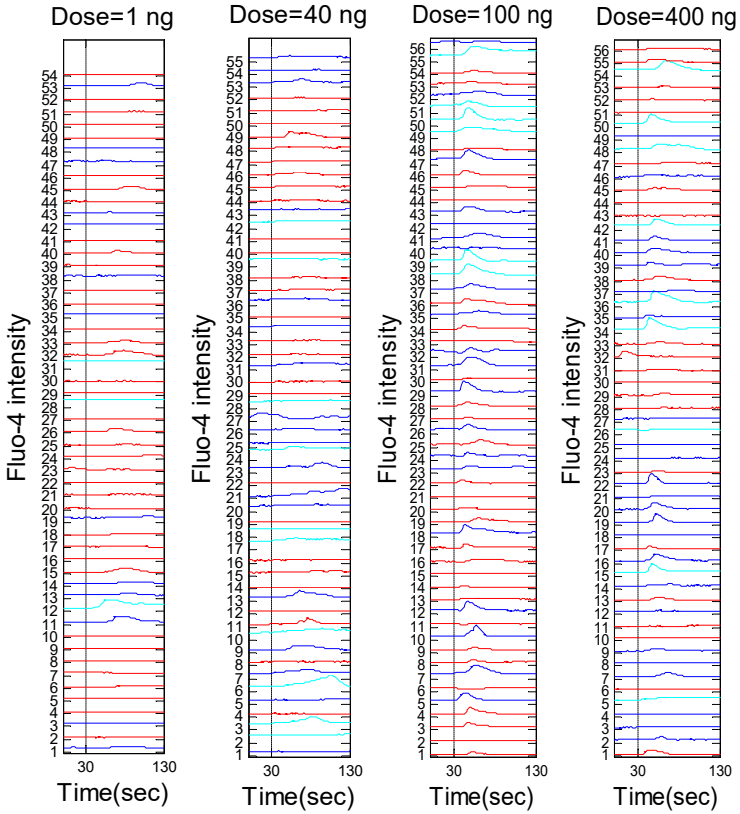
Cell State Visualization through PCA and K-means



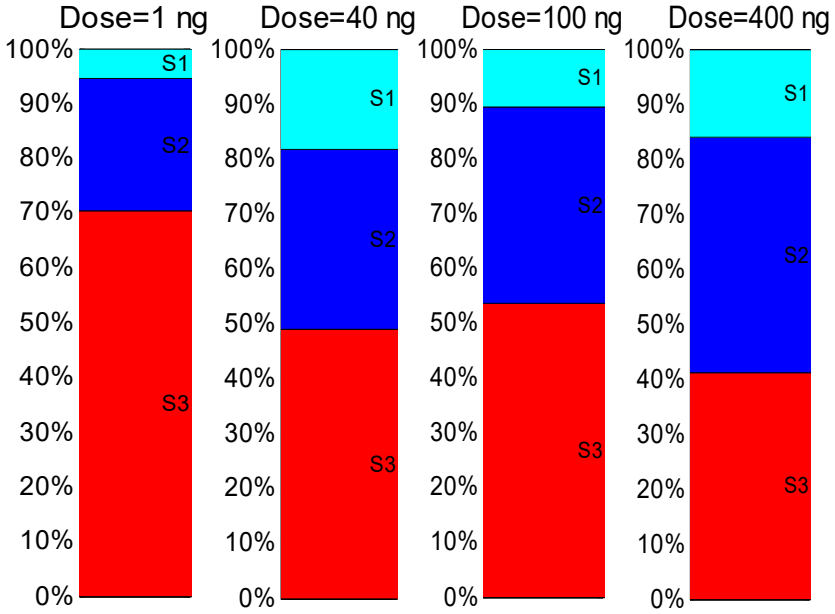
Dividing cell population based on Ca^{2+} amplitude.

