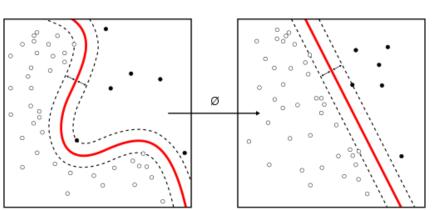
Best-fit subspaces and Singular Value Decomposition

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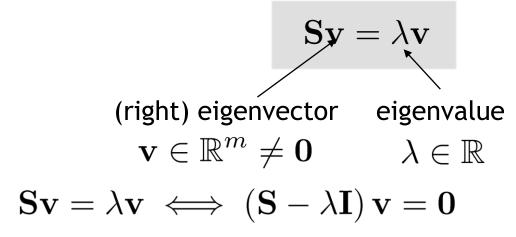
Mathematical background

Singular vector decomposition

Principle component analysis

Eigenvalues & Eigenvectors

Eigenvectors (for a square m×m matrix S)



Example
$$\begin{pmatrix} 6 & -2 \\ 4 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{pmatrix} 2 \\ 4 \end{pmatrix} = 2 \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

How many eigenvalues are there at most?

only has a non-zero solution if $|\mathbf{S} - \lambda \mathbf{I}| = 0$

this is a m-th order equation in λ which can have at most m distinct solutions (roots of the characteristic polynomial) - $\underline{\text{can be}}$ $\underline{\text{complex even though } S$ is real.

Matrix-vector multiplication

$$S = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$
 has eigenvalues 3, 2, 0 with corresponding eigenvectors

$$v_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad v_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad v_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

On each eigenvector, S acts as a multiple of the identity matrix: but as a different multiple on each.

Any vector (say
$$x = \begin{pmatrix} 2 \\ 4 \\ 6 \end{pmatrix}$$
) can be viewed as a combination of the eigenvectors: $x = 2v_1 + 4v_2 + 6v_3$

Matrix vector multiplication

 Thus a matrix-vector multiplication such as Sx (S, x as in the previous slide) can be rewritten in terms of the eigenvalues/vectors:

$$Sx = S(2v_1 + 4v_2 + 6v_3)$$

 $Sx = 2Sv_1 + 4Sv_2 + 6Sv_3 = 2\lambda_1 v_1 + 4\lambda_2 v_2 + 6\lambda_3 v_3$

- Even though x is an arbitrary vector, the action of S on x is determined by the eigenvalues/vectors.
- Suggestion: the effect of "small" eigenvalues is small.

Eigenvalues & Eigenvectors

For symmetric matrices, eigenvectors for distinct eigenvalues are orthogonal

$$Sv_{\{1,2\}} = \lambda_{\{1,2\}}v_{\{1,2\}}$$
, and $\lambda_1 \neq \lambda_2 \implies v_1 \bullet v_2 = 0$

All eigenvalues of a real symmetric matrix are real.

for complex
$$\lambda$$
, if $|S - \lambda I| = 0$ and $S = S^T \Rightarrow \lambda \in \Re$

All eigenvalues of a positive semidefinite matrix are non-negative

$$\forall w \in \Re^n, w^T S w \ge 0$$
, then if $S v = \lambda v \Rightarrow \lambda \ge 0$

Example

• Let
$$S = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$
 Real, symmetric.

• Then
$$S - \lambda I = \begin{bmatrix} 2 - \lambda & 1 \\ 1 & 2 - \lambda \end{bmatrix} \Rightarrow (2 - \lambda)^2 - 1 = 0.$$

- The eigenvalues are 1 and 3 (nonnegative, real).
- The eigenvectors are orthogonal (and real):

$$\begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

 $\begin{pmatrix} 1 \\ -1 \end{pmatrix} \qquad \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \begin{array}{c} \text{Plug in these values} \\ \text{and solve for} \\ \text{eigenvectors.} \end{array}$ eigenvectors.

