

# Big Data Computing

Master's Degree in Computer Science

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# Recap from Last Lecture(s)

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

# DIMENSIONALITY REDUCTION

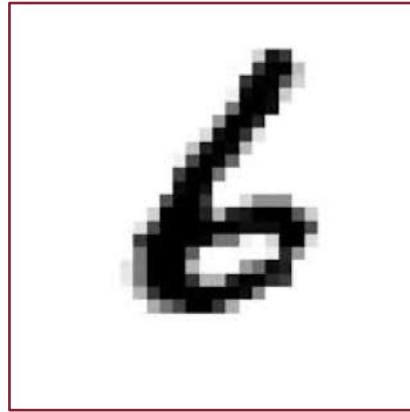
# Modeled vs. True Dimensionality

## Example

Handwritten digit recognition

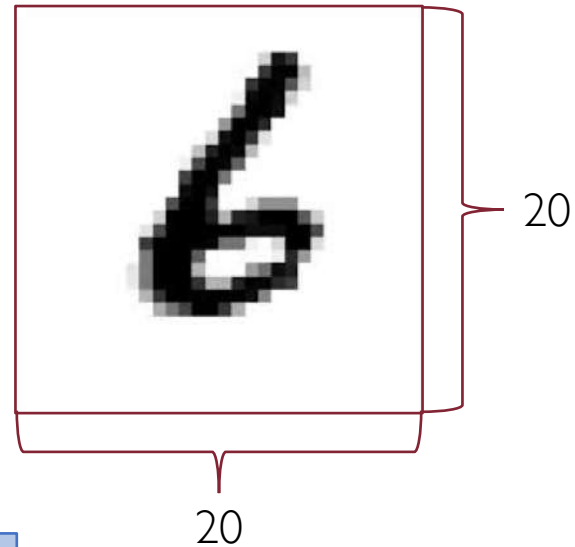


# Modeled vs. True Dimensionality





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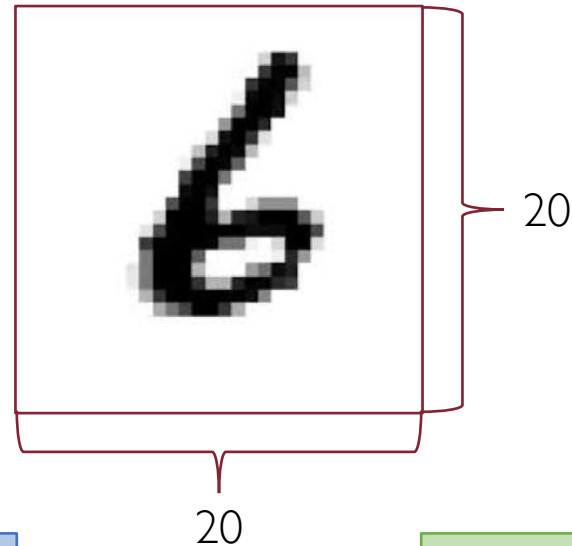


Modeled dimensionality

Each digit represented by **20x20** bitmap

**400**-dimensional binary vector

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Modeled dimensionality

Each digit represented by **20x20** bitmap

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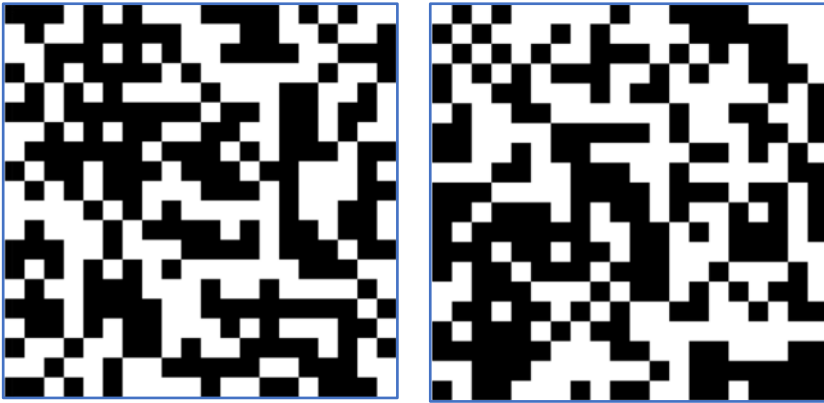
True dimensionality

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

Small variations of the pen-stroke

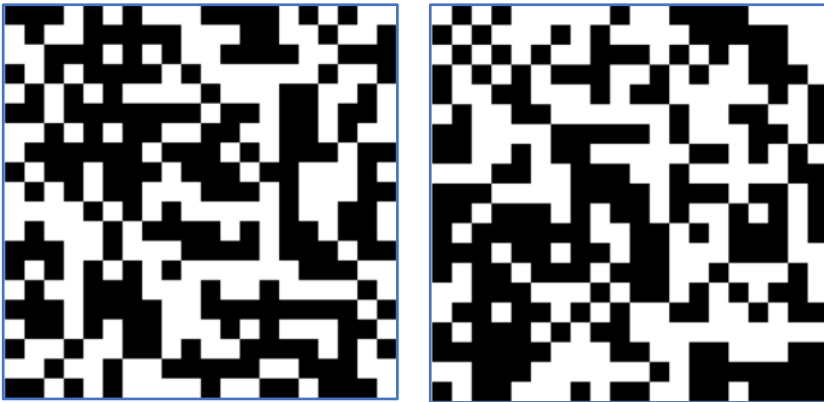
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Random samples from  
400-d space



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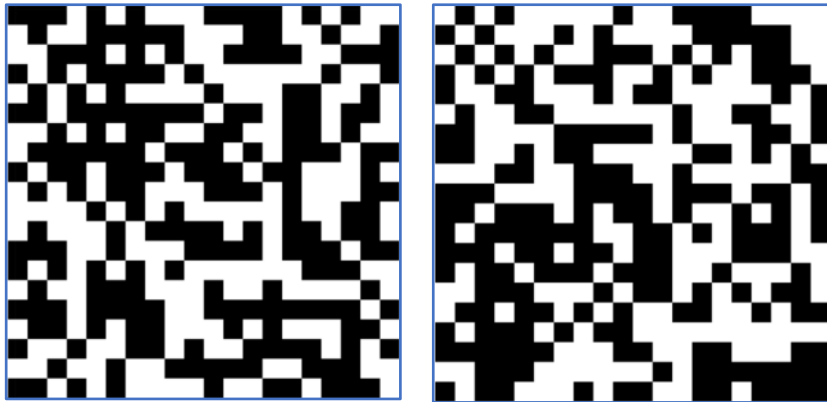


