

# Introduction to Neural Computation

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MIT BCS 9.40 — 2017

Lecture 17  
Principal Components Analysis

# Learning Objectives for Lecture 17

- Eigenvectors and eigenvalues
- Variance and multivariate Gaussian distributions
- Computing a covariance matrix from data
- Principal Components Analysis (PCA)

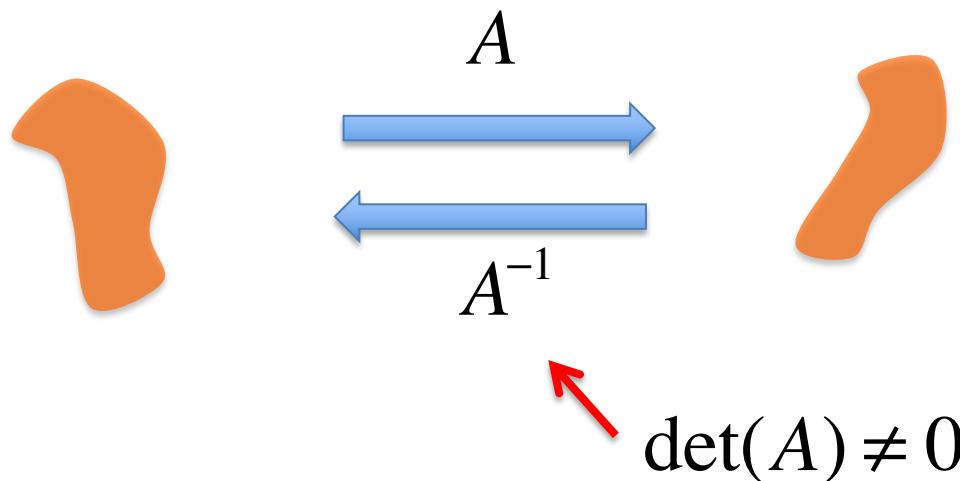
# Learning Objectives for Lecture 17

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# Matrix transformations

$$\vec{y} = A\vec{x}$$

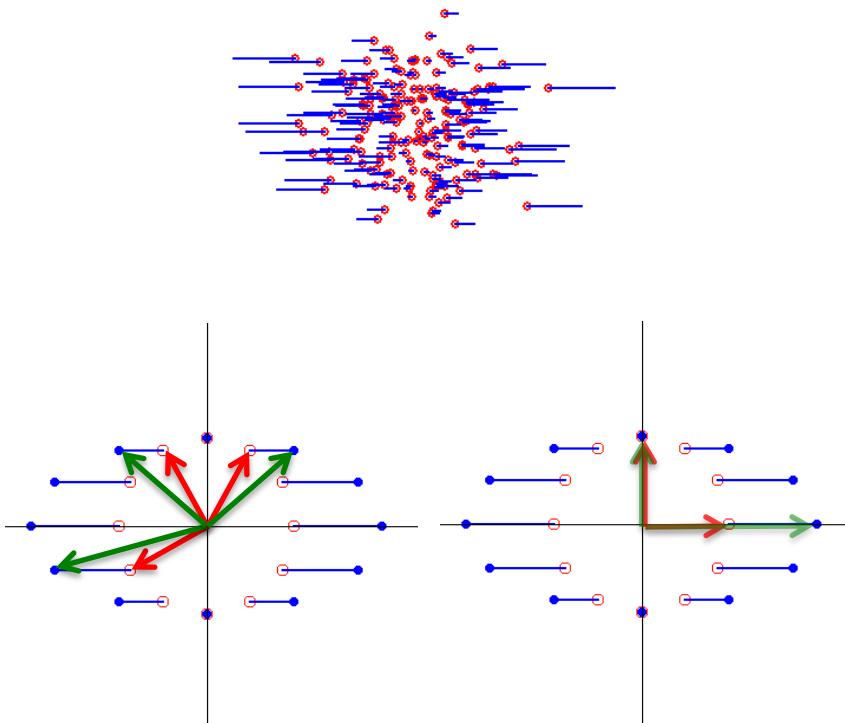
- In general A maps the set of vectors in  $\mathbb{R}^2$  onto another set of vectors in  $\mathbb{R}^2$ .



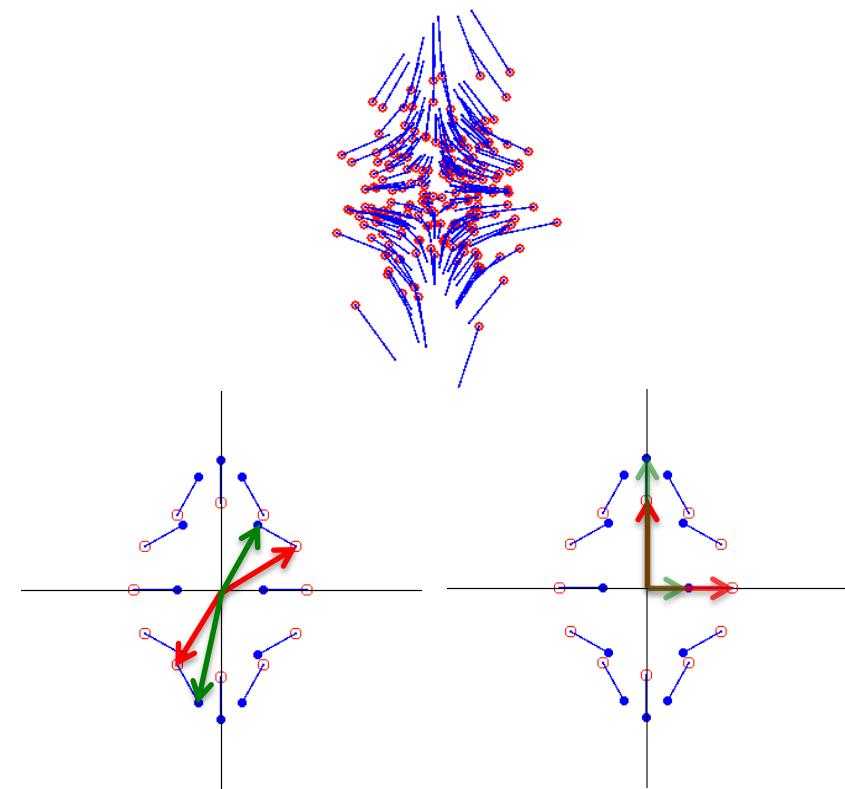
# Eigenvectors and eigenvalues

- Matrix transformations have special directions

$$A = \begin{pmatrix} 1+\delta & 0 \\ 0 & 1 \end{pmatrix}$$



$$A = \begin{pmatrix} 1-\delta & 0 \\ 0 & 1+\delta \end{pmatrix}$$

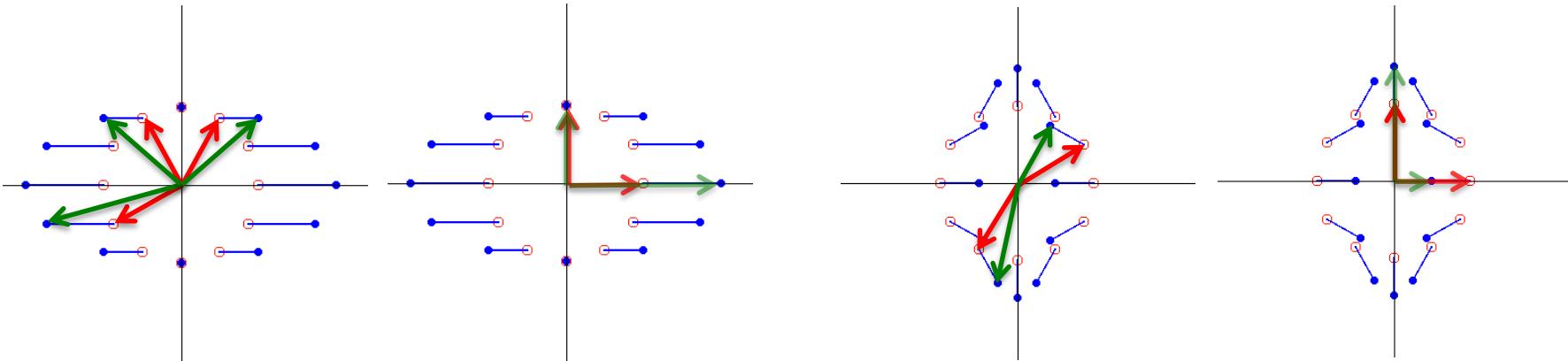


These are all diagonal matrices

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

# Eigenvectors and eigenvalues

- Some vectors are rotated, some are not.



- For a diagonal matrix, vectors along the axes are scaled, but not rotated.

$$\begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \lambda_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \Lambda \hat{e}_1 = \lambda_1 \hat{e}_1$$

$$\begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \lambda_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \Lambda \hat{e}_2 = \lambda_2 \hat{e}_2$$

# Eigenvectors and eigenvalues

- Diagonal matrices have the property that they map any vector parallel to a standard basis vector into another vector along that standard basis vector.

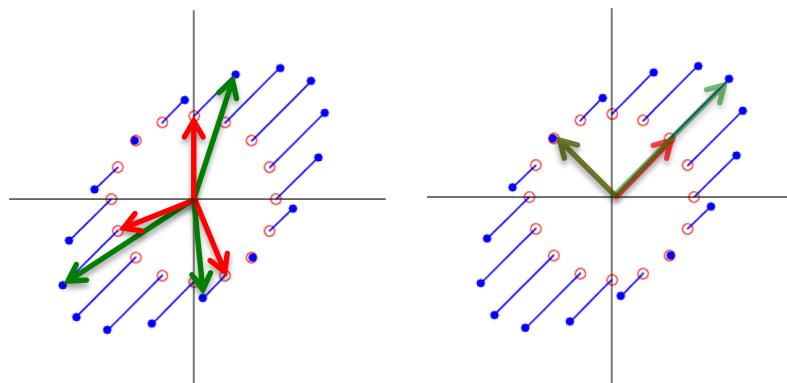
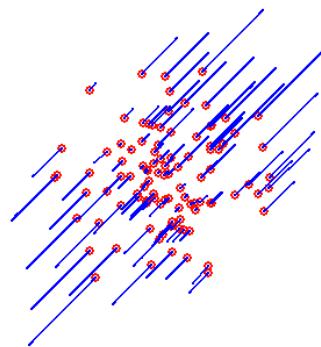
$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix} \quad \text{eigenvalue equation}$$
$$\Lambda \hat{e}_i = \lambda_i \hat{e}_i , \quad i=1,2,\dots,n$$

- Any vector  $\vec{v}$  that is mapped by matrix  $A$  onto a parallel vector  $\lambda \vec{v}$  is called an eigenvector of  $A$ . The scale factor  $\lambda$  is called the eigenvalue of vector  $\vec{v}$ .
- A matrix in  $\mathbb{R}^n$  has  $n$  eigenvectors and  $n$  eigenvalues.