Cell Subpopulation Profile trough PCA and K-means

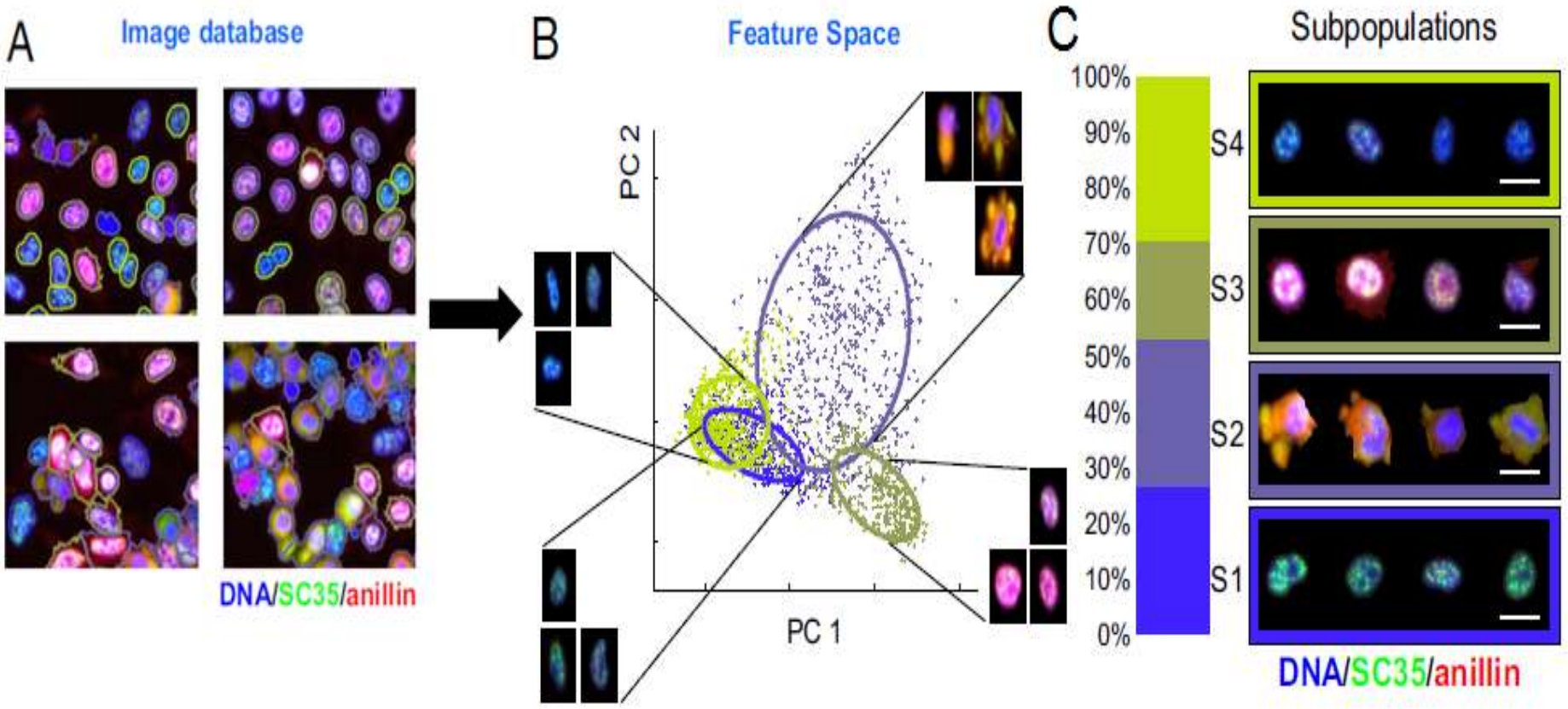
a



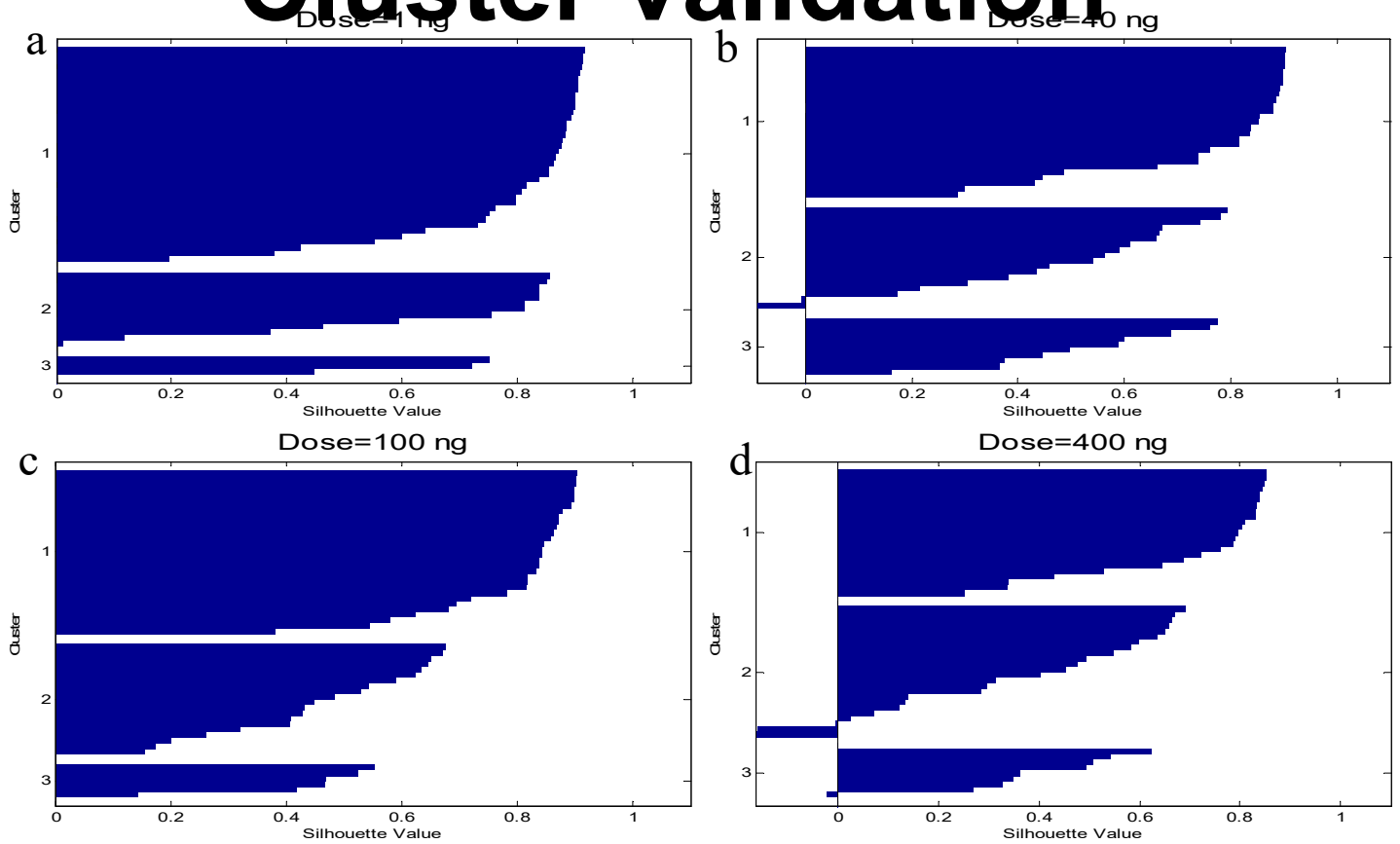
b



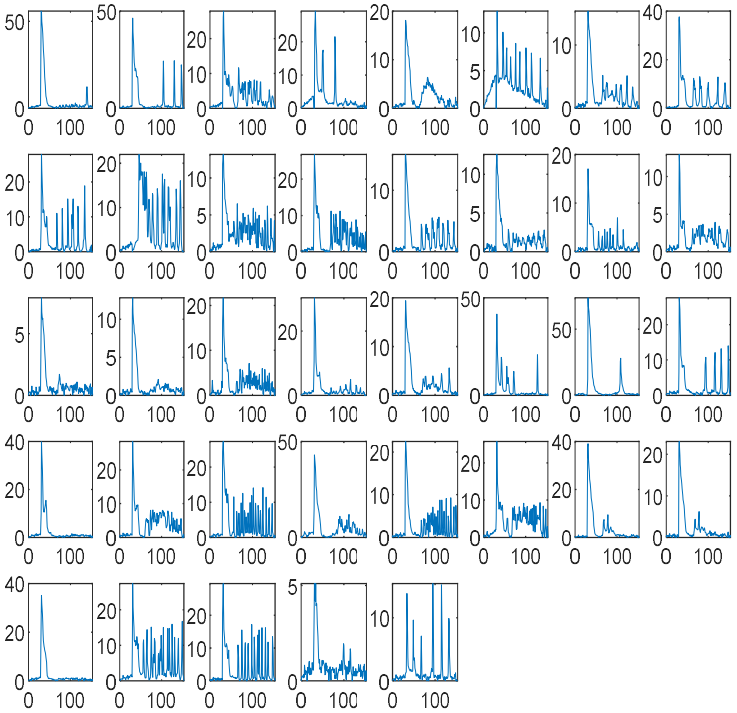
Dimension reduction

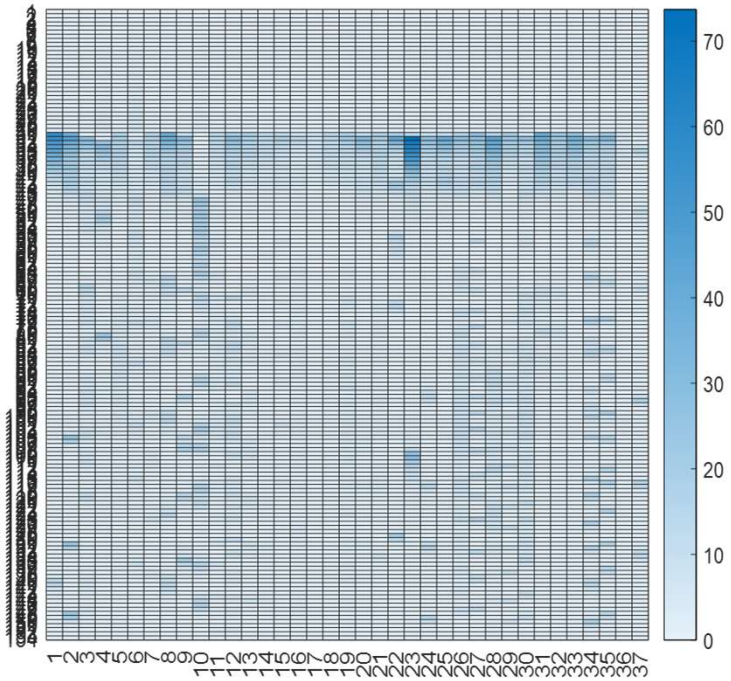


Silhouette Clustering: Cluster validation

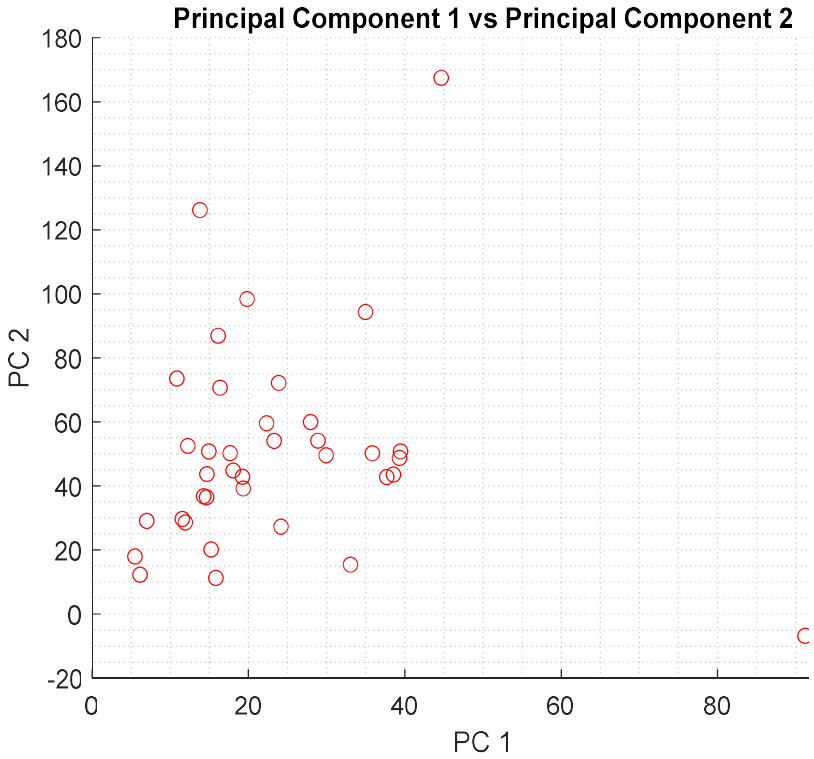


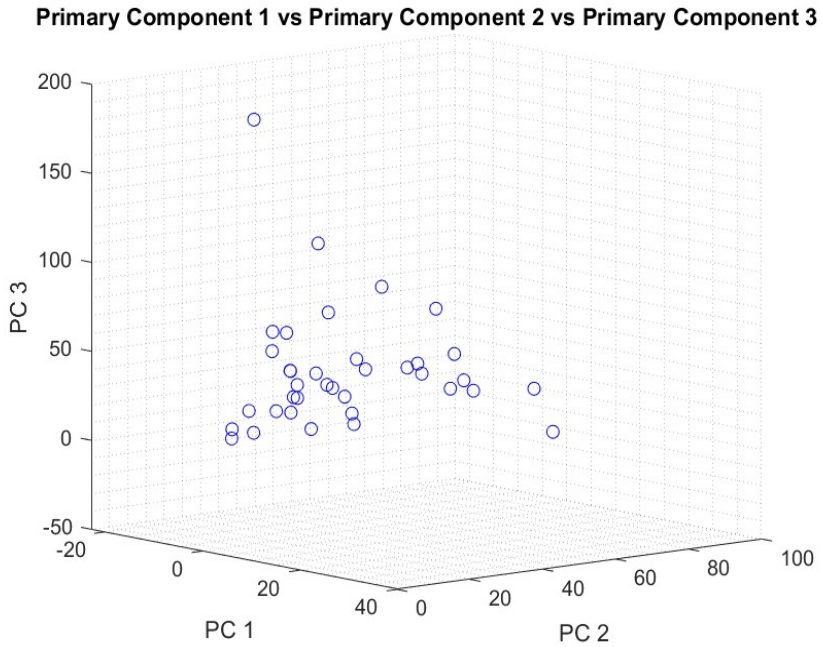
Assignment





Presentation in 2D and 3D

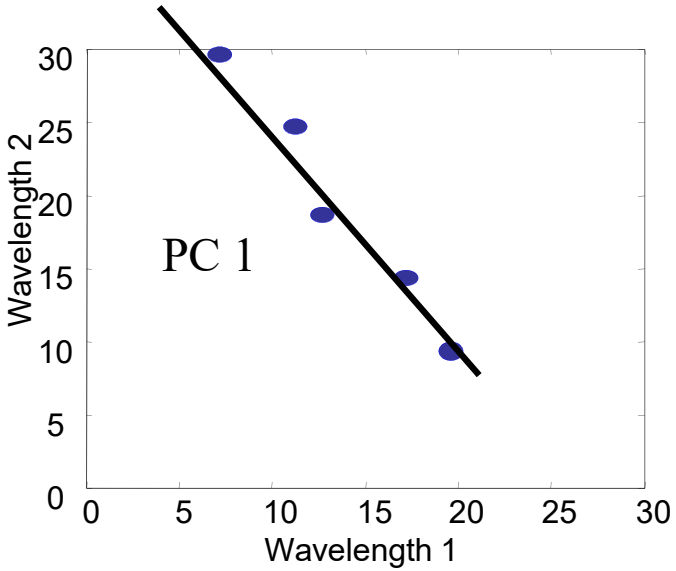


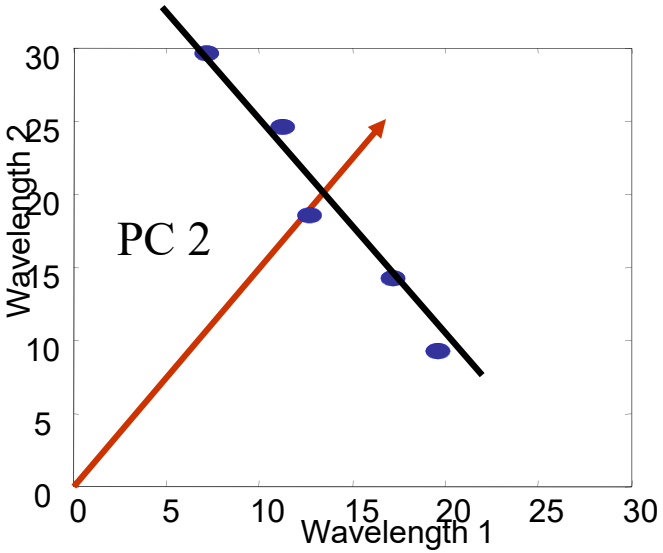


Principal Components

PCA , 1901, Karl Pearson

- All principal components (PCs) start at the origin of the ordinate axes.
- First PC is direction of maximum variance from origin
- Subsequent PCs are orthogonal to 1st PC and describe maximum residual variance