True digits living in a  
400-d space



# 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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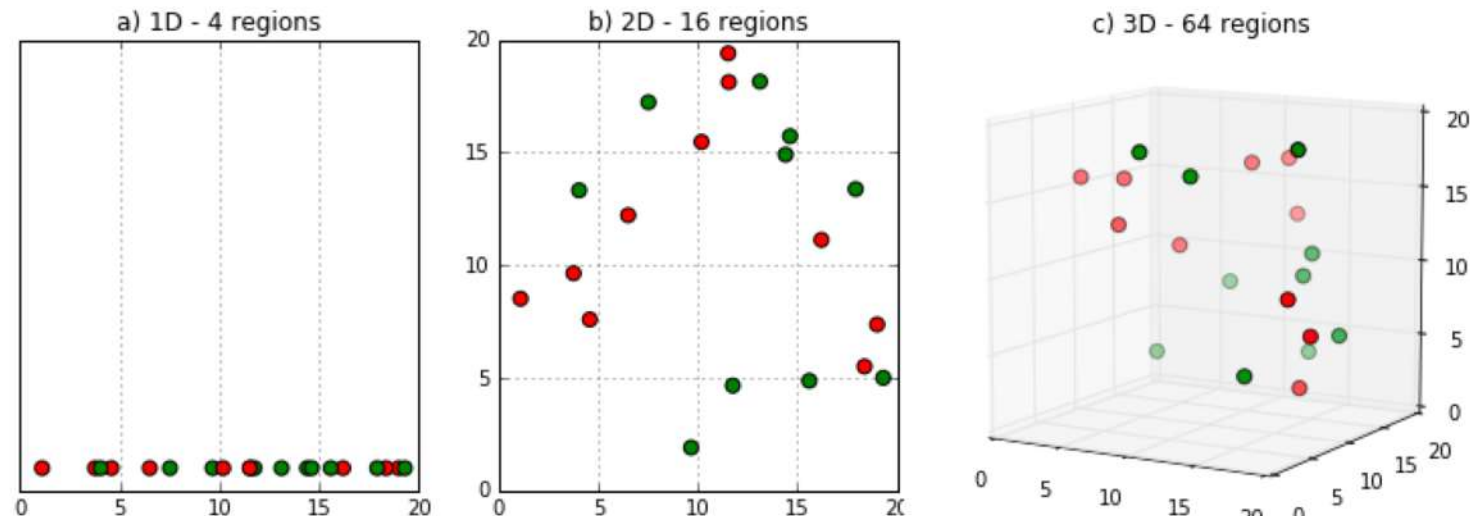
Put it another way:  
The number of examples must grow exponentially with dimensionality if we want to  
maintain the same "density"

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Put it another way:

The number of examples must grow exponentially with dimensionality if we want to maintain the same "density"





# Dealing with High Dimensionality

3 possible approaches



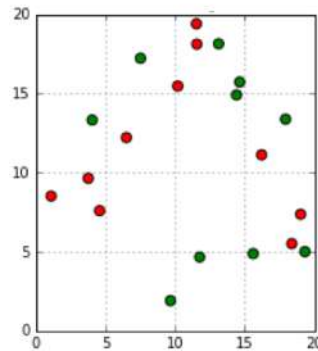
Feature Engineering  
(using domain knowledge)  
e.g., SIFT in computer vision

# Dealing with High Dimensionality

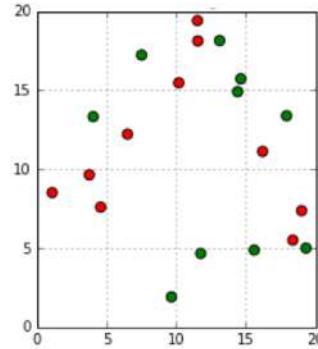
3 possible approaches

**Feature Engineering**  
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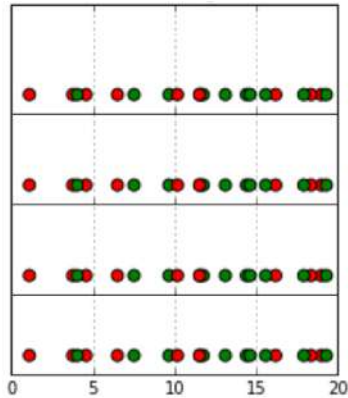
**Making Assumptions**



# Dealing with High Dimensionality: Assumptions



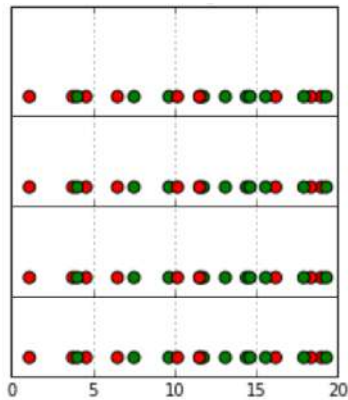
independence



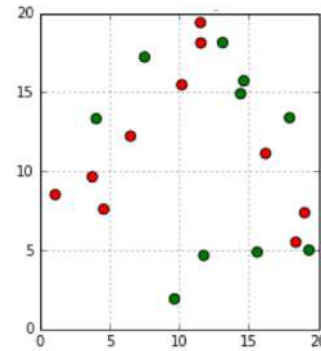
Count along each dimension separately

# Dealing with High Dimensionality: Assumptions

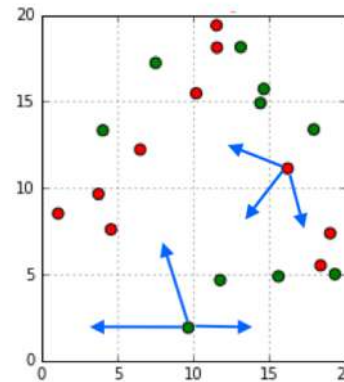
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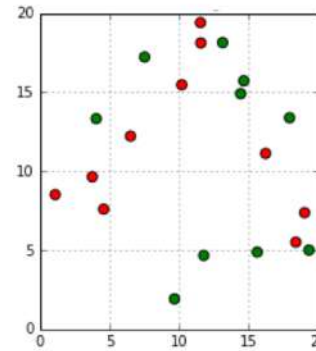