# Eigenvectors and eigenvalues

- What are the special directions of our rotated transformations?

$$A = \Phi \Lambda \Phi^T = \begin{pmatrix} 1.5 & 0.5 \\ 0.5 & 1.5 \end{pmatrix} \quad \Lambda = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix} \quad \Phi(45^\circ) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$



# Eigenvectors and eigenvalues

- What are the eigenvectors and eigenvalues of our rotated transformation  $\Phi \Lambda \Phi^T$ ?

$$A \vec{x}_i = a_i \vec{x}_i$$

$$\Phi \Lambda \Phi^T \vec{x}_i = a_i \vec{x}_i$$

$$\Phi^T \Phi \Lambda \Phi^T \vec{x}_i = \Phi^T (a_i \vec{x}_i)$$

$$\Lambda \Phi^T \vec{x}_i = a_i \Phi^T \vec{x}_i$$

$\hat{e}_i$        $\hat{e}_i$

Remember...

$$\Lambda \hat{e}_i = \lambda_i \hat{e}_i \quad \Lambda = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

So we know the solution if  $\Phi^T \vec{x}_i = \hat{e}_i$

$$\Lambda \hat{e}_i = a_i \hat{e}_i$$

$$\Rightarrow a_i = \lambda_i$$

So the solution to the eigenvalue equation  $\Phi \Lambda \Phi^T \vec{x}_i = a_i \vec{x}_i$  is:

eigenvalues

$$a_i = \lambda_i$$

eigenvectors

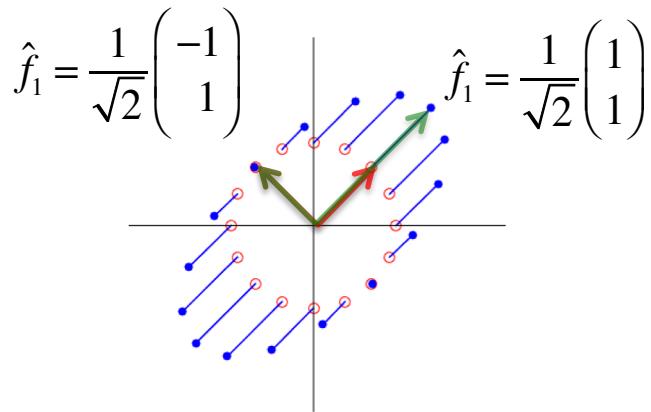
$$\vec{x}_i = \Phi \hat{e}_i$$

what is this?

# Eigenvectors and eigenvalues

- The eigenvectors are just the standard basis vectors rotated by the matrix  $\Phi$  !

$$\vec{x}_i = \Phi \hat{e}_i$$



$$\Phi(45^0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

$$\vec{x}_1 = \Phi \hat{e}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\vec{x}_2 = \Phi \hat{e}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

The eigenvectors are just the columns of  $\Phi$ !

# Eigenvectors and eigenvalues

- In summary, a symmetric matrix  $A$  can always be written as follows:

$$A = \Phi \Lambda \Phi^T$$

where  $\Phi$  is a rotation matrix and  $\Lambda$  is a diagonal matrix

- The eigenvectors of  $A$  are the columns of  $\Phi$  (the basis vectors,  $\hat{f}_i$ )

$$\Phi = \left( \begin{array}{c|c} \hat{f}_1 & \hat{f}_2 \end{array} \right)$$

- The eigenvalue associated with each eigenvector  $\hat{f}_i$  is the diagonal element  $\lambda_i$  of  $\Lambda$ .

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

# Eigenvectors and eigenvalues

- Note that eigenvectors are not unique...

If  $\vec{x}_i$  is an eigenvector of A      then so is  $a\vec{x}_i$

$$A\vec{x}_i = \lambda_i \vec{x}_i \quad A(a\vec{x}_i) = \lambda_i(a\vec{x}_i)$$

... so we usually write eigenvectors as unit vectors

- For a matrix in n-dimensions... there are n different unit eigenvectors
- For a symmetric matrix, the eigenvectors of A are orthogonal (and we write them as unit vectors)...  
... the eigenvectors of A form a complete orthonormal basis set!

# Eigenvectors and eigenvalues

- What are the eigenvalues of a general 2-dim matrix  $A$  ?

$$A\vec{x} = \lambda\vec{x}$$

we only want solutions where

$$A\vec{x} = \lambda I\vec{x}$$

$$\vec{x} \neq 0$$

$$(A - \lambda I)\vec{x} = 0$$

$$\det(A - \lambda I) = 0$$

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad A - \lambda I = \begin{pmatrix} a - \lambda & b \\ c & d - \lambda \end{pmatrix} \quad \det(A - \lambda I) = (a - \lambda)(d - \lambda) - bc$$

$$\det(A - \lambda I) = (a - \lambda)(d - \lambda) - bc = 0$$

$$ad - \lambda(a + d) + \lambda^2 - bc = 0$$

Characteristic equation of matrix  $A$

$$\lambda^2 - (a + d)\lambda + (ad - bc) = 0$$

# Eigenvectors and eigenvalues

- What are the eigenvalues of a general 2-dim matrix?

Characteristic equation of matrix A

$$\lambda^2 - (a+d)\lambda + (ad - bc) = 0$$

- Solutions are given by the quadratic formula

$$\lambda_{\pm} = \frac{1}{2}(a+d) \pm \frac{1}{2}\sqrt{(a-d)^2 + 4bc}$$


eigenvalues can be real, complex, imaginary

# Eigenvectors and eigenvalues

$$\lambda_{\pm} = \frac{1}{2}(a+d) \pm \frac{1}{2}\sqrt{(a-d)^2 + 4bc}$$

- For a symmetric matrix

$$A = \begin{pmatrix} a & b \\ b & d \end{pmatrix}$$

$$\lambda_{\pm} = \frac{1}{2}(a+d) \pm \frac{1}{2}\sqrt{(a-d)^2 + 4b^2}$$

$\underbrace{\phantom{(a-d)^2}}_{\geq 0}$

$$A = \begin{pmatrix} 3/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}$$

$$\lambda_{\pm} = \frac{1}{2}\left(\frac{3}{2} + \frac{1}{2}\right) \pm \frac{1}{2}\sqrt{\left(\frac{3}{2} - \frac{1}{2}\right)^2 + 4\left(\frac{1}{2}\right)^2}$$

The eigenvalues of a symmetric matrix are always real.

$$\lambda_{\pm} = 1 \pm \frac{\sqrt{2}}{2}$$

# Eigenvectors and eigenvalues

- Let's consider a special case of a symmetric matrix

$$A = \begin{pmatrix} a & b \\ b & a \end{pmatrix}$$

$$\lambda_{\pm} = \frac{1}{2}(a+d) \pm \frac{1}{2}\sqrt{(a-d)^2 + 4b^2}$$

$$\lambda_+ = a+b \quad \lambda_- = a-b$$

$$A\vec{x}_+ = \lambda_+\vec{x}_+$$

$$\begin{pmatrix} a & b \\ b & a \end{pmatrix}\vec{x}_+ = (a+b)\vec{x}_+$$

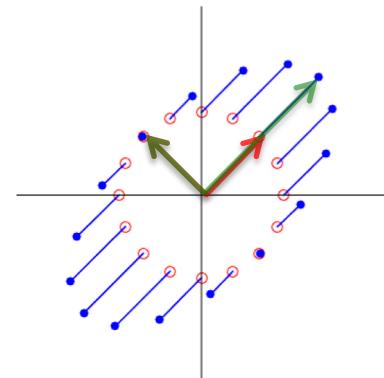
$$\begin{pmatrix} a & b \\ b & a \end{pmatrix}\vec{x}_+ = \begin{pmatrix} a+b & 0 \\ 0 & a+b \end{pmatrix}\vec{x}_+$$

$$\begin{pmatrix} -b & b \\ b & -b \end{pmatrix}\vec{x}_+ = 0$$

$$\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0$$

$$\begin{aligned} x_1 &= s \\ x_2 &= s \end{aligned}$$

$$\vec{x}_+ = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \vec{x}_- = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$



# Eigen-decomposition

- The process of writing a matrix  $A$  as  $A = \Phi\Lambda\Phi^T$  is called eigen-decomposition. It works for any symmetric matrix.
  - the eigenvalues  $\lambda_i$  are real numbers
  - the eigenvectors  $\hat{f}_i$  form an orthogonal basis set

- Let's rewrite...

$$A = \Phi\Lambda\Phi^T \quad \Lambda = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$
$$A\Phi = \Phi\Lambda\Phi^T\Phi$$

- Eigenvalue equation

$$A\Phi = \Phi\Lambda$$

is equivalent to the set of equations

$$A\hat{f}_i = \lambda_i \hat{f}_i$$

# Eigenvectors and eigenvalues

- Matlab has a function 'eig' to calculate eigenvectors and eigenvalues

$$A = FVF^T$$

```
>> A=[1.5 0.5;0.5 1.5]
A =
    1.5000    0.5000
    0.5000    1.5000
```

```
>> [F,V]=eig(A)
```

```
F =
```

-0.7071	0.7071
0.7071	0.7071

```
V =
```

1	0
0	2

```
>> F*V*F'
```

```
ans =
```

1.5000	0.5000
0.5000	1.5000

# Learning Objectives for Lecture 17

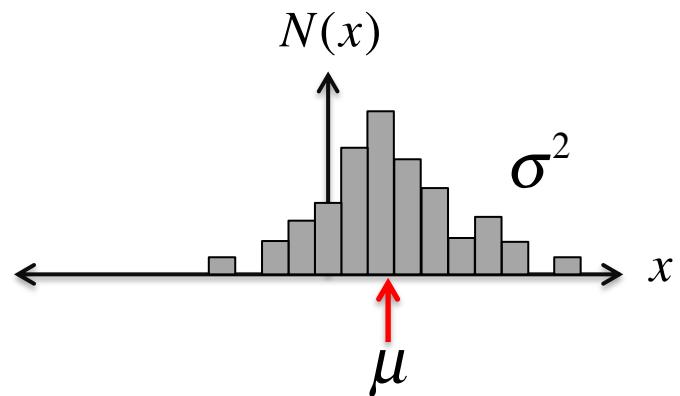
- Eigenvectors and eigenvalues
- Variance and multivariate Gaussian distributions
- Computing a covariance matrix from data
- Principal Components Analysis (PCA)

# Variance

- Let's say we have  $m$  observations of a variable  $x$

$$x^{(j)}, j=1,2,3,\dots,m$$

$\downarrow$   
 $j^{\text{th}}$  observation of  $x$

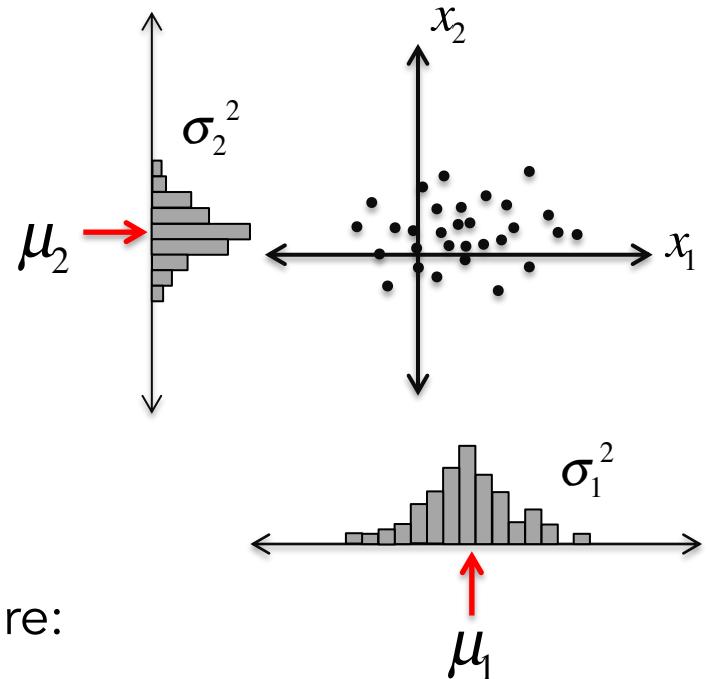


- The mean of these observations is  $\mu = \langle x \rangle = \frac{1}{m} \sum_{i=1}^m x^{(i)}$
- The variance is  $\sigma^2 = \frac{1}{m} \sum_{i=1}^m (x^{(i)} - \mu)^2$

# Variance

- Now let's say we have m simultaneous observations of variables and .

