Teoria degli Algoritmi

Corso di Laurea Magistrale in Matematica Applicata

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SAPIENZA
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Recap from Last Lecture(s)

- High-dimensional naïve representation (i.e., feature space) of data

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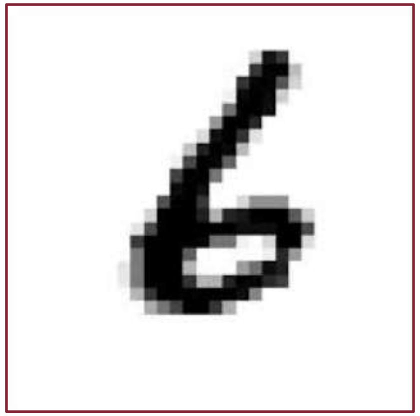
- High-dimensional naïve representation (i.e., feature space) of data
- Clustering high-dimensional data may be problematic
  - Due to the curse of dimensionality
- Many data sources (e.g., text, images) have this issue
- Good news! High-dimensionality is often not real!
  - Due to the way in which we observe/collect data

Modeled vs. True Dimensionality

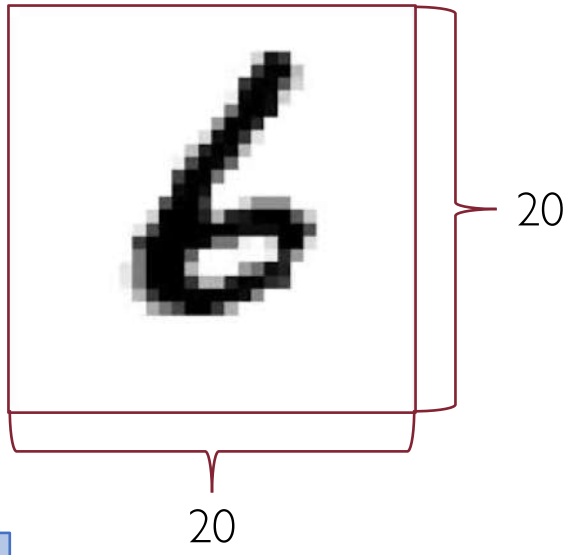
Example

Handwritten digit recognition

Modeled vs. True Dimensionality



Modeled vs. True Dimensionality

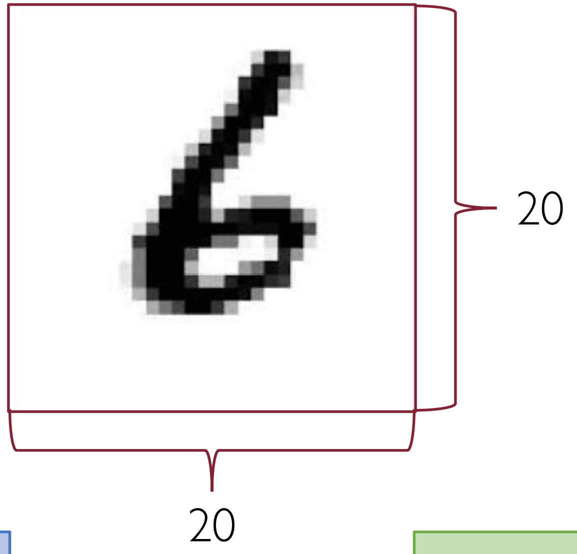


Modeled dimensionality

Each digit represented by 20x20 bitmap

400-dimensional binary vector

Modeled vs. True Dimensionality



Modeled dimensionality

Each digit represented by 20x20 bitmap

400-dimensional binary vector

True dimensionality

Actual digits just cover a tiny fraction of all this huge space

Small variations of the pen-stroke

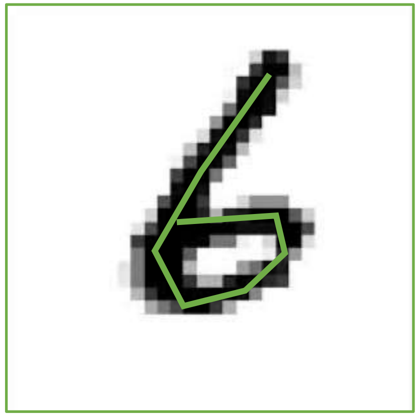
Modeled vs. True Dimensionality

Random samples from
400-d space


Modeled vs. True Dimensionality

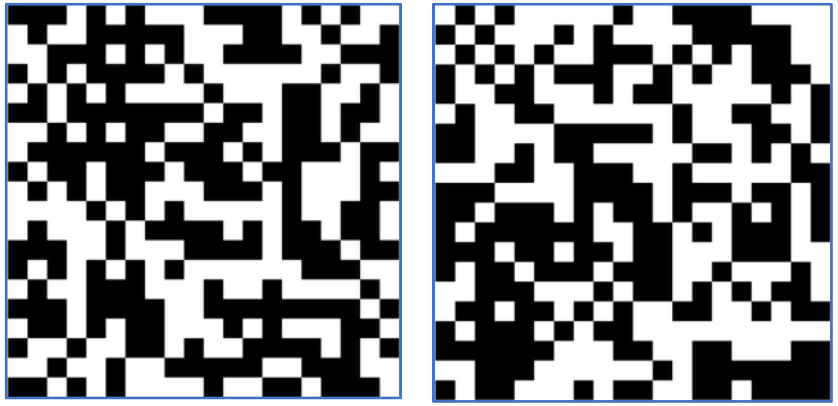
Random samples from 400-d space

True digits living in a 400-d space

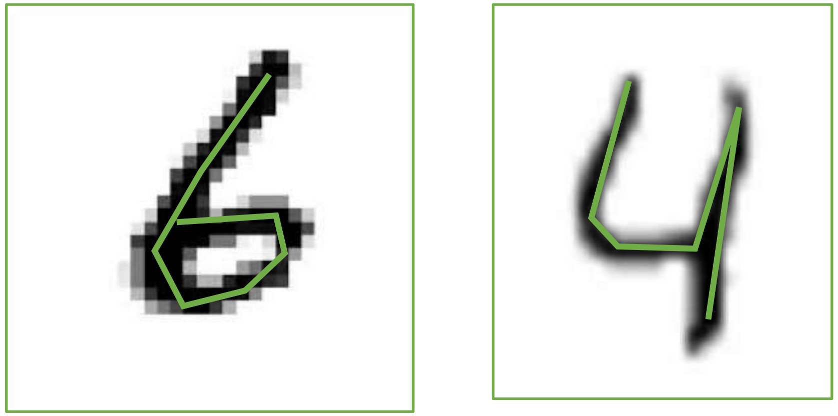


Modeled vs. True Dimensionality

Random samples from 400-d space



True digits living in a 400-d space



We model data (i.e., digits) as very high dimensional…

… In fact, they are not so

The Curse of Dimensionality

As dimensionality grows fewer examples in each region of the feature space
(assuming # examples is constant)

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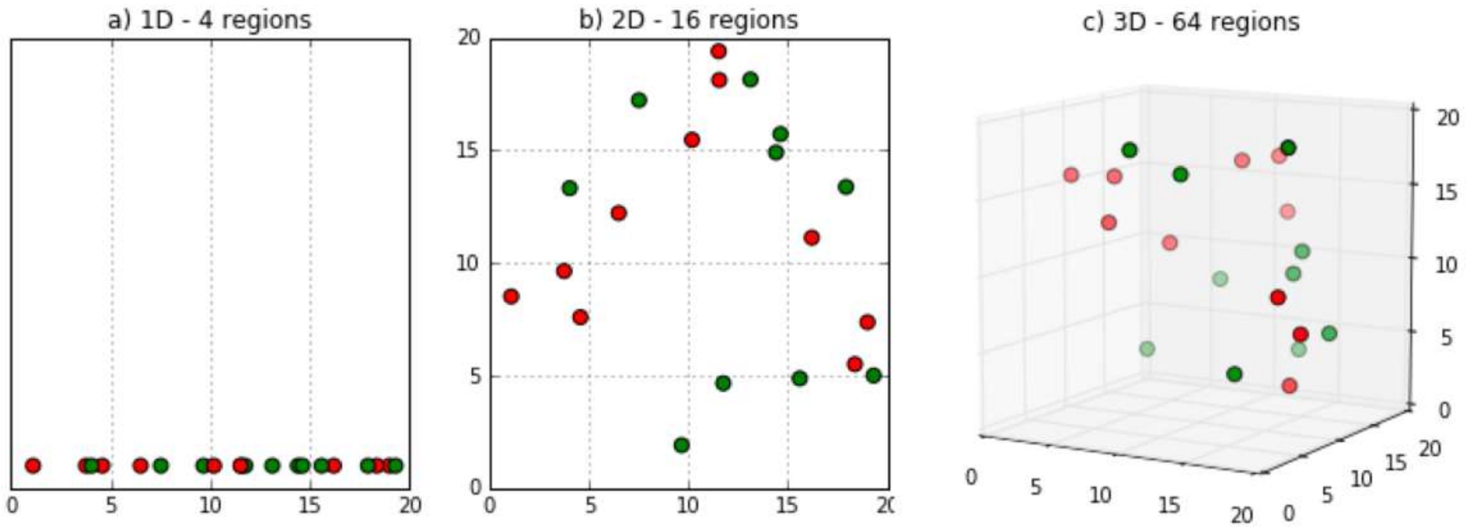

Dimensionality Reduction

- A technique to unveil the actual (i.e., meaningful) dimensions of data
- A pre-processing step for representing data with fewer features
- Preserve as much "structure" of the data as possible
- Retained structure must be discriminative affecting data separability

"structure" here means variance

Dimensionality Reduction

$\boxed{\text{2 main approaches}}$

Dimensionality Reduction

2 main approaches

Feature Selection

Pick a subset of the original dimensions that are good predictors (e.g., using information gain)

$x_1, x_2, \ldots, x_{j-1}, x_j, x_{j+1}, \ldots, x_{d-1}, x_d$

Dimensionality Reduction

2 main approaches

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Feature Extraction

Build a new set of $k < d$ dimensions as a (linear) combination of the originals

$e_1, e_2, \ldots, e_k$

$e_i = f(x_1, x_2, \ldots, x_d)$

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Principal Component Analysis (PCA)

Dimensionality reduction technique based on feature extraction

High-dimensional data is in fact embedded into some lower dimensional space

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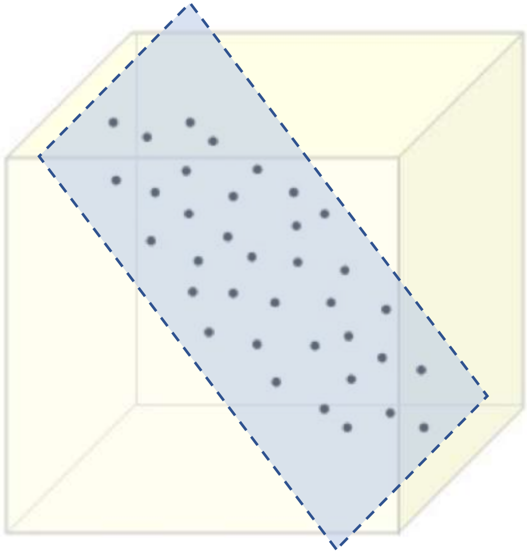
Example

A 3-d set of points embedded into a 2-d hyperplane



Principal Component Analysis (PCA)

PCA defines a set of principal components as follows:

- 1st: direction of the greatest variance of data
- 2nd: perpendicular to 1st and greatest variance of what's left
- … and so on until d

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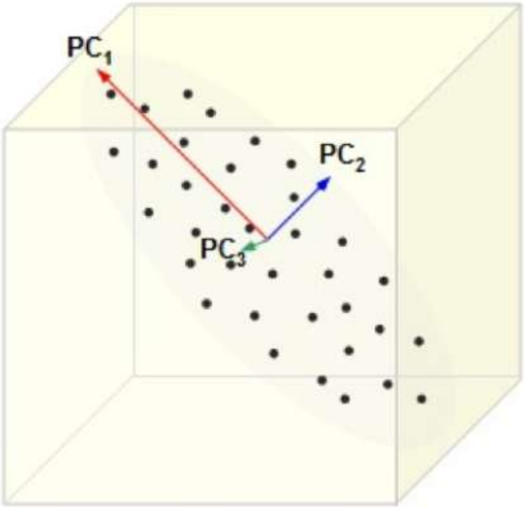
The top k < d components become the new dimensions



$\boxed{\text{e.g., } k = 2}$

Principal Component Analysis (PCA)

PC_1 and PC_2 are the top-2 principal components

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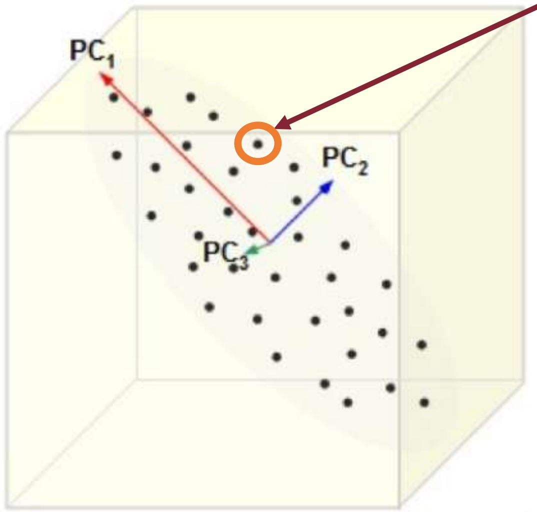
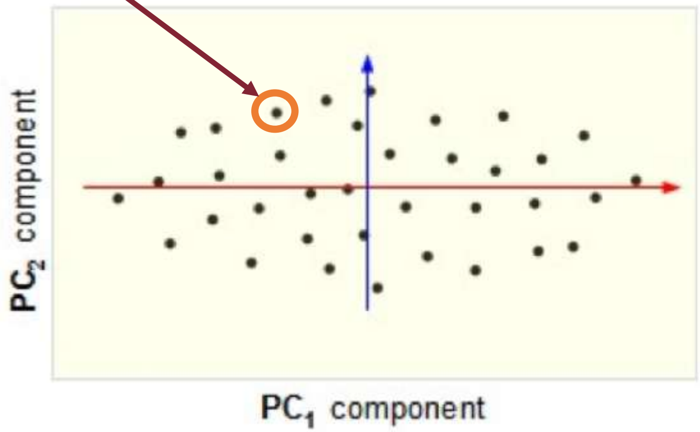
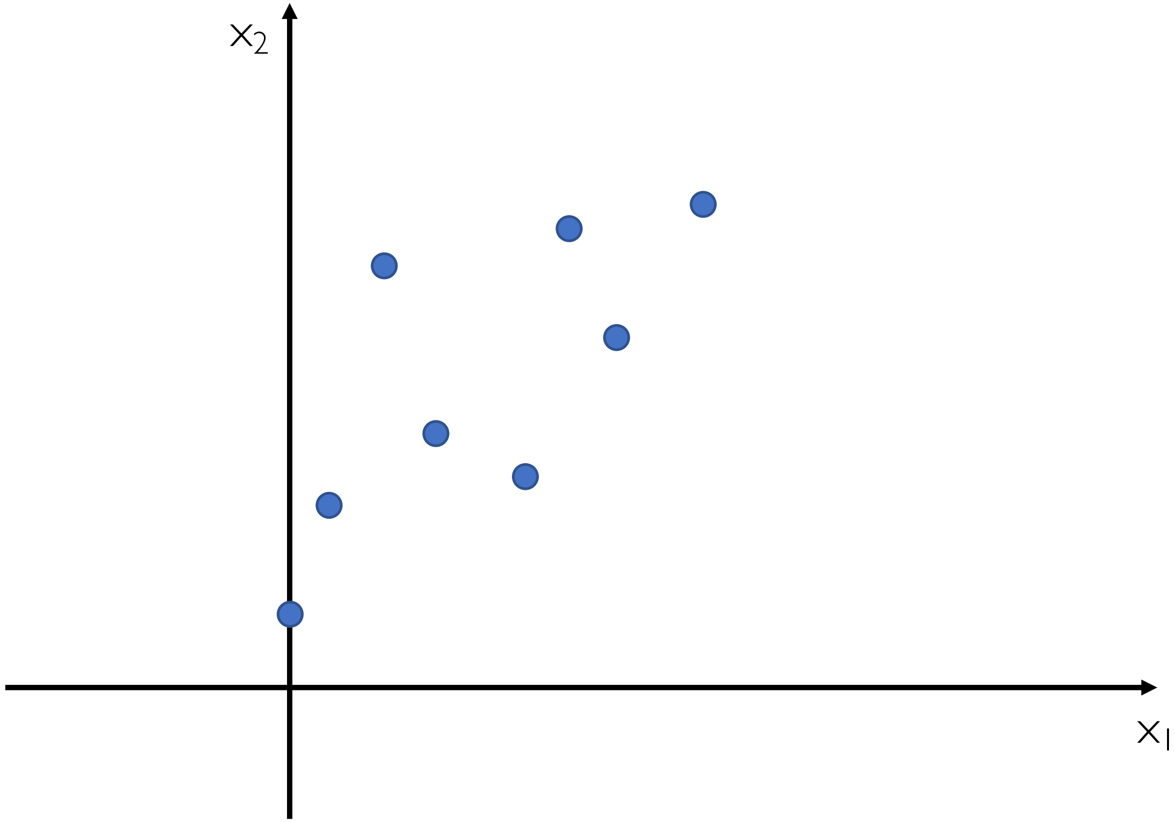
Change the coordinates of every point according to the new dimensions





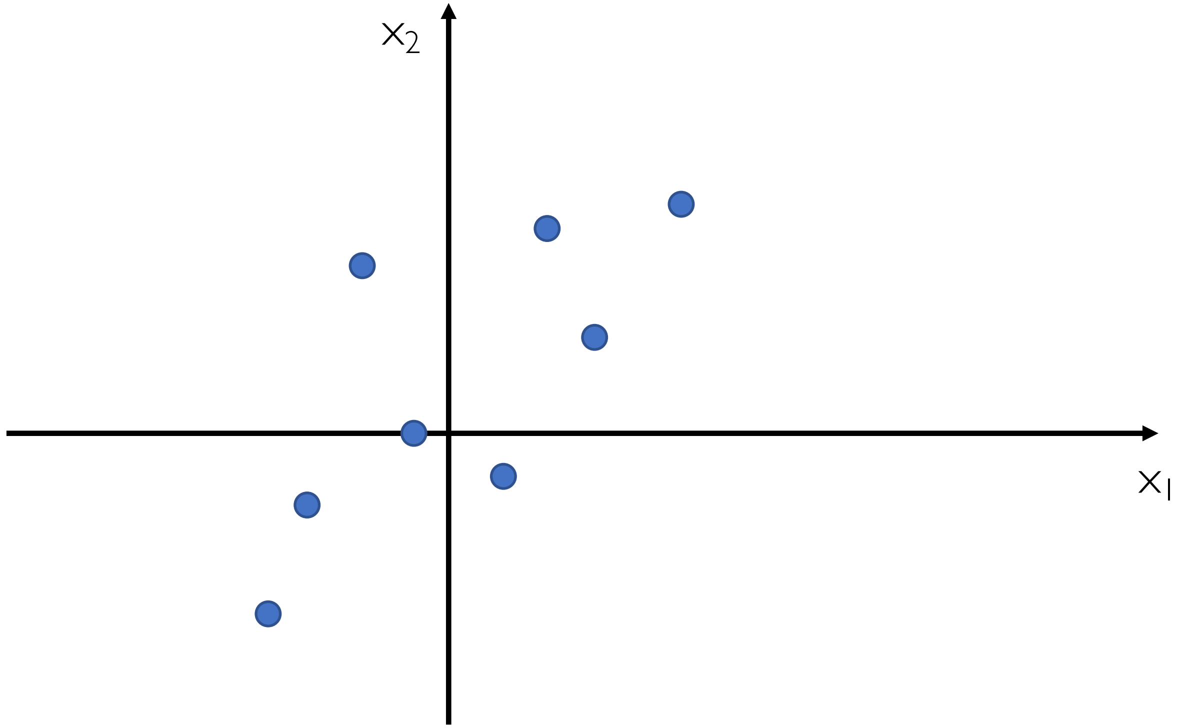
Why Do We Look for Greatest Variance?

Example: Reduce 2-dimensional data to 1-d



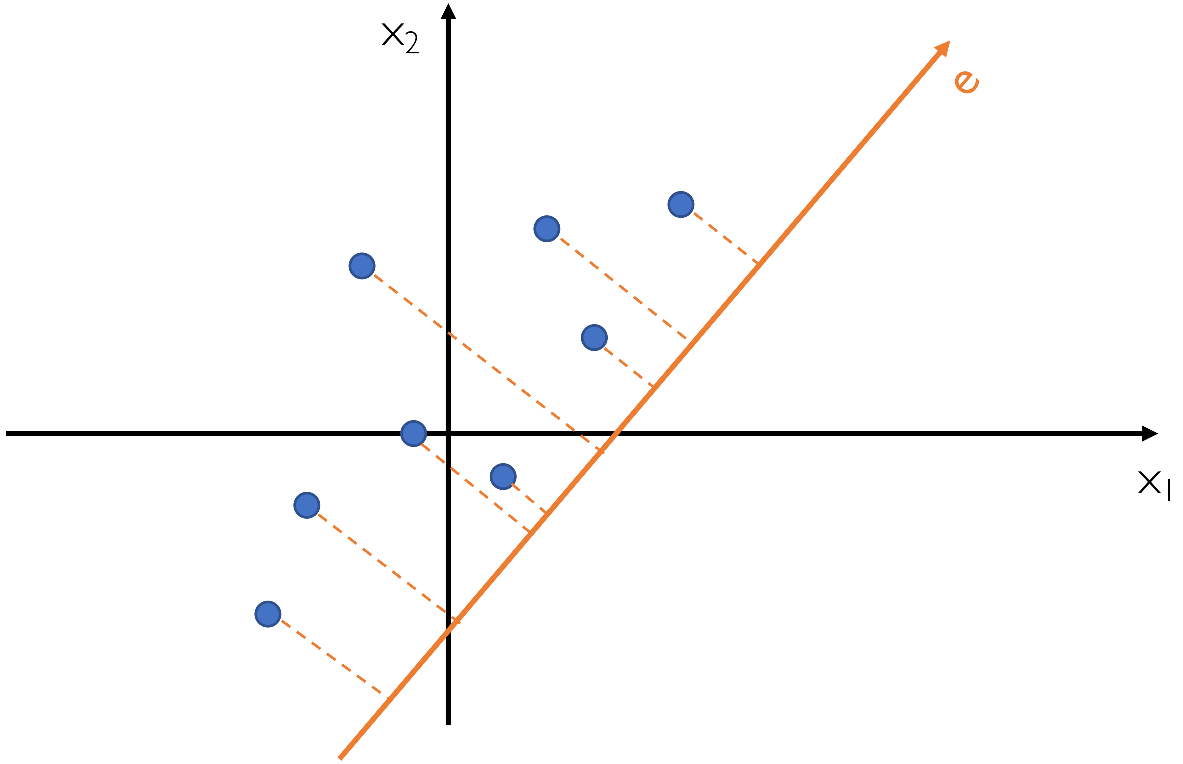
Why Do We Look for Greatest Variance?