smoothness

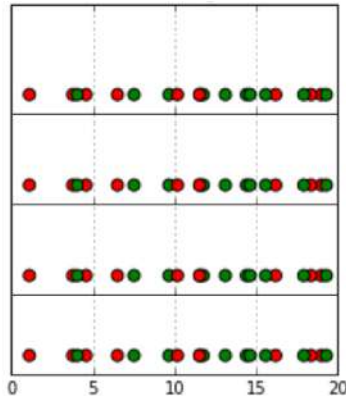


Propagate counts to neighboring regions

# Dealing with High Dimensionality: Assumptions

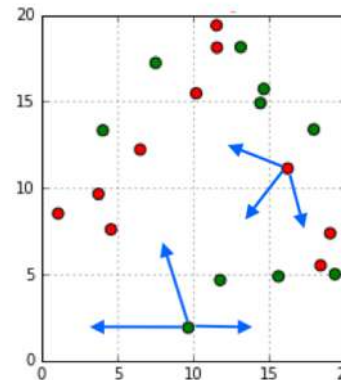


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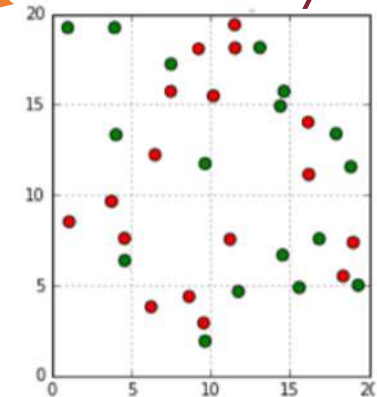
Count along each dimension separately

smoothness



Propagate counts to neighboring regions

simmetry



Invariance to the order of dimensions

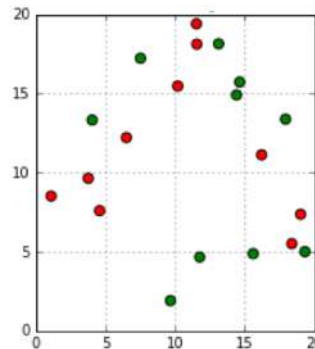
# Dealing with High Dimensionality

3 possible approaches

## Feature Engineering

(using domain knowledge)  
e.g., SIFT in computer vision

## Making Assumptions



## Reduce Dimensionality

Create a new set of  
dimensions (i.e., variables)

# 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

2 main approaches



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## Feature Selection

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

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

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## Feature Extraction

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

$e_1, e_2, \dots, e_k$

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

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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

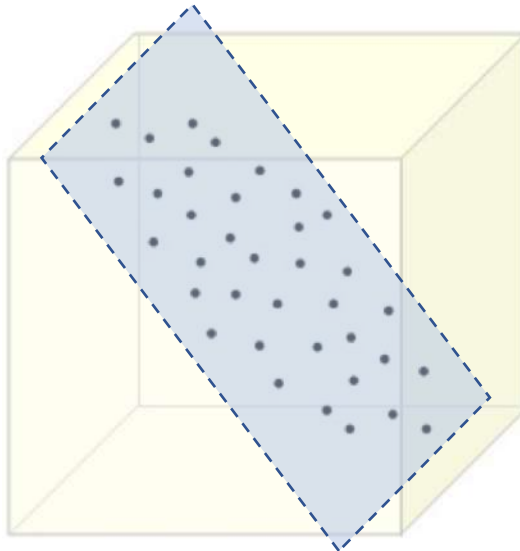
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## Example

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:

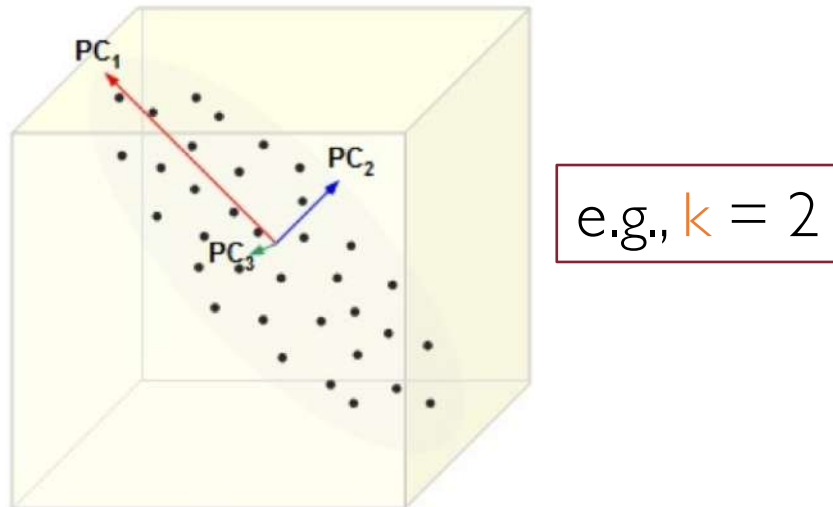
- 1st: direction of the greatest variance of data
- 2nd: perpendicular to 1st and greatest variance of what's left
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The top  $k < d$  components become the new dimensions