$$\begin{pmatrix} x_1^{(j)} \\ x_2^{(j)} \end{pmatrix}, j = 1, 2, 3, \dots, m$$



- The mean and variance of  $x_1$  and  $x_2$  are:

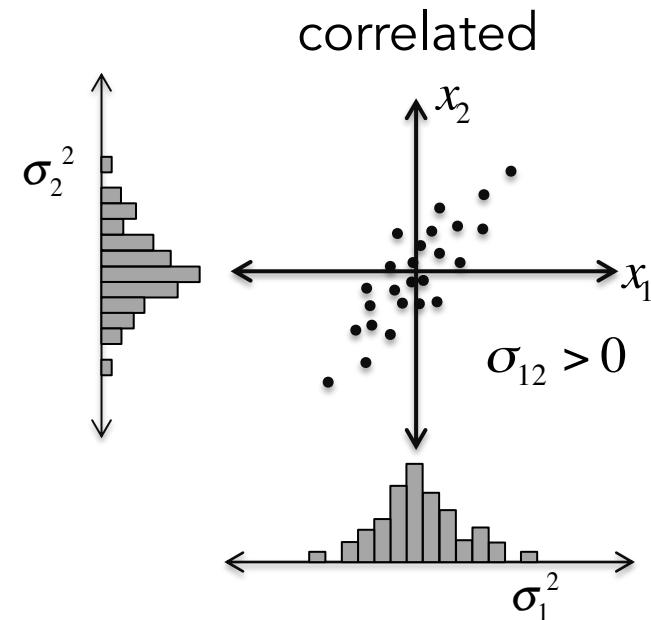
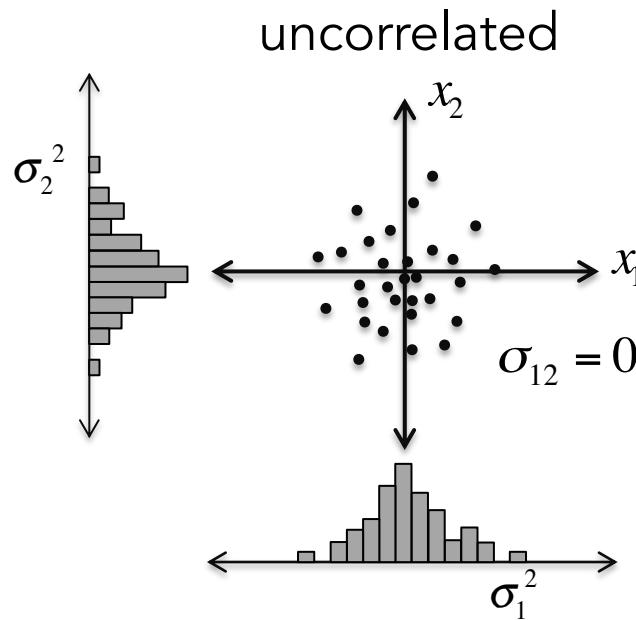
$$\mu_1 = \frac{1}{m} \sum_{j=1}^m x_1^{(j)}$$

$$\mu_2 = \frac{1}{m} \sum_{j=1}^m x_2^{(j)}$$

$$\sigma_1^2 = \frac{1}{m} \sum_{j=1}^m (x_1^{(j)} - \mu_1)^2$$

$$\sigma_2^2 = \frac{1}{m} \sum_{j=1}^m (x_2^{(j)} - \mu_2)^2$$

# Covariance



- $x_1$  has the same variance in both of these cases... also  $x_2$
- So we need another measure to describe the relation between  $x_1$  and  $x_2$ .

covariance

$$\sigma_{12} = \frac{1}{m} \sum_{j=1}^m (x_1^{(j)} - \mu_1)(x_2^{(j)} - \mu_2)$$

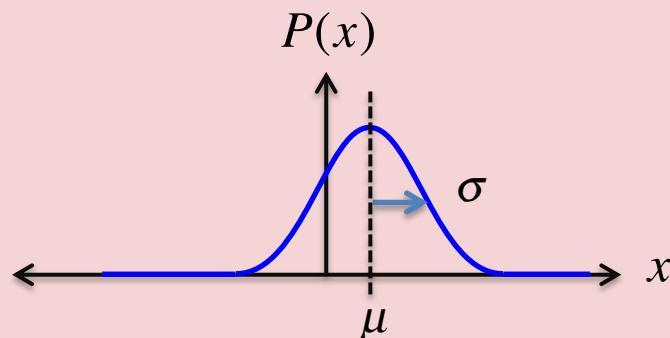
correlation

$$\rho = \frac{\sigma_{12}}{\sqrt{\sigma_1^2 \sigma_2^2}}$$

# Gaussian distribution

- Many kinds of data can be fit by a Gaussian distribution

If  $x$  is a Gaussian random variable



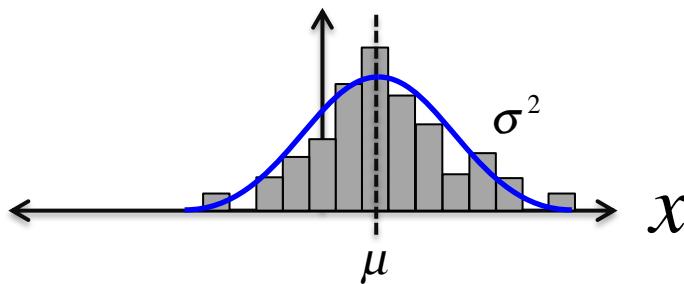
probability 'density'

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

- Gaussian is defined by only its mean and variance.

To find the Gaussian that best fits our data –

Just measure the mean and variance!



# Gaussian distribution

- We are going develop a description of Gaussian distributions in higher dimensions
- Develop deep insights into high-dimensional data
- We will develop this description using vector and matrix notation
  - vectors and matrices are the natural format to manipulate data sets
  - very compact notation
  - manipulations are trivial in Matlab

# Multivariate Gaussian distribution

- We can create a Gaussian distribution in two dimensions

Two independent Gaussian random variables  $x_1$  and  $x_2$

$$P(x_1, x_2) = P(x_1)P(x_2)$$

$$= \beta e^{-\frac{1}{2}x_1^2} e^{-\frac{1}{2}x_2^2}$$

normalization to

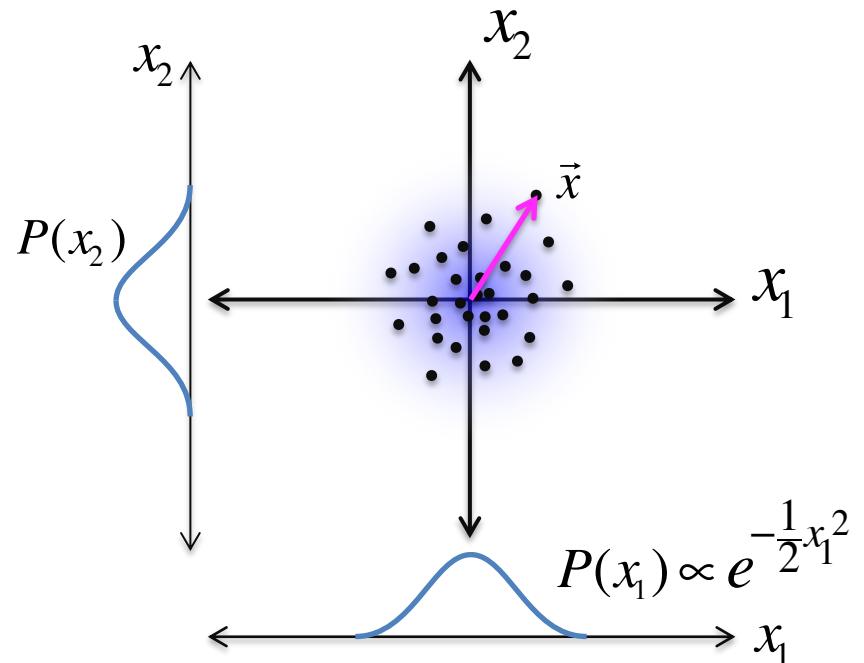
make total prob = 1

$$= \beta e^{-\frac{1}{2}(x_1^2+x_2^2)}$$

$$P(\vec{x}) = \beta e^{-\frac{1}{2}d^2}$$

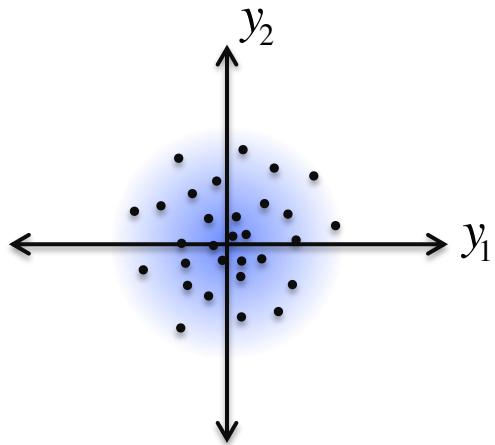
$$d^2 = |\vec{x}|^2 = \vec{x}^T \vec{x}$$

$d$  = Mahalanobis Distance



Isotropic multivariate Gaussian distribution

# Multivariate Gaussian distribution

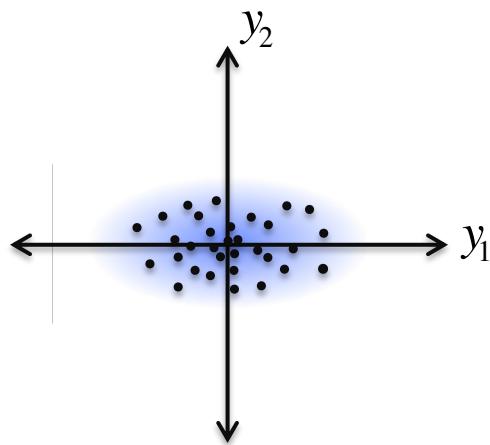


Isotropic

$$P(\vec{y}) = \beta e^{-\frac{1}{2\sigma^2} \vec{y}^T \vec{y}}$$

$$\sigma^2$$

variance

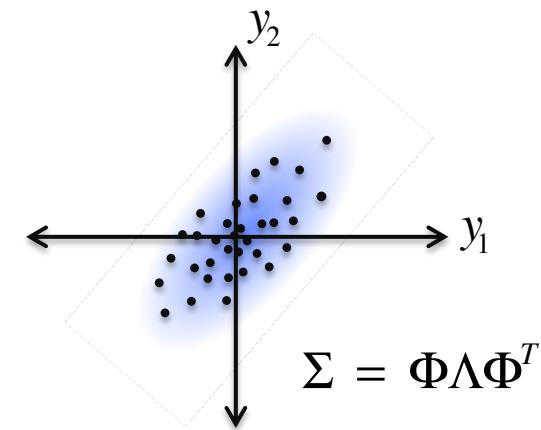


Non-isotropic:  
no correlation

$$P(\vec{y}) = \beta e^{-\frac{1}{2} \vec{y}^T \Lambda^{-1} \vec{y}}$$

$$\Lambda = \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix}$$

variance matrix



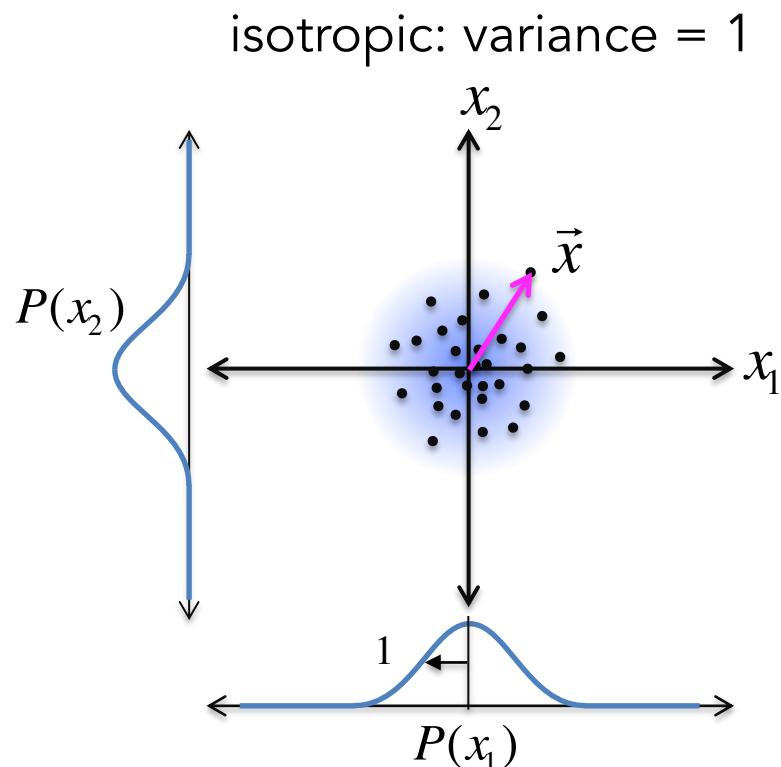
Non-isotropic:  
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$$P(\vec{y}) = \beta e^{-\frac{1}{2} \vec{y}^T \Sigma^{-1} \vec{y}}$$