The Goal

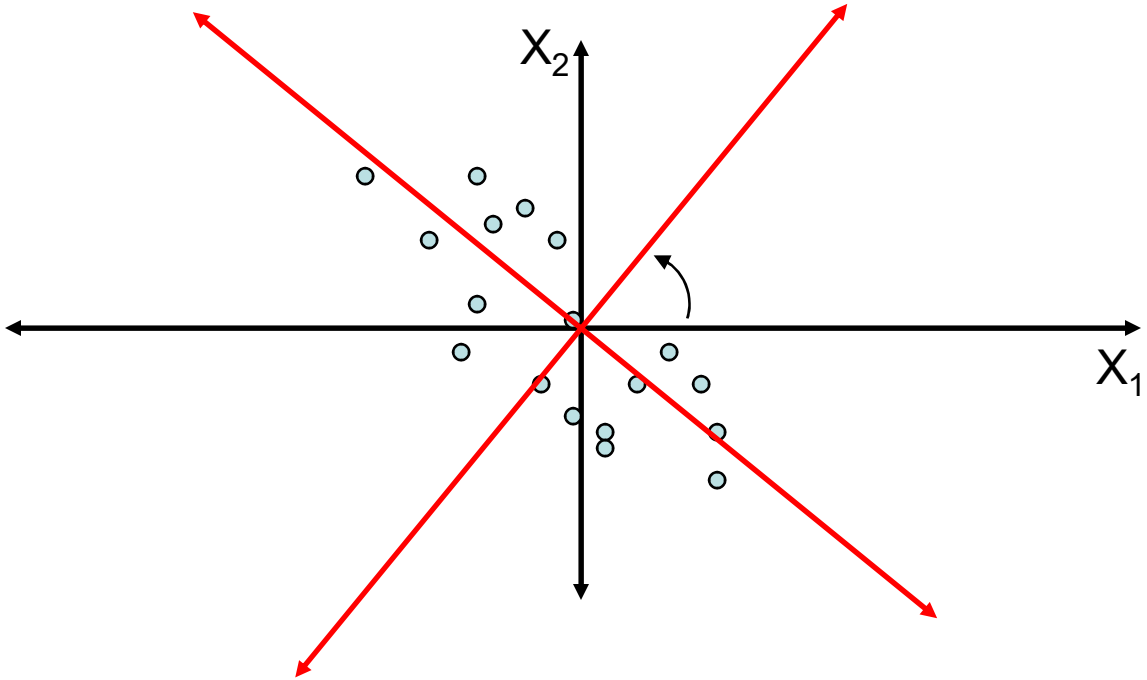
We wish to explain/summarize the underlying variance-covariance structure of a large set of variables through a few linear combinations of these variables.

Applications

- Uses:
  - Data Visualization
  - Data Reduction
  - Data Classification
  - Trend Analysis
  - Factor Analysis
  - Noise Reduction
- Examples:
  - How many unique “sub-sets” are in the sample?
  - How are they similar / different?
  - What are the underlying factors that influence the samples?
  - Which time / temporal trends are (anti)correlated?
  - Which measurements are needed to differentiate?
  - How to best present what is “interesting”?
  - Which “sub-set” does this new sample rightfully belong?