First of all, let's center the points around the mean along x_1 and x_2



Why Do We Look for Greatest Variance?

Map, i.e., project (x_1, x_2) to a new single dimension axis e



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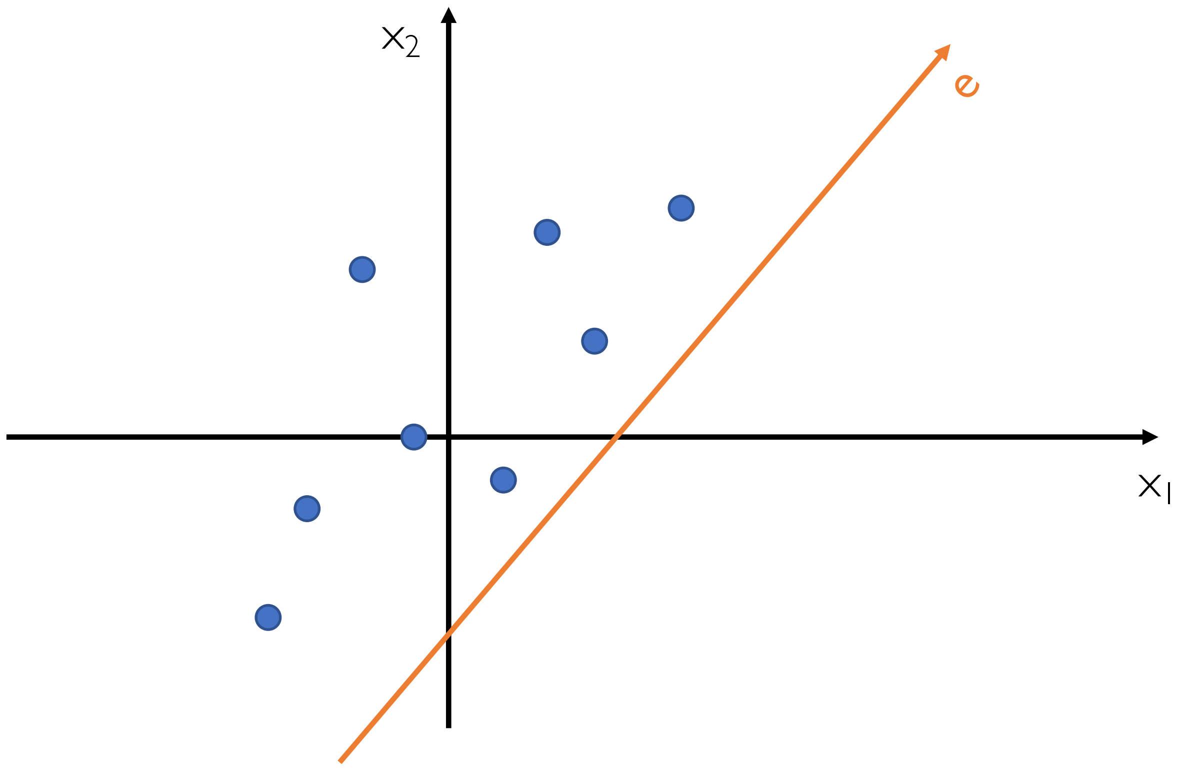

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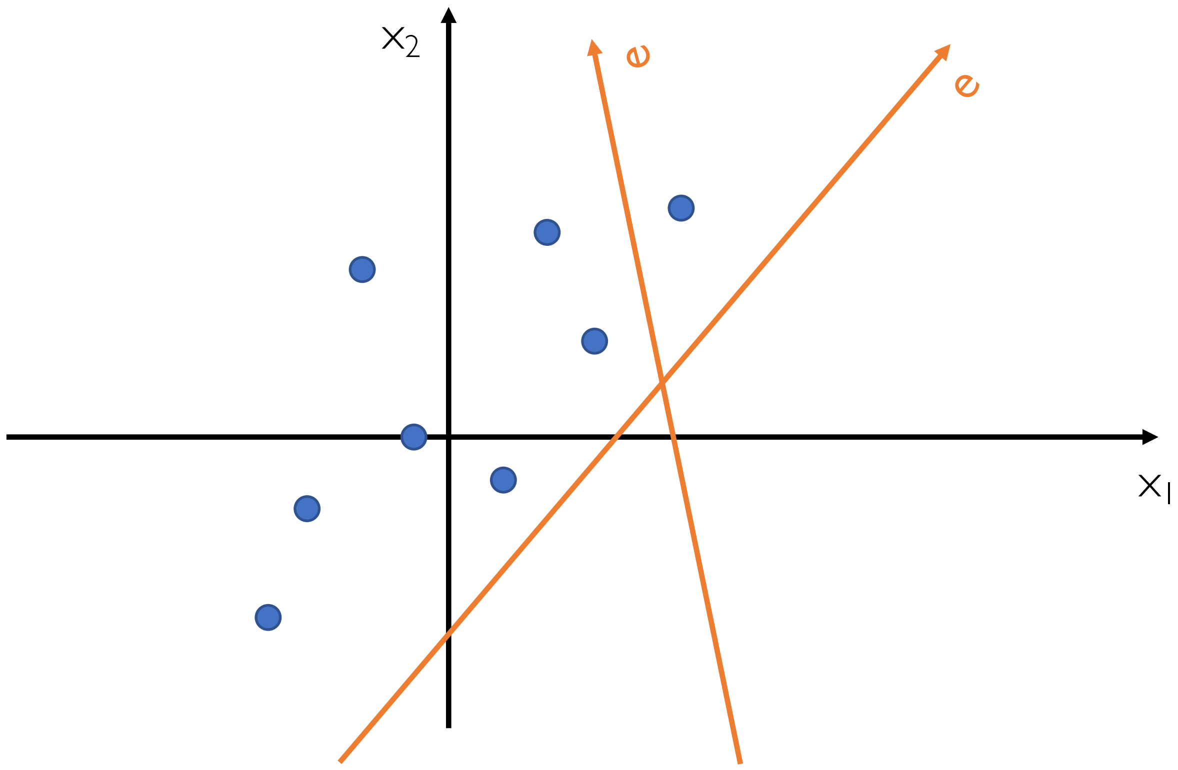

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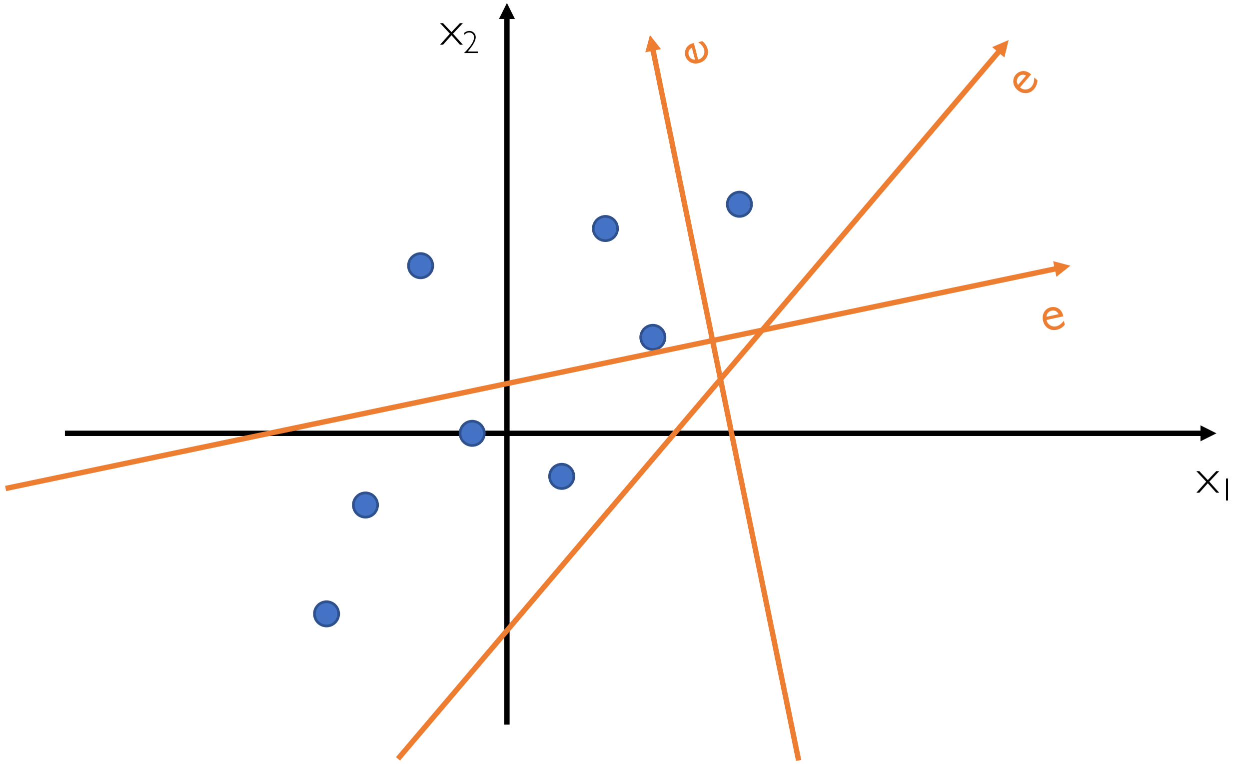

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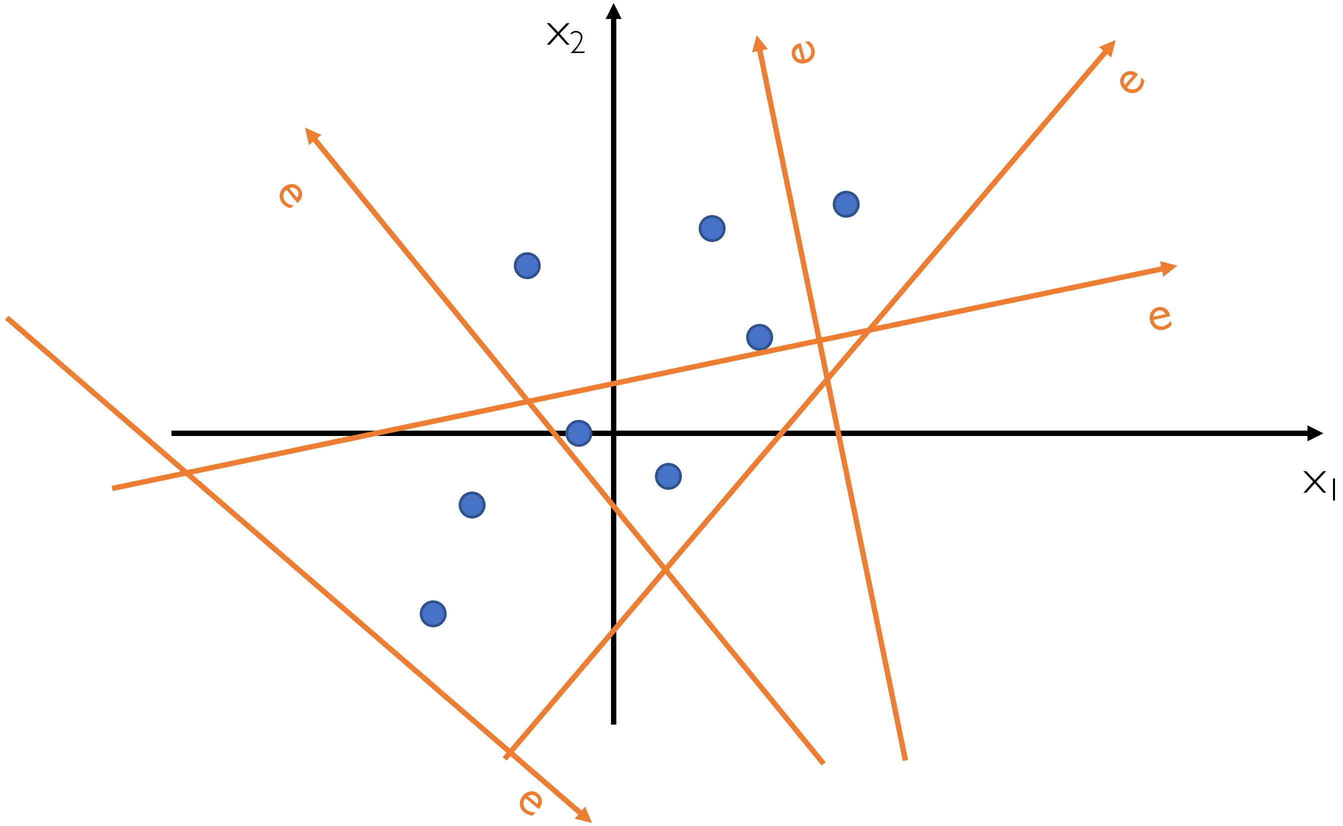
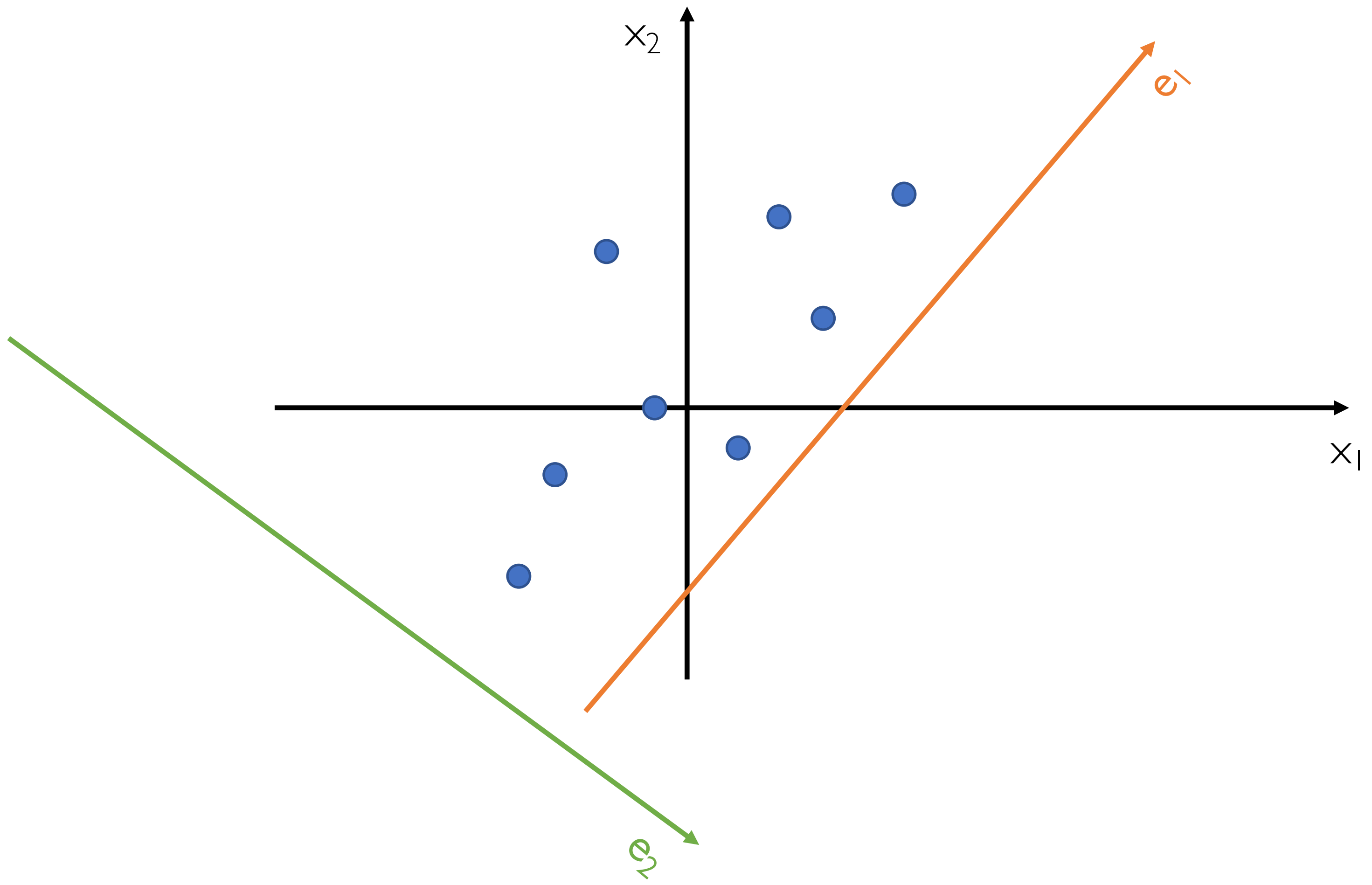


infinitely many mappings from (x_1, x_2) to a new axis e

Why Do We Look for Greatest Variance?

Let's consider 2 different mappings e_1 and e_2



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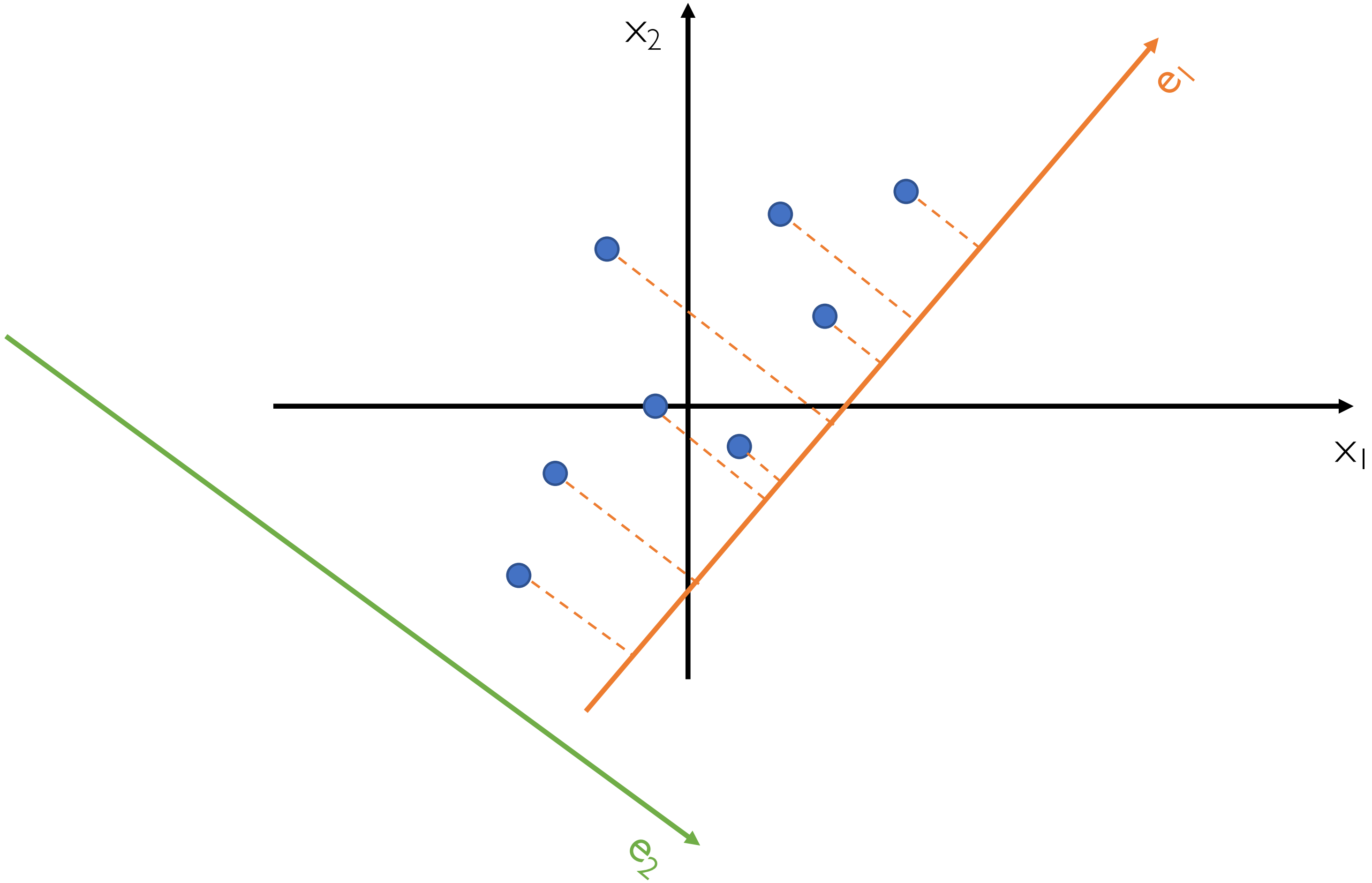