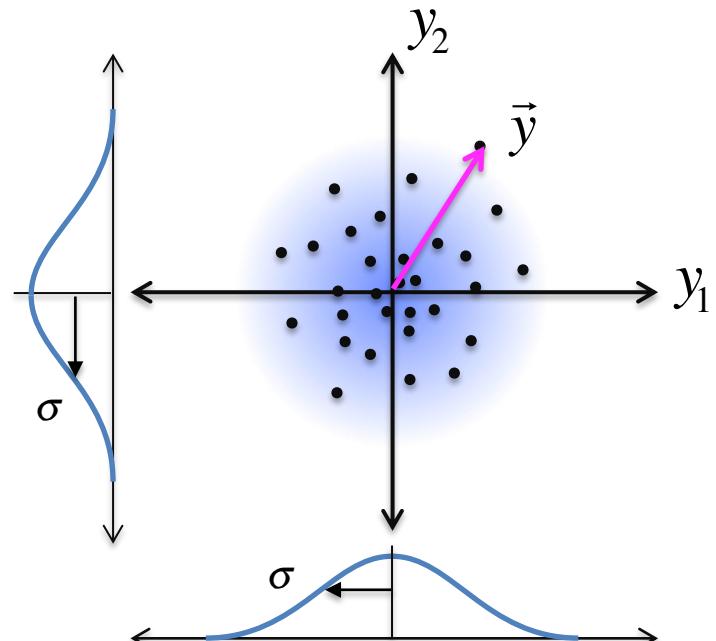
$$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{pmatrix}$$

covariance matrix

# Multivariate Gaussian distribution



isotropic: variance =  $\sigma^2$



$$\vec{y} = \sigma \vec{x}$$

# Multivariate Gaussian distribution

$$P(\vec{y}) = ?$$

$$\vec{y} = \boldsymbol{\sigma} \vec{x}$$

$$P(\vec{x}) = \beta e^{-\frac{1}{2}\vec{x}^T \vec{x}}$$

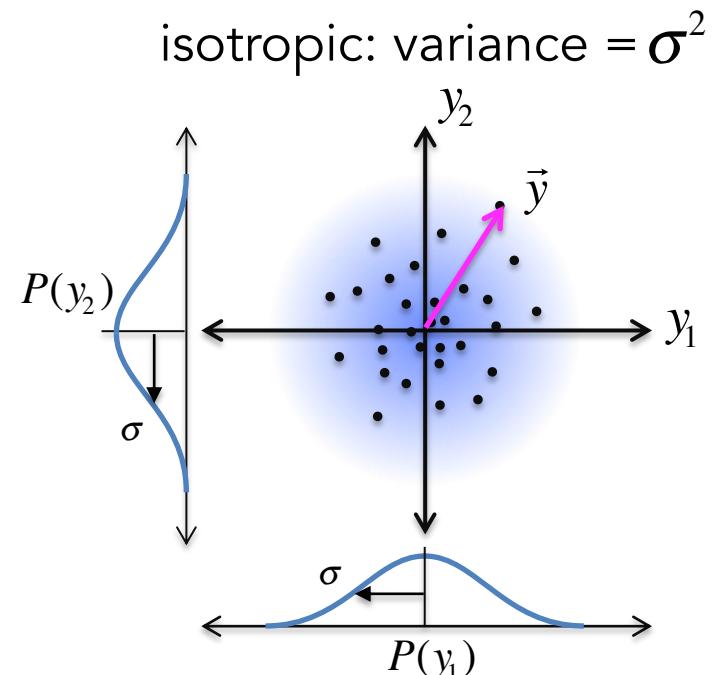
$$\vec{x} = \boldsymbol{\sigma}^{-1} \vec{y}$$

What is the Mahalanobis distance?

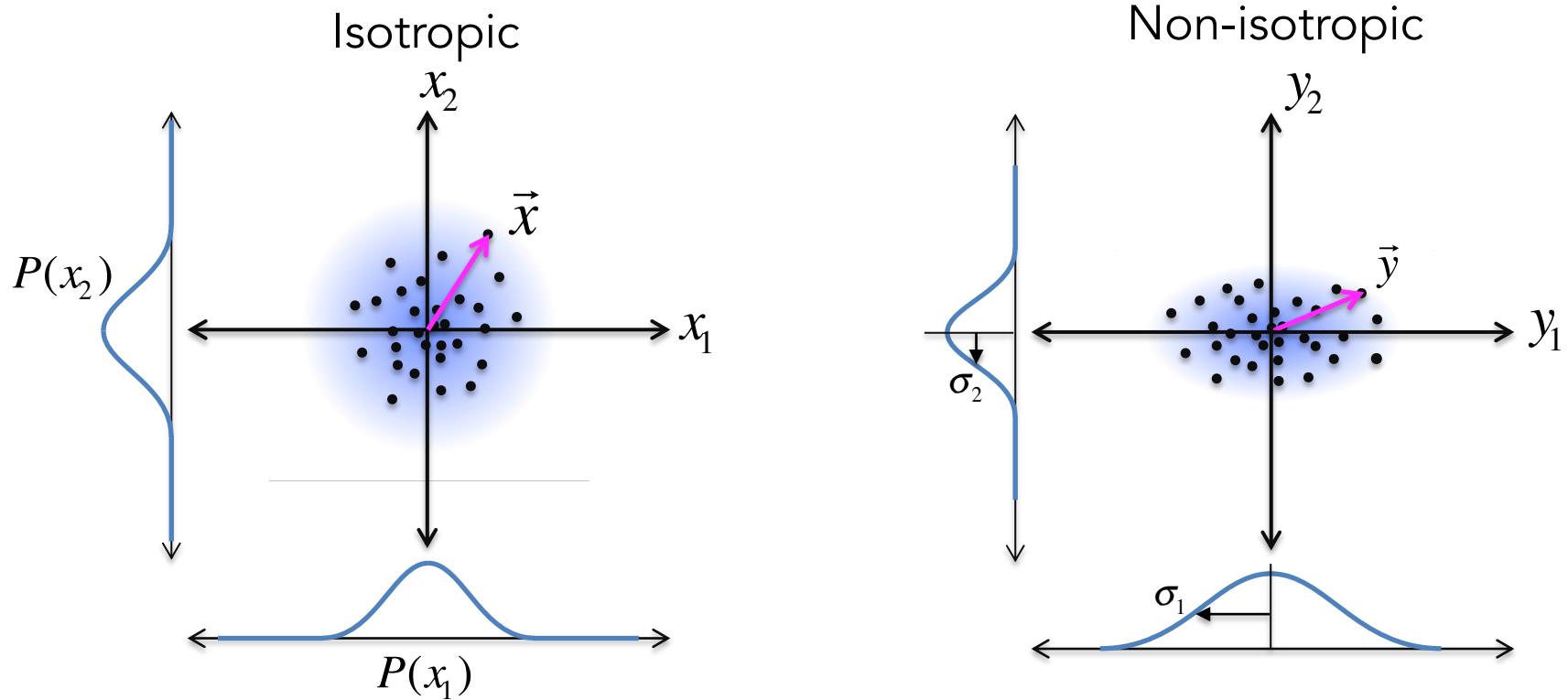
$$\begin{aligned} d^2 &= \vec{x}^T \vec{x} = (\boldsymbol{\sigma}^{-1} \vec{y})^T (\boldsymbol{\sigma}^{-1} \vec{y}) \\ &= \vec{y}^T \boldsymbol{\sigma}^{-1} \boldsymbol{\sigma}^{-1} \vec{y} \end{aligned}$$

$$d^2 = \vec{y}^T \boldsymbol{\sigma}^{-2} \vec{y}$$

$$\begin{aligned} P(\vec{y}) &= \beta e^{-\frac{1}{2} \left( \frac{\vec{y}^T \vec{y}}{\sigma^2} \right)} \\ &= \beta e^{-\frac{1}{2} \frac{|\vec{y}|^2}{\sigma^2}} \end{aligned}$$



# Multivariate Gaussian distribution



$$\vec{y} = S \vec{x}$$

$$S = \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{pmatrix}$$

# Multivariate Gaussian distribution

$$\vec{y} = S\vec{x} \quad \vec{x} = S^{-1}\vec{y}$$

What is the Mahalanobis distance?

$$d^2 = \vec{x}^T \vec{x} = \left( S^{-1} \vec{y} \right)^T \left( S^{-1} \vec{y} \right)$$

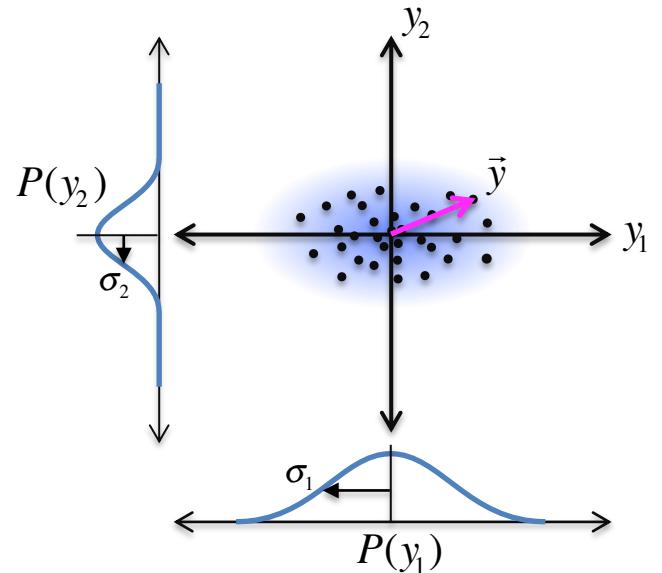
$$= \vec{y}^T S^{-1} S^{-1} \vec{y}$$

$$= \vec{y}^T S^{-2} \vec{y}$$

$$d^2 = \vec{y}^T \Lambda^{-1} \vec{y}$$

$$\Lambda^{-1} = S^{-2} = \begin{pmatrix} \sigma_1^{-2} & 0 \\ 0 & \sigma_2^{-2} \end{pmatrix}$$