# Principal Component Analysis (PCA)

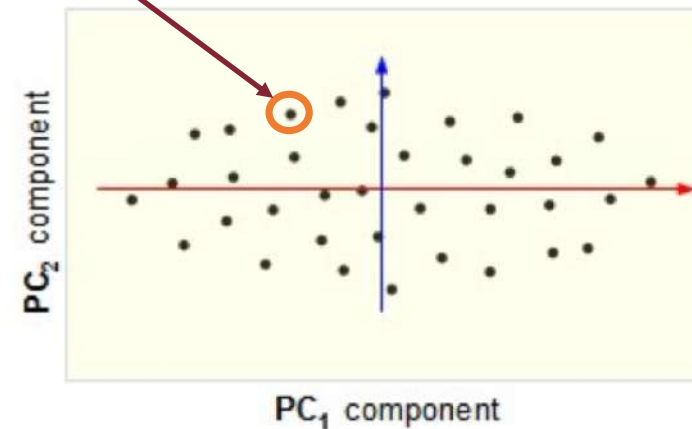
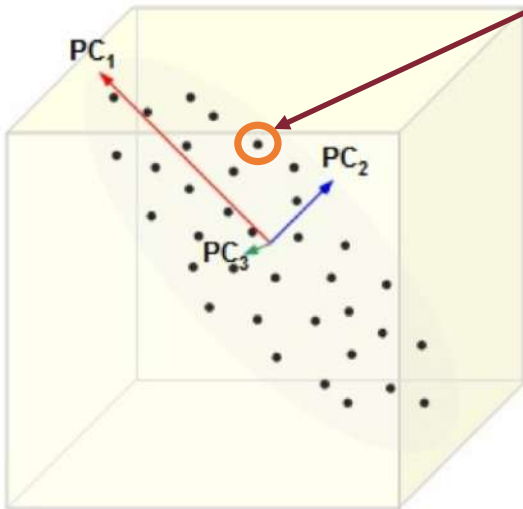
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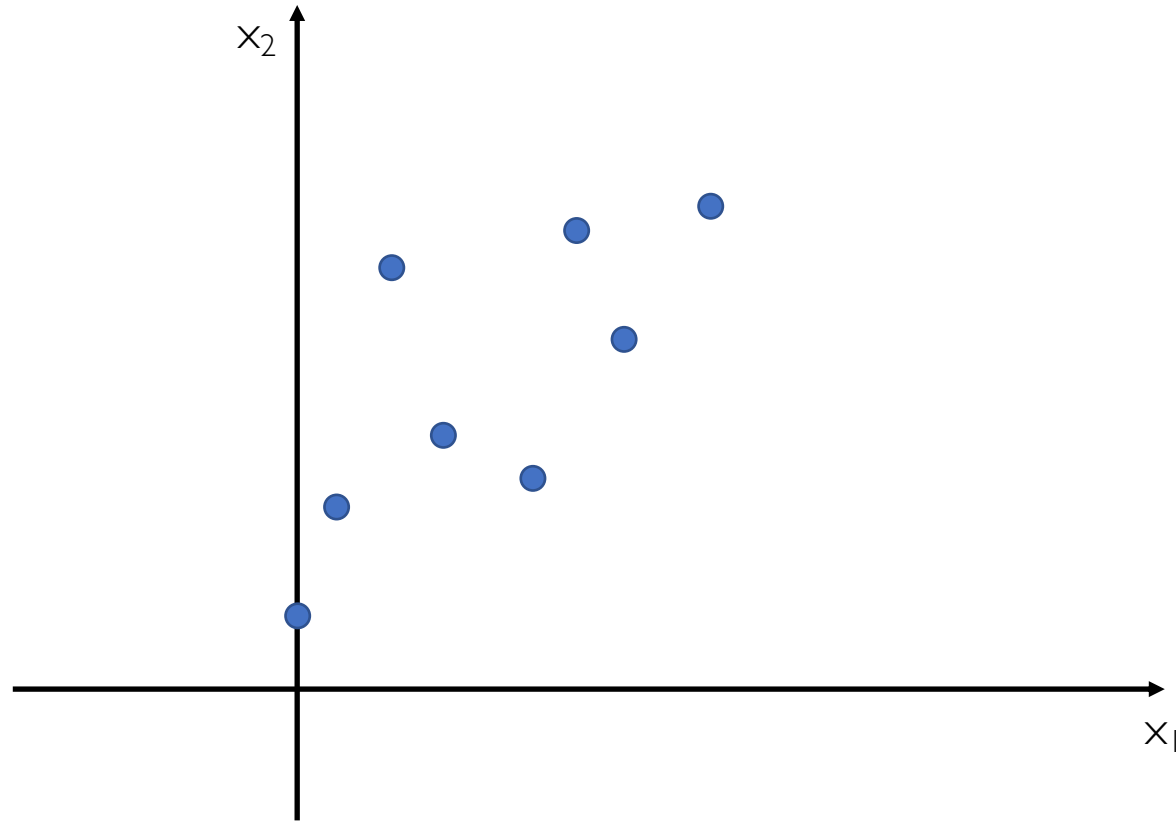
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Change the coordinates of every point according to the new dimensions



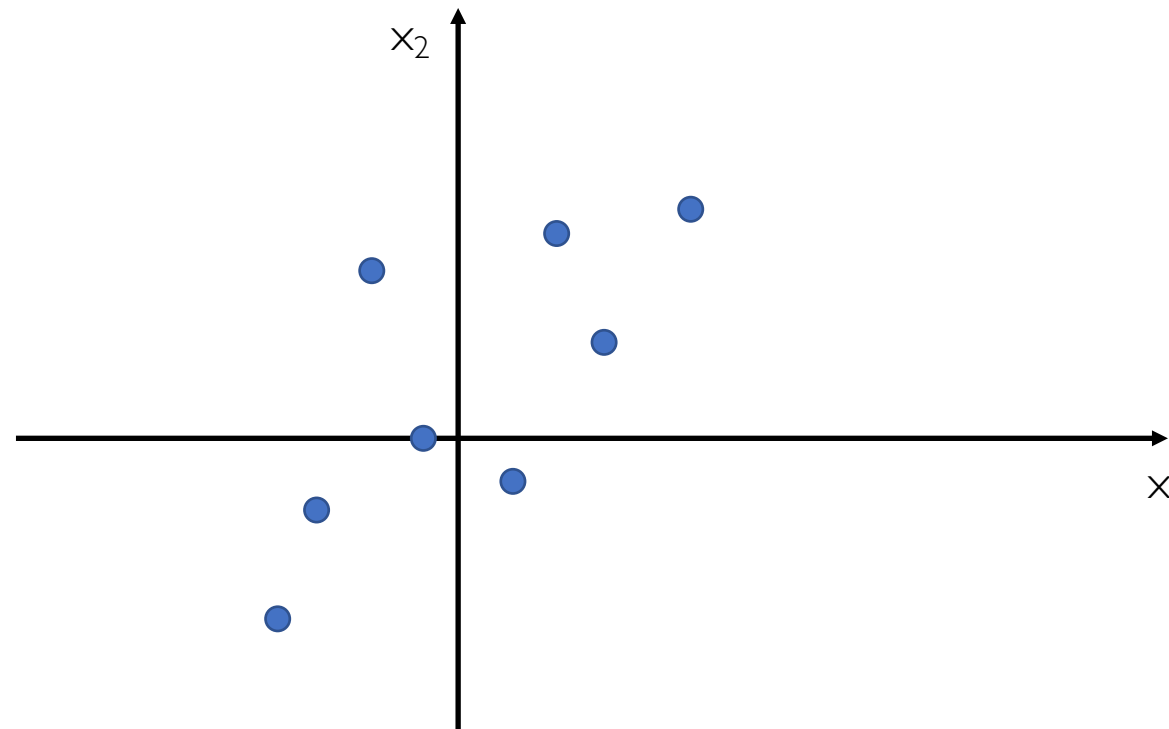
# Why Do We Look for Greatest Variance?