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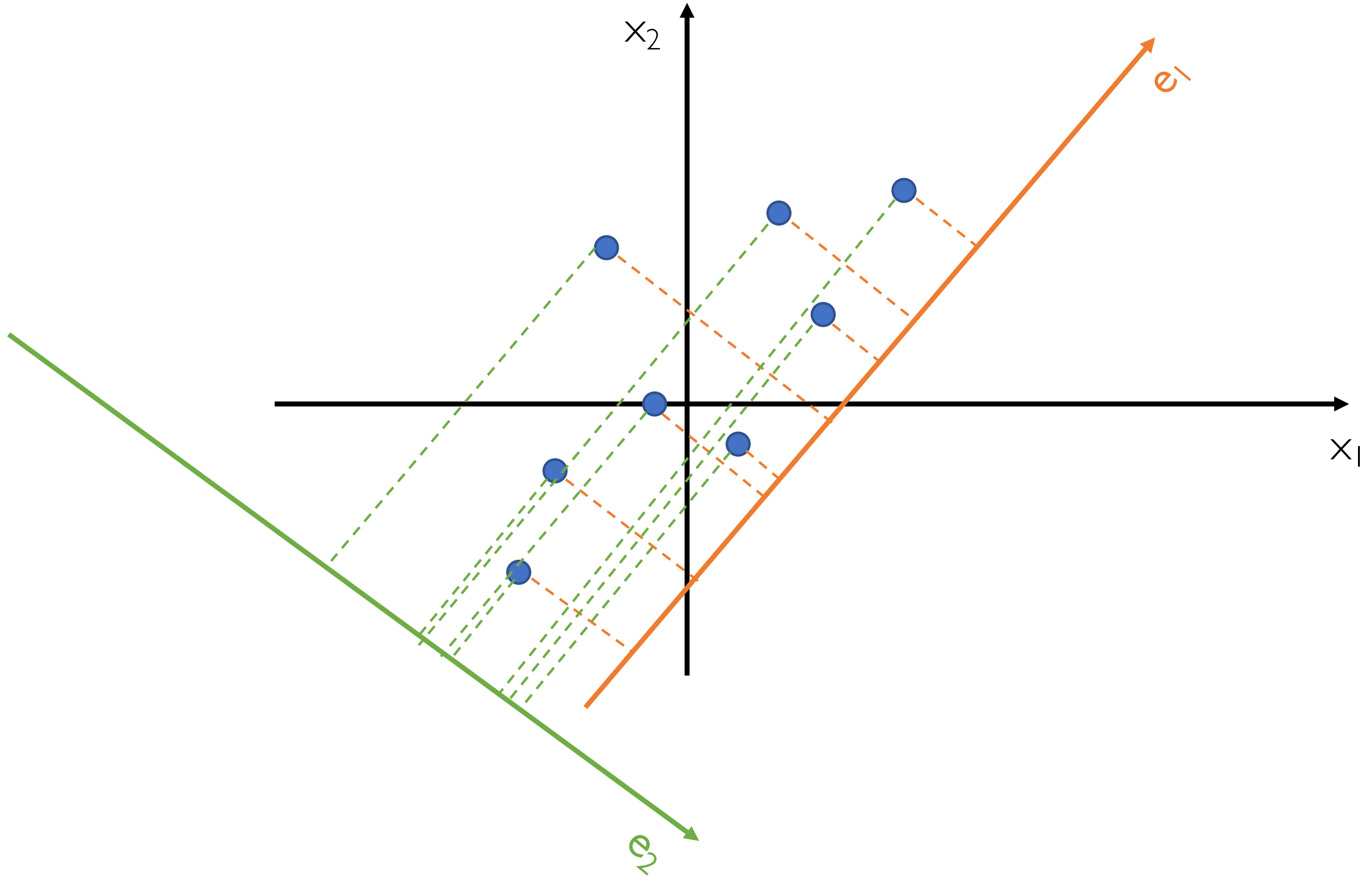
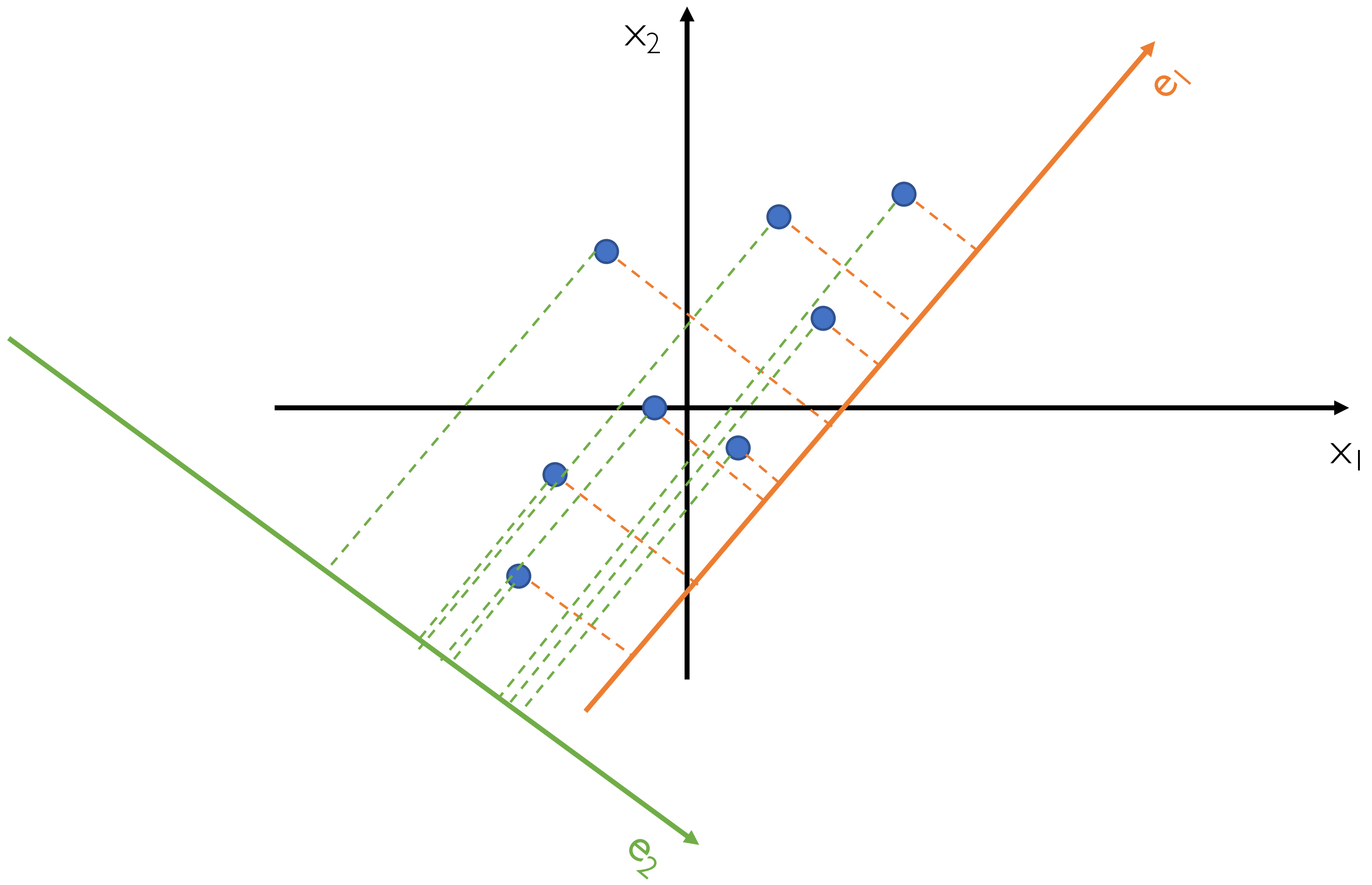


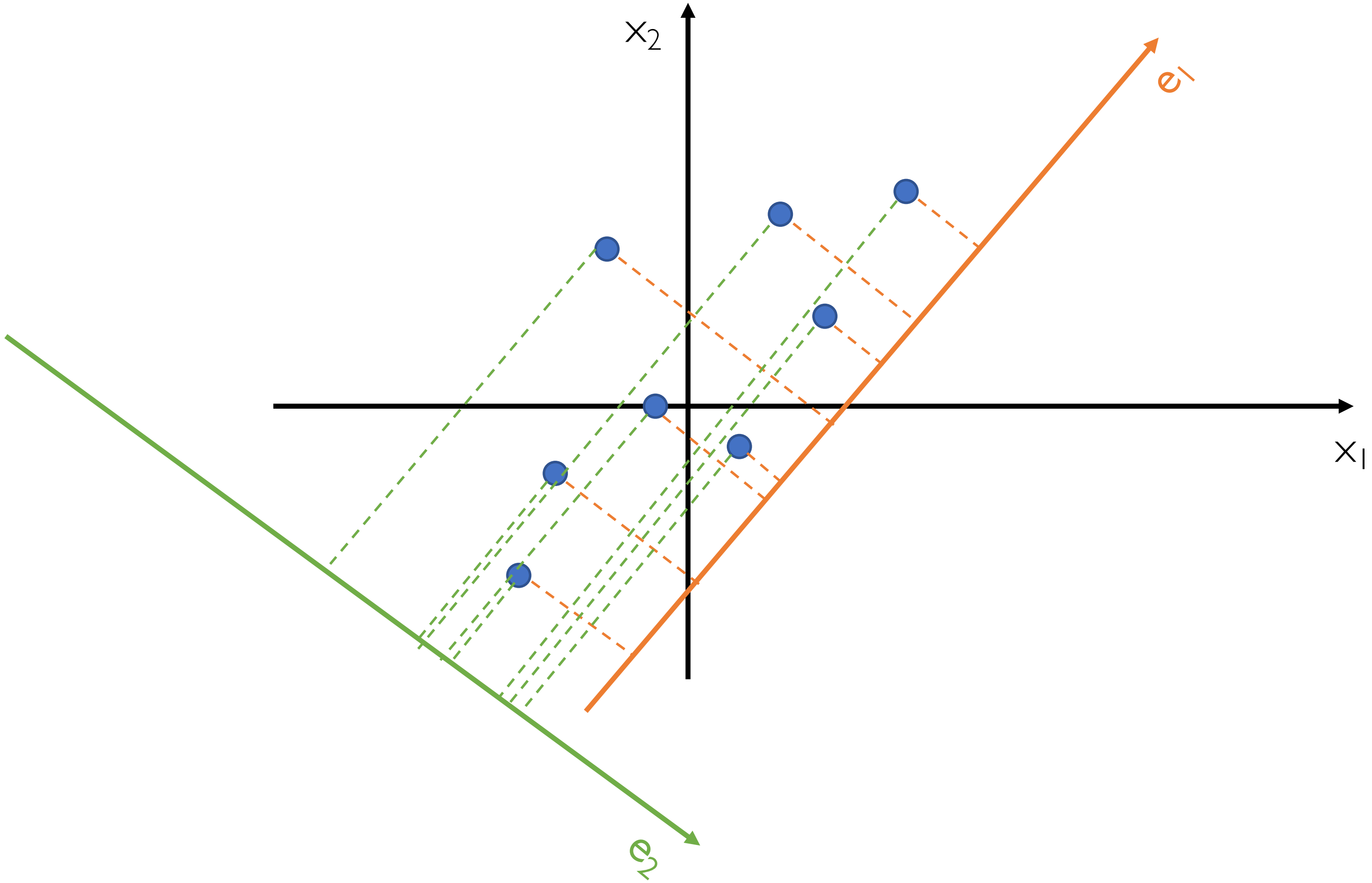
Why Do We Look for Greatest Variance?

Which one is better?



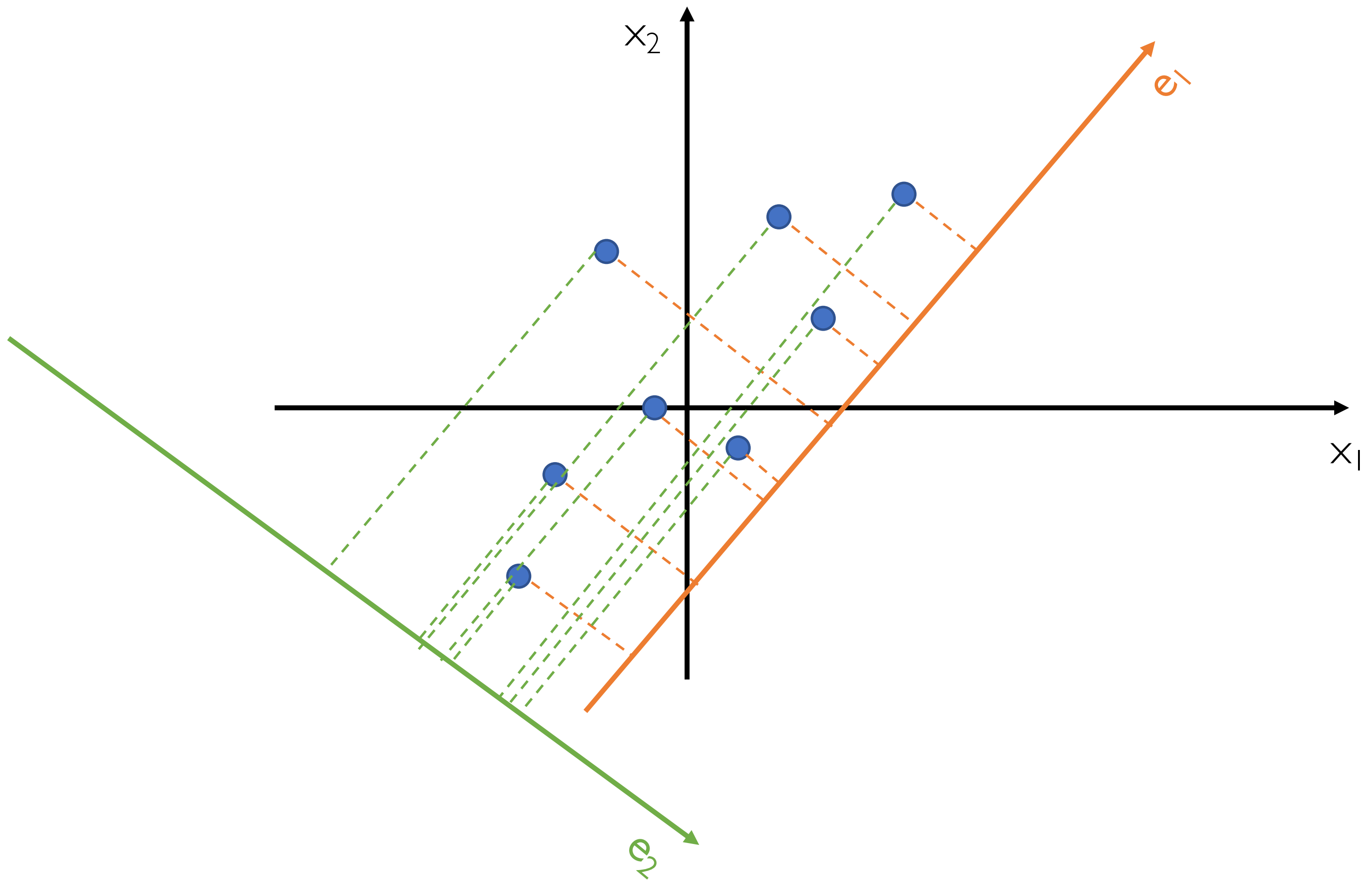
Why Do We Look for Greatest Variance?

Points projected onto e_1 look more spread-out than onto e_2



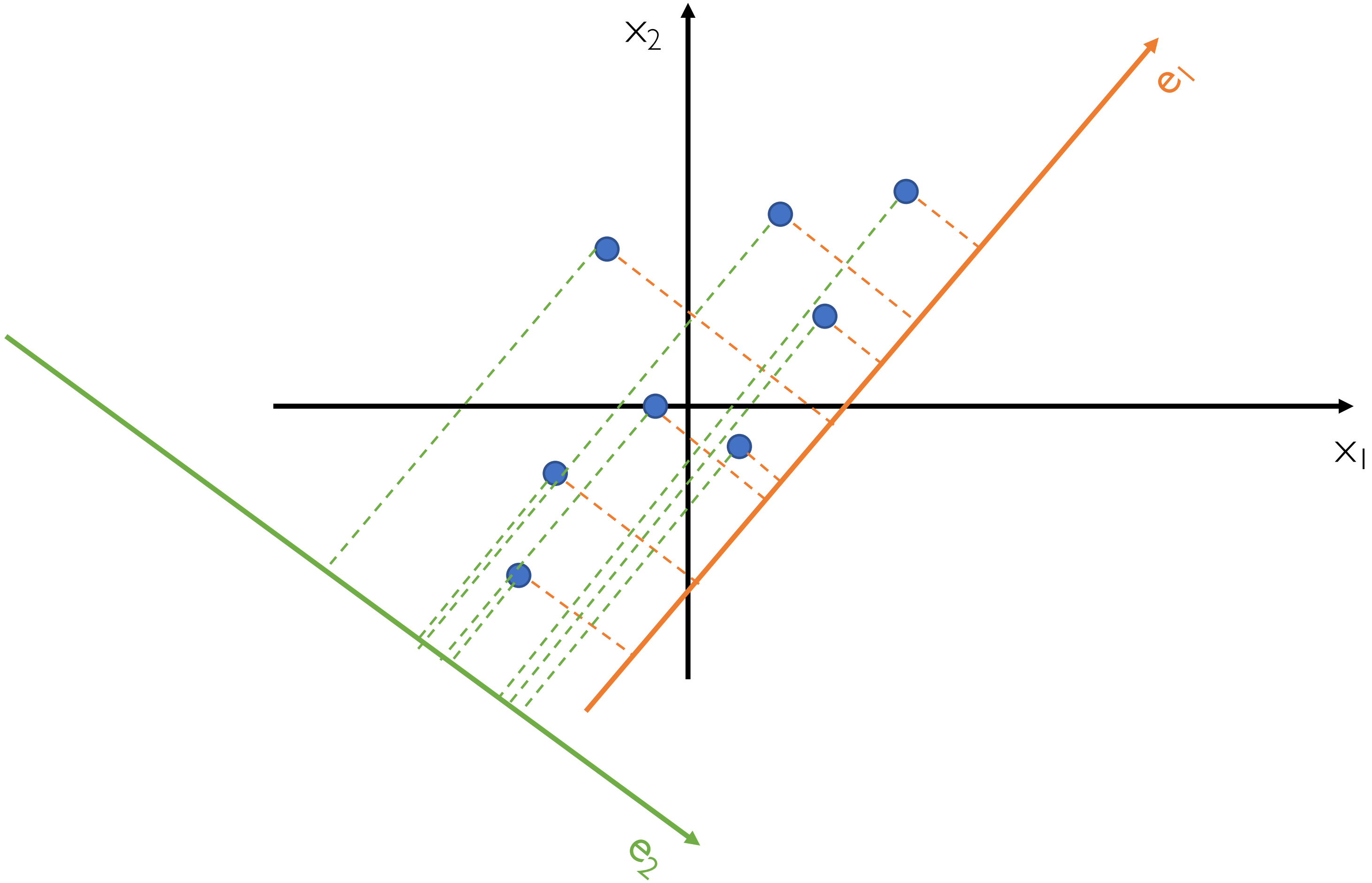
Why Do We Look for Greatest Variance?

The variance along e_1 is larger than along e_2



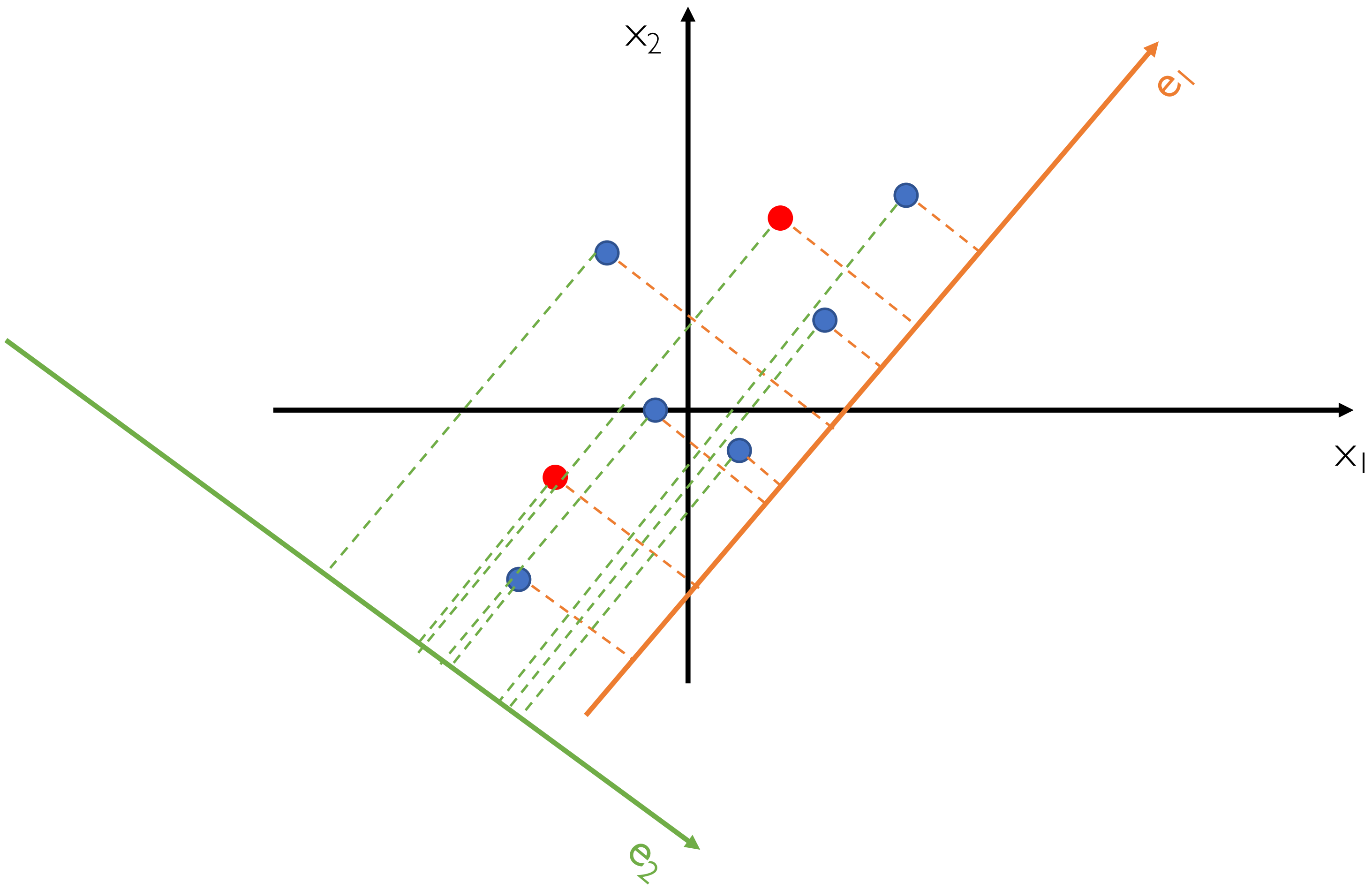
Why Do We Look for Greatest Variance?