Trick: Rotate Coordinate Axes

Suppose we have a population measured on p random variables $X_1,\ldots,X_p$. Note that these random variables represent the p-axes of the Cartesian coordinate system in which the population resides. Our goal is to develop a new set of p axes (linear combinations of the original p axes) in the directions of greatest variability:



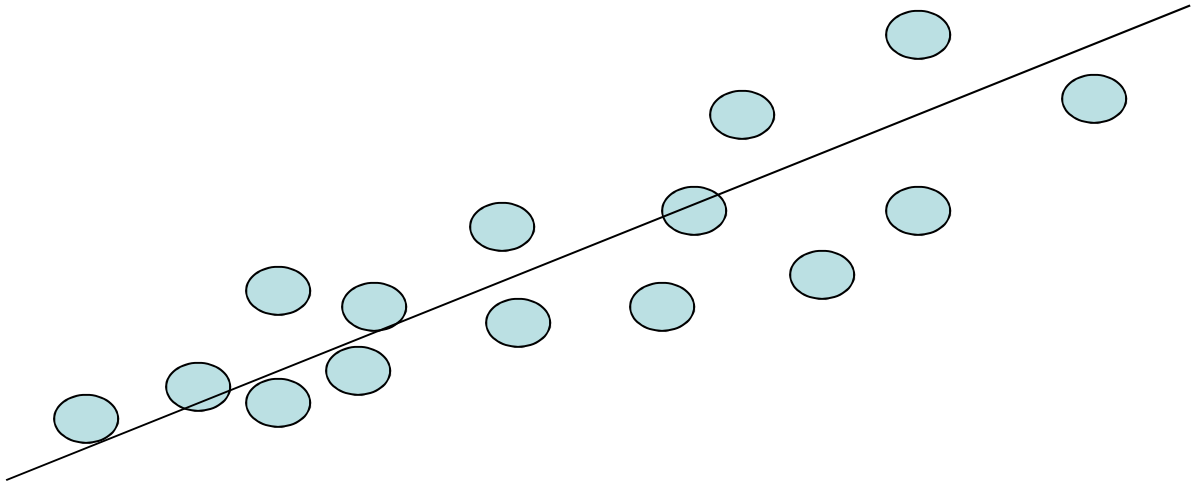
This is accomplished by rotating the axes.

Algebraic Interpretation

- Given m points in a n dimensional space, for large n, how does one project on to a low dimensional space while preserving broad trends in the data and allowing it to be visualized?

Algebraic Interpretation – 1D

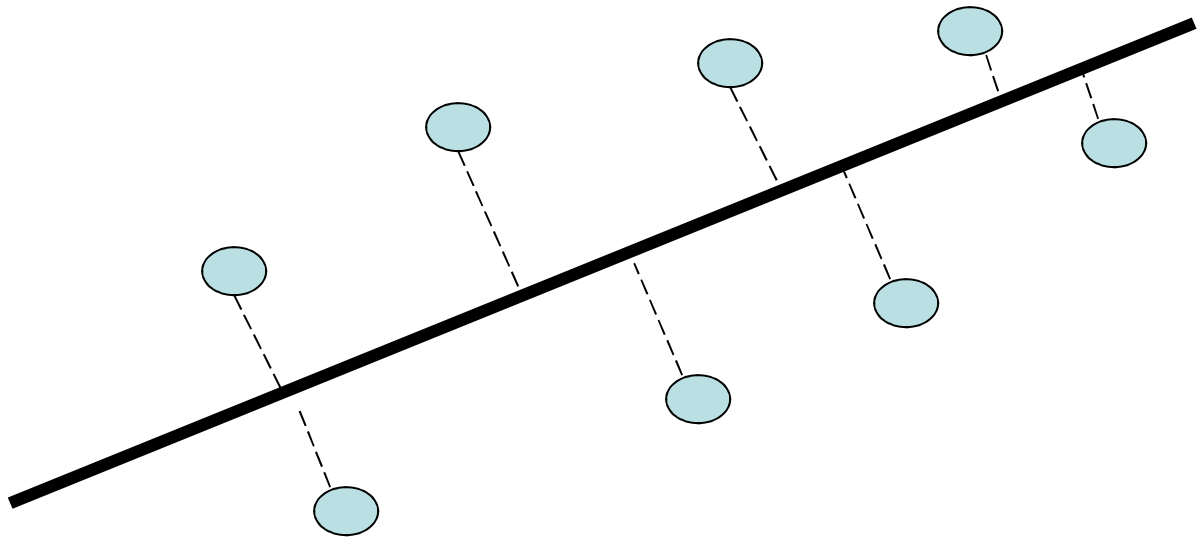
- Given m points in a n dimensional space, for large n, how does one project on to a 1 dimensional space?



- Choose a line that fits the data so the points are spread out well along the line

Algebraic Interpretation – 1D

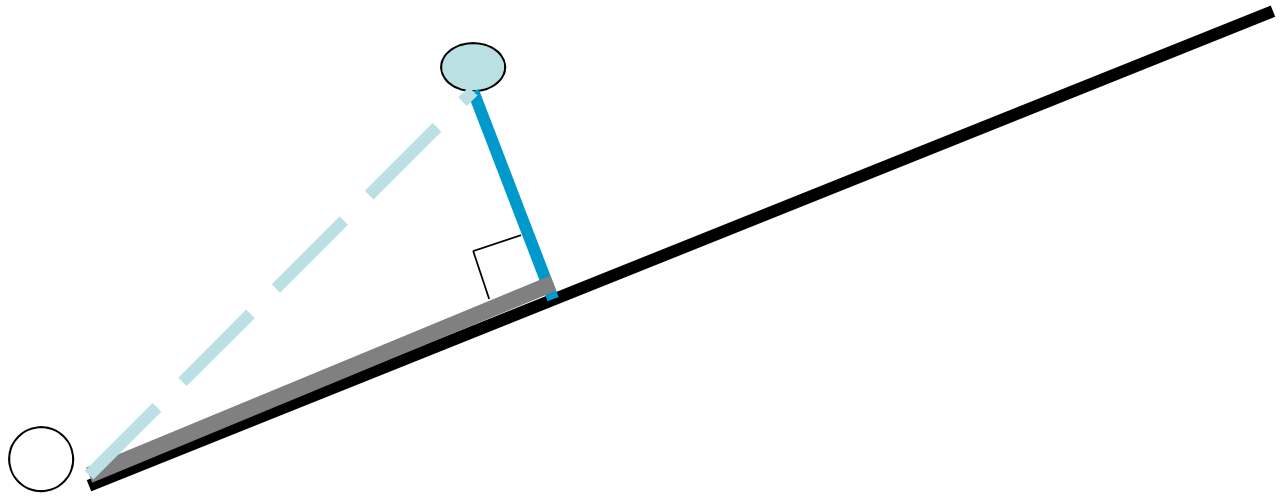
- Formally, minimize sum of squares of distances to the line.