Example: Reduce 2-dimensional data to 1-d



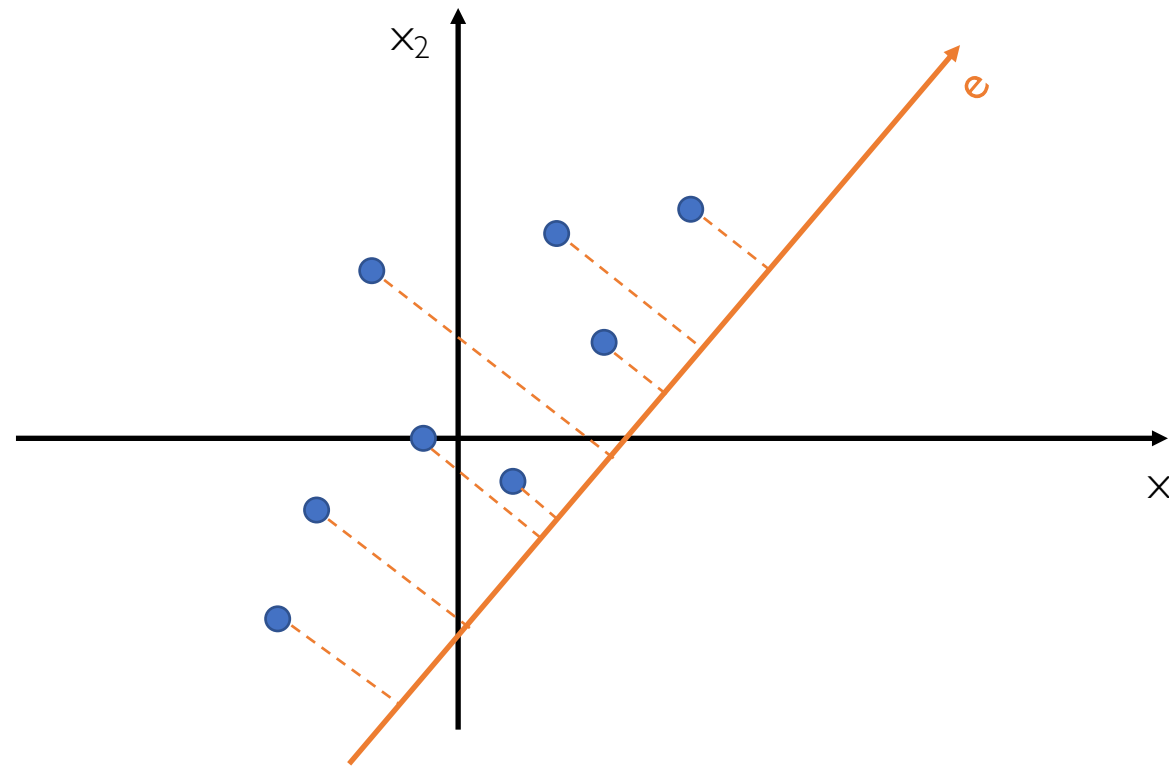
# Why Do We Look for Greatest Variance?

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



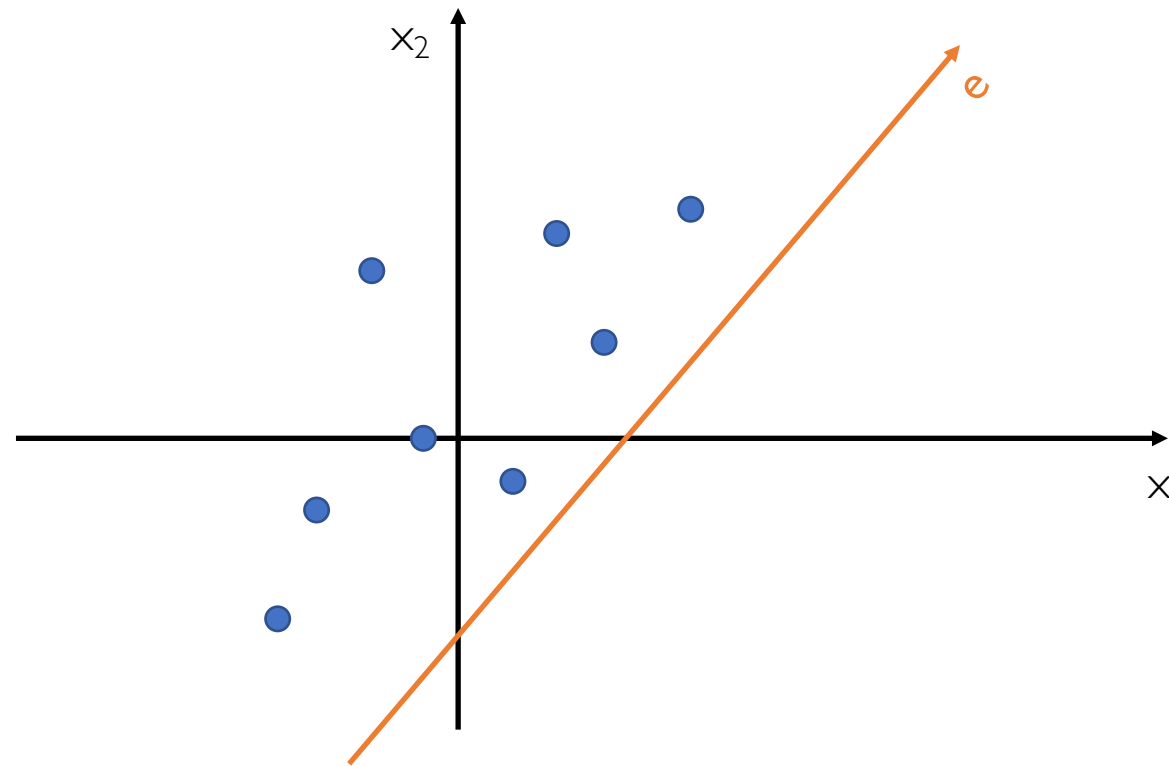
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Map, i.e., project  $(x_1, x_2)$  to a new single dimension axis  $e$