Eigen/diagonal Decomposition

- Let $S \in \mathbb{R}^{m \times m}$ be a square matrix with m linearly independent eigenvectors (a "non-defective" matrix)
- Theorem: Exists an eigen decomposition

$$\mathbf{S} = \mathbf{U} \mathbf{\Lambda} \mathbf{U}^{-1}$$
 diagonal

- Columns of *U* are eigenvectors of *S*
- Diagonal elements of A are eigenvalues S of

$$\mathbf{\Lambda} = \operatorname{diag}(\lambda_1, \dots, \lambda_m), \ \lambda_i \geq \lambda_{i+1}$$

Diagonal decomposition: why/how

Let \boldsymbol{U} have the eigenvectors as columns: $U = \begin{bmatrix} v_1 & \dots & v_n \end{bmatrix}$

Then, **SU** can be written

$$SU = S \begin{bmatrix} v_1 & \dots & v_n \end{bmatrix} = \begin{bmatrix} \lambda_1 v_1 & \dots & \lambda_n v_n \end{bmatrix} = \begin{bmatrix} v_1 & \dots & v_n \end{bmatrix} \begin{bmatrix} \lambda_1 & \dots & \lambda_n \end{bmatrix}$$

Thus $SU=U\Lambda$, or $U^{-1}SU=\Lambda$

And **S=U\(\Omega\)U**-1.

Diagonal decomposition - example

Recall
$$S = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$
; $\lambda_1 = 1, \lambda_2 = 3.$

The eigenvectors
$$\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$
 and $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ form $U = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$

Inverting, we have
$$U^{-1} = \begin{bmatrix} 1/2 & -1/2 \\ 1/2 & 1/2 \end{bmatrix}$$
 Recall UU-1 =I.

Then, **S=U/
$$U^{-1}$$
=**

$$\begin{bmatrix}
1 & 1 \\
-1 & 1
\end{bmatrix}
\begin{bmatrix}
1 & 0 \\
0 & 3
\end{bmatrix}
\begin{bmatrix}
1/2 & -1/2 \\
1/2 & 1/2
\end{bmatrix}$$

Example continued

Symmetric Eigen Decomposition

- If $\mathbf{S} \in \mathbb{R}^{m \times m}$ is a symmetric matrix:
- Theorem: Exists a (unique) eigen decomposition $S = Q\Lambda Q^T$
- where Q is orthogonal:
 - $\mathbf{Q}^{-1} = \mathbf{Q}^T$
 - Columns of **Q** are normalized eigenvectors
 - Columns are orthogonal.
 - (everything is real)

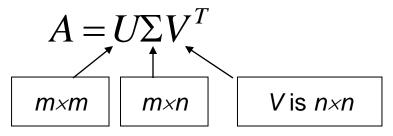
Mathematical background

Singular vector decomposition

Principle component analysis

Singular Value Decomposition

For an $m \times n$ matrix \mathbf{A} of rank r there exists a factorization (Singular Value Decomposition = SVD) as follows:



The columns of U are orthogonal eigenvectors of AA^{T} .

The columns of V are orthogonal eigenvectors of A^TA .

Eigenvalues $\lambda_1 \dots \lambda_r$ of $\mathbf{A}\mathbf{A}^T$ are the eigenvalues of $\mathbf{A}^T\mathbf{A}$.

$$\sigma_{\scriptscriptstyle i} = \sqrt{\lambda_{\scriptscriptstyle i}}$$

$$\Sigma = diag(\sigma_1...\sigma_{\scriptscriptstyle r})$$
 Singular values.

$AA^{T}, A^{T}A$

 $Rank(\mathbf{A})=Ran(\mathbf{A}\mathbf{A}^T)=rank(\mathbf{A}^T\mathbf{A}).$

Eigenvalues $\lambda_1 \dots \lambda_r$ of AA^T are the eigenvalues of A^TA .

Lemma. $\lambda \neq 0$ be the eigenvalue of AA^T , α_1 , ..., α_r are pairwise orthogonal unit eigenvectors corresponds to λ , then $A^T\alpha_1$, $A^T\alpha_2$, ..., $A^T\alpha_r$ are pairwise orthogonal eigenvectors of A^TA , and $\sqrt{(A^T\alpha_j, A^T\alpha_j)} = \sqrt{\lambda_j}$.