Why is that good?



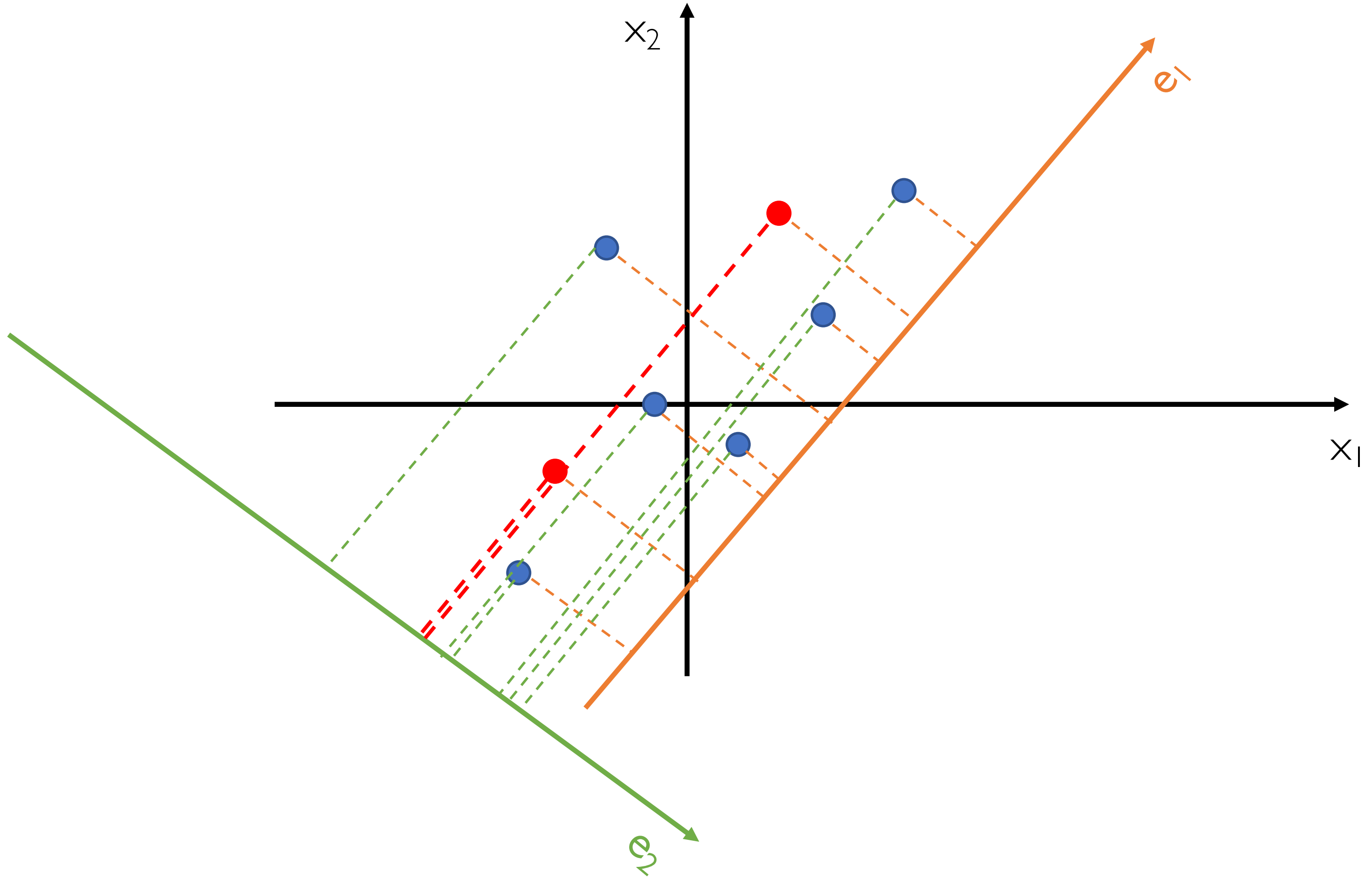
Why Do We Look for Greatest Variance?

Consider the 2 red points below



Why Do We Look for Greatest Variance?

On (x_1, x_2) far away from each other, end up close if projected onto e_2



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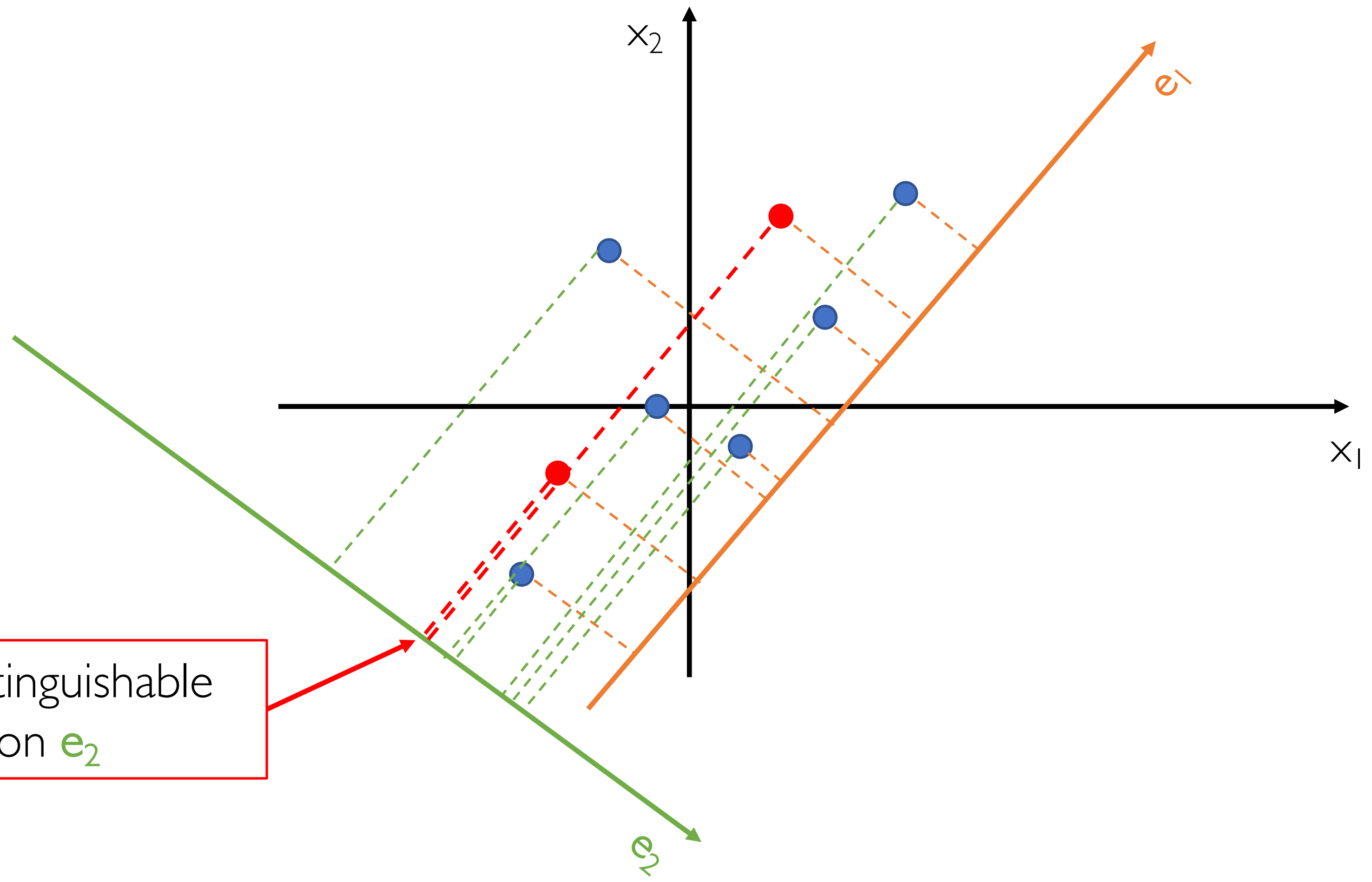
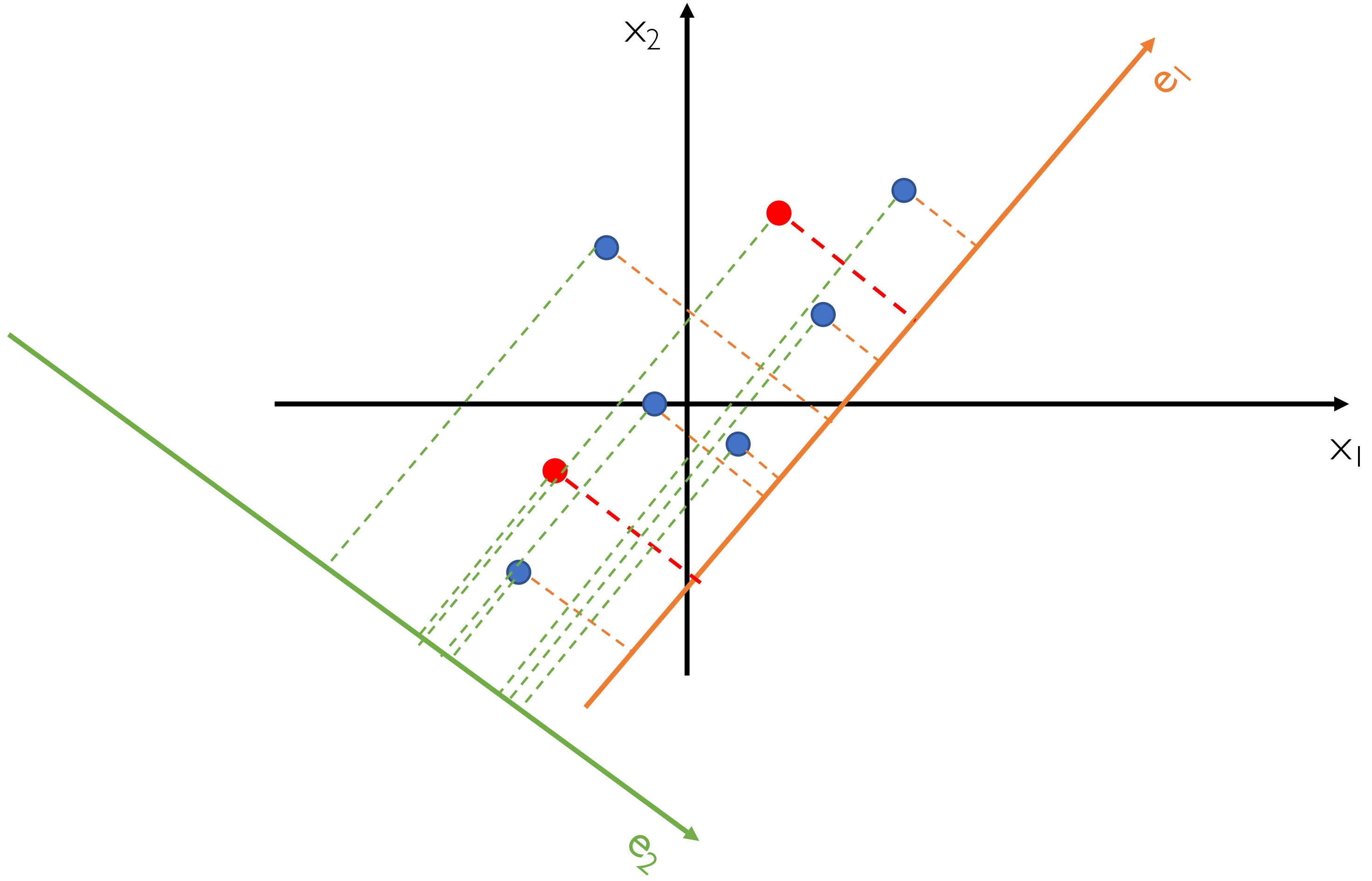


Almost indistinguishable points on e_2

Why Do We Look for Greatest Variance?

If projected onto e_1 they better preserve their distance



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⇩

Solution

Pick e so as to maximize variance of projected data

Variance of a Random Variable

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- Formally, it is the expected value of the squared deviation from its mean

$$\mathrm{Var}(X) = \mathrm{E}[(X - \mu)^2]$$

$$\text{where } \mu = \mathrm{E}[X]$$

Covariance of Two Random Variables

- A measure of the joint variability of two random variables X and Y
  - Do X and Y increase/decrease together, or when one increases/decreases the other decreases/increases?

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$$\mathrm{Cov}(X, Y) = \mathrm{E}[(X - \mu_X)(Y - \mu_Y)]$$

$$\boxed{\mathrm{Cov}(X, X) = \mathrm{Var}(X)}$$

$$\text{where } \mu_X = \mathrm{E}[X] \text{ and } \mu_Y = \mathrm{E}[Y]$$

Covariance Matrix

- Given a random vector $\mathbf{X} = (X_1, \ldots, X_d)$ its covariance matrix K is a dxd square matrix with the covariance between each pair of elements

Covariance Matrix

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- In the matrix diagonal there are variances, i.e., the covariance of each element with itself

$$\mathrm{K}[i, j] = \mathrm{Cov}(X_i, X_j)$$

Covariance Matrix of Original Dimensions

- The original set of dimensions is a random vector $\mathbf{X} = (X_1, \ldots, X_d)$

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Covariance Matrix of Original Dimensions

- The original set of dimensions is a random vector $\mathbf{X} = (X_1, \ldots, X_d)$
- In our example, d = 2 and $\mathbf{X} = (X_1, X_2)$
- The covariance matrix K is a 2-by-2 matrix
- To ease the covariance computation, we center each data point at zero
  - Subtracting the mean of each attribute/dimension
  - The mean of each dimension becomes then 0

Covariance Matrix of Original Dimensions

Let n be the total number of data points: $\mathbf{x}_1, \ldots, \mathbf{x}_n$

Each data point is represented by a (x_1, x_2) pair

$\mathbf{x}_i = (x_{i,1}, x_{i,2})$

We associate 2 random variables X_1, X_2 to each dimension, and we compute:

$$\mu_1 = \mathrm{E}[X_1] = \frac{1}{n}\sum_{i=1}^{n} x_{i,1}$$

$$\mu_2 = \mathrm{E}[X_2] = \frac{1}{n}\sum_{i=1}^{n} x_{i,2}$$

$$\mathbf{x}_i = (x_{i,1} - \mu_1, x_{i,2} - \mu_2)$$

Covariance Matrix of Original Dimensions

Let us rewrite each data point $\mathbf{x}_i$ as follows:
$\mathbf{x}_i = (x'_{i,1}, x'_{i,2})$ where:
$x'_{i,1} = x_{i,1} - \mu_1; x'_{i,2} = x_{i,2} - \mu_2$

$$\mu_1^{\text{new}} = \mathrm{E}[X_1] = \frac{1}{n}\sum_{i=1}^{n} x'_{i,1} = \frac{1}{n}\sum_{i=1}^{n}(x_{i,1} - \mu_1)$$

$$\mu_2^{\text{new}} = \mathrm{E}[X_2] = \frac{1}{n}\sum_{i=1}^{n} x'_{i,2} = \frac{1}{n}\sum_{i=1}^{n}(x_{i,2} - \mu_2)$$

Covariance Matrix of Original Dimensions

$$\mu_1^{\text{new}} = \frac{1}{n}\sum_{i=1}^{n}(x_{i,1}-\mu_1) = \frac{1}{n}\Bigg(\underbrace{\sum_{i=1}^{n} x_{i,1}}_{n\mu_1} - \underbrace{\sum_{i=1}^{n} \mu_1}_{n\mu_1}\Bigg) = 0$$

$$\mu_2^{\text{new}} = \frac{1}{n}\sum_{i=1}^{n}(x_{i,2}-\mu_2) = \frac{1}{n}\Bigg(\underbrace{\sum_{i=1}^{n} x_{i,2}}_{n\mu_2} - \underbrace{\sum_{i=1}^{n} \mu_2}_{n\mu_2}\Bigg) = 0$$

0-mean

Covariance Matrix of Original Dimensions

Scaling data so as to have 0-mean on all dimensions
allow computing covariance much easily

$$\mathrm{Cov}(X_1, X_2) = \mathrm{E}[(X_1 - \underbrace{\mu_1^{\mathrm{new}}}_{=0})(X_2 - \underbrace{\mu_2^{\mathrm{new}}}_{=0})] = \mathrm{E}[X_1 X_2]$$

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As a consequence, the covariance matrix is also easier to compute!

Covariance Matrix of Original Dimensions

Let's assume the following is our 2-by-2 covariance matrix

$$\begin{array}{cc} & \begin{array}{cc} x_1 & x_2 \end{array} \\ \begin{array}{c} x_1 \\ x_2 \end{array} & \begin{bmatrix} 2 & 4/5 \\ 4/5 & 3/5 \end{bmatrix} \end{array}$$

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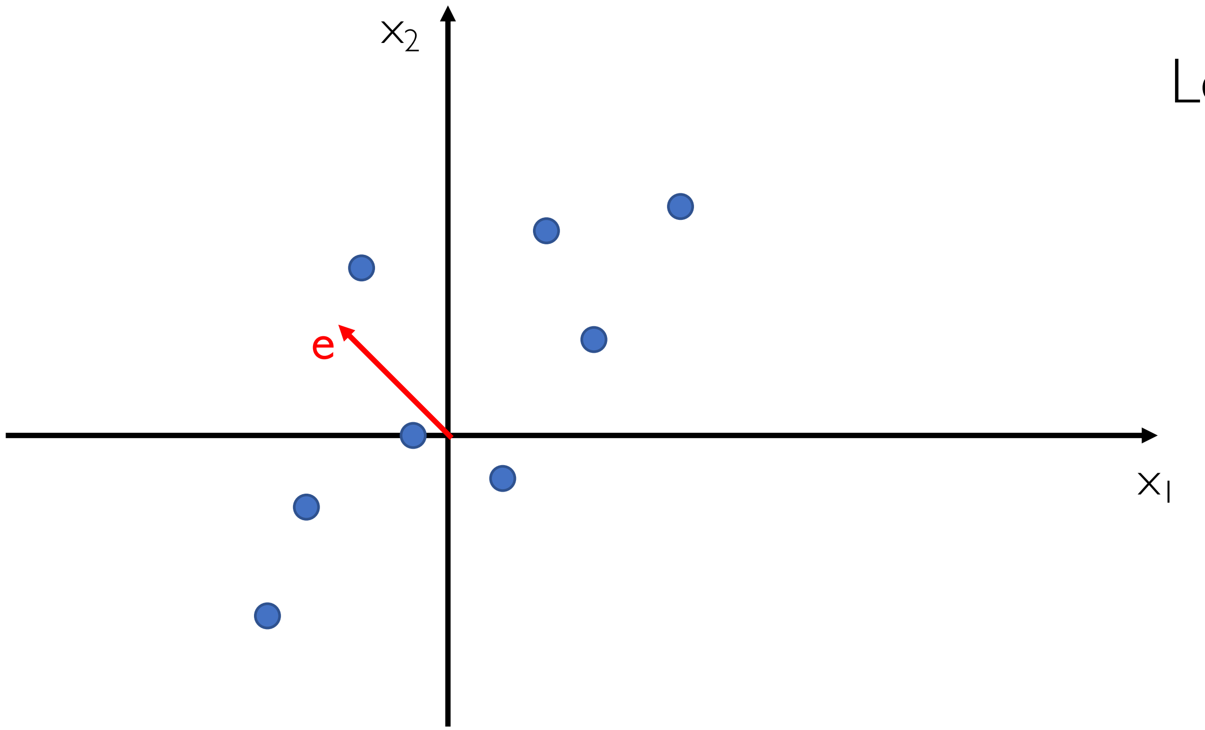
$$\boxed{\mathrm{Cov}(X_2, X_2) = \mathrm{Var}(X_2) = \frac{1}{n}\sum_{i=1}^{n} (x'_{i,2})^2}$$

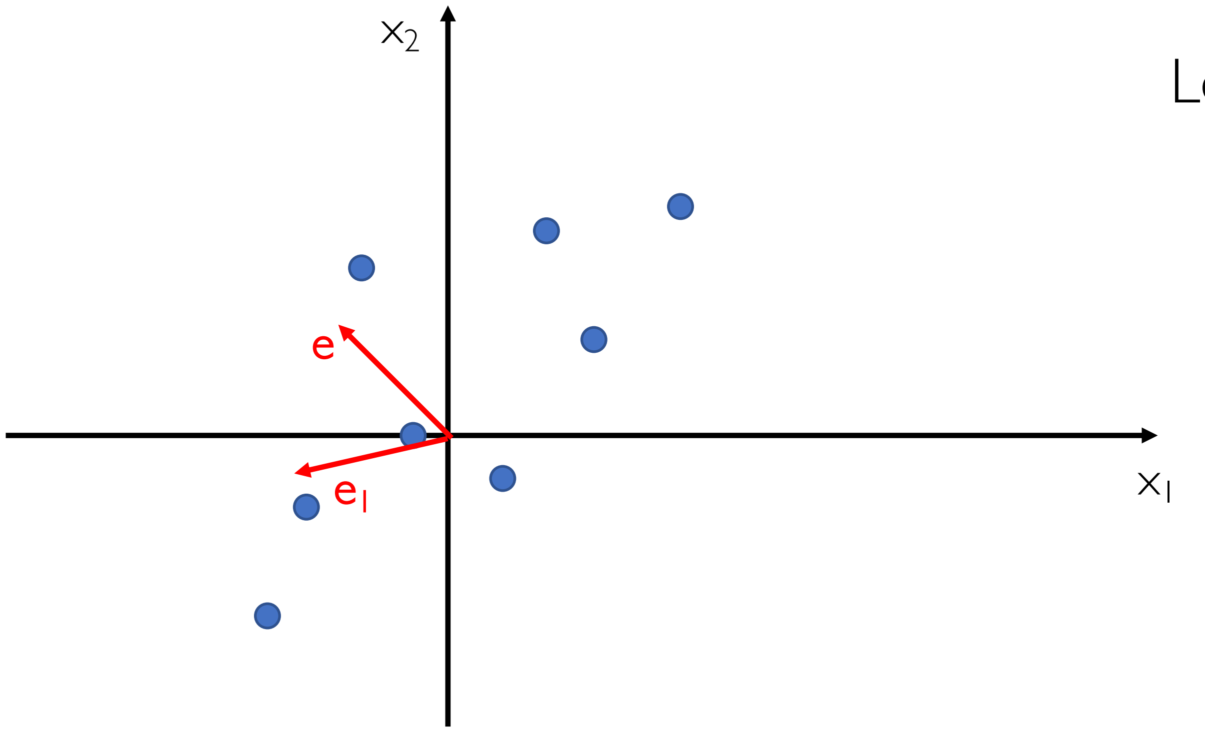
Covariance Matrix of Original Dimensions