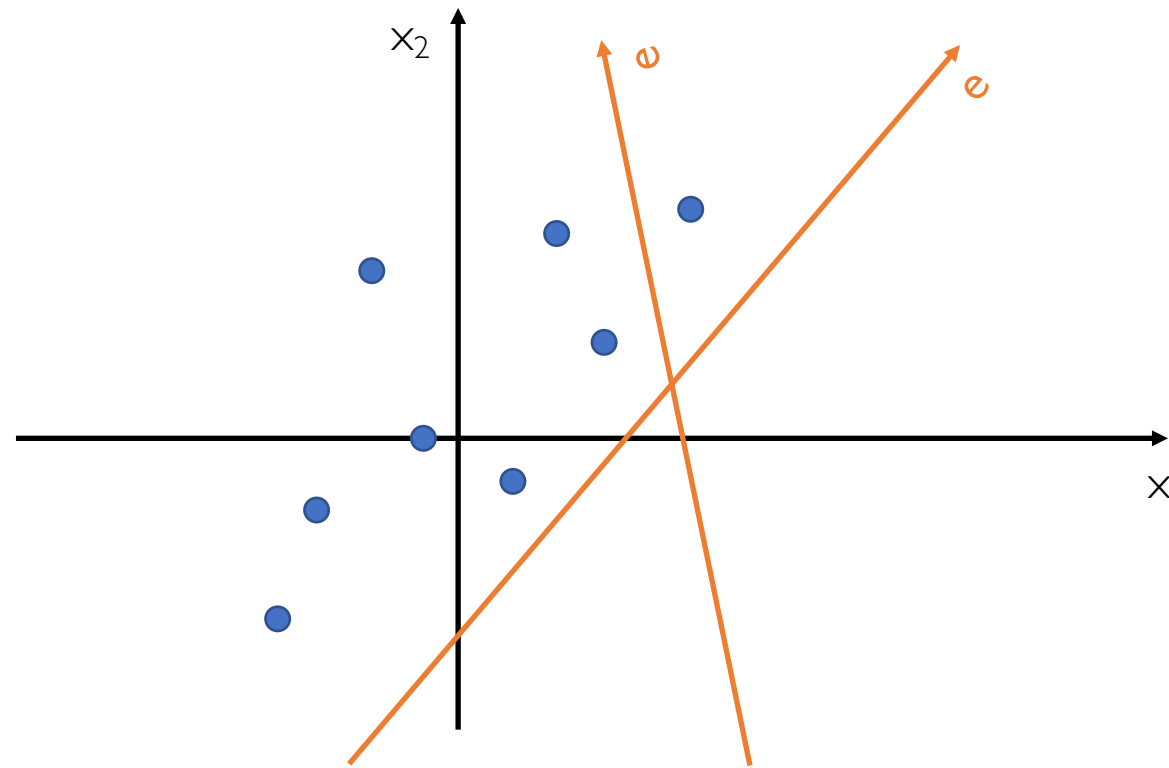
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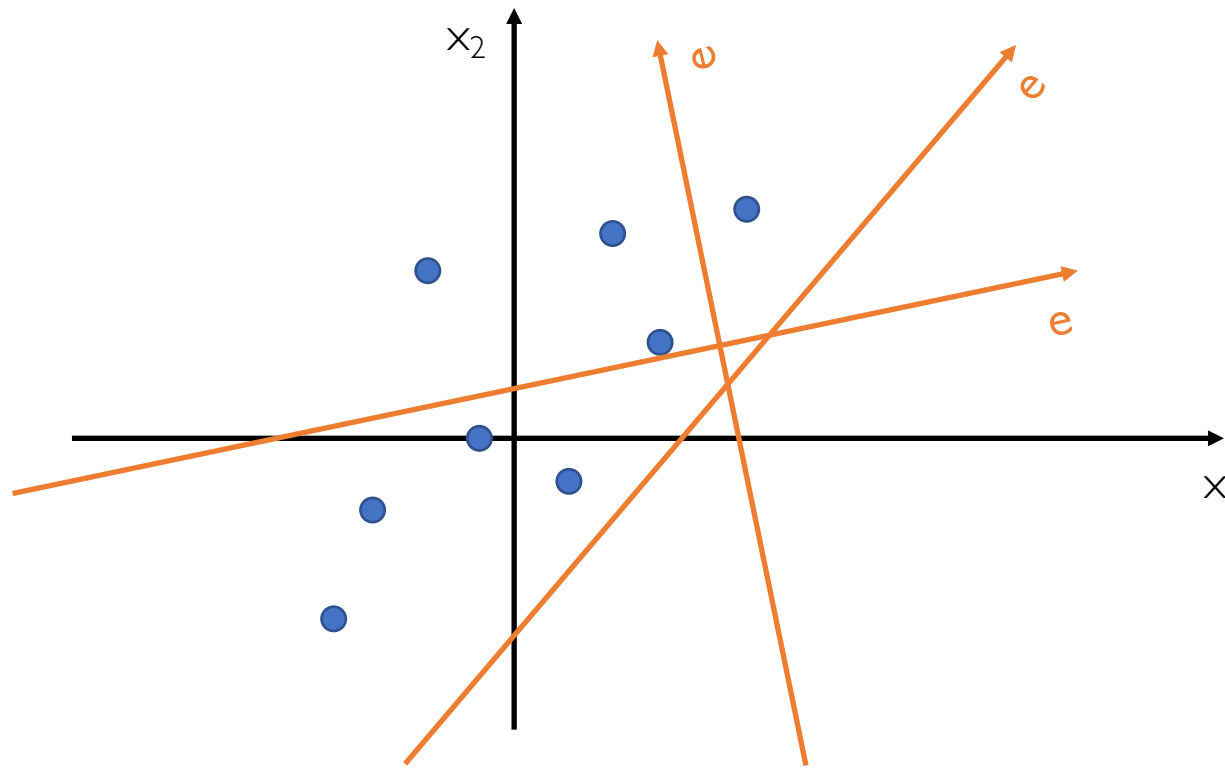
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