- Why sum of squares? Because it allows fast minimization, assuming the line passes through 0

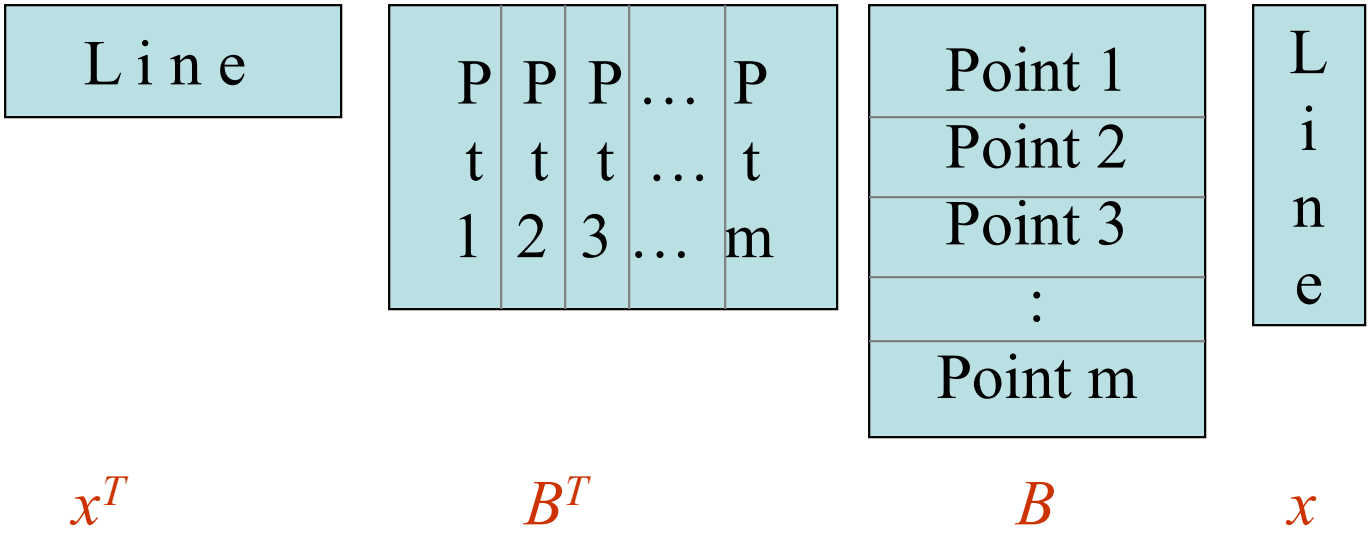
Algebraic Interpretation – 1D

- Minimizing sum of squares of distances to the line is the same as maximizing the sum of squares of the projections on that line.



Algebraic Interpretation – 1D

- How is the sum of squares of projection lengths expressed in algebraic terms?



Algebraic Interpretation – 1D

- How many eigenvectors are there?
- For Real Symmetric Matrices

  – except in degenerate cases when eigenvalues repeat, there are n eigenvectors

  $x_1 \ldots x_n$ are the eigenvectors

  $e_1 \ldots e_n$ are the eigenvalues

  – all eigenvectors are mutually orthogonal and therefore form a new basis
    - Eigenvectors for distinct eigenvalues are mutually orthogonal
    - Eigenvectors corresponding to the same eigenvalue have the property that any linear combination is also an eigenvector with the same eigenvalue; one can then find as many orthogonal eigenvectors as the number of repeats of the eigenvalue.

Algebraic Interpretation – 1D

- For matrices of the form B^TB
  - All eigenvalues are non-negative (show this)

PCA: *General*

From k original variables: $x_1,x_2,\ldots,x_k$:

Produce k new variables: $y_1,y_2,\ldots,y_k$:

$$y_1 = a_{11}x_1 + a_{12}x_2 + \ldots + a_{1k}x_k$$

$$y_2 = a_{21}x_1 + a_{22}x_2 + \ldots + a_{2k}x_k$$

$$\ldots$$

$$y_k = a_{k1}x_1 + a_{k2}x_2 + \ldots + a_{kk}x_k$$

PCA: *General*

From k original variables: $x_1,x_2,\ldots,x_k$:

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$y_1 = a_{11}x_1 + a_{12}x_2 + \ldots + a_{1k}x_k$

$y_2 = a_{21}x_1 + a_{22}x_2 + \ldots + a_{2k}x_k$

...

$y_k = a_{k1}x_1 + a_{k2}x_2 + \ldots + a_{kk}x_k$

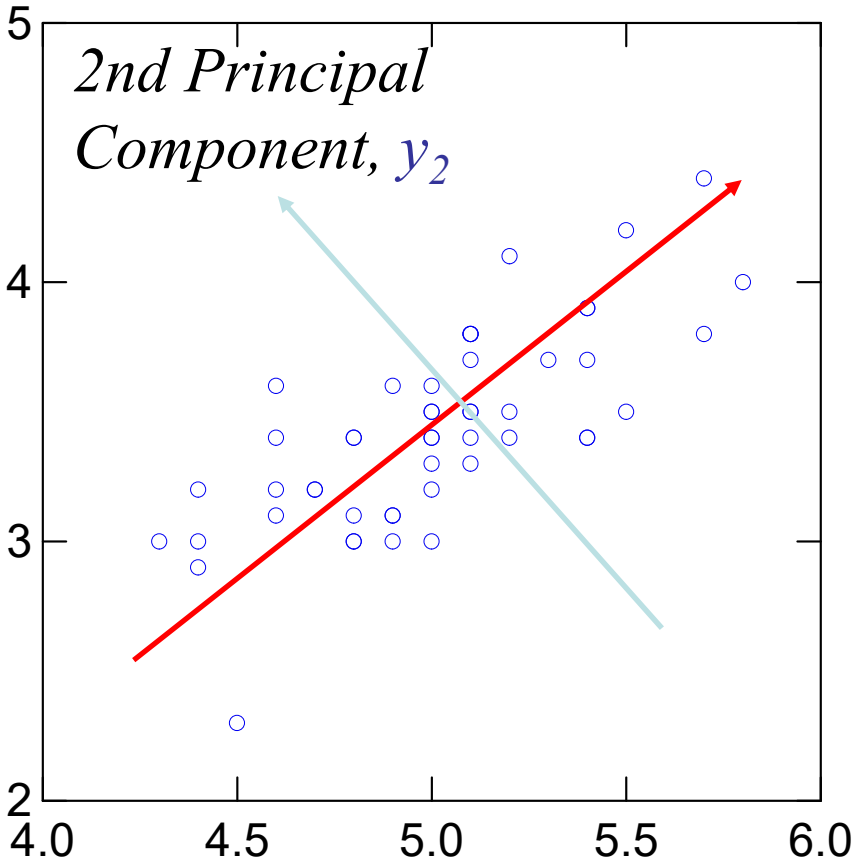
such that:

y_k's are uncorrelated (orthogonal)

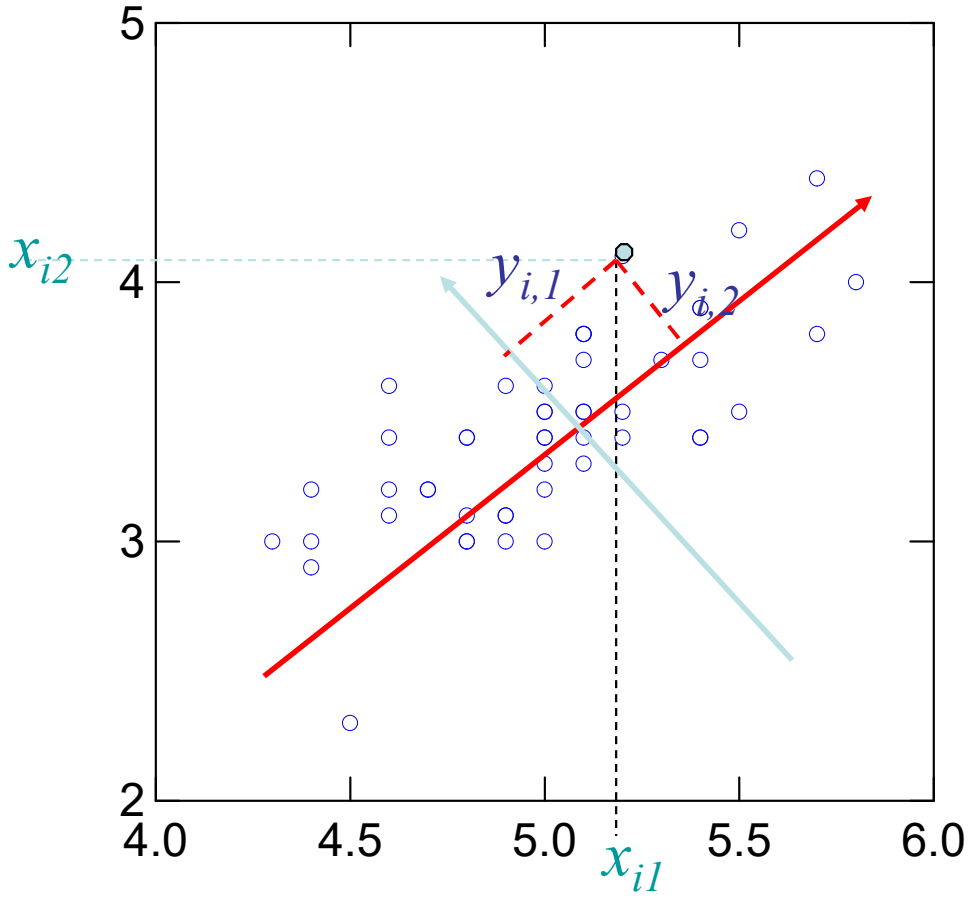
y_1 explains as much as possible of original variance in data set