Let's multiply our 2-by-2 covariance matrix K by a random vector e = (-1,1)

$$\underbrace{\begin{bmatrix} 2 & 4/5 \\ 4/5 & 3/5 \end{bmatrix}}_{K} \underbrace{\begin{bmatrix} -1 \\ 1 \end{bmatrix}}_{\mathbf{e}} =$$

Covariance Matrix of Original Dimensions



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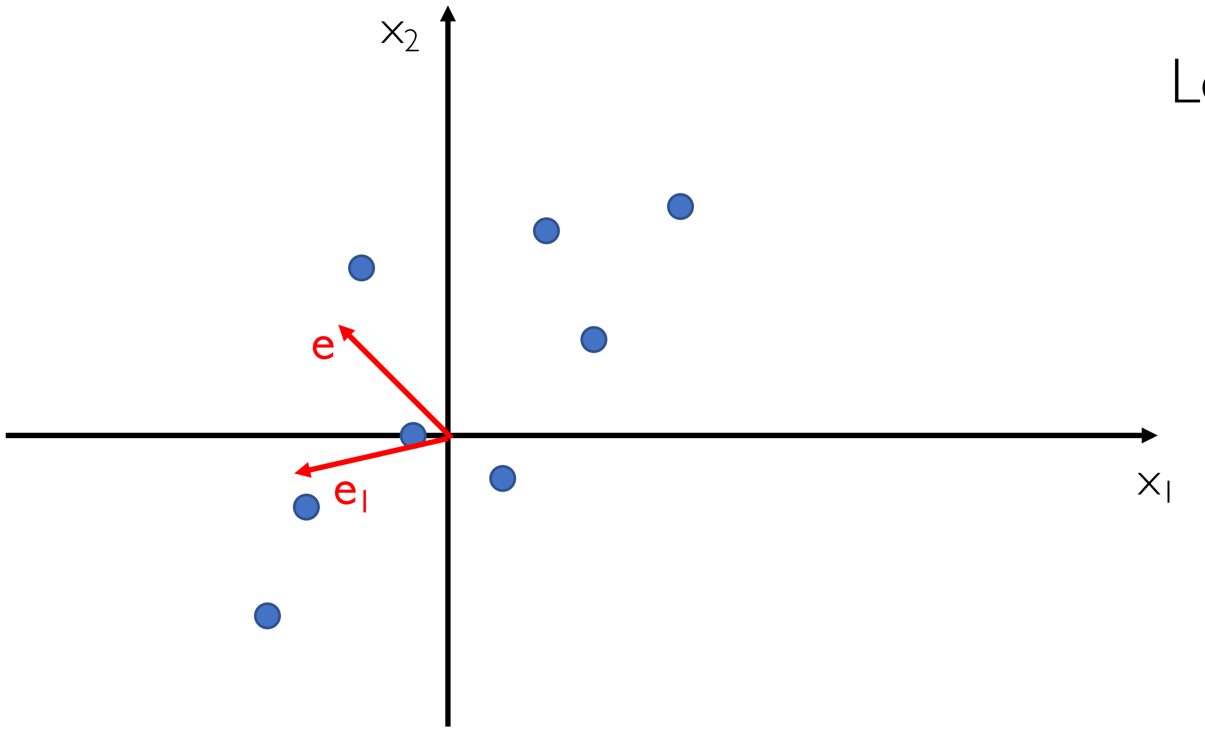

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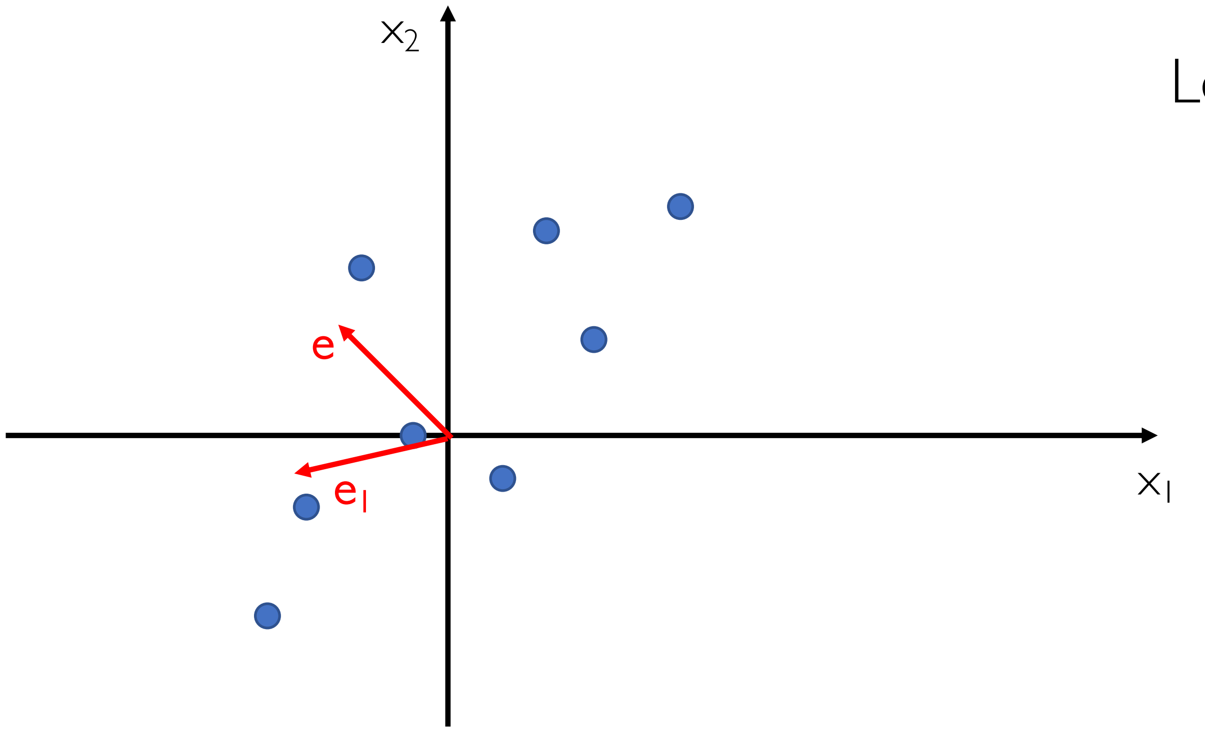
slope = 1/-1 = -1

Covariance Matrix of Original Dimensions



Let's multiply our 2-by-2 covariance matrix K by a random vector **e** = (-1,1)

$$\underbrace{\begin{bmatrix} 2 & 4/5 \\ 4/5 & 3/5 \end{bmatrix}}_{K} \underbrace{\begin{bmatrix} -1 \\ 1 \end{bmatrix}}_{\mathbf{e}} = \underbrace{\begin{bmatrix} -6/5 \\ -1/5 \end{bmatrix}}_{\mathbf{e_1}}$$

slope = 1/-1 = -1

new slope = -(1/5)/-(6/5) = 1/6

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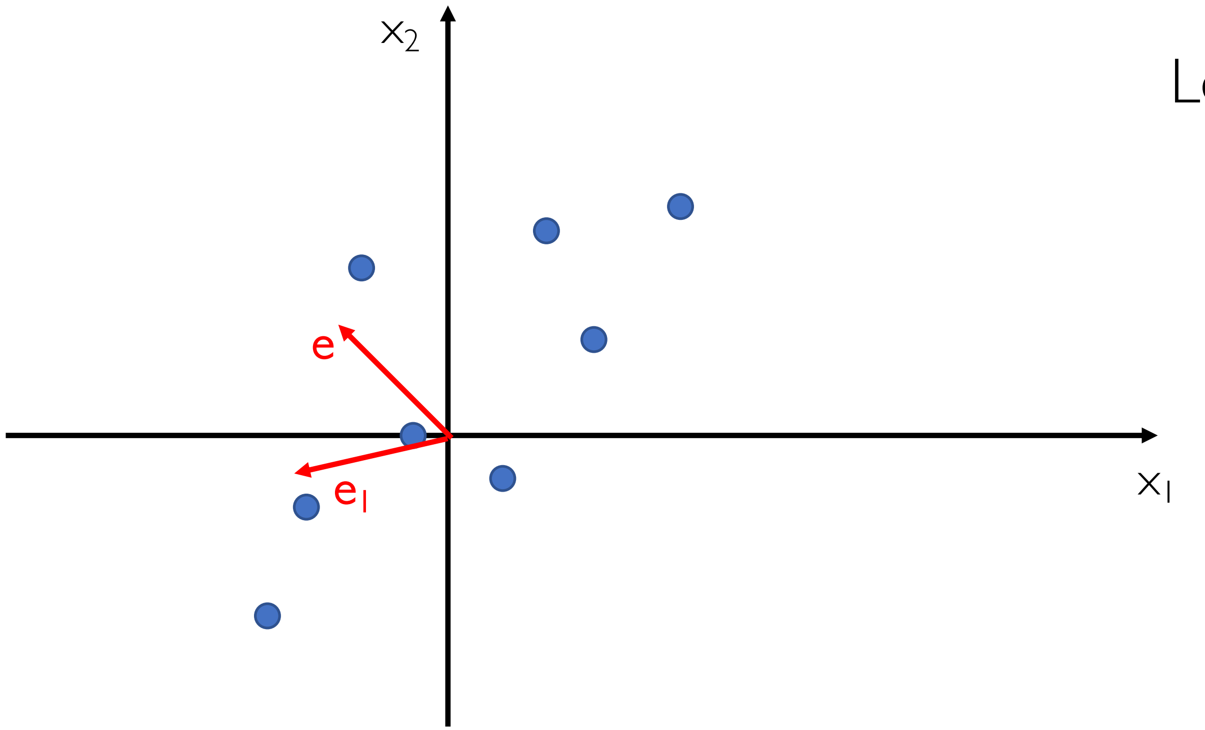

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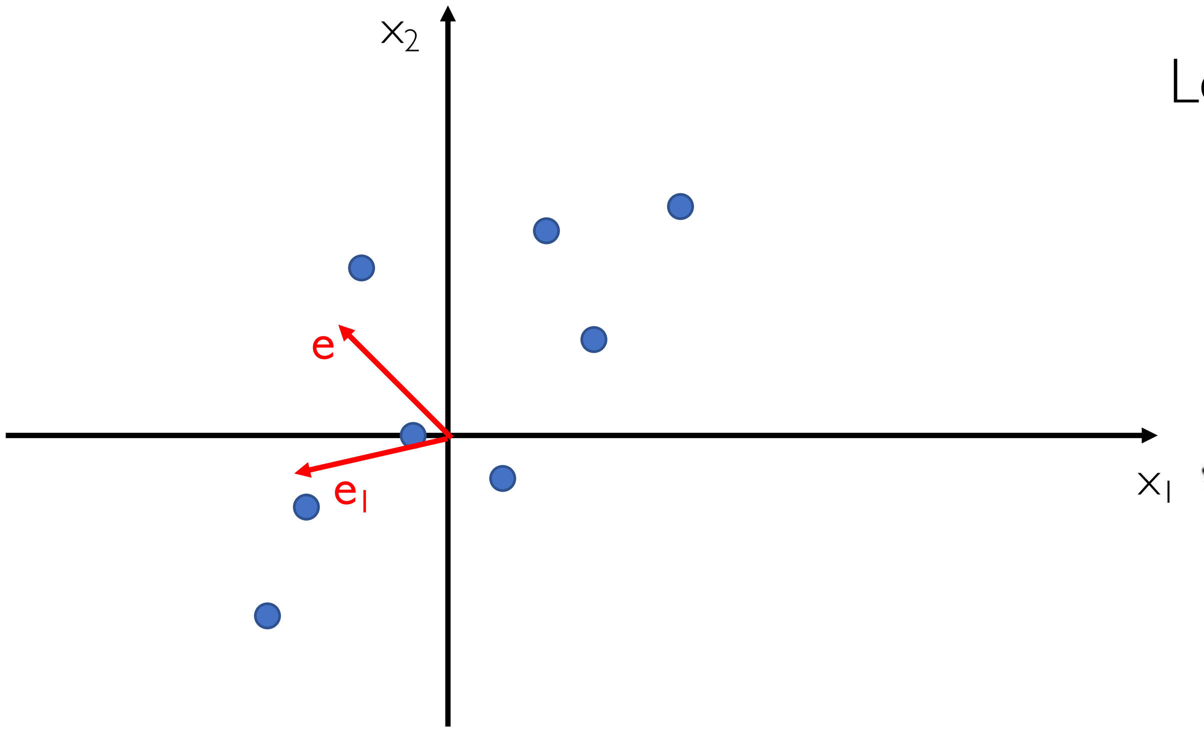

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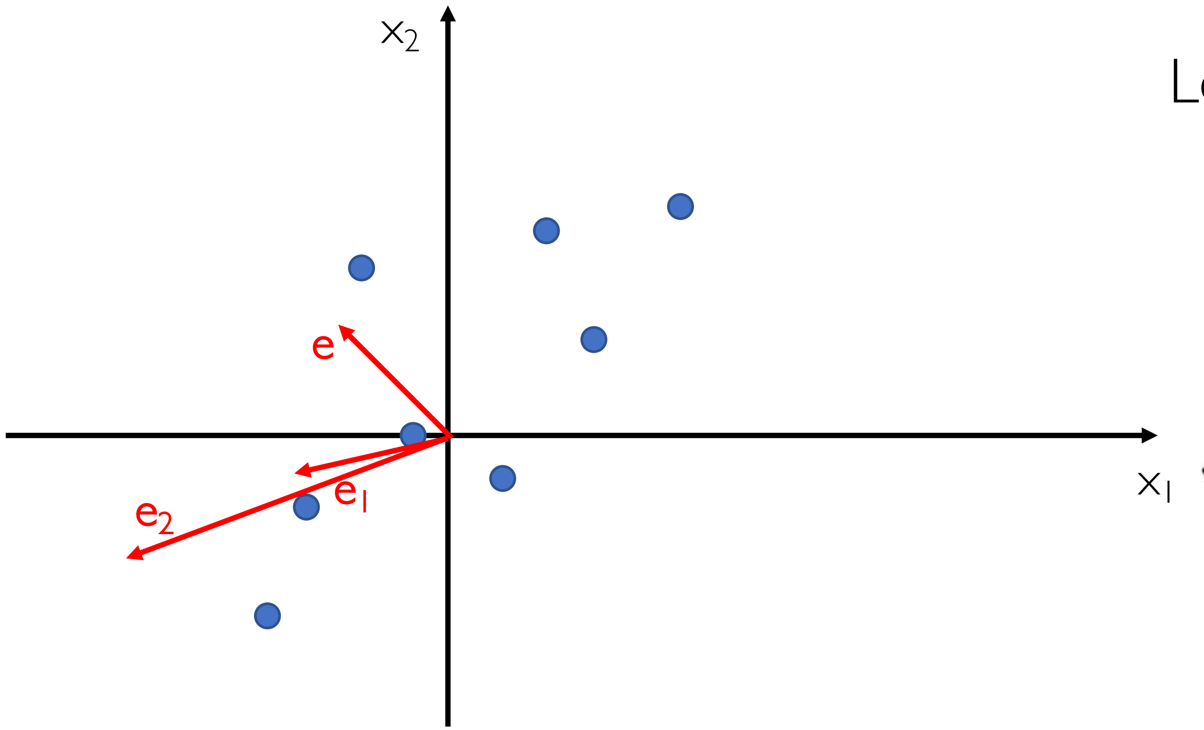

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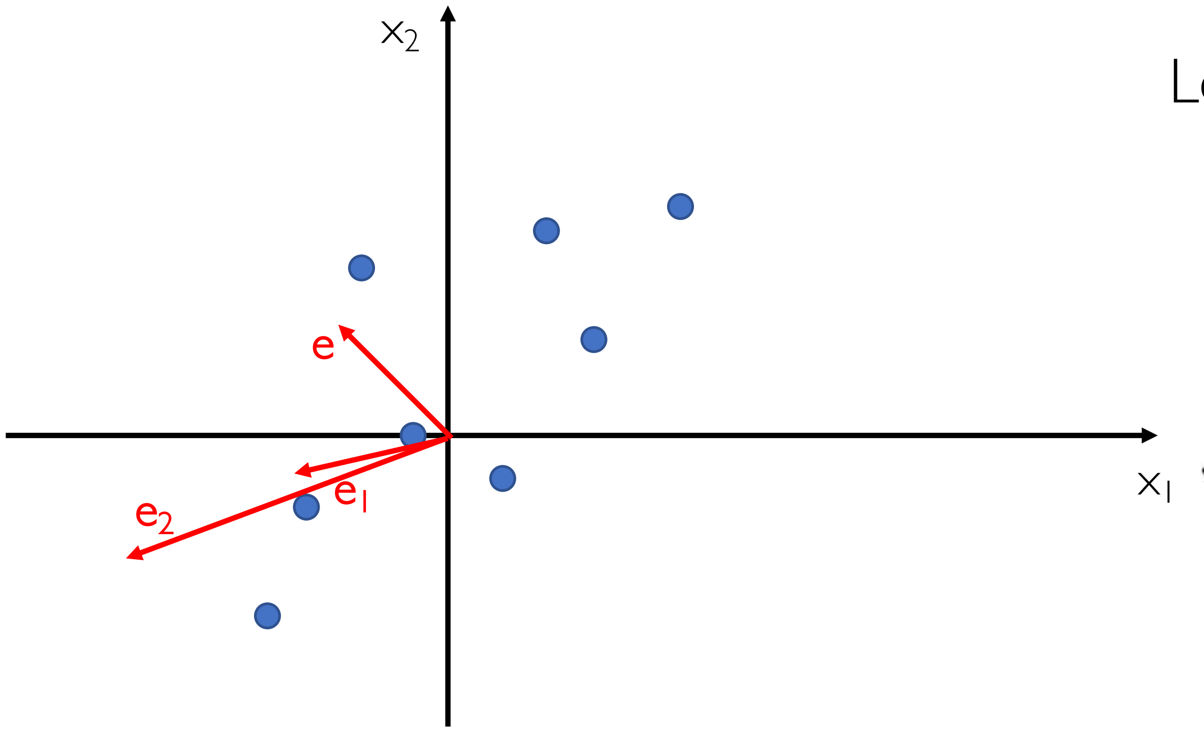

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slope = 1/6

new slope = 27/64

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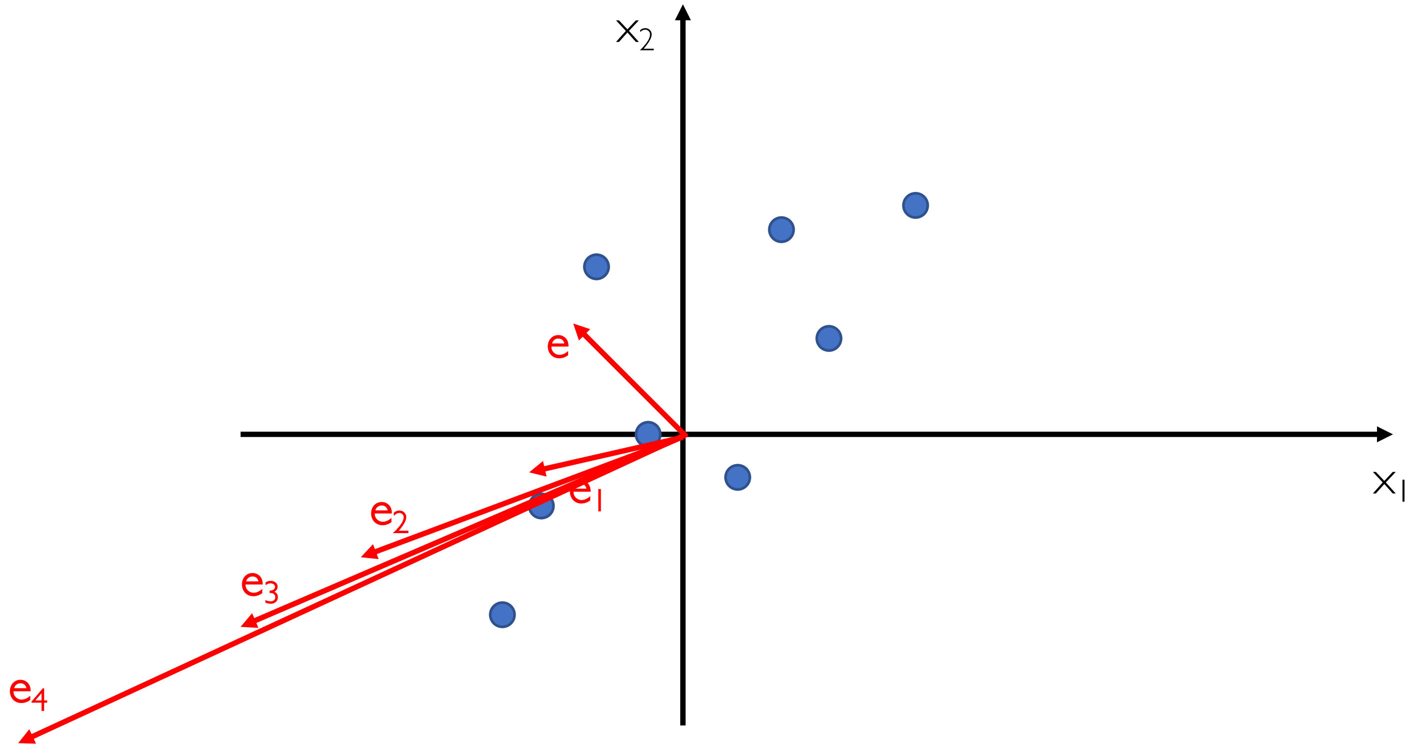
Covariance Matrix of Original Dimensions