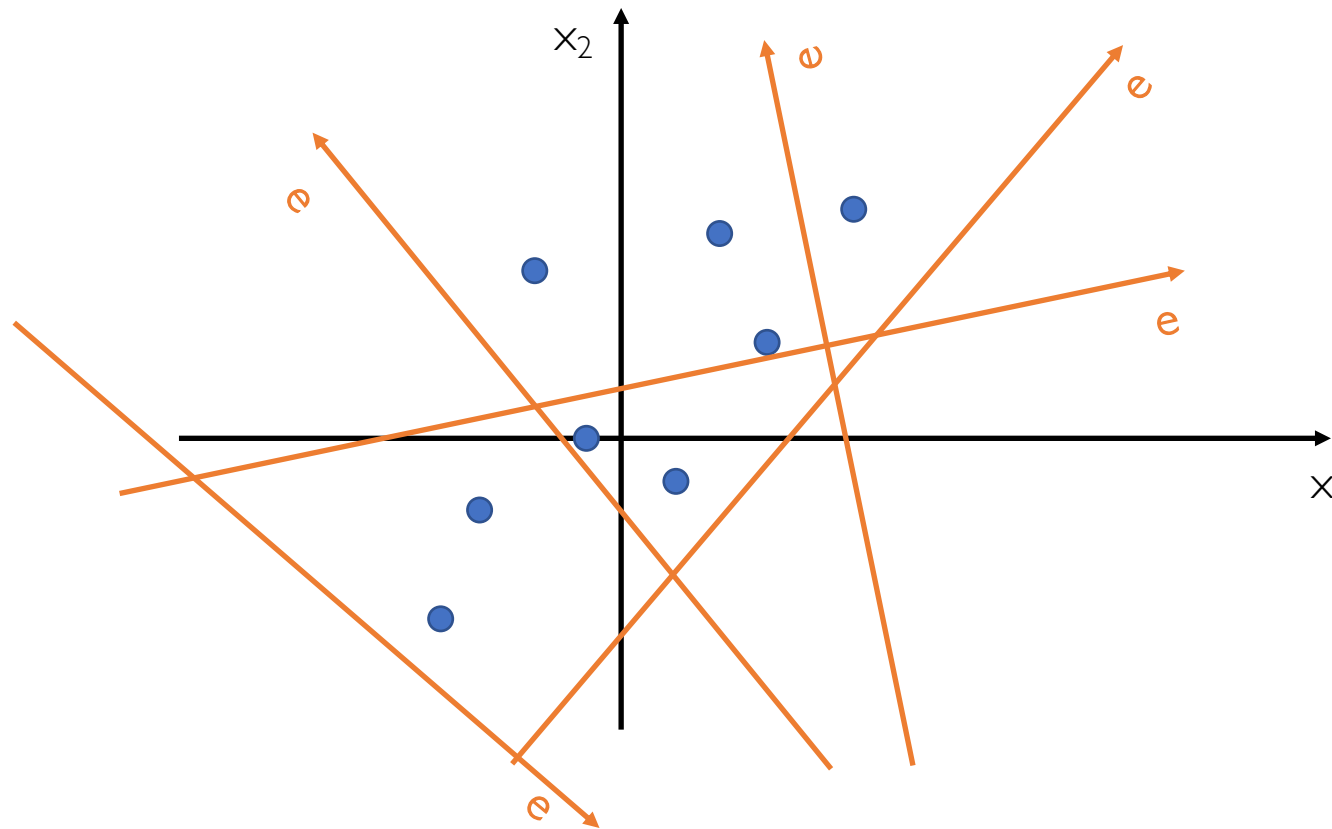
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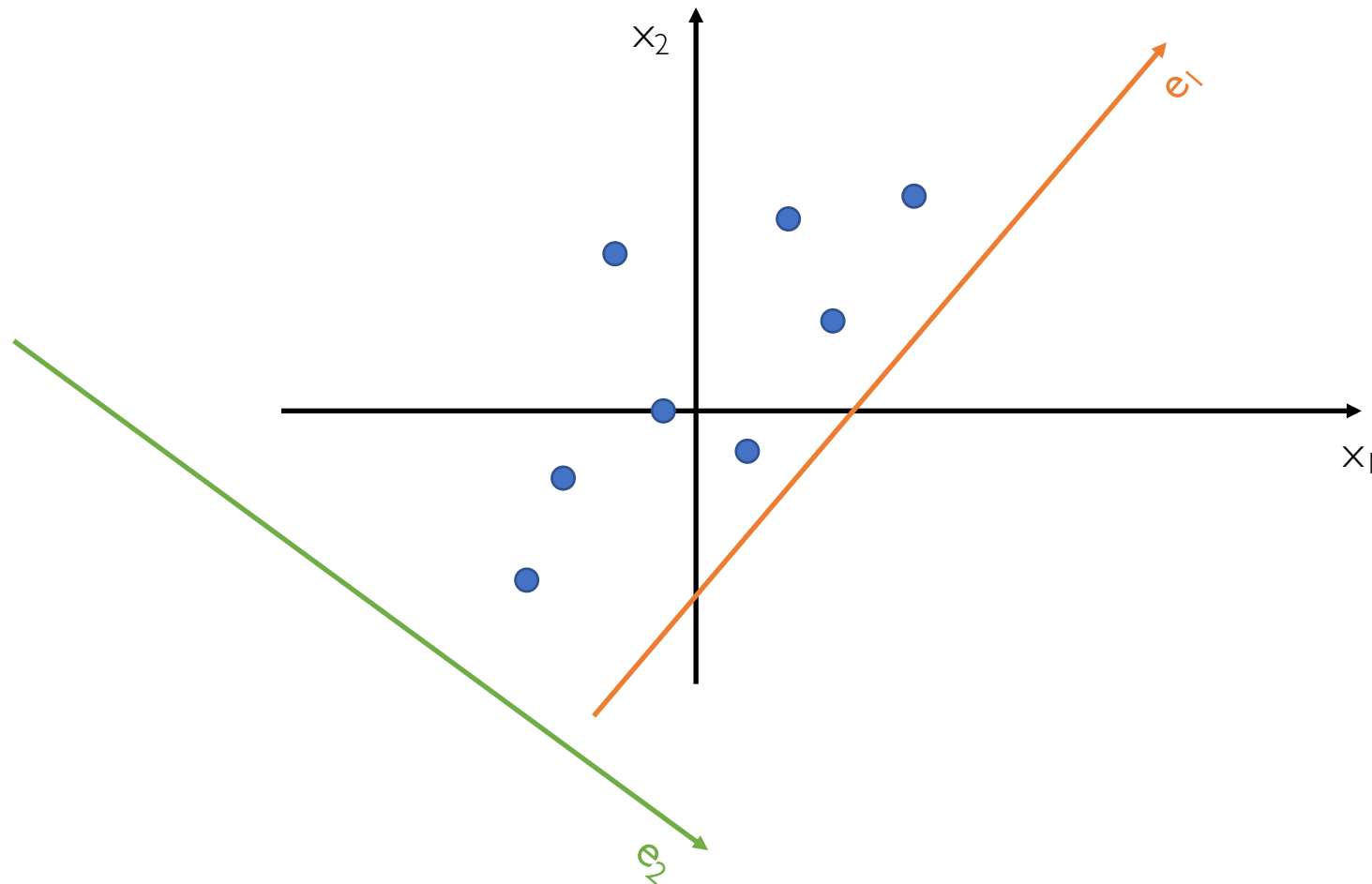