y_2 explains as much as possible of remaining variance

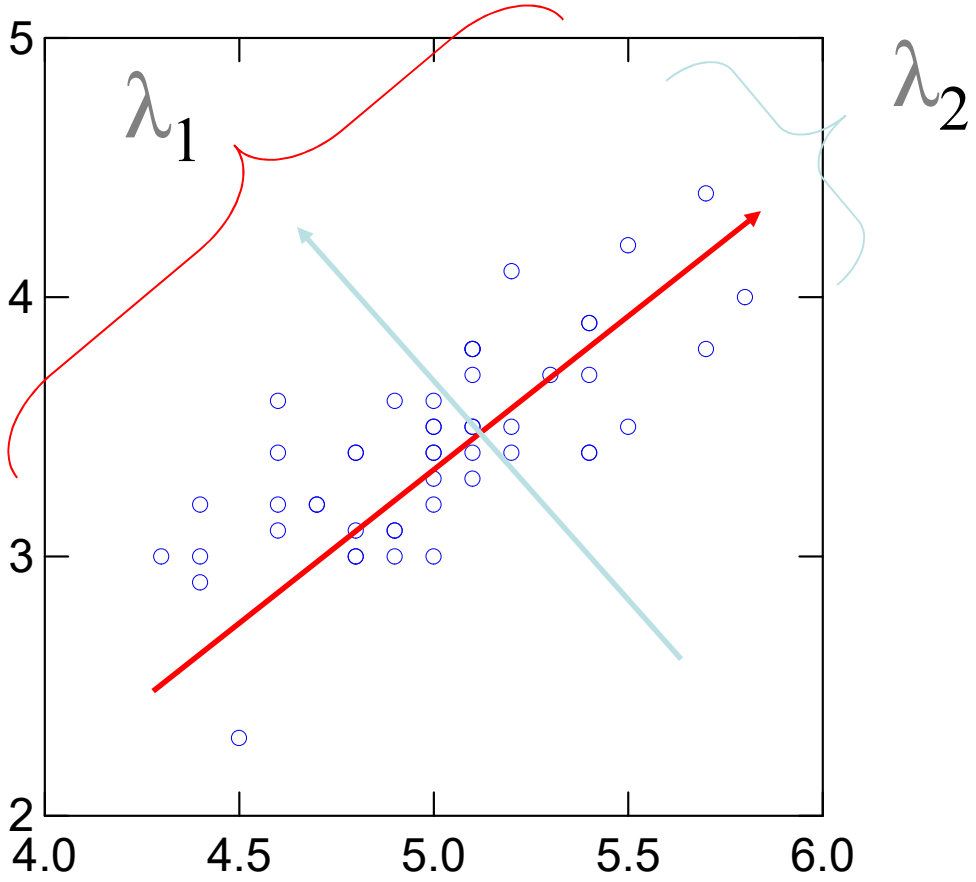
etc.


2nd Principal
Component, y_2
1st Principal
Component, y_1
5
4
3
2
4.0
4.5
5.0
5.5
6.0

PCA Scores



PCA Eigenvalues



PCA

From *k* original variables: $x_1,x_2,\ldots,x_k$:

Produce *k* new variables: $y_1,y_2,\ldots,y_k$:

$$y_1 = a_{11}x_1 + a_{12}x_2 + \ldots + a_{1k}x_k$$
$$y_2 = a_{21}x_1 + a_{22}x_2 + \ldots + a_{2k}x_k$$
$$\ldots$$
$$y_k = a_{k1}x_1 + a_{k2}x_2 + \ldots + a_{kk}x_k$$

y_k's are **Principal Components**

such that:

y_k's are uncorrelated (orthogonal)

y_1 explains as much as possible of original variance in data set

y_2 explains as much as possible of remaining variance

etc.

Principal Components Analysis on:

- *Covariance Matrix:*
  - Variables must be in same units
  - Emphasizes variables with most variance
  - Mean eigenvalue ≠1.0

- *Correlation Matrix:*
  - Variables are standardized (mean 0.0, SD 1.0)
  - Variables can be in different units
  - All variables have same impact on analysis
  - Mean eigenvalue = 1.0

PCA: *General*

$\{a_{11},a_{12},...,a_{1k}\}$ is 1st **Eigenvector** of correlation/covariance matrix, and **coefficients** of first principal component

$\{a_{21},a_{22},...,a_{2k}\}$ is 2nd **Eigenvector** of correlation/covariance matrix, and **coefficients** of 2nd principal component

…

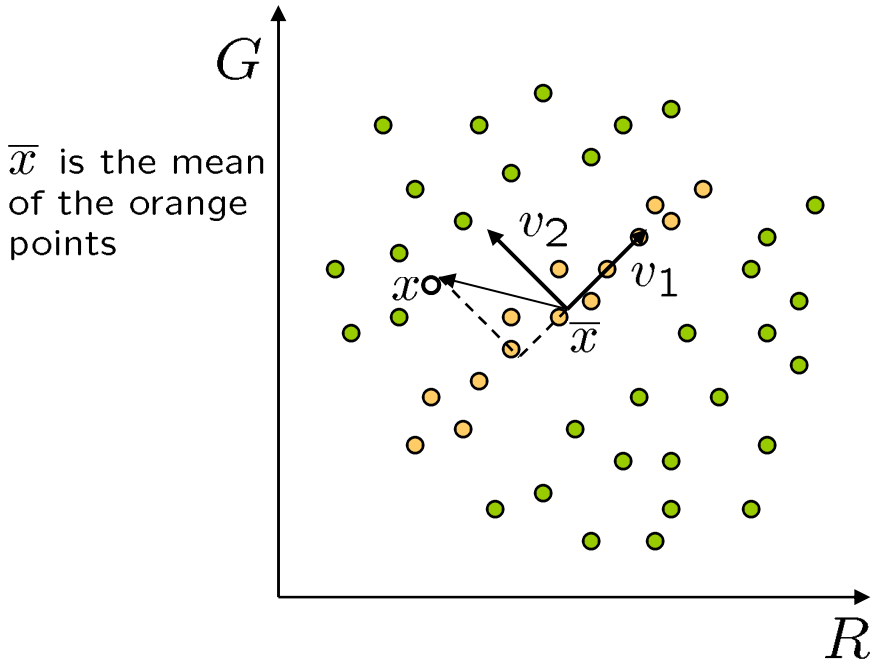
$\{a_{k1},a_{k2},...,a_{kk}\}$ is *k*th **Eigenvector** of correlation/covariance matrix, and **coefficients** of *k*th principal component

PCA Summary until now

- Rotates multivariate dataset into a new configuration which is easier to interpret

- Purposes
  - simplify data
  - look at relationships between variables
  - look at patterns of units

Classification in Subspace



convert **x** into $\mathbf{v_1}$, $\mathbf{v_2}$ coordinates

$$\mathbf{x} \rightarrow ((\mathbf{x} - \overline{x}) \cdot \mathbf{v_1}, (\mathbf{x} - \overline{x}) \cdot \mathbf{v_2})$$

What does the $\mathbf{v_2}$ coordinate measure?