Theorem. $\mathbf{A} = \begin{bmatrix} \mathbf{a}_{ij} \end{bmatrix}_{\mathbf{m} \times \mathbf{n}}$ and $\sqrt{\lambda}_1, \sqrt{\lambda}_2, \ldots, \sqrt{\lambda}_r$ be the singular value of \mathbf{A} , then $\mathbf{A} = \mathbf{U} \mathbf{\Sigma} V^T$, where $\mathbf{U} \mathbf{U}^T = \mathbf{I}, \ \mathbf{V} \mathbf{V}^T = \mathbf{I}, \ \mathbf{\Sigma} = \begin{bmatrix} \sqrt{\lambda}_1 & & & & \\ & \sqrt{\lambda}_2 & & & \\ & & & \sqrt{\lambda}_r & & \\ & & & & \ddots & \vdots \\ & & & & & \ddots & \vdots \\ & & & & & & \ddots & \vdots \\ & & & & & & \ddots & \vdots \\ & & & & & & & \ddots & \vdots \\ & & & & & & & \ddots & \vdots \\ & & & & & & & & & & \end{bmatrix}.$

Singular Value Decomposition

 Illustration of SVD dimensions and sparseness

Image of unit ball under linear transformation

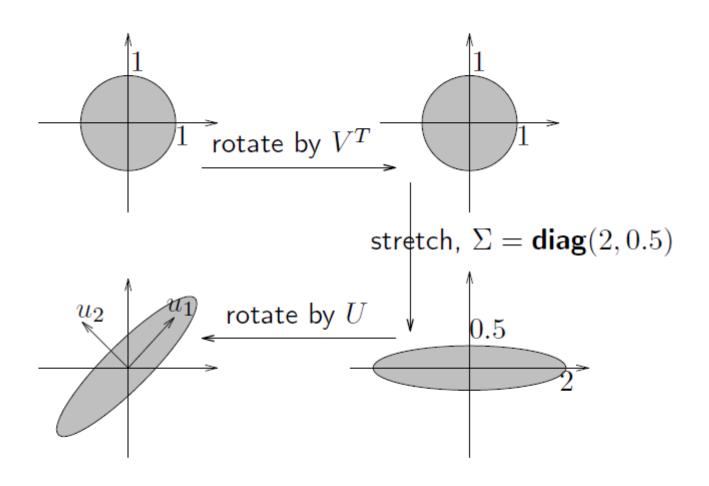
full SVD:

$$A = U\Sigma V^T$$

gives interretation of y = Ax:

- rotate (by V^T)
- stretch along axes by σ_i ($\sigma_i = 0$ for i > r)
- ullet zero-pad (if m>n) or truncate (if m< n) to get m-vector
- rotate (by U)

Image of unit ball under A



SVD example

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

Thus m=3, n=2. Its SVD is

$$\begin{bmatrix} 0 & 2/\sqrt{6} & 1/\sqrt{3} \\ 1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ 1/\sqrt{2} & 1/\sqrt{6} & -1/\sqrt{3} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \sqrt{3} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{bmatrix}$$

Typically, the singular values arranged in decreasing order.

Low-rank Approximation

- SVD can be used to compute optimal lowrank approximations.
- Approximation problem: Find A_k of rank k
 such that

$$A_k = \min_{X: rank(X) = k} \left\| A - X \right\|_F \leftarrow Frobenius norm \\ \left\| A \right\|_F \equiv \sqrt{\sum_{i=1}^m \sum_{j=1}^n |a_{ij}|^2}.$$

 A_k and X are both $m \times n$ matrices.

Typically, want $k \ll r$.