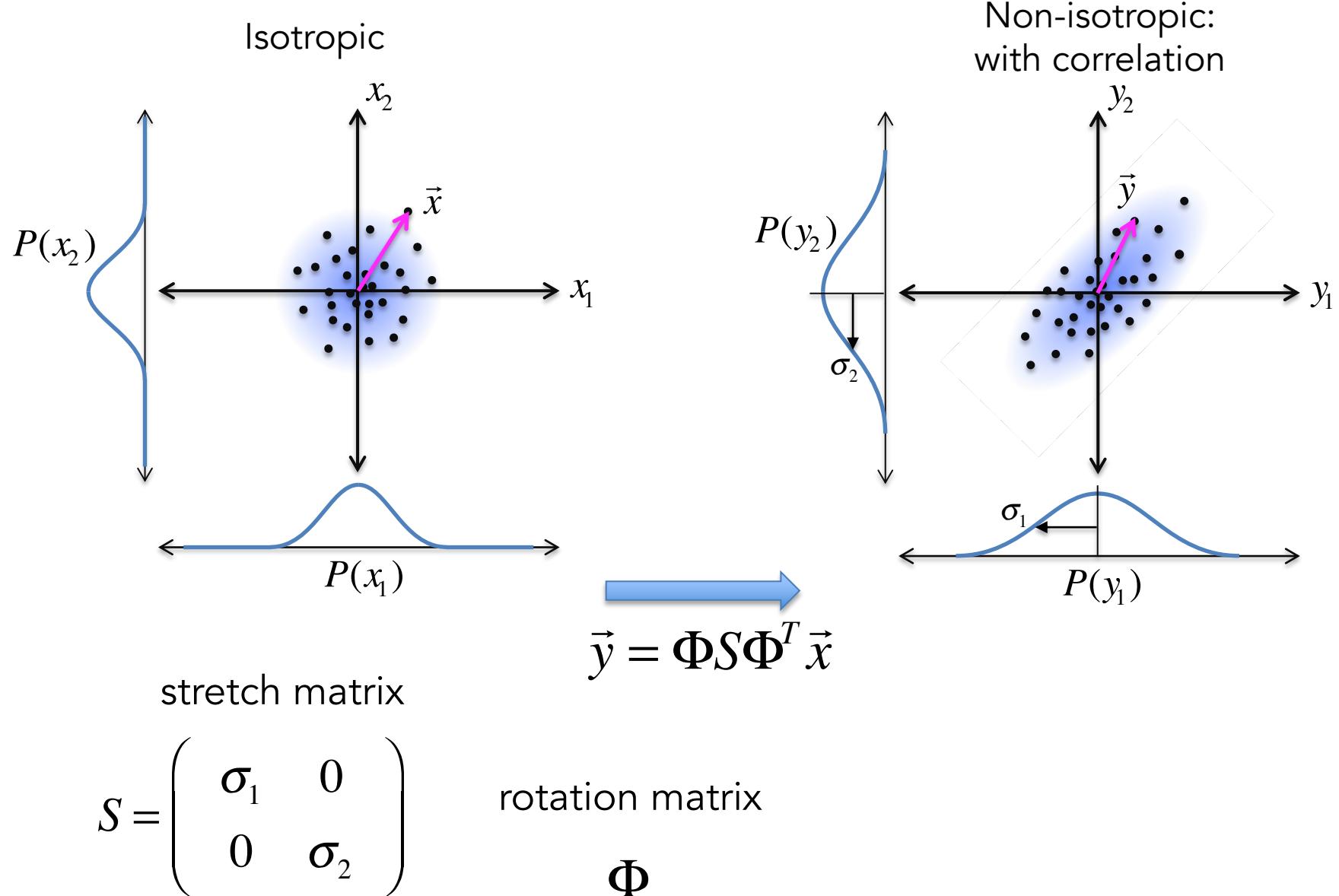
$$P(\vec{y}) = \beta e^{-\frac{1}{2}\vec{y}^T \Lambda^{-1} \vec{y}} = \beta e^{-\frac{1}{2}\left(\frac{y_1^2}{\sigma_1^2} + \frac{y_2^2}{\sigma_2^2}\right)}$$



$$\Lambda = \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix}$$

matrix of variances

# Multivariate Gaussian distribution



# Covariance matrix

$$\vec{y} = \Phi S \Phi^T \vec{x} \quad \vec{x} = \Phi S^{-1} \Phi^T \vec{y}$$

What is the Mahalanobis distance?

$$d^2 = \vec{x}^T \vec{x} = (\Phi S^{-1} \Phi^T \vec{y})^T (\Phi S^{-1} \Phi^T \vec{y})$$

$$= \vec{y}^T \Phi S^{-1} \Phi^T \Phi S^{-1} \Phi^T \vec{y}$$

$$= \vec{y}^T \Phi S^{-2} \Phi^T \vec{y}$$

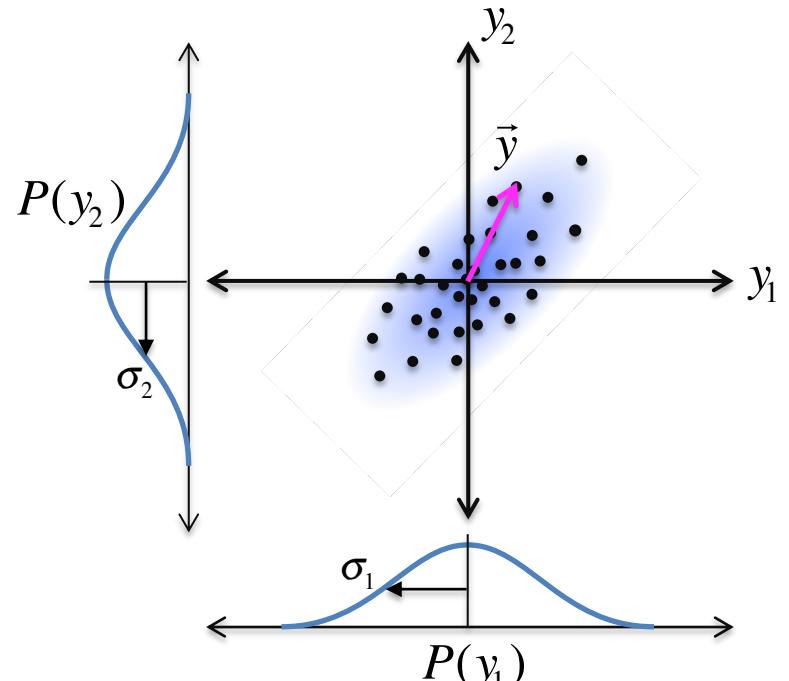
$$= \vec{y}^T \Phi \Lambda^{-1} \Phi^T \vec{y}$$

$$d^2 = \underbrace{\vec{y}^T \Sigma^{-1} \vec{y}}$$

$$P(\vec{y}) = \beta e^{-\frac{1}{2} \vec{y}^T \Sigma^{-1} \vec{y}}$$

$$\Sigma^{-1} = \Phi \Lambda^{-1} \Phi^T$$

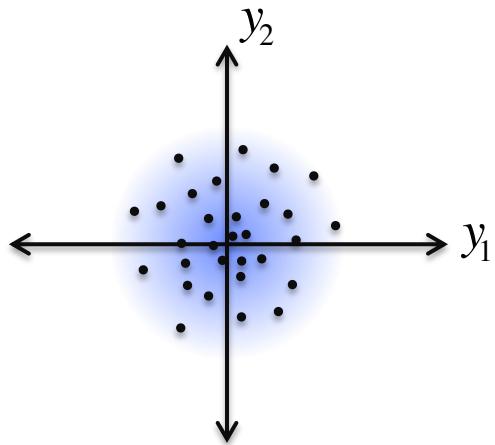
$$\Sigma = \Phi \Lambda \Phi^T$$



$$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{pmatrix}$$

covariance matrix

# Multivariate Gaussian distribution

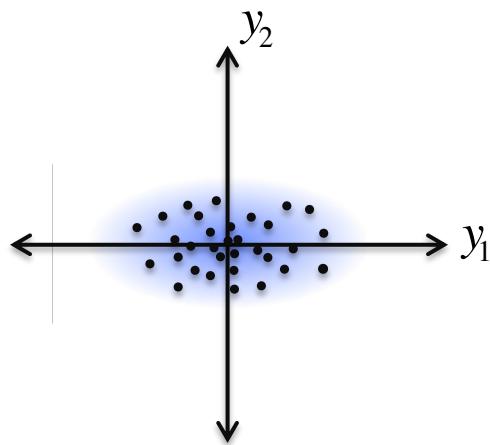


Isotropic

$$P(\vec{y}) = \beta e^{-\frac{1}{2\sigma^2} \vec{y}^T \vec{y}}$$

$$\sigma^2$$

variance

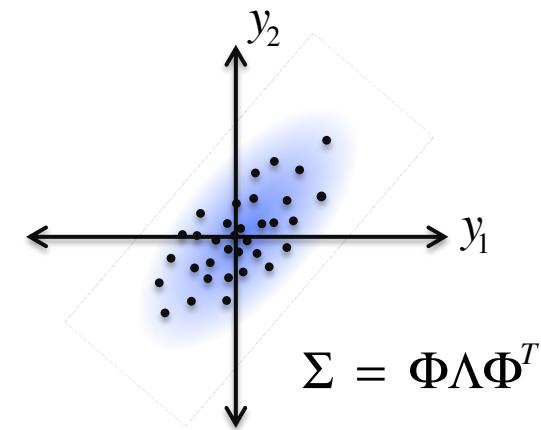


Non-isotropic:  
no correlation

$$P(\vec{y}) = \beta e^{-\frac{1}{2} \vec{y}^T \Lambda^{-1} \vec{y}}$$

$$\Lambda = \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix}$$

variance matrix



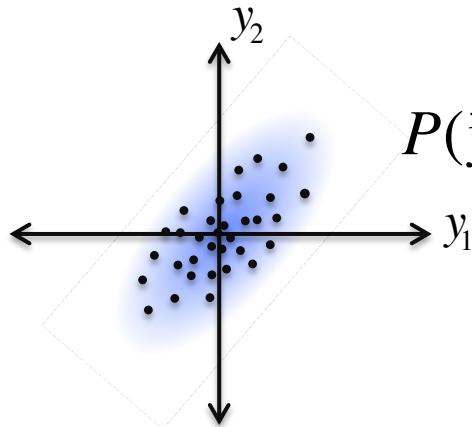
Non-isotropic:  
with correlation

$$P(\vec{y}) = \beta e^{-\frac{1}{2} \vec{y}^T \Sigma^{-1} \vec{y}}$$

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{pmatrix}$$

covariance matrix

# Eigen-decomposition of the covariance matrix



$$P(\vec{y}) = \beta e^{-\frac{1}{2}\vec{y}^T \Sigma^{-1} \vec{y}}$$

$$\Sigma^{-1} = \Phi \Lambda^{-1} \Phi^T$$

$$\Sigma = \Phi \Lambda \Phi^T$$

- Thus, our covariance matrix is just a transformation matrix that turns an isotropic Gaussian distribution (of variance 1) into non-isotropic multivariate Gaussian.
- The eigenvectors of the covariance matrix are just the basis vectors of the rotated transformation.
- And the eigenvalues of the covariance matrix are the variances of the Gaussian in the directions of these basis vectors.

# Learning Objectives for Lecture 17

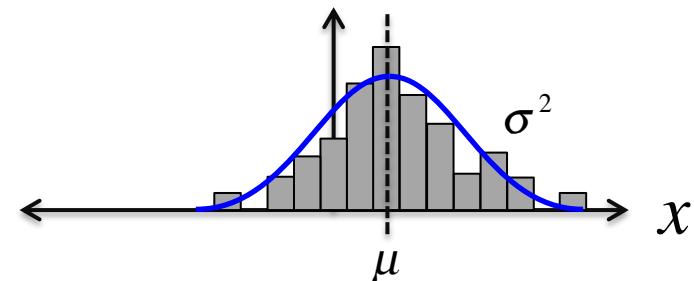
- Eigenvectors and eigenvalues
- Variance and multivariate Gaussian distributions
- Computing a covariance matrix from data
- Principal Components Analysis (PCA)

# How do we fit a Gaussian to multivariate data?

- In 1-dimension

To find the Gaussian that best fits our data –

Just measure the mean and variance!