If we keep doing this the resulting vector is getting longer and turns towards the direction of the largest variance



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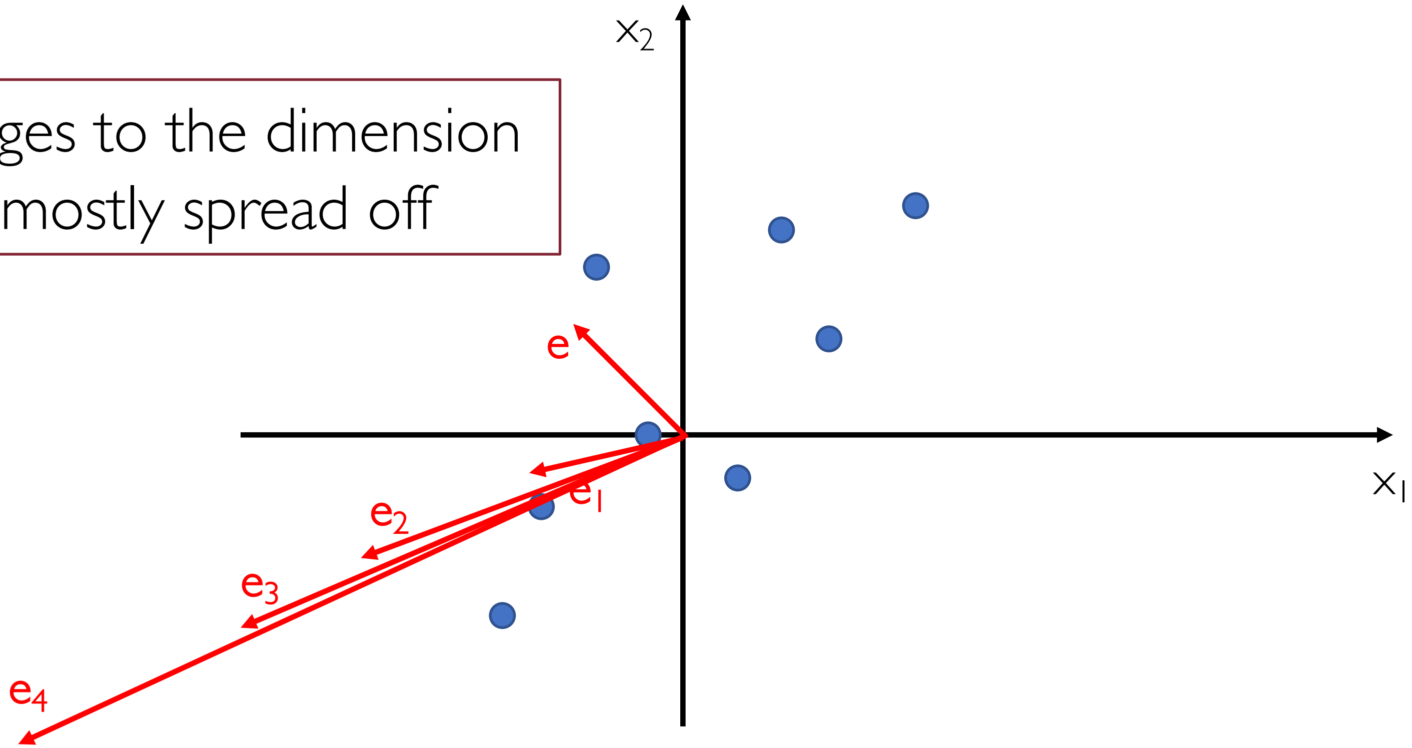
The slope converges to the dimension where data is mostly spread off



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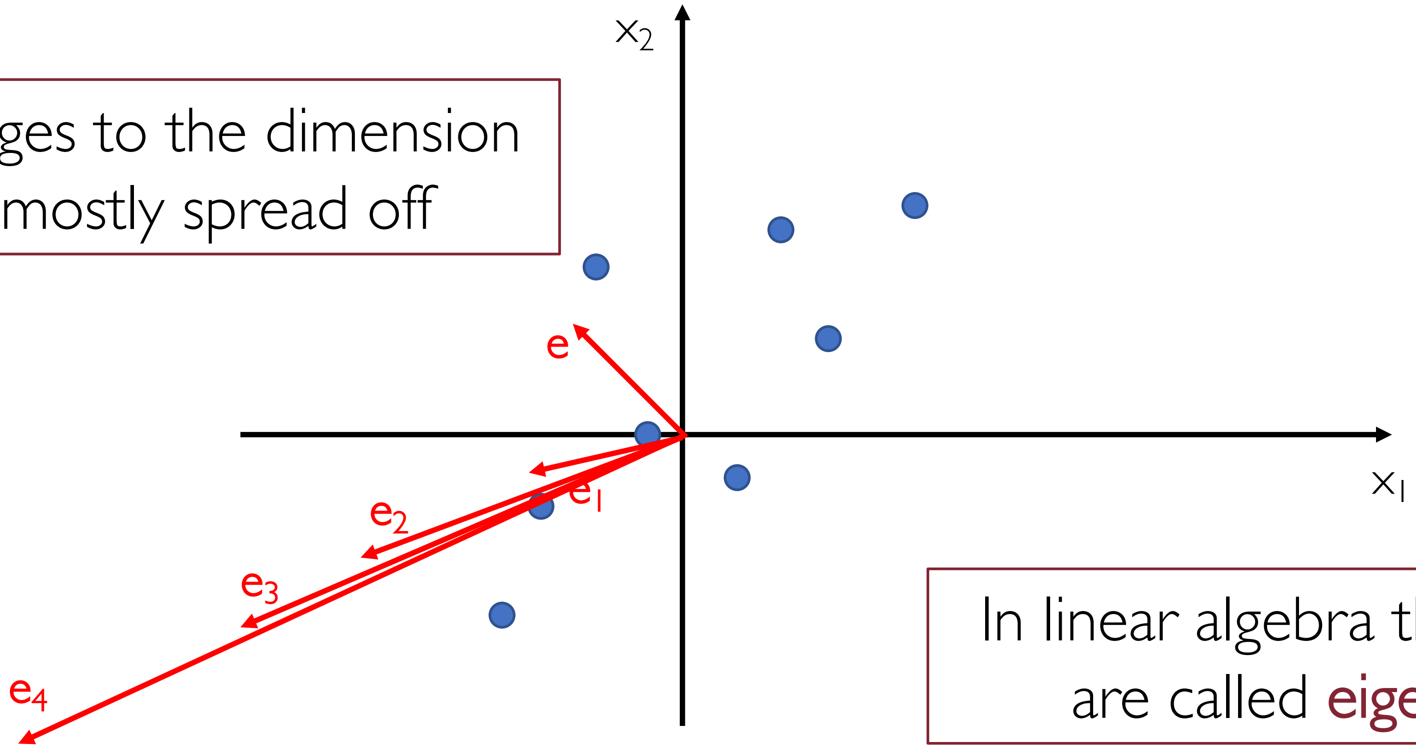

In linear algebra those vectors are called eigenvectors

Eigenvectors of the Covariance Matrix

$$\boxed{K\mathbf{e} = \lambda\mathbf{e}}$$

Eigenvectors of the Covariance Matrix

linear transformation

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When you multiply a matrix by an eigenvector **e** the resulting vector does not change its direction, but it is only scaled by a factor λ (eigenvalue)

Eigenvectors of the Covariance Matrix

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In other words, eigenvectors encapsulate all the relevant information to describe a linear transformation (in our case, represented by the covariance matrix K)

Eigenvectors of the Covariance Matrix

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When you multiply a matrix by an eigenvector e the resulting vector does not change its direction, but it is only scaled by a factor λ (eigenvalue)

Principal Components

eigenvectors of the covariance matrix with the largest eigenvalues

How Do We Compute Eigenvectors?

Remember that we want to solve for **e** the following:

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$$K\mathbf{e} = \lambda\mathbf{e}$$

We can rewrite the system of equations above as:

$$K\mathbf{e} - \lambda\mathbf{e} = 0 \Rightarrow (K - \lambda I)\mathbf{e} = 0$$

I is the identity matrix

How Do We Compute Eigenvectors?

We therefore resort to solve the following homogeneous system:

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e = 0

The only way for the homogeneous system above to have a non-trivial solution is for its matrix (K – λI) to be non-invertible, otherwise:

$$\cancel{(K - \lambda I)}\cancel{(K - \lambda I)^{-1}}\boxed{\mathbf{e} = 0}\cancel{(K - \lambda I)^{-1}}$$

How Do We Compute Eigenvectors?

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If the determinant of the matrix $(K - \lambda I)$ is equal to 0, it is non-invertible

The corresponding homogeneous system will have a non-trivial solution

How Do We Compute Eigenvectors?

1. Find the eigenvalues by solving for λ: det(K – λI) = 0

$$\det\left(\underbrace{\begin{bmatrix} 2-\lambda & 4/5 \\ 4/5 & 3/5-\lambda \end{bmatrix}}_{K-\lambda I}\right) = 0$$

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characteristic equation of K

$$\boxed{\lambda_1 = \tfrac{13+\sqrt{113}}{10} \approx 2.36;} \quad \boxed{\lambda_2 = \tfrac{13-\sqrt{113}}{10} \approx 0.24}$$

How Do We Compute Eigenvectors?

2. Plug each eigenvalue in to find the corresponding eigenvector

$$\underbrace{\begin{bmatrix} 2 & 4/5 \\ 4/5 & 3/5 \end{bmatrix}}_{K} \underbrace{\begin{bmatrix} e_{1,1} \\ e_{1,2} \end{bmatrix}}_{\mathbf{e_1}} = \lambda_1 \underbrace{\begin{bmatrix} e_{1,1} \\ e_{1,2} \end{bmatrix}}_{\mathbf{e_1}}$$

$$\underbrace{\begin{bmatrix} 2 & 4/5 \\ 4/5 & 3/5 \end{bmatrix}}_{K} \underbrace{\begin{bmatrix} e_{2,1} \\ e_{2,2} \end{bmatrix}}_{\mathbf{e_2}} = \lambda_2 \underbrace{\begin{bmatrix} e_{2,1} \\ e_{2,2} \end{bmatrix}}_{\mathbf{e_2}}$$

How Do We Compute Eigenvectors?

Let's see what happens for λ_1

$$\begin{cases} 2e_{1,1} + 4/5e_{1,2} = \frac{13+\sqrt{113}}{10}e_{1,1} \\ 4/5e_{1,1} + 3/5e_{1,2} = \frac{13+\sqrt{113}}{10}e_{1,2} \end{cases}$$

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$$\begin{cases} 2e_{1,1} + 0.8e_{1,2} = 2.36e_{1,1} \\ 0.8e_{1,1} + 0.6e_{1,2} = 2.36e_{1,2} \end{cases}$$

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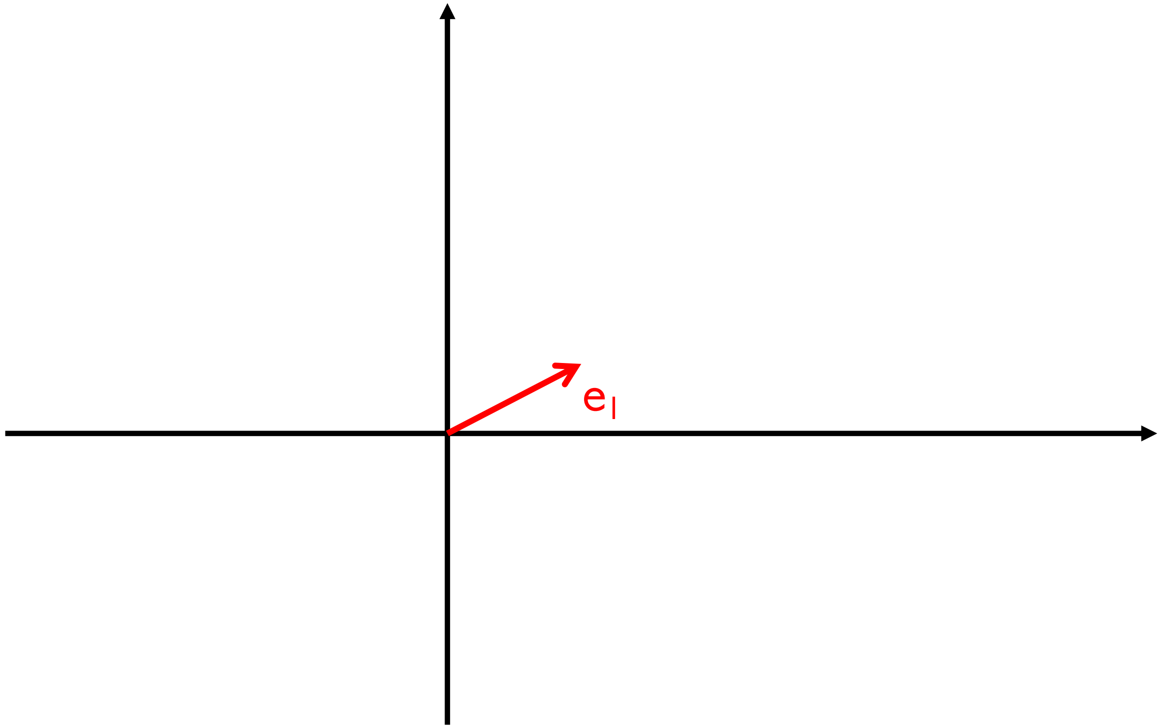
The system has infintely many solutions

How Do We Compute Eigenvectors?

Any vector which satisfies the relationship above works!



$$\begin{bmatrix} 1.1 \\ 0.5 \end{bmatrix}$$

$$e_{1,1} \approx 2.2 e_{1,2}$$

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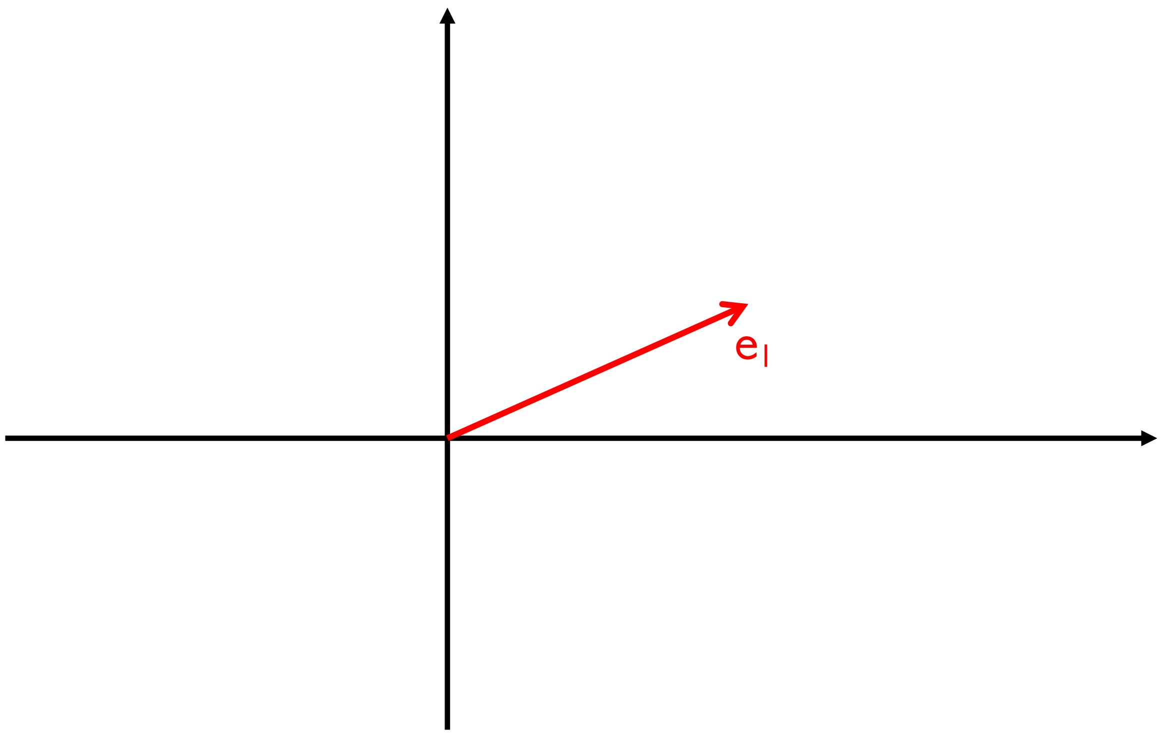

$$\begin{bmatrix} 2.2 \\ 1 \end{bmatrix}$$

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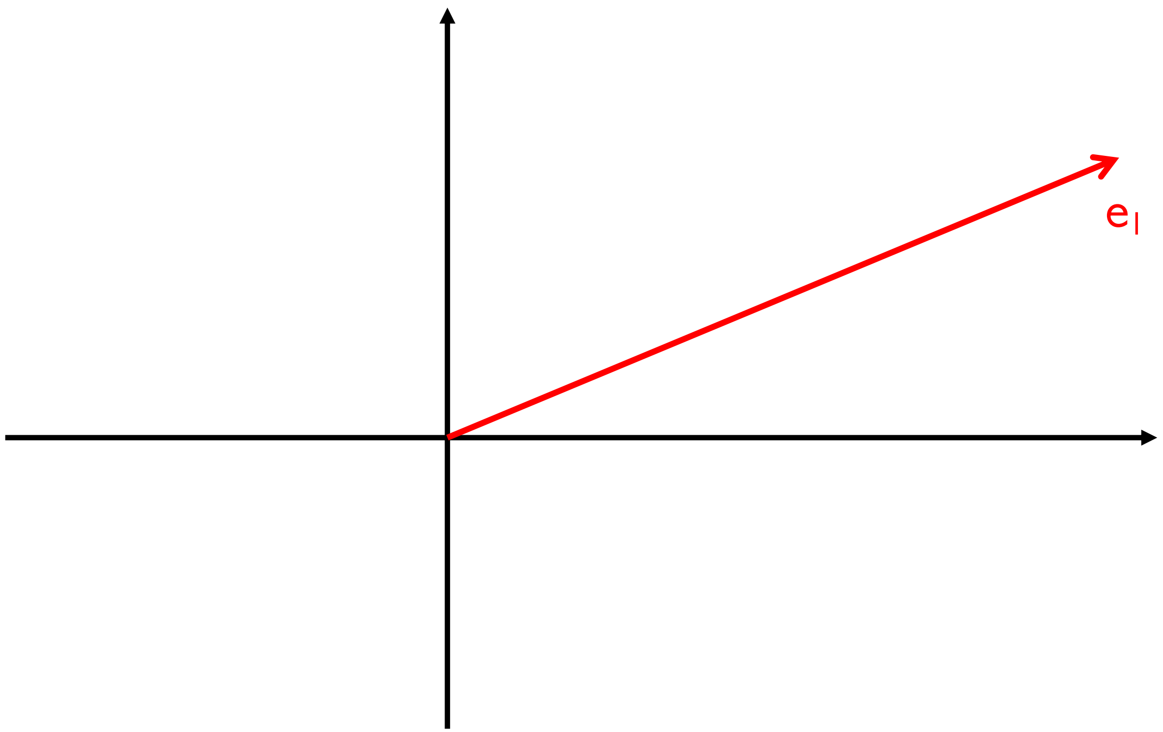
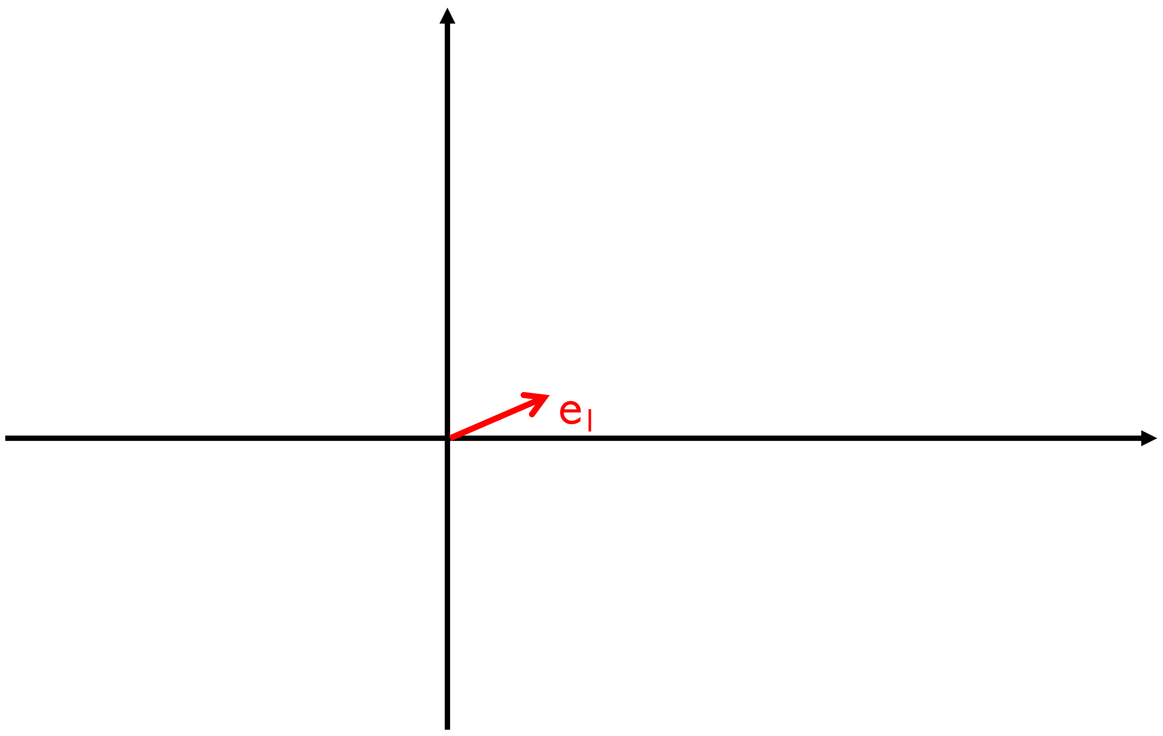


$$\begin{bmatrix} 4.4 \\ 2 \end{bmatrix}$$

$$e_{1,1} \approx 2.2 e_{1,2}$$

How Do We Compute Eigenvectors?