Low-rank Approximation

Solution via SVD

$$A_k = U \operatorname{diag}(\sigma_1, ..., \sigma_k, 0, ..., 0)V^T$$

$$set smallest r-k$$

$$singular values to zero$$

$$\begin{bmatrix}
* & * & * & * & * \\
* & * & * & * & * \\
* & * & * & * & *
\end{bmatrix} = \begin{bmatrix}
\star & \star & \star \\
\star & \star & \star
\end{bmatrix}$$

$$\begin{bmatrix}
\star & \star & \star & \star \\
\star & \star & \star & \star
\end{bmatrix}$$

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\end{bmatrix}$$

$$\begin{bmatrix}
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\star & \star & \star & \star & \star
\end{bmatrix}$$

$$A_k = \sum_{i=1}^k \sigma_i u_i v_i^T - column notation: sum of rank 1 matrices$$

Approximation error

- How good (bad) is this approximation?
- It's the best possible, measured by the Frobenius norm of the error:

$$\min_{X:rank(X)=k} ||A - X||_F = ||A - A_k||_F = \sigma_{k+1}$$

where the σ_i are ordered such that $\sigma_i \geq \sigma_{i+1}$. Suggests why Frobenius error drops as k increased.

Recall random projection

- Completely different method for low-rank approximation
- Was data-oblivious
 - SVD-based approximation is data-dependent
- Error for random projection depended only on start/finish dimensionality
 - For every distance
- Error for SVD-based approximation is for the Frobenius norm, not for individual distances

SVD Low-rank approximation

- Whereas the term-doc matrix A may have m=50000, n=10 million (and rank close to 50000)
- We can construct an approximation A₁₀₀ with rank 100.
 - Of all rank 100 matrices, it would have the lowest Frobenius error.

Power Method for SVD

- $A = \sum_{i} \delta_{i} u_{i} v_{i}^{T}$
- $B = A^T A$ $= (\sum_i \delta_i v_i u_i^T) (\sum_j \delta_j u_j v_j^T) = \sum_i \delta_i^2 v_i v_i^T$

. . .

- $\bullet \ B^k = \sum_i \delta_i^{2k} v_i v_i^T$
- If $\delta_1 > \delta_2$ then the first term in the summation dominates. i.e., $B^k \to \delta_1^{2k} v_1 v_1^T$
- To estimate v_1 : take the first column of B^k and normalize it to an unit vector.

Power Method for SVD

- $A = \sum_{i} \delta_{i} u_{i} v_{i}^{T}$, A is large and sparse
- $B^k = \sum_i \delta_i^{2k} v_i v_i^T$ could be very cost.
- Improve:
 - Randomly select $x = \sum_{i=1}^{d} c_i v_i$
 - $B^k \cdot x \approx (\delta_1^{2k} v_1 v_1^T) x = c_1 \delta_1^{2k} v_1 = y$
 - Normalize y will get v_1 .
 - Trick: $B^k \cdot x = A^T A \cdots A^T A x$

Matrix Approximation

$$A_{i} = U\Sigma_{i}V^{T}$$

 Σ_i : the rank *i* version of Σ (by setting last $m-i\sigma$'s to zero)

 A_i : the best rank i approximation to A in the sence of Euclidean distance

$$A = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \dots + \sigma_m u_m v_m^T$$

Storage save : rank one matrix (m+n) numbers

Operation save : m + n

making small σ 's to zero and back substitute (see next page for application in image compression)

Image Compression

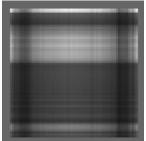
- As described in text p.352
- For grey scale images: m×n bytes

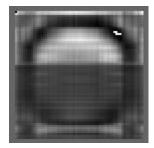
After SVD, taking the most significant r terms:

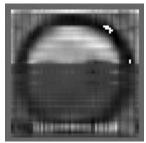
$$A = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \dots + \sigma_r u_r v_r^T$$

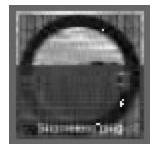
Only need to store r×(m+n+1)













Original 64×64

r = 1,3,5,10,16 (no perceivable difference afterwards)

Mathematical background

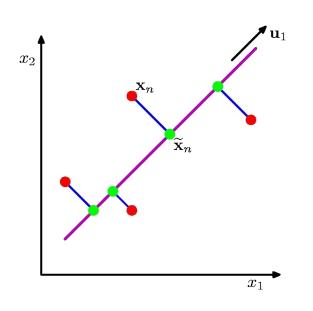
Singular vector decomposition

Principle component analysis

PCA Applications

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

Principle Component Analysis



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)