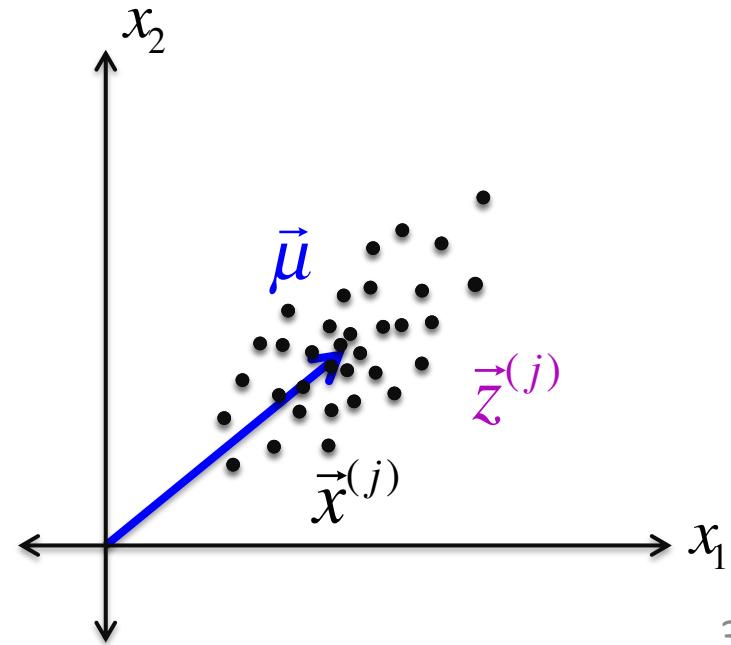


- Compute the covariance matrix!

$$\vec{x}^{(j)}, j = 1, 2, 3, \dots, m$$

- First we subtract the mean

$$\vec{z}^{(j)} = \vec{x}^{(j)} - \vec{\mu} \quad \vec{\mu} = \frac{1}{m} \sum_{j=1}^m \vec{x}^{(j)}$$



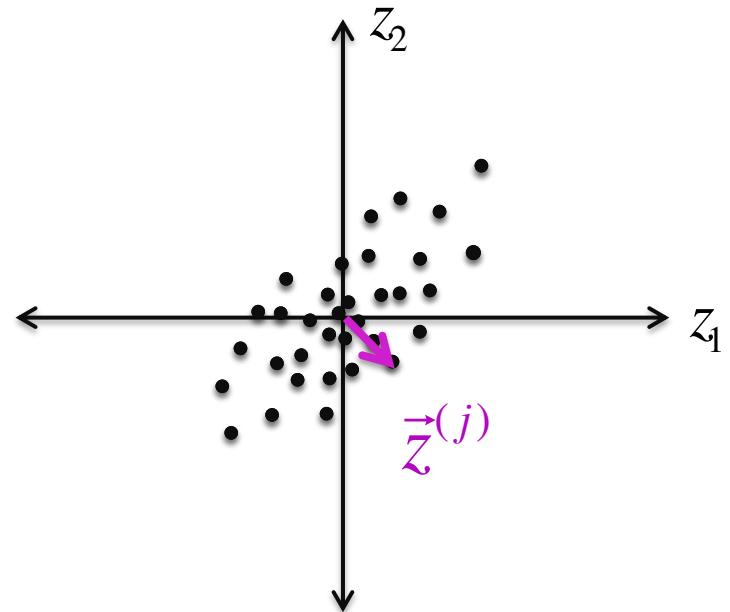
# Computing the covariance matrix from data

- Compute the covariance matrix of a set of multivariate observations

$$\vec{x}^{(j)}, j = 1, 2, 3, \dots, m$$

- First we subtract the mean

$$\vec{z}^{(j)} = \vec{x}^{(j)} - \vec{\mu} \quad \vec{\mu} = \frac{1}{m} \sum_{j=1}^m \vec{x}^{(j)}$$



$$\sum = \begin{pmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{21} & \sigma_2^2 \end{pmatrix} = \begin{pmatrix} \sigma_1^2 = \frac{1}{m} \sum_{j=1}^m z_1^{(j)} z_1^{(j)} & \sigma_{12} = \frac{1}{m} \sum_{j=1}^m z_1^{(j)} z_2^{(j)} \\ \sigma_{21} = \frac{1}{m} \sum_{j=1}^m z_2^{(j)} z_1^{(j)} & \sigma_2^2 = \frac{1}{m} \sum_{j=1}^m z_2^{(j)} z_2^{(j)} \end{pmatrix}$$

# Outer product

- We are going to implement a useful trick called the vector 'outer product'.

Inner product

$$\vec{z}^T \vec{z} = \begin{pmatrix} z_1 & z_2 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = |\vec{z}|^2$$

1 x 2      2 x 1      1 x 1

$$\vec{z} = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}$$

Outer product

$$\vec{z} \vec{z}^T = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \begin{pmatrix} z_1 & z_2 \end{pmatrix} = \begin{pmatrix} z_1 z_1 & z_1 z_2 \\ z_1 z_2 & z_2 z_2 \end{pmatrix}$$

2 x 1      1 x 2      2 x 2

# Computing the covariance matrix

- The covariance matrix has a simpler form using outer product.

$$\vec{z}^{(j)} = \begin{pmatrix} z_1^{(j)} \\ z_2^{(j)} \end{pmatrix}$$

$$\frac{1}{m} \sum_{j=1}^m \vec{z}^{(j)} (\vec{z}^{(j)})^T = \frac{1}{m} \sum_{j=1}^m \begin{pmatrix} z_1^{(j)} z_1^{(j)} & z_1^{(j)} z_2^{(j)} \\ z_2^{(j)} z_1^{(j)} & z_2^{(j)} z_2^{(j)} \end{pmatrix}$$

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{21} & \sigma_{22}^2 \end{pmatrix}$$

# Computing the covariance matrix

- Representing data as a matrix
- We have  $m$  observations of vector  $\vec{z}$
- Put them in matrix form as follows

$$\vec{z}^{(j)} = \begin{pmatrix} z_1^{(j)} \\ z_2^{(j)} \end{pmatrix}, j = 1 \dots m$$

$$Z = (\vec{z}^{(1)} \ \vec{z}^{(2)} \ \vec{z}^{(3)} \ \dots \ \vec{z}^{(m)})$$

$j = 1 \quad 2 \quad 3 \quad \dots \quad m$  = number of samples

$$Z = \begin{pmatrix} z_{11} & z_{12} & z_{13} & \cdots & z_{1m} \\ z_{21} & z_{22} & z_{23} & \cdots & z_{2m} \end{pmatrix} n$$

$n \times m$

dimension of  
data vector = 2

# Computing the covariance matrix

- Now finding the covariance matrix is trivial!

$$\Sigma = \frac{1}{m} Z Z^T$$

$$= \frac{1}{m} \begin{pmatrix} z_{11} & z_{12} & z_{13} & \cdots & z_{1m} \\ z_{21} & z_{22} & z_{23} & \cdots & z_{2m} \end{pmatrix} \begin{pmatrix} z_{11} & z_{21} \\ z_{12} & z_{22} \\ z_{13} & z_{23} \\ \vdots & \vdots \\ z_{1m} & z_{2m} \end{pmatrix} = \begin{pmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{21} & \sigma_{22}^2 \end{pmatrix}$$

$2 \times m$                                      $m \times 2$                                      $2 \times 2$

# Subtracting the mean

- The covariance calculation we just did assumes the data were mean-subtracted. How to subtract the mean?
- We have  $m$  observations of vector  $\vec{x}$

$$X = \begin{pmatrix} x_{11} & x_{12} & x_{13} & \cdots & x_{1m} \\ x_{21} & x_{22} & x_{23} & \cdots & x_{2m} \end{pmatrix}_{n \times m} \rightarrow \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}$$

- First compute the mean in matrix notation and make a matrix with  $m$  copies of this column vector.

`Mu=mean(X,2);`

`MU=repmat(mu,1,m);`

$$M = \begin{pmatrix} \mu_1 & \mu_1 & \mu_1 & \cdots & \mu_1 \\ \mu_2 & \mu_2 & \mu_2 & \cdots & \mu_2 \end{pmatrix}_{n \times m}$$

- Now subtract this from  $X$  to get  $Z$

$$Z=X-MU;$$

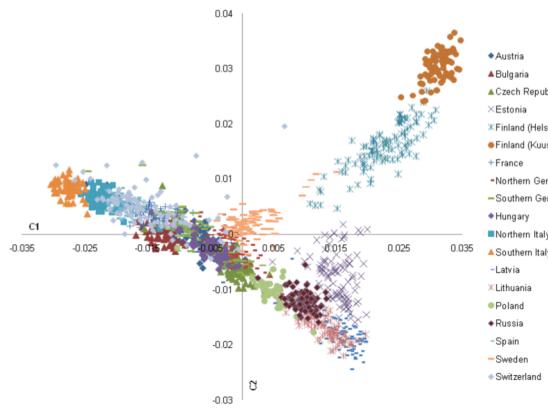
# Learning Objectives for Lecture 17

- Eigenvectors and eigenvalues
- Variance and multivariate Gaussian distributions
- Computing a covariance matrix from data
- Principal Components Analysis (PCA)

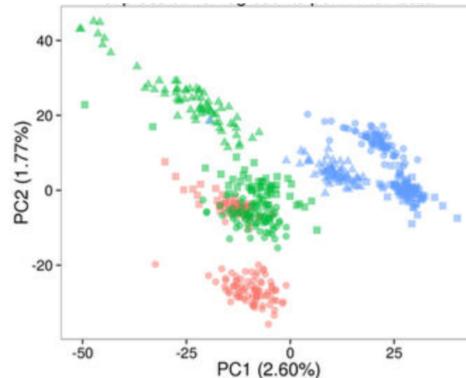
# Principal Components Analysis

- A method for finding the directions in high-dimensional data that contain information.