By convention, we restrict to $||\mathbf{e}_1|| = 1$



$$\begin{bmatrix} 0.91 \\ 0.41 \end{bmatrix}$$

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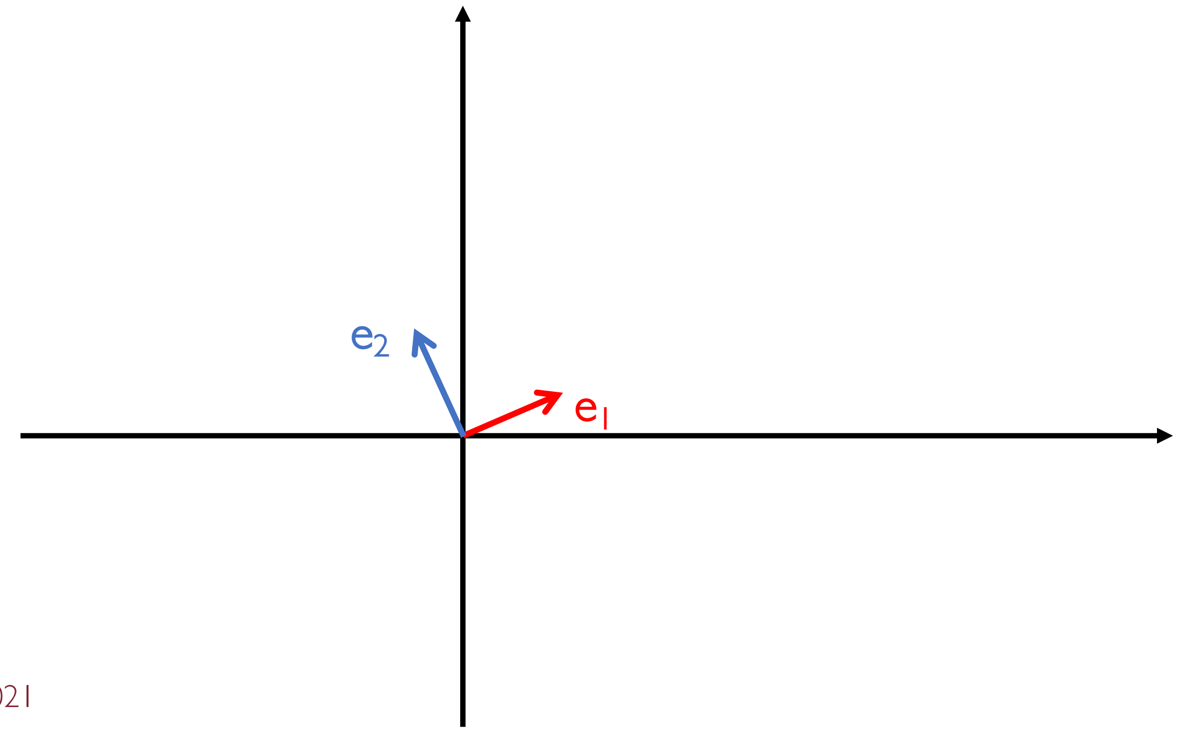
How Do We Compute Eigenvectors?

The second eigenvector e_2 can be found by plugging in the smaller eigenvalue λ_2



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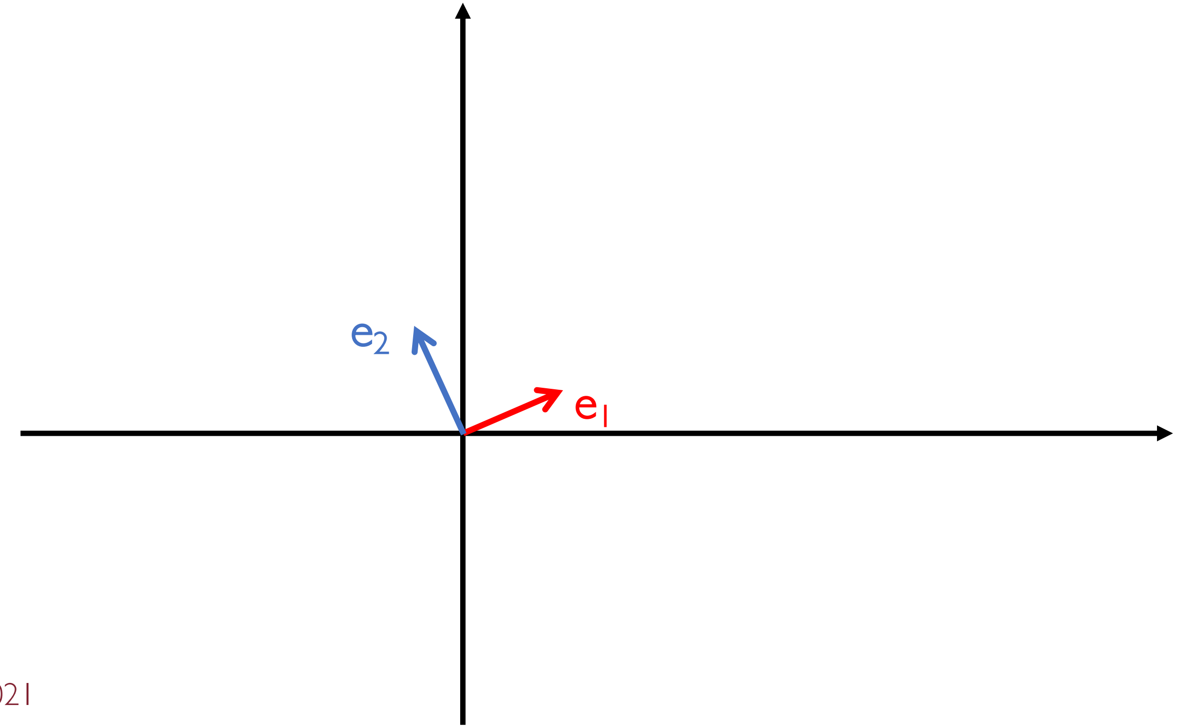
This is just orthogonal to the previously found e_1



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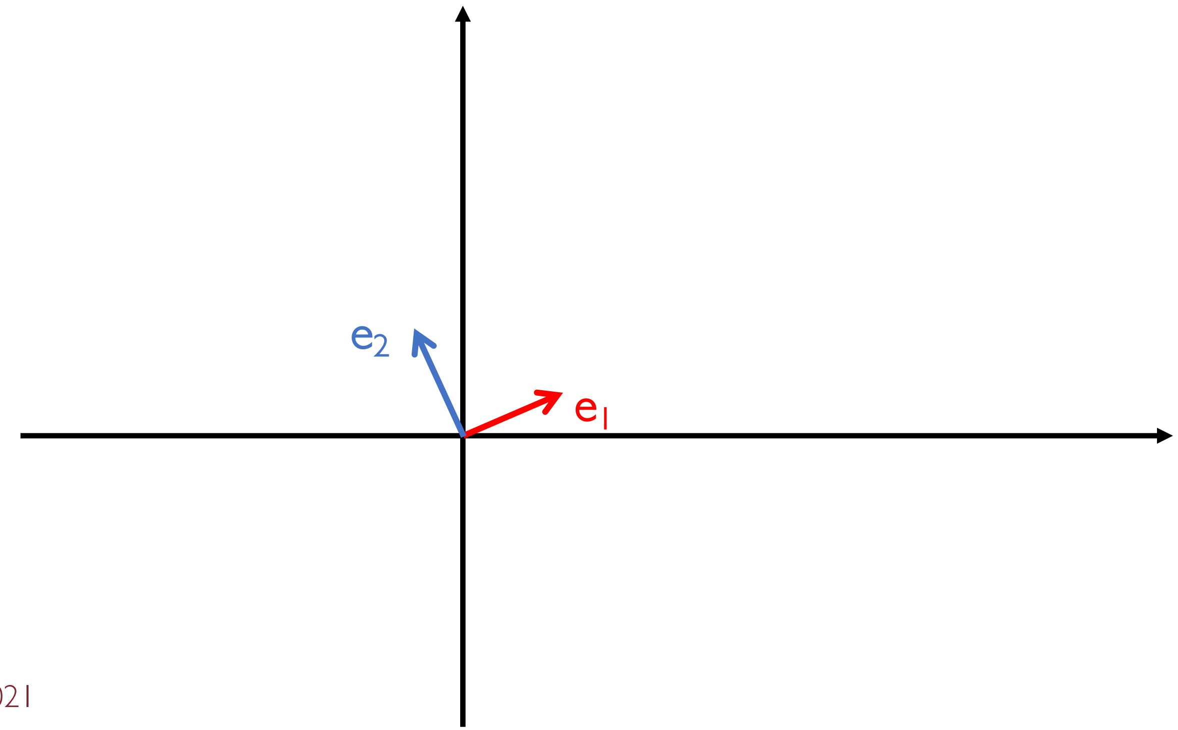

e_1 and e_2 are the new coordinate system replacing the original x_1 and x_2

$$\mathbf{e_1} = \begin{bmatrix} 0.91 \\ 0.41 \end{bmatrix} \mathbf{e_2} = \begin{bmatrix} -0.41 \\ 0.91 \end{bmatrix}$$

Principal Components

$$\mathbf{e}_1 = \begin{bmatrix} 0.91 \\ 0.41 \end{bmatrix} \mathbf{e}_2 = \begin{bmatrix} -0.41 \\ 0.91 \end{bmatrix}$$

e_1 is the 1st principal component as it is the eigenvector corresponding to the largest eigenvalue

e_2 is the 2nd principal component as it is the eigenvector corresponding to the smallest eigenvalue

Projecting to New Dimensions: 2-d Case

- e_1 and e_2 identify our new coordinate system (principal components)

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$\Downarrow$

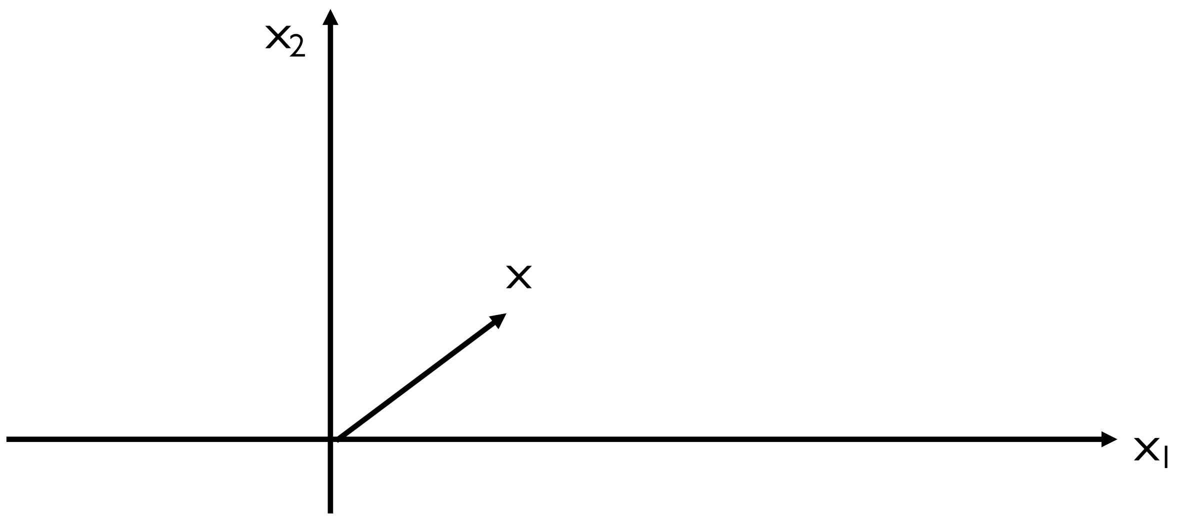
Goal

We want to represent $\mathbf{x}$ in the new $(\mathbf{e}_1, \mathbf{e}_2)$-coordinate system

Projecting to New Dimensions: 2-d Case

1. Center $\mathbf{x}$ around the mean of each dimension

$$\mathbf{x}' = \mathbf{x} - \boldsymbol{\mu} = (x_1 - \mu_1, x_2 - \mu_2)$$



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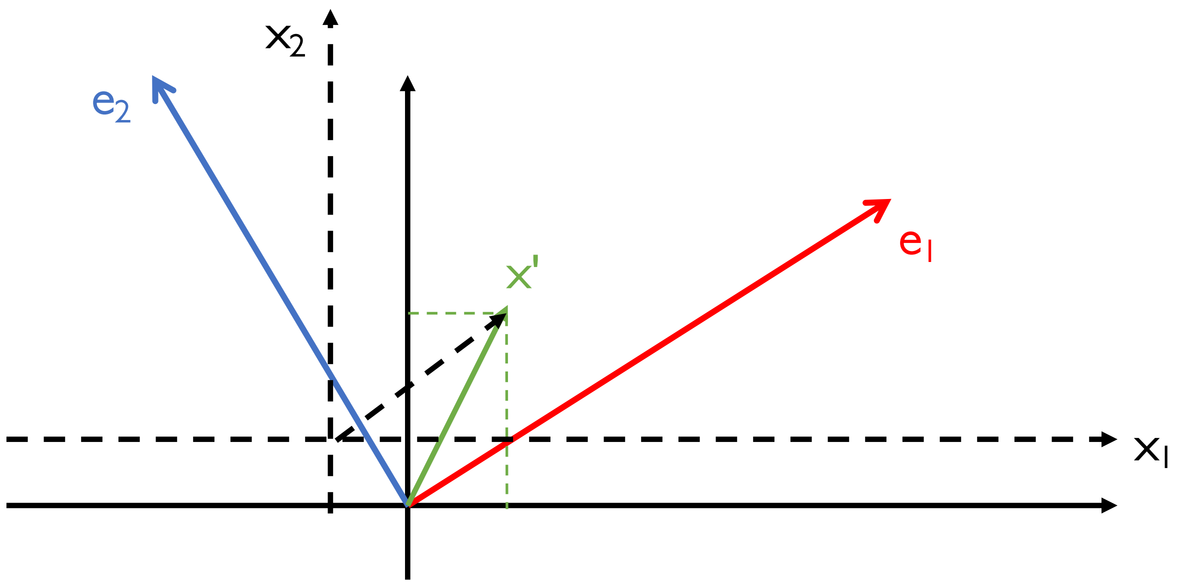
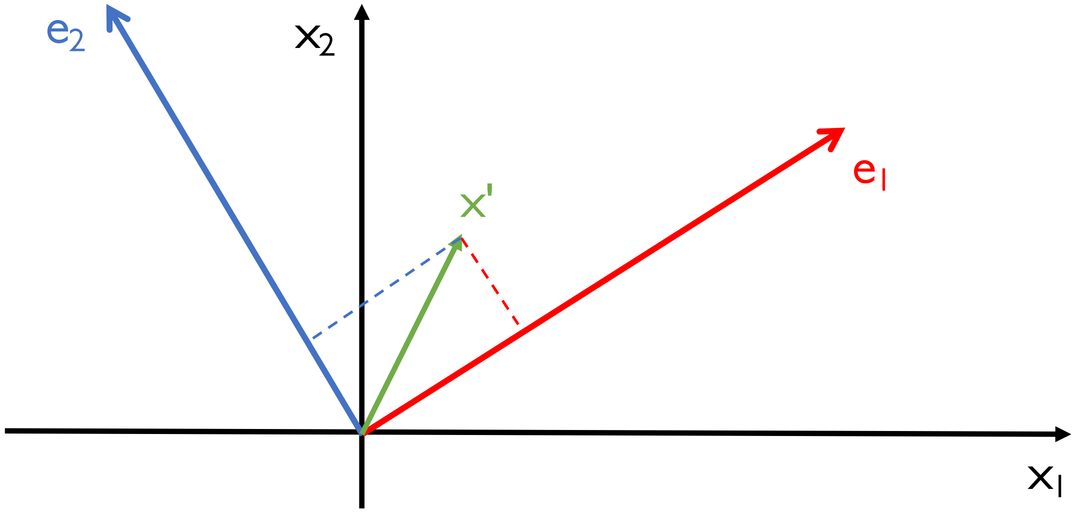


Projecting to New Dimensions: 2-d Case

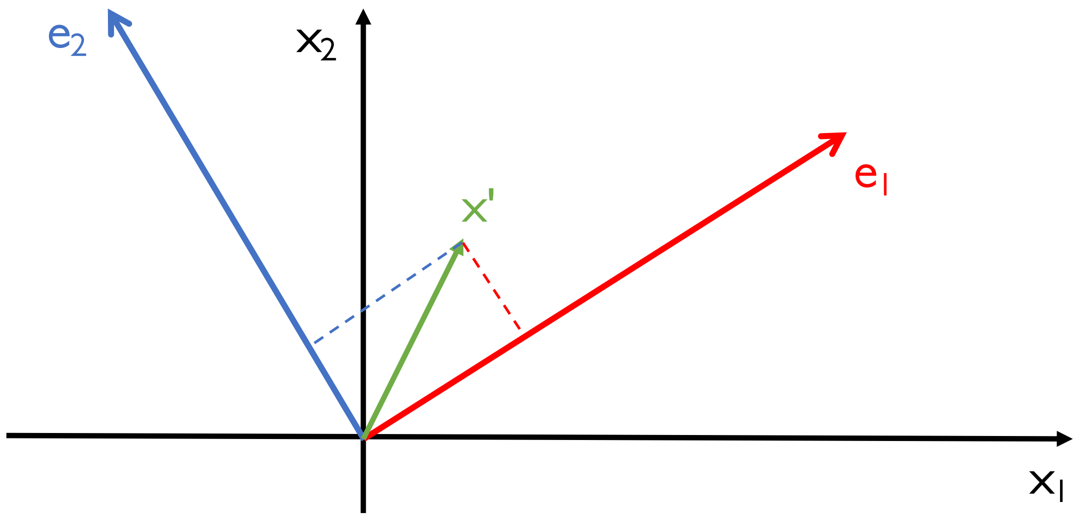
2. Project **x'** on each dimension $\mathbf{e}_1$ and $\mathbf{e}_2$

$$\mathbf{x}' = \underbrace{(x'_1, x'_2)}_{\text{coordinates of } \mathbf{x}' \text{ in the } (\mathbf{e}_1, \mathbf{e}_2)\text{-space}} = (\mathbf{x}'^T\mathbf{e}_1, \mathbf{x}'^T\mathbf{e}_2)$$



Projecting to New Dimensions: 2-d Case

Why the dot product?