Principle Components Analysis

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

Covariance

 Variance – measure of the deviation from the mean for points in one dimension e.g. heights

$$Var(X) = E((x - \mu)^2)$$

 Covariance as a measure of how much each of the dimensions vary from the mean with respect to each other.

$$Cov(X,Y) = E[((X - E(X)(Y - E(Y)))]$$

- Covariance is measured between 2 dimensions to see if there is a relationship between the 2 dimensions e.g. number of hours studied & marks obtained.
- The covariance between one dimension and itself is the variance

Covariance Matrix

 Representing Covariance between dimensions as a matrix e.g. for 3 dimensions:

$$C = \begin{bmatrix} cov(x,x) & cov(x,y) & cov(x,z) \\ cov(y,x) & cov(y,y) & cov(y,z) \\ cov(z,x) & cov(z,y) & cov(z,z) \end{bmatrix}$$

- Diagonal is the variances of x, y and z
- cov(x,y) = cov(y,x) hence matrix is symmetrical about the diagonal
- n-dimensional data will result in $n \times n$ covariance matrix.

Covariance

- Exact value is not as important as it's sign.
- A <u>positive value</u> of covariance indicates both dimensions increase or decrease together
 - e.g. as the number of hours studied increases, the marks in that subject increase.
- A <u>negative value</u> indicates while one increases the other decreases, or vice-versa
 - e.g. active social life at WoL vs performance in CS dept.
- If <u>covariance is zero</u>: the two dimensions are independent of each other
 - e.g. heights of students vs the marks obtained in a subject.

PCA

- Principal Components Analysis (PCA) is a technique that can be used to simplify a dataset.
- It is a linear transformation that chooses a new coordinate system for the data set such that
 - greatest variance by any projection of the data set comes to lie on the first axis (then called the first principal component),
 - the second greatest variance on the second axis, and so on.
- PCA can be used for reducing dimensionality by eliminating the later principal components.

PCA

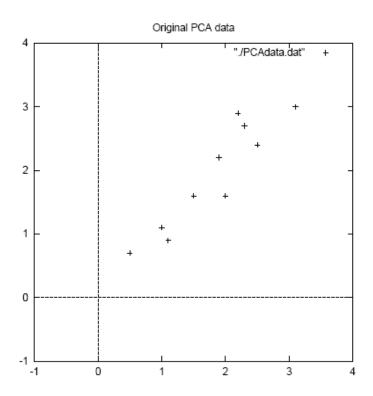
- By finding the eigenvalues and eigenvectors of the covariance matrix, we find that the eigenvectors with the largest eigenvalues correspond to the dimensions that have the strongest correlation in the dataset.
- This is the principal component.
- PCA is a useful statistical technique that has found application in:
 - fields such as face recognition and image compression
 - finding patterns in data of high dimension

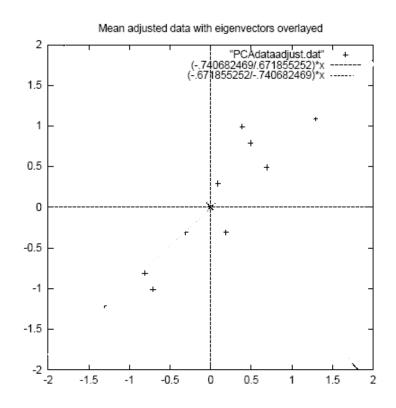
Subtract the mean

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.