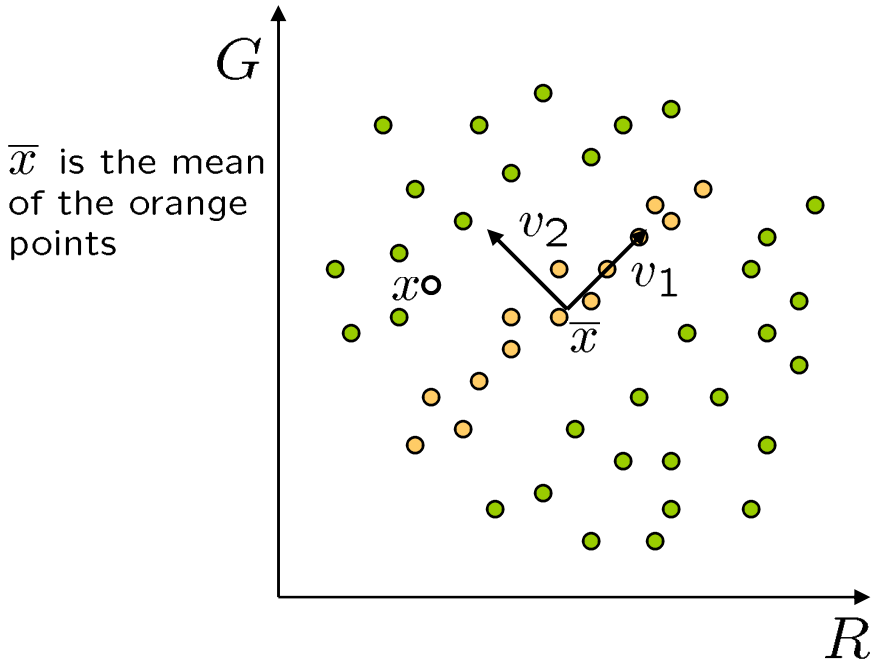
- distance to line
- use it for classification—near 0 for orange pts

What does the $\mathbf{v_1}$ coordinate measure?

- position along line
- use it to specify which orange point it is

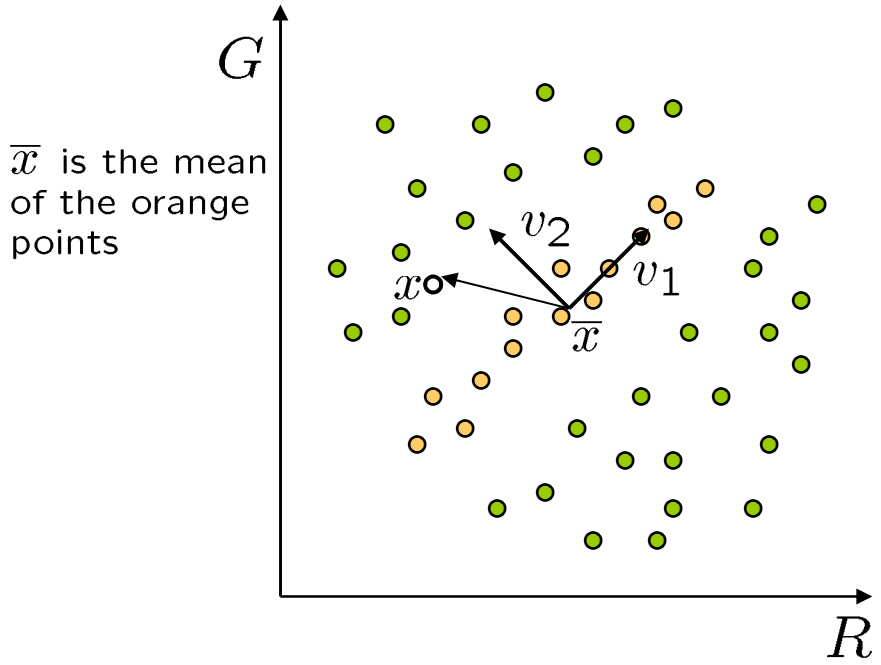
- Classification can be expensive
  - Must either search (e.g., nearest neighbors) or store large probability density functions.
- Suppose the data points are arranged as above
  - Idea—fit a line, classifier measures distance to line

Dimensionality Reduction



- Dimensionality reduction
  - We can represent the orange points with *only* their $\mathbf{v}_1$ coordinates
    - since $\mathbf{v}_2$ coordinates are all essentially 0
  - This makes it much cheaper to store and compare points
  - A bigger deal for higher dimensional problems

Linear Subspaces



Consider the variation along direction **v** among all of the orange points:

$$var(\mathbf{v}) = \sum_{\text{orange point } \mathbf{x}} \|(\mathbf{x} - \overline{\mathbf{x}})^{\mathbf{T}} \cdot \mathbf{v}\|^2$$

What unit vector **v** minimizes *var*?

$$\mathbf{v}_2 = min_{\mathbf{v}} \{var(\mathbf{v})\}$$

What unit vector **v** maximizes *var*?

$$\mathbf{v}_1 = max_{\mathbf{v}} \{var(\mathbf{v})\}$$

$$\begin{aligned} var(\mathbf{v}) &= \sum_{\mathbf{x}} \|(\mathbf{x} - \overline{\mathbf{x}})^{\mathbf{T}} \cdot \mathbf{v}\| \\ &= \sum_{\mathbf{x}} \mathbf{v}^{\mathbf{T}} (\mathbf{x} - \overline{\mathbf{x}})(\mathbf{x} - \overline{\mathbf{x}})^{\mathbf{T}} \mathbf{v} \\ &= \mathbf{v}^{\mathbf{T}} \left[\sum_{\mathbf{x}} (\mathbf{x} - \overline{\mathbf{x}})(\mathbf{x} - \overline{\mathbf{x}})^{\mathbf{T}} \right] \mathbf{v} \\ &= \mathbf{v}^{\mathbf{T}} \mathbf{A} \mathbf{v} \quad \text{where } \mathbf{A} = \sum_{\mathbf{x}} (\mathbf{x} - \overline{\mathbf{x}})(\mathbf{x} - \overline{\mathbf{x}})^{\mathbf{T}} \end{aligned}$$

Solution: $\mathbf{v}_1$ is eigenvector of **A** with *largest* eigenvalue
$\mathbf{v}_2$ is eigenvector of **A** with *smallest* eigenvalue

Higher Dimensions

- Suppose each data point is N-dimensional
  - Same procedure applies:

$$\begin{aligned} var(\mathbf{v}) &= \sum_{\mathbf{x}} \|(\mathbf{x}-\bar{\mathbf{x}})^{\mathrm{T}} \cdot \mathbf{v}\| \\ &= \mathbf{v}^{\mathrm{T}}\mathbf{A}\mathbf{v} \quad \text{where } \mathbf{A} = \sum_{\mathbf{x}} (\mathbf{x}-\bar{\mathbf{x}})(\mathbf{x}-\bar{\mathbf{x}})^{\mathrm{T}} \end{aligned}$$

  - The eigenvectors of **A** define a new coordinate system
    - eigenvector with largest eigenvalue captures the most variation among training vectors **x**
    - eigenvector with smallest eigenvalue has least variation
  - We can compress the data by only using the top few eigenvectors
    - corresponds to choosing a “linear subspace”
      - represent points on a line, plane, or “hyper-plane”
    - these eigenvectors are known as the ***principal components***

A 2D Numerical Example

PCA Example –STEP 1

- Subtract the mean

  from each of the data dimensions. All the x values have $\bar{x}$ subtracted and y values have $\bar{y}$ 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