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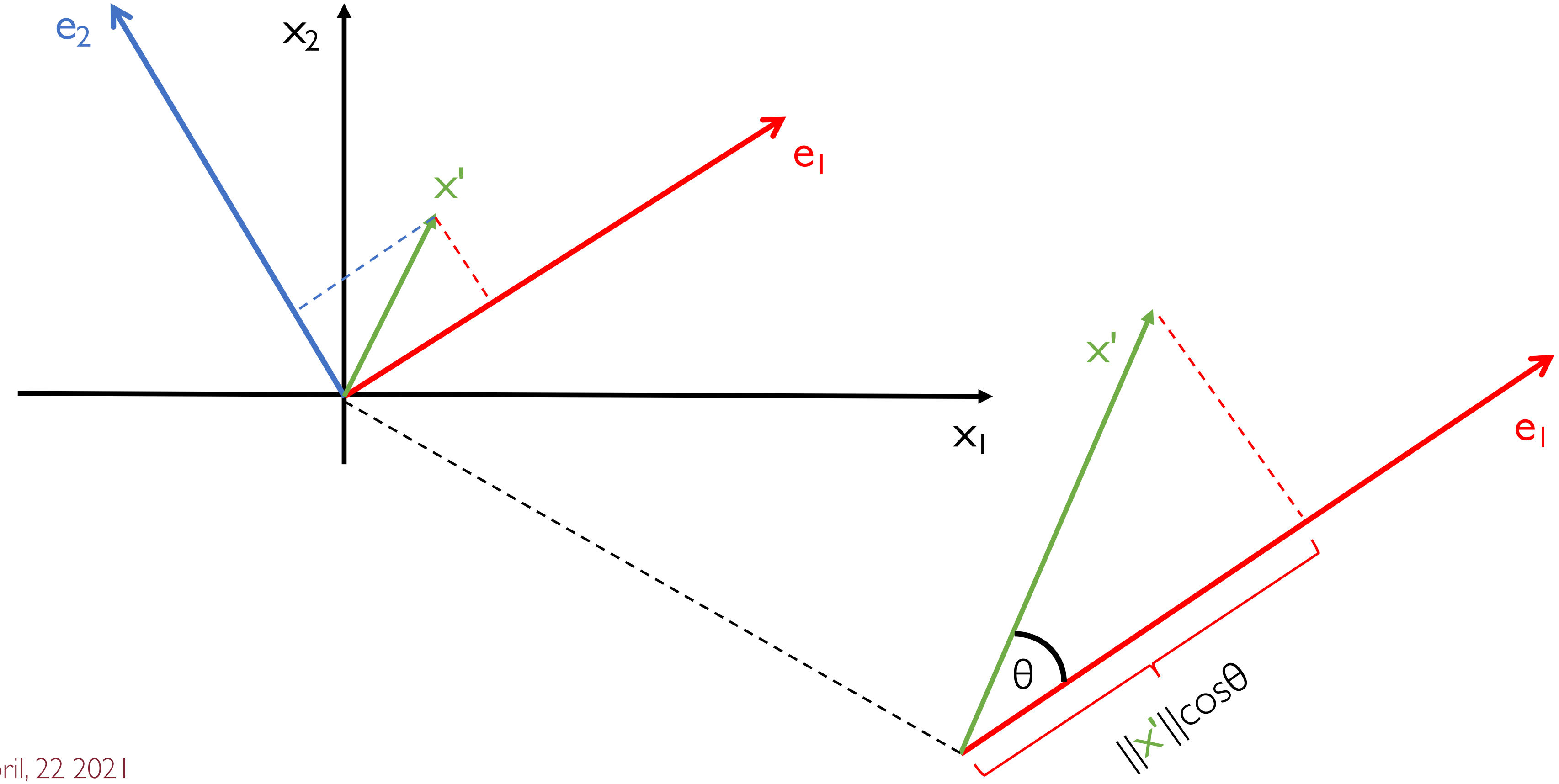
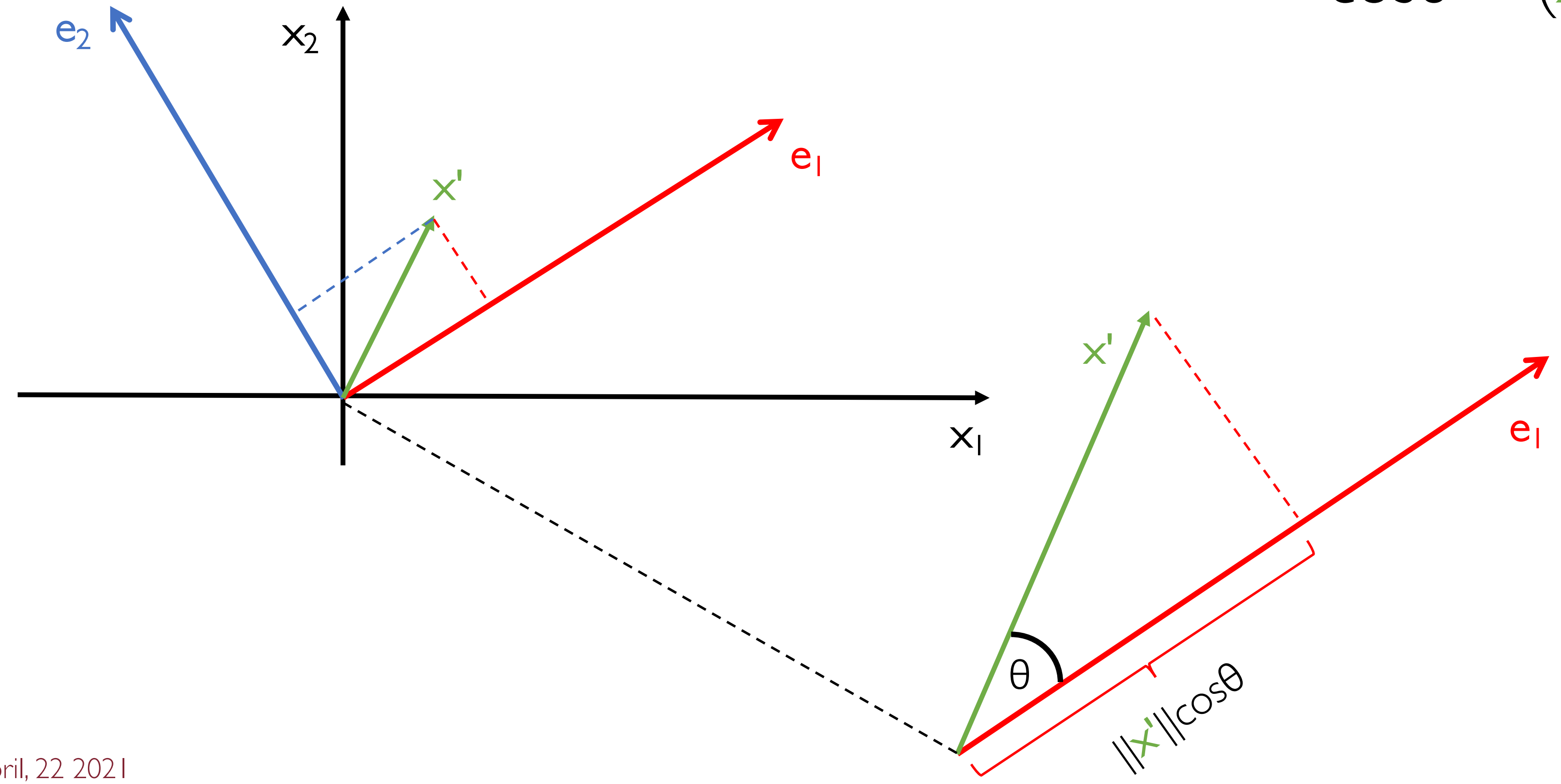


Projecting to New Dimensions: 2-d Case

Why the dot product?

$$\cos\theta = (x'e_1)/||x'||||e_1||$$



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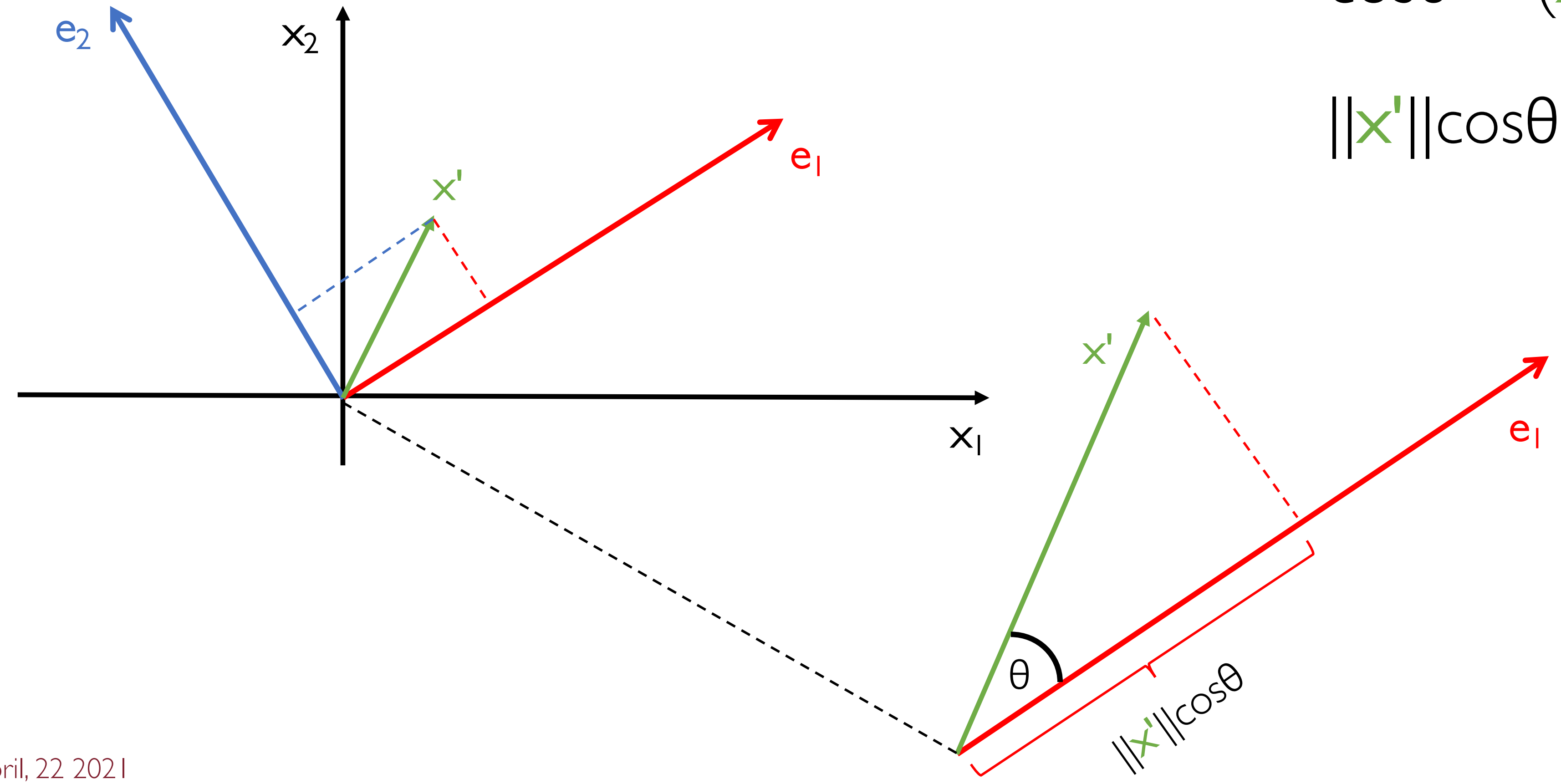

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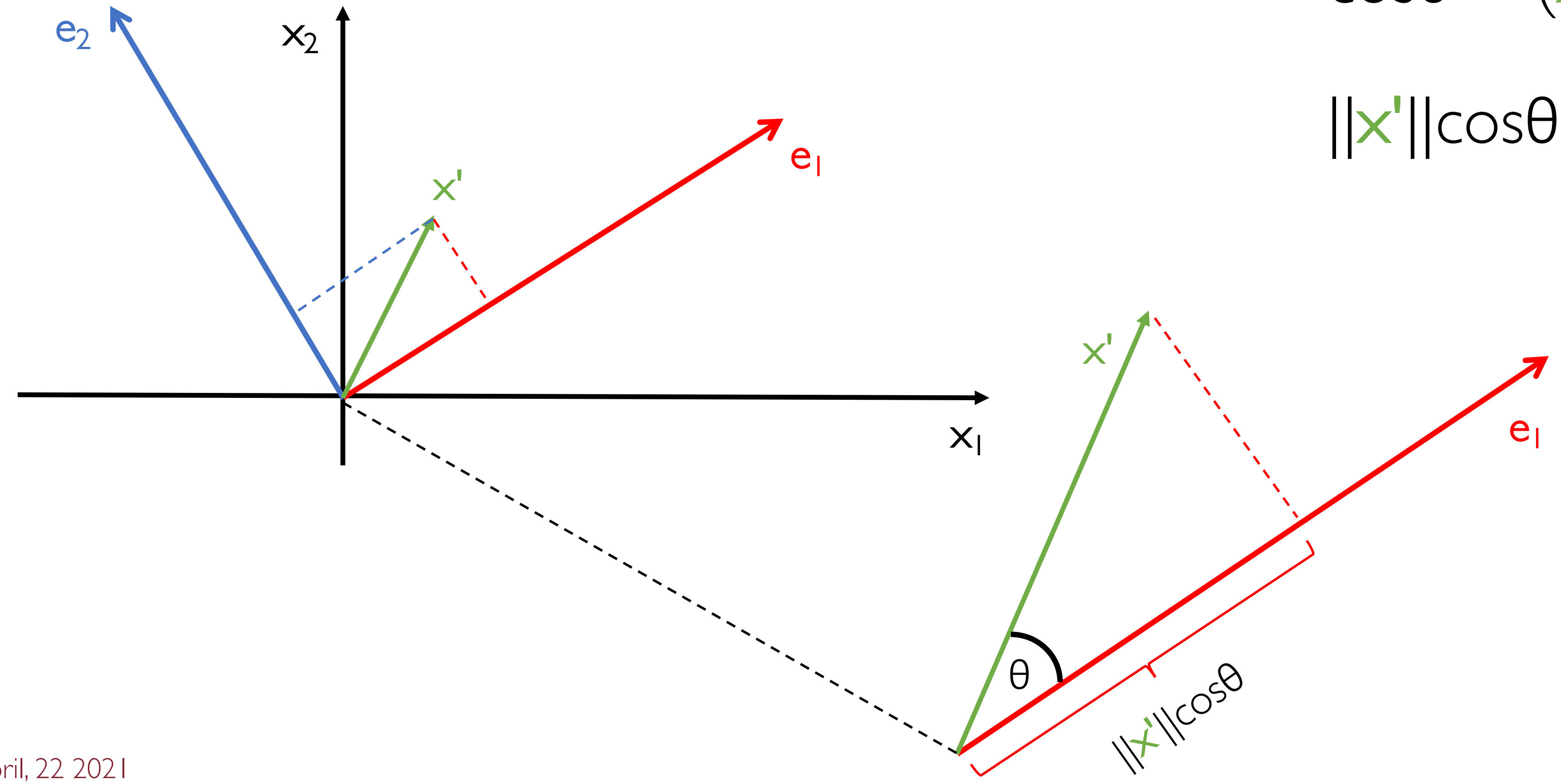

$||e_1|| = 1$

Projecting to New Dimensions: 2-d Case

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$$\cos\theta = (x'e_1)/\|x'\|\|e_1\|$$

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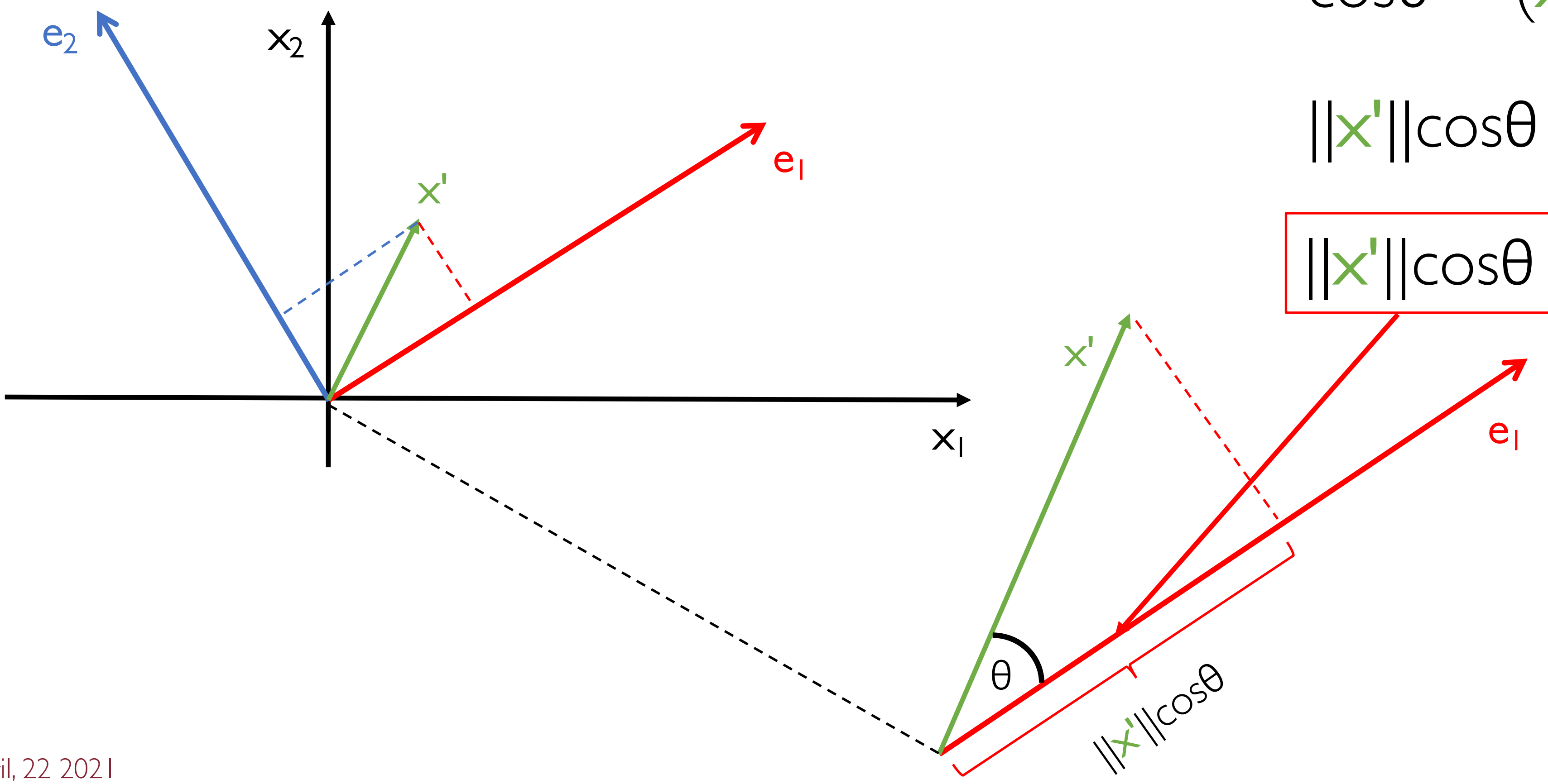
$$\boxed{\|x'\|\cos\theta = x'e_1}$$

$$\boxed{\|e_1\| = 1}$$



Projecting to New Dimensions: 2-d Case

The new coordinates of the original data point **x** according to the eigenvectors e_1 and e_2 are as follows:

$$\mathbf{x}' = \begin{bmatrix} x'_1 \\ x'_2 \end{bmatrix} = \begin{bmatrix} \mathbf{x}'^T \mathbf{e}_1 \\ \mathbf{x}'^T \mathbf{e}_2 \end{bmatrix} = \begin{bmatrix} (x_1 - \mu_1)e_{1,1} + (x_2 - \mu_2)e_{1,2} \\ (x_1 - \mu_1)e_{2,1} + (x_2 - \mu_2)e_{2,2} \end{bmatrix}$$

Projecting to New Dimensions: *d*-dimensions

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix}$$

Original d-dimensional data point

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$$\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_k$$
$$k \ll d, \ \ \mathbf{e}_i \in \mathbb{R}^d$$

k << d
principal components

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k << d principal components

1. Mean centering

$$\mathbf{x}' = \mathbf{x} - \boldsymbol{\mu} = \begin{bmatrix} x_1 - \mu_1 \\ x_2 - \mu_2 \\ \vdots \\ x_d - \mu_d \end{bmatrix}$$

Projecting to New Dimensions: *d*-dimensions

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k << d
principal components

2. Projection to principal components

$$\mathbf{x}' = \begin{bmatrix} x'_1 \\ x'_2 \\ \vdots \\ x'_k \end{bmatrix} = \begin{bmatrix} (\mathbf{x}-\boldsymbol{\mu})^T\mathbf{e}_1 \\ (\mathbf{x}-\boldsymbol{\mu})^T\mathbf{e}_2 \\ \vdots \\ (\mathbf{x}-\boldsymbol{\mu})^T\mathbf{e}_k \end{bmatrix} = \begin{bmatrix} (x_1-\mu_1)e_{1,1} + (x_2-\mu_2)e_{1,2} + \ldots + (x_d-\mu_d)e_{1,d} \\ (x_1-\mu_1)e_{2,1} + (x_2-\mu_2)e_{2,2} + \ldots + (x_d-\mu_d)e_{2,d} \\ \vdots \\ (x_1-\mu_1)e_{k,1} + (x_2-\mu_2)e_{k,2} + \ldots + (x_d-\mu_d)e_{k,d} \end{bmatrix}$$

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More details available here:
https://github.com/gtolomei/theory-of-algorithms/raw/main/extras/Notes_on_Principal_Component_Analysis.pdf

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- We want to select k dimensions ($k \ll d$)
- We know that eigenvalue λ_i is the variance along e_i and the overall variance of the data is given by the sum of all the eigenvalues

How Many Dimensions?

- In a d-dimensional space we may have $e_1, \ldots, e_d$ length-1 eigenvectors
- We want to select k dimensions ($k << d$)
- We know that eigenvalue λ_i is the variance along e_i and the overall variance of the data is given by the sum of all the eigenvalues

⇓

Pick the subset of k eigenvectors that "explain" the most variance

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1. Sort eigenvectors by eigenvalues such that $\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_d$

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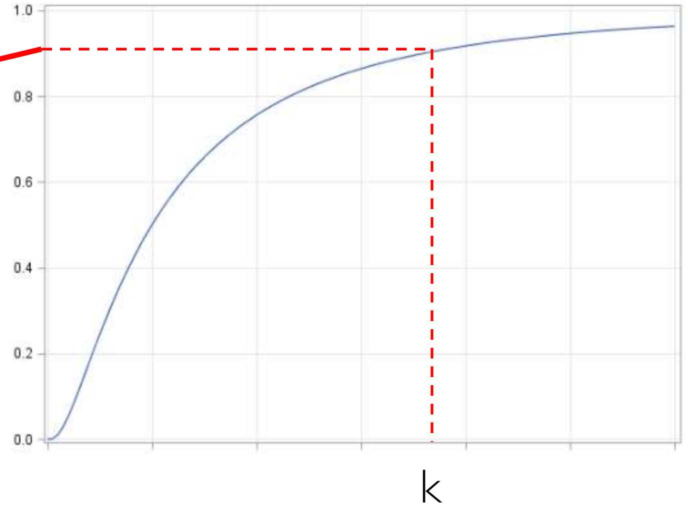
2. Pick the first k eigenvectors that explain x% of the total variance

$$\boxed{\frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{d} \lambda_i} \leq 1}$$

e.g., x = 90÷95%



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<u>Solution</u>

Normalize each dimension to 0-mean and 1-std-deviation

$$z = \frac{x - \mu}{\sigma}$$

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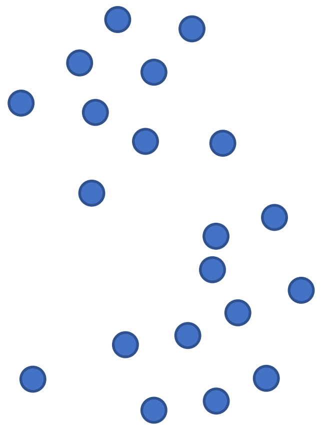

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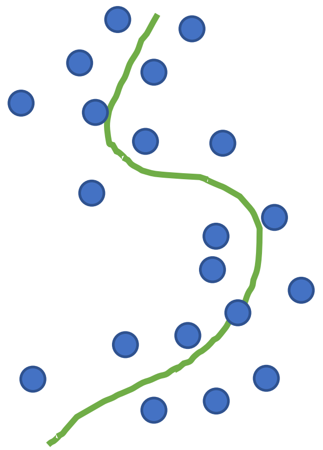

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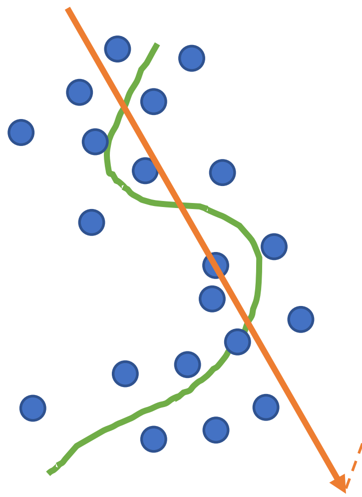

PCA will find a straight line and will not mimic non-linearity

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- PCA is a dimensionality reduction technique which allows representing high-dimensional data into low-dimensional linear subspace
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  - The original space is rotated to make dimensions uncorrelated (i.e., independent)
- Reduced size of data means faster processing and smaller storage
- PCA can be very expensive for many very large-scale applications
- If data do not live on a linear subspace PCA may not work well