DATA:		ZERO MEAN DATA:	
X	У	X	у
2.5	2.4	.69	.49
0.5	0.7	-1.31	-1.21
2.2	2.9	.39	.99
1.9	2.2	.09	.29
3.1	3.0	1.29	1.09
2.3	2.7	.49	.79
2	1.6	.19	31
1	1.1	81	81
1.5	1.6	31	31
1.1	0.9	71	-1.01



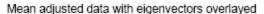


Calculate the covariance matrix

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

 Calculate the eigenvectors and eigenvalues of the covariance matrix

```
eigenvalues = .0490833989
1.28402771
eigenvectors = -.735178656 -.677873399
.677873399 -.735178656
```



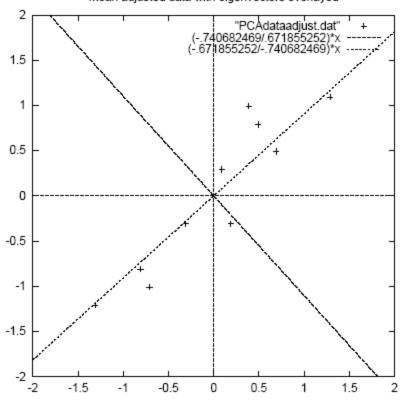


Figure 3.2: A plot of the normalised data (mean subtracted) with the eigenvectors of the covariance matrix overlayed on top.

•eigenvectors are plotted as diagonal dotted lines on the plot.

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.

- 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.

- 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.

Feature Vector

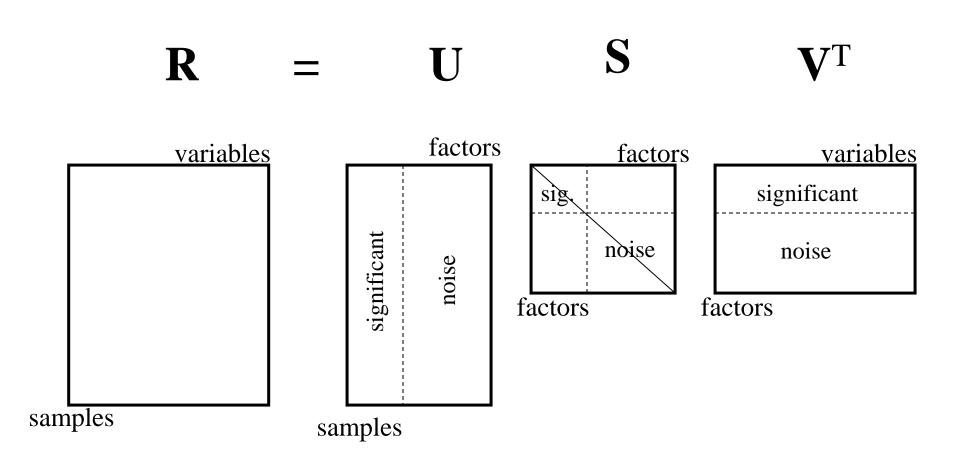
FeatureVector = (eig1 eig2 eig3 ... eign)
We can either form a feature vector with both of the eigenvectors:

```
-.677873399 -.735178656
-.735178656 .677873399
or, we can choose to leave out the smaller, less
```

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

```
- .677873399- .735178656
```

- 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.



- FinalData is the final data set, with data items in columns, and dimensions along rows.
- What will this give us?
 - It will give us the original data solely in terms of the vectors we chose.
- We have changed our data from being in terms of the axes x and y, and now they are in terms of our 2 eigenvectors.