Genetic profiling



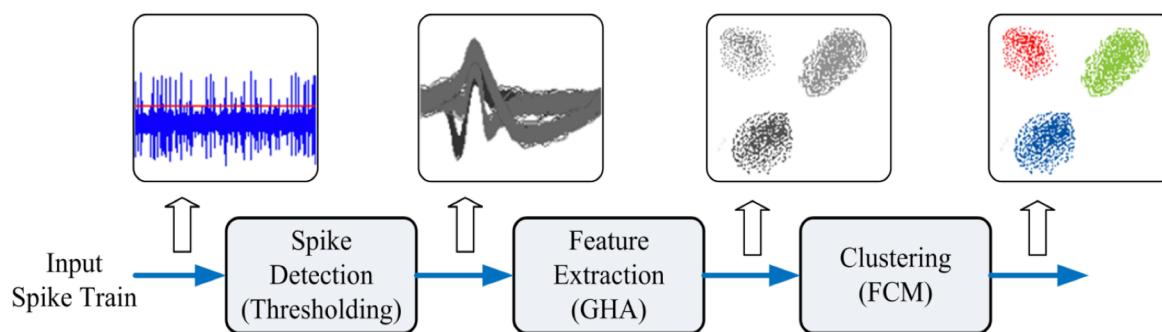
Single-cell transcriptional profiling



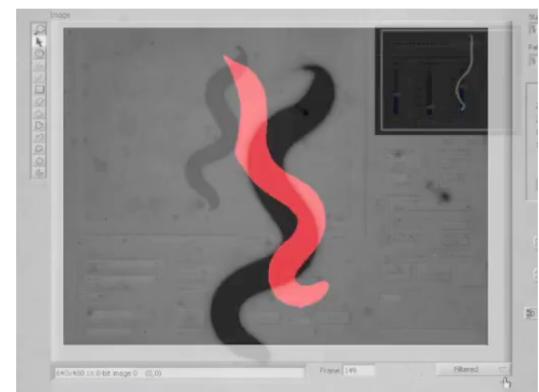
Eigenfaces



Spike Sorting

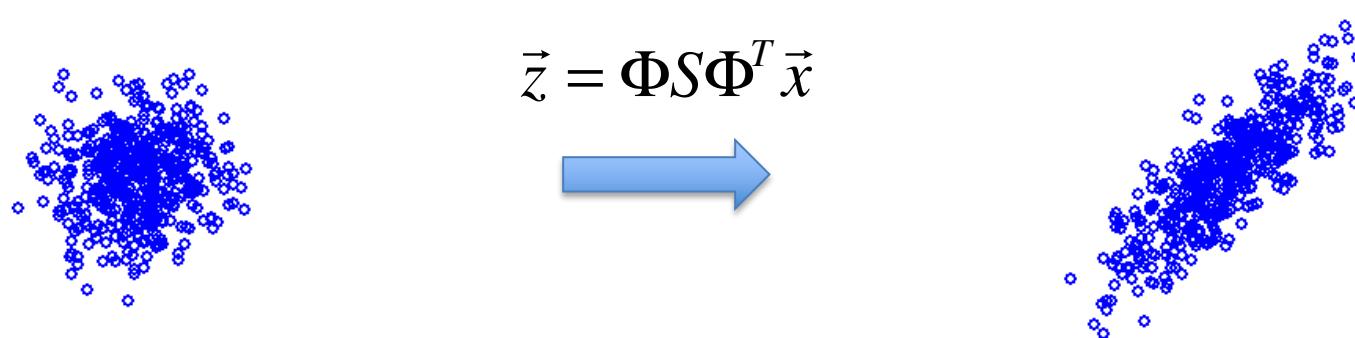


Eigenworm



# PCA demo on Gaussian points

$$\Phi = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \quad S = \begin{pmatrix} \sqrt{3} & 0 \\ 0 & (\sqrt{3})^{-1} \end{pmatrix}$$



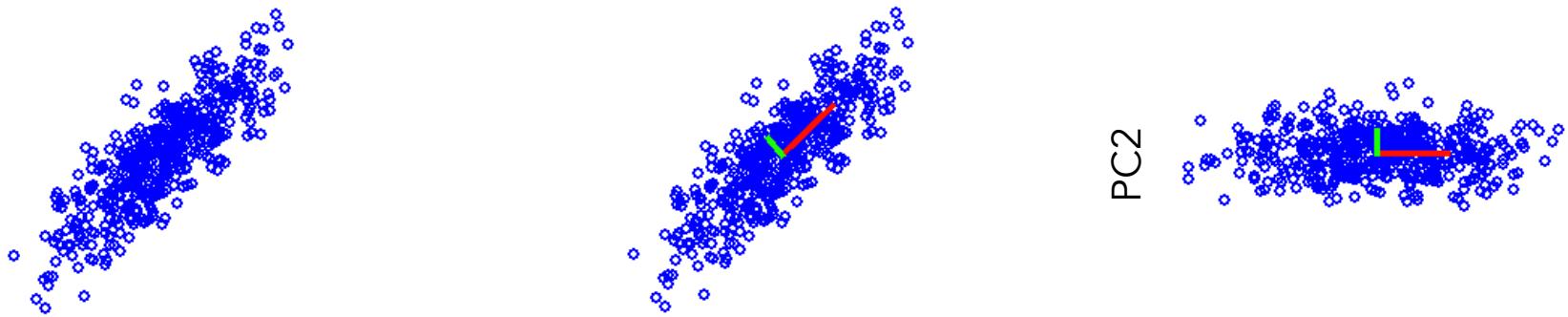
$X$

m=500;  
X=randn(2,m);

$Z$

```
R=[1 -1;1 1]/sqrt(2);
S=[1.73 0 ; 0  0.577];
%
Z=R*S*R'*X;
```

# PCA demo on Gaussian points



$$\Sigma = \frac{1}{m} Z Z^T$$

$$\Sigma = F V F^T$$

$Q = Z^* Z' / m;$   
 $[F, V] = \text{eig}(Q);$

$$F = \begin{pmatrix} 0.72 & -0.70 \\ 0.70 & 0.72 \end{pmatrix}$$

$$V = \begin{pmatrix} 3.28 & 0 \\ 0 & 0.31 \end{pmatrix}$$

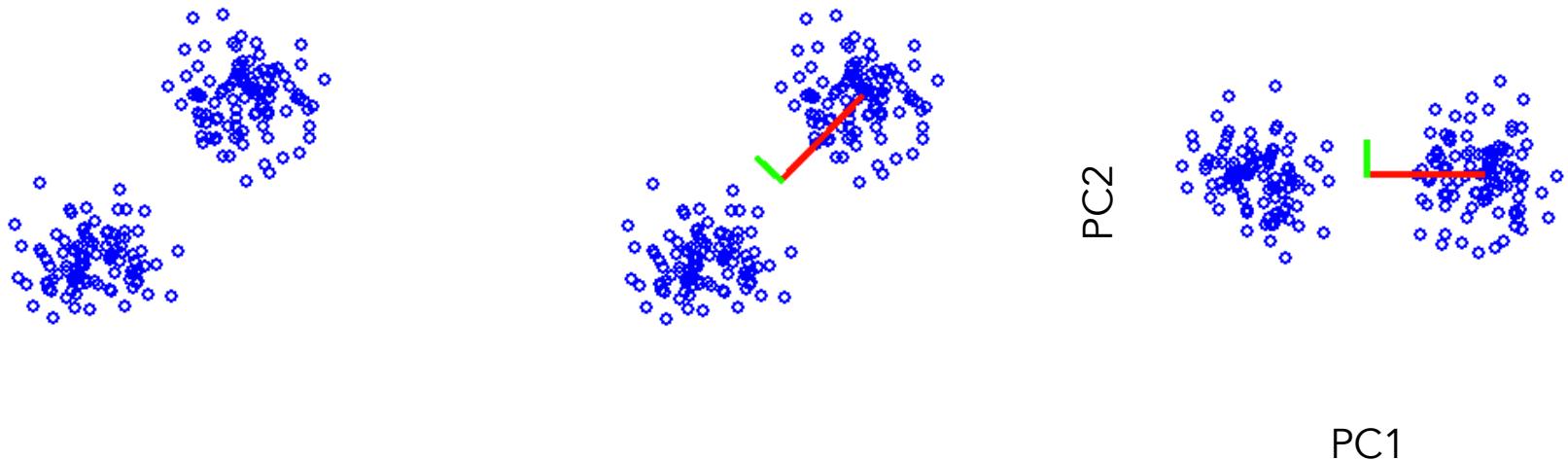
PC1

$$\vec{z}_f = F^T \vec{z}$$

$F = -\text{fliplr}(F);$   
 $V = \text{flip}(\text{sum}(V));$

$Z_f = F'^* Z;$

# Clustering

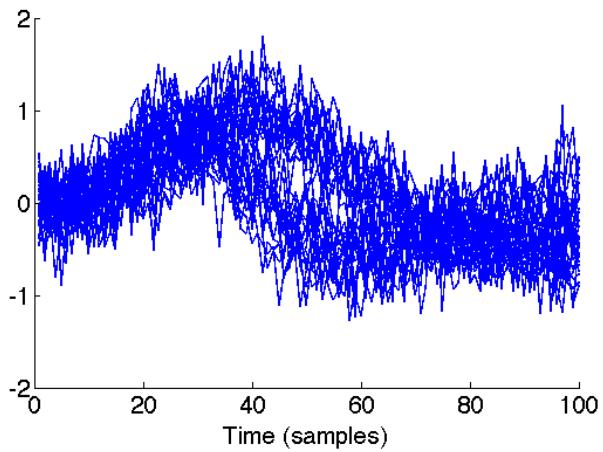


$$Q = Z^* Z' / m; \\ [F, V] = \text{eig}(Q);$$

$$Zf = F'^* Z;$$

# PCA on time-domain signals

- Let's look at a problem in the time domain.
- Here we have many examples of a noisy signal in time.



Each example has 100 time points

$$\vec{x}^j = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \quad n = 100$$

There are 200 different vectors

$$X = (\vec{x}^{(1)} \ \vec{x}^{(2)} \ \vec{x}^{(3)} \ \dots \ \vec{x}^{(m)})$$

$m = 200$

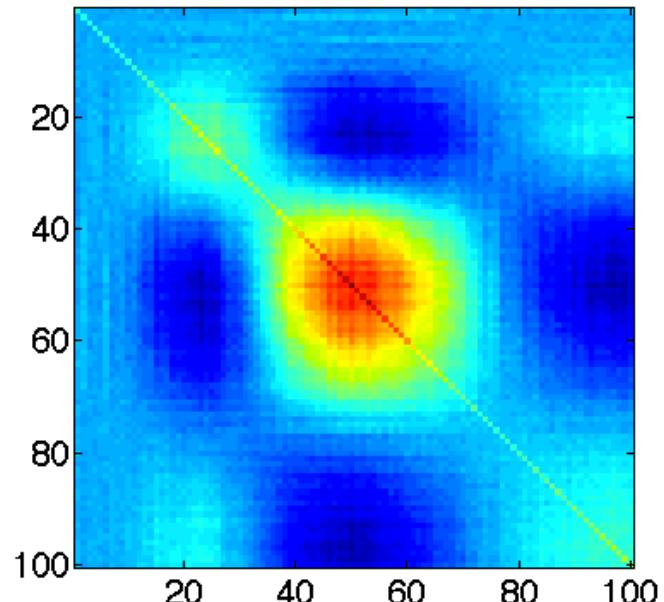
$$X = \begin{pmatrix} & n & x & m \\ & 200 & & \end{pmatrix} 100$$

# Covariance matrix

- Do PCA
  - Subtract the mean
  - Compute the covariance matrix
  - Find the eigenvectors and eigenvalues