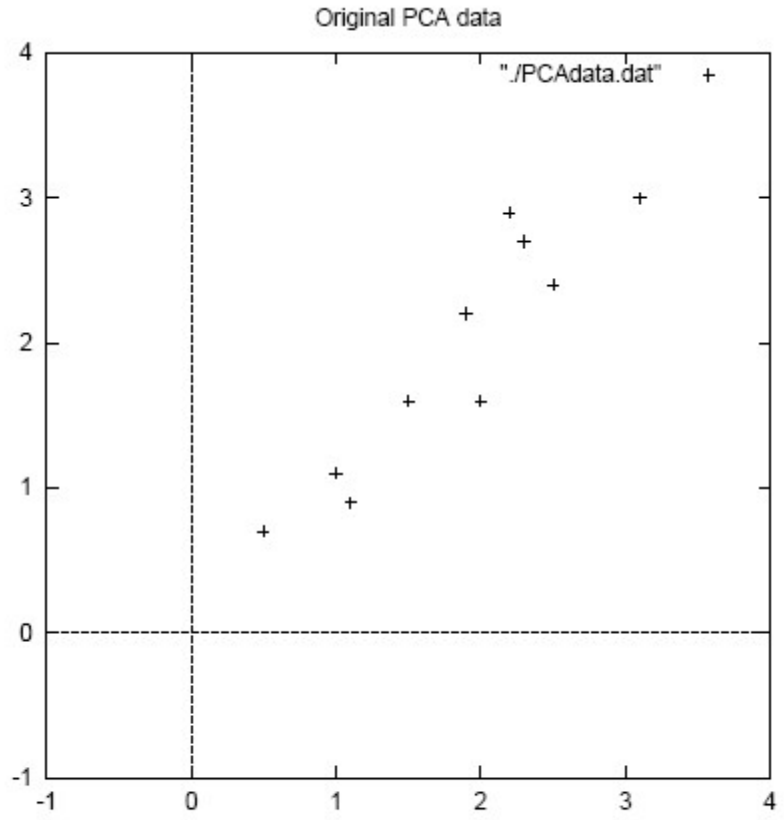


Figure 3.1: PCA example data, original data on the left, data with the means subtracted on the right, and a plot of the data

PCA Example –STEP 2

- Calculate the covariance matrix

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

- 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

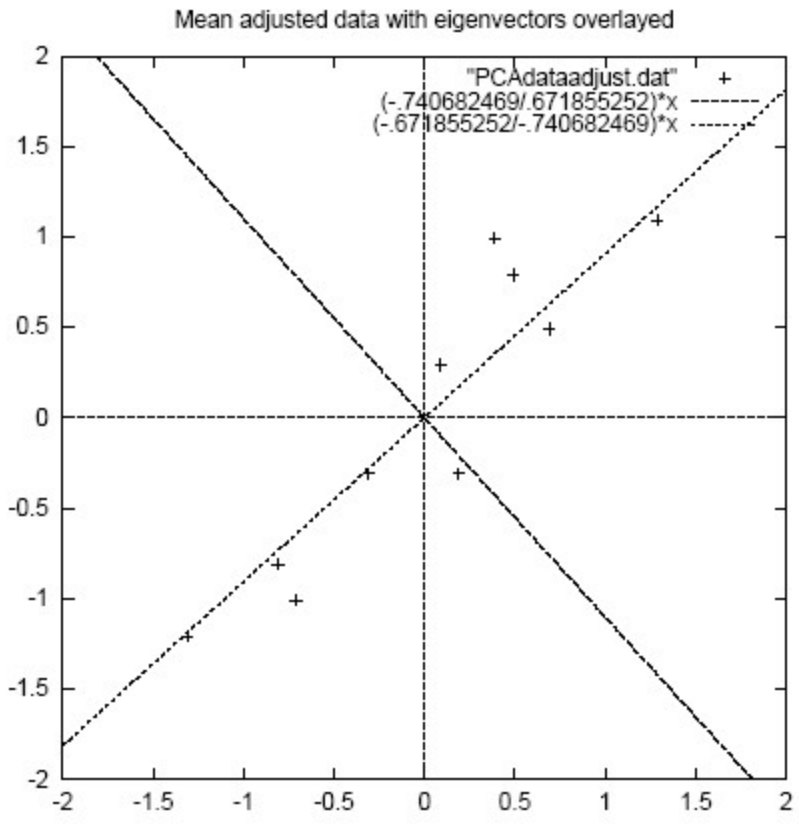


Figure 3.2: A plot of the normalised data (mean subtracted) with the eigenvectors of the covariance matrix overlayed on top.

- 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

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

PCA Example –STEP 4

- Feature Vector

  FeatureVector = (eig_1 eig_2 eig_3 … 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

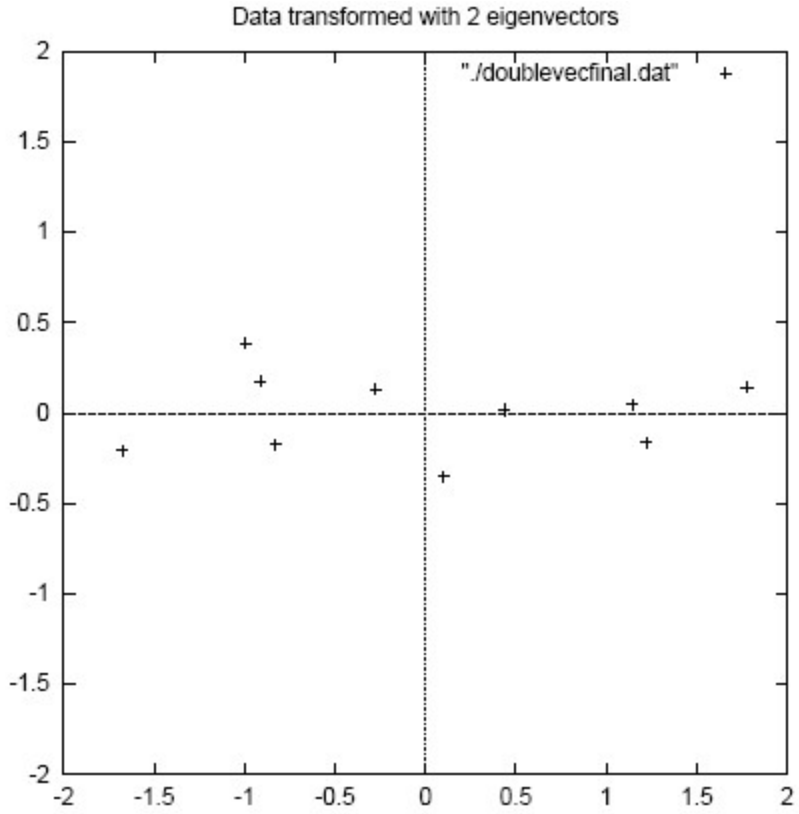


Figure 3.3: The table of data by applying the PCA analysis using both eigenvectors, and a plot of the new data points.

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

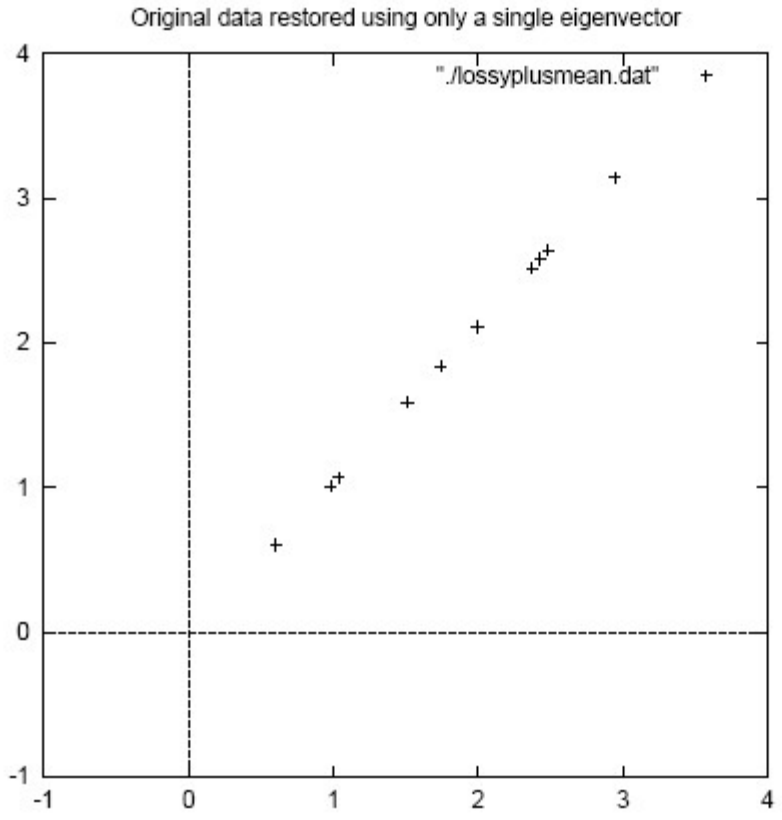


Figure 3.5: The reconstruction from the data that was derived using only a single eigenvector