FinalData transpose: dimensions along columns

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

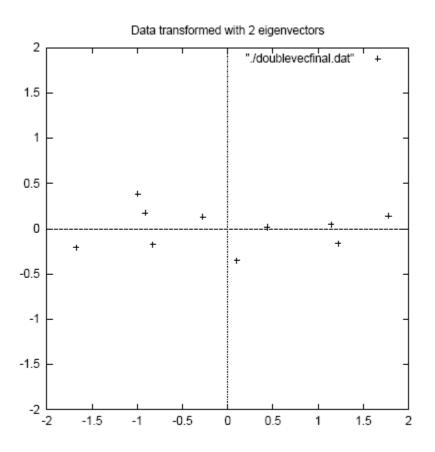


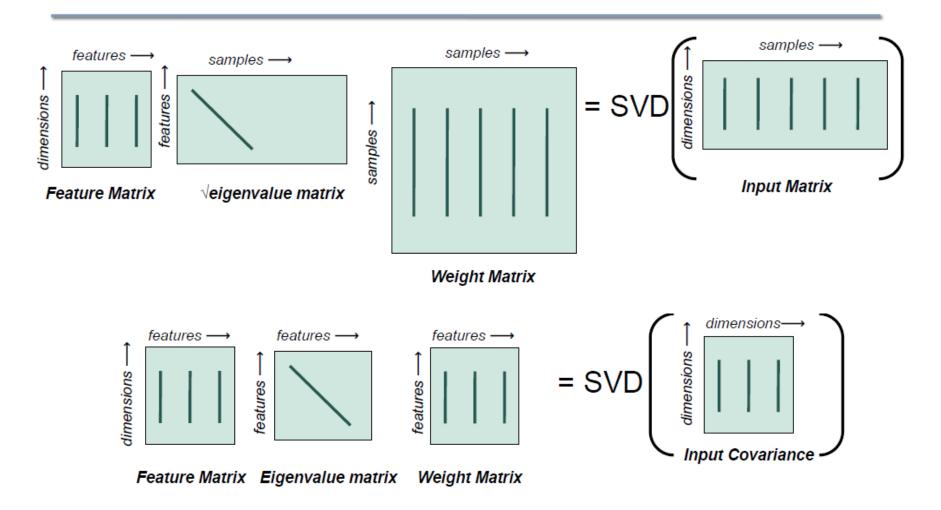
Figure 3.3: The table of data by applying the PCA analysis using both eigenvectors, and a plot of the new data points.

PCA vs SVD

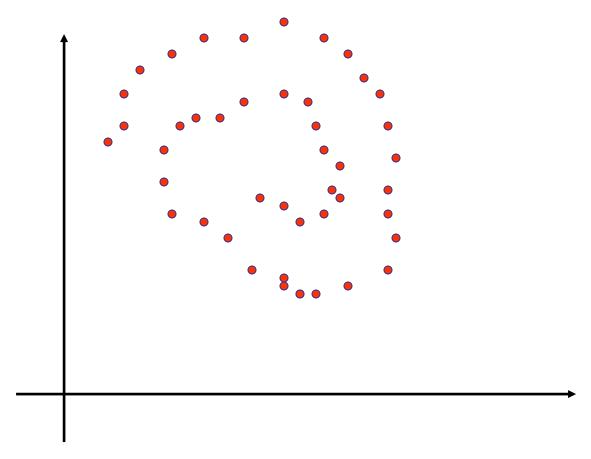
A better way to compute PCA

- SVD
- Why?
 - More stable, robust and fancy extensions!

PCA through the SVD

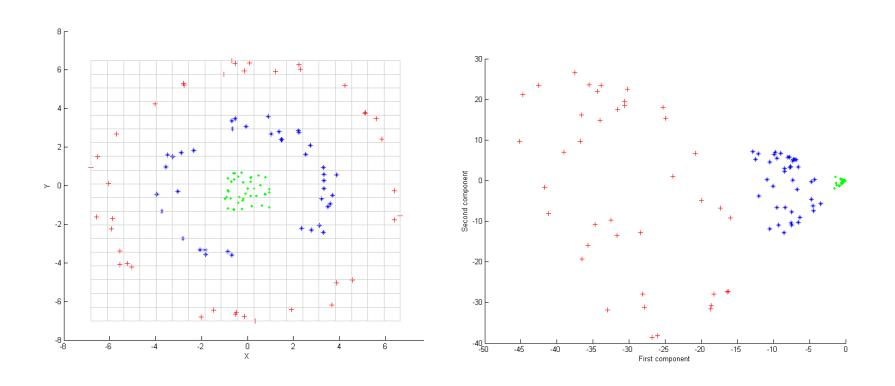


PCA, a Problematic Data Set



PCA cannot capture NON-LINEAR structure!

Kernel PCA



PCA Conclusions

- PCA
 - finds orthonormal basis for data
 - Sorts dimensions in order of "importance"
 - Discard low significance dimensions
- Uses:
 - Get compact description
 - Ignore noise
 - Improve classification (hopefully)
- Not magic:
 - Doesn't know class labels
 - Can only capture linear variations
- One of many tricks to reduce dimensionality!