$$\Sigma = \frac{1}{m} ZZ^T$$

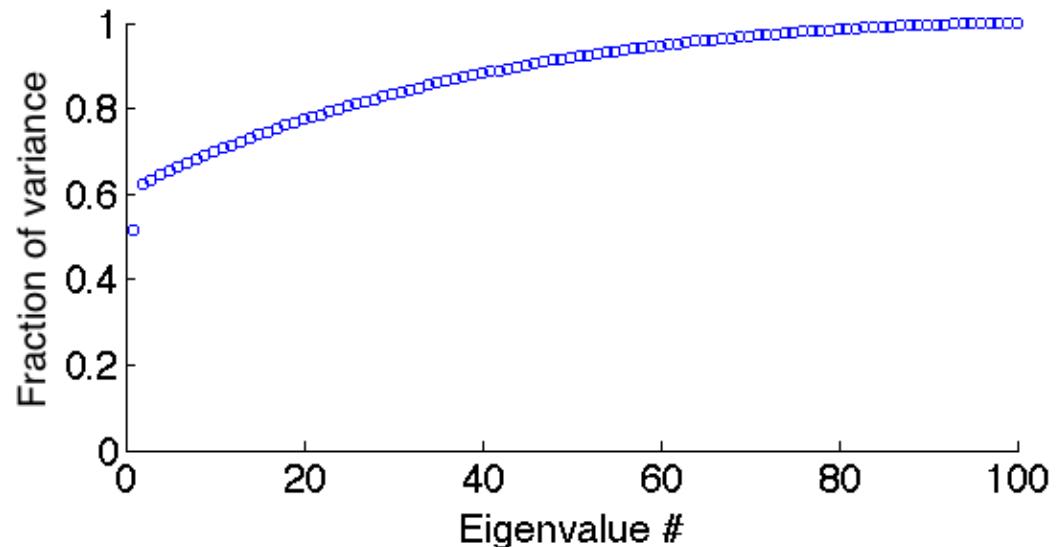
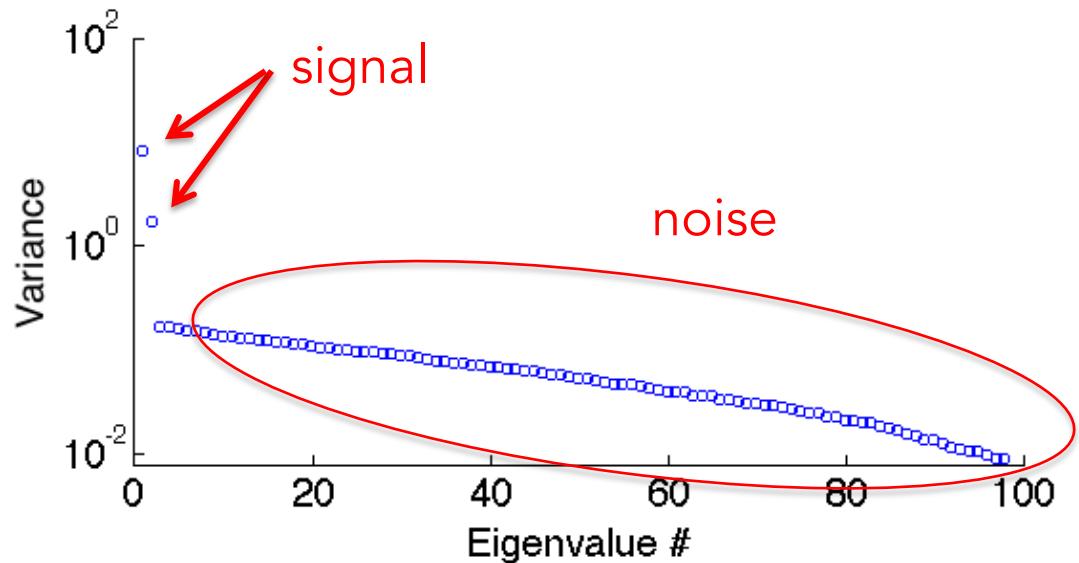
```
Mu=mean(X,2);  
MU=repmat(mu,1,m);  
Z=X-MU;  
Q=Z*Z'/m;  
  
[F,V]=eig(cov);
```



# Eigenvalues

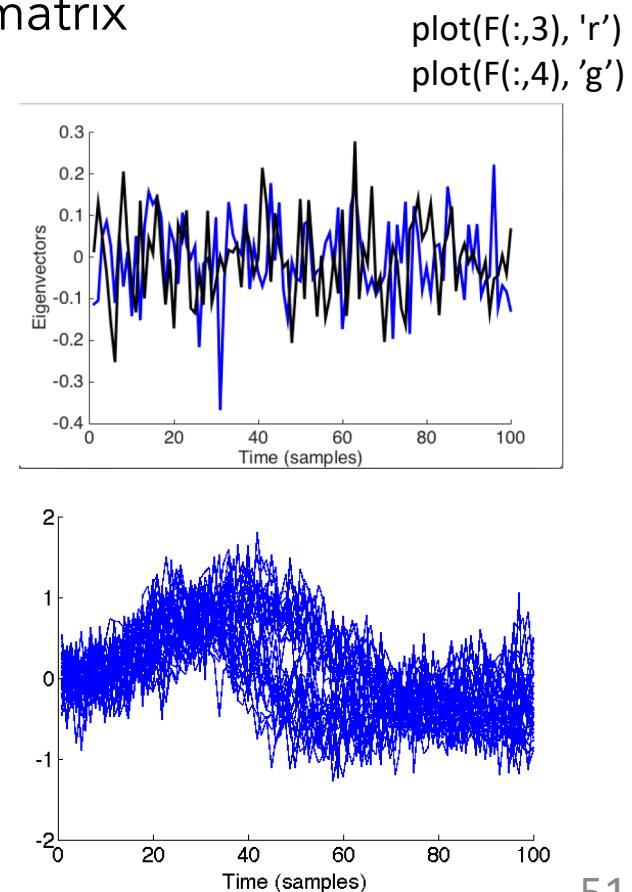
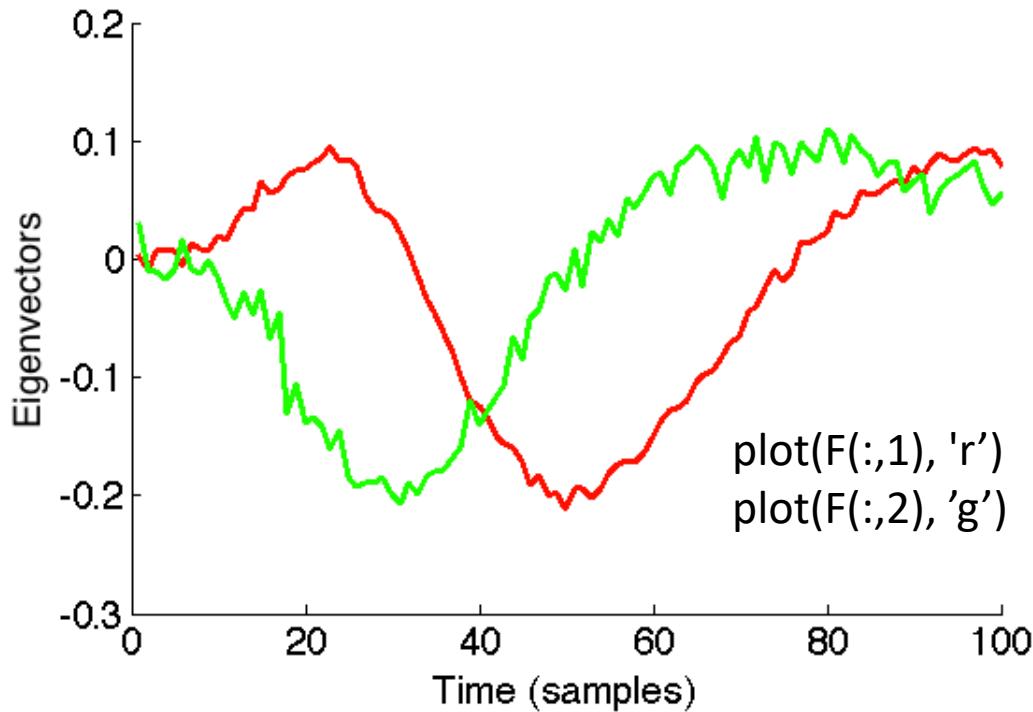
```
[F,V]=eig(cov);  
var=flip(sum(V));
```

- The first two eigenvalues are much larger than all the rest
- The first two eigenvalues explain over 60% of the total variance.



# Eigenvectors

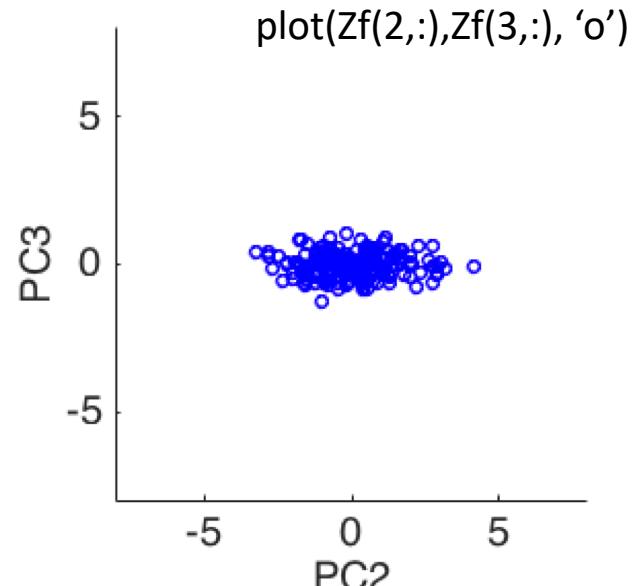
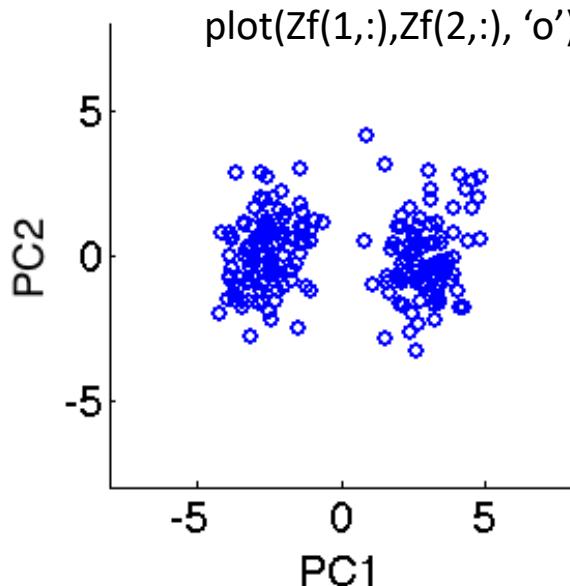
- Since there were only two large eigenvalues, we look at the eigenvectors associated with these eigenvalues
- These are just the first two columns of the F matrix



# Principal components

- Principal components are just the projections of each of the original data vectors onto the two principal eigenvectors.
- Remember, this is just a change of basis using the matrix  $F$

$$\vec{z}_f = F^T \vec{z} \quad Zf = F^*Z;$$



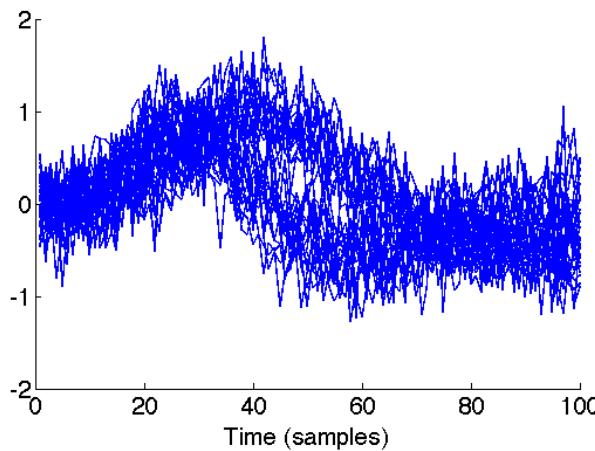
# Filtering using PCA

- Only the first two entries in the column vectors  $Z_f$  (in the rotated basis) have signal. So keep only the first two and set the rest to zero.

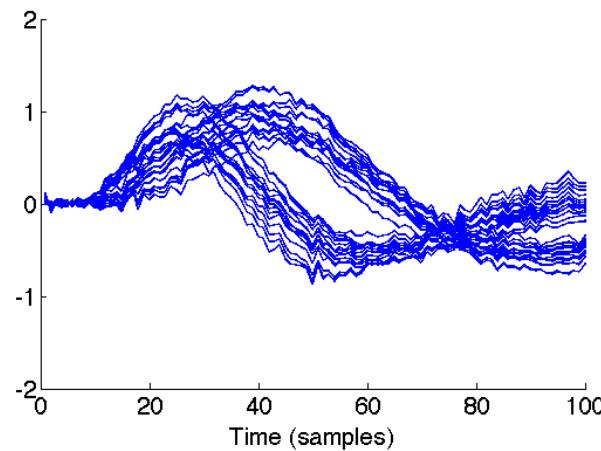
```
Zf=F'*Z;  
Zffilt=Zf;  
Zffilt(3:end,:)=0;  
Zfilt=F*Zffilt;  
Xfilt=Zfilt+MU;
```

- Then rotate back to the original basis set

Before filtering



After filtering



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