infinitely many mappings from  $(x_1, x_2)$  to a new axis **e**



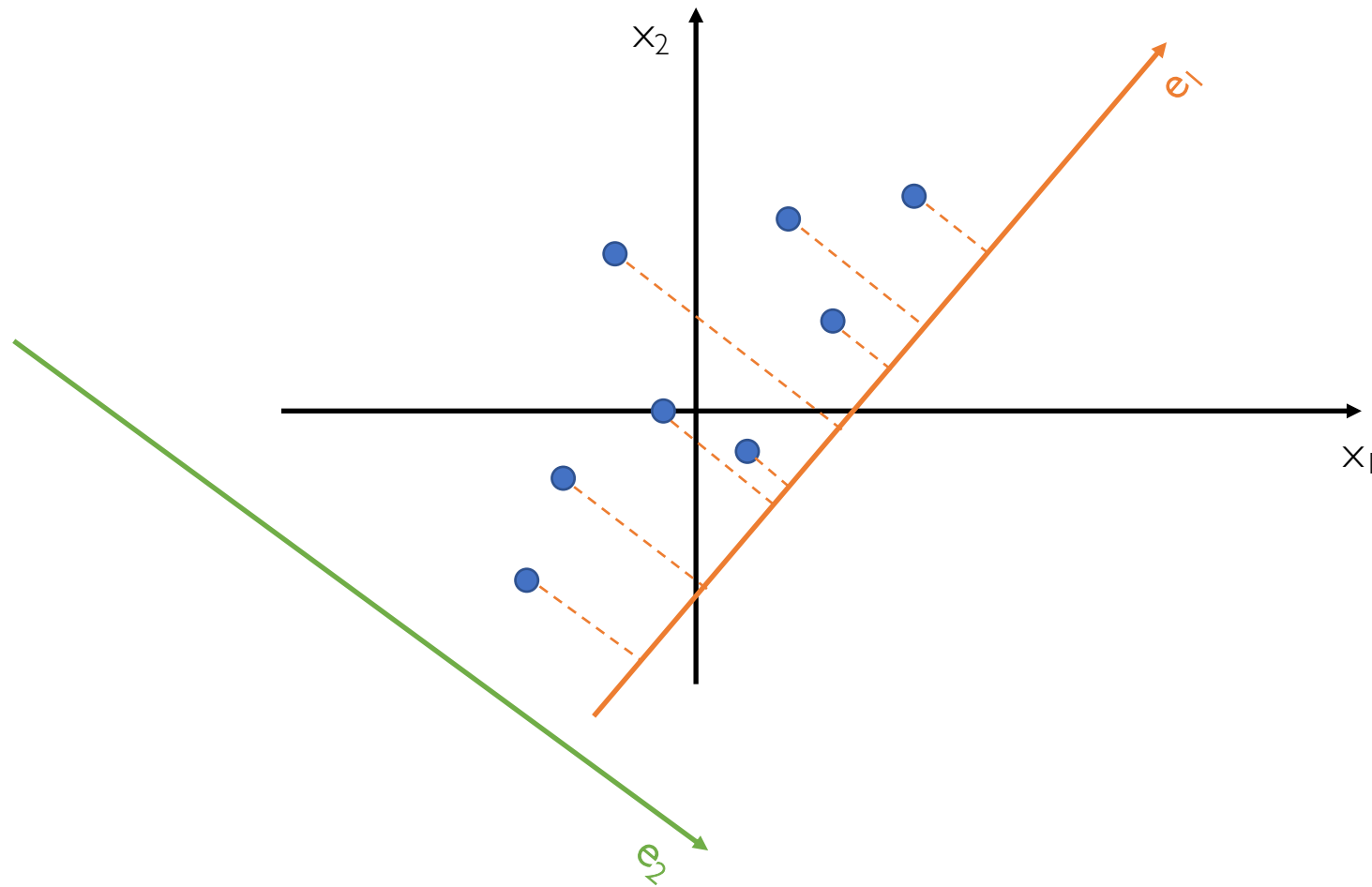
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Let's consider 2 different mappings  $e_1$  and  $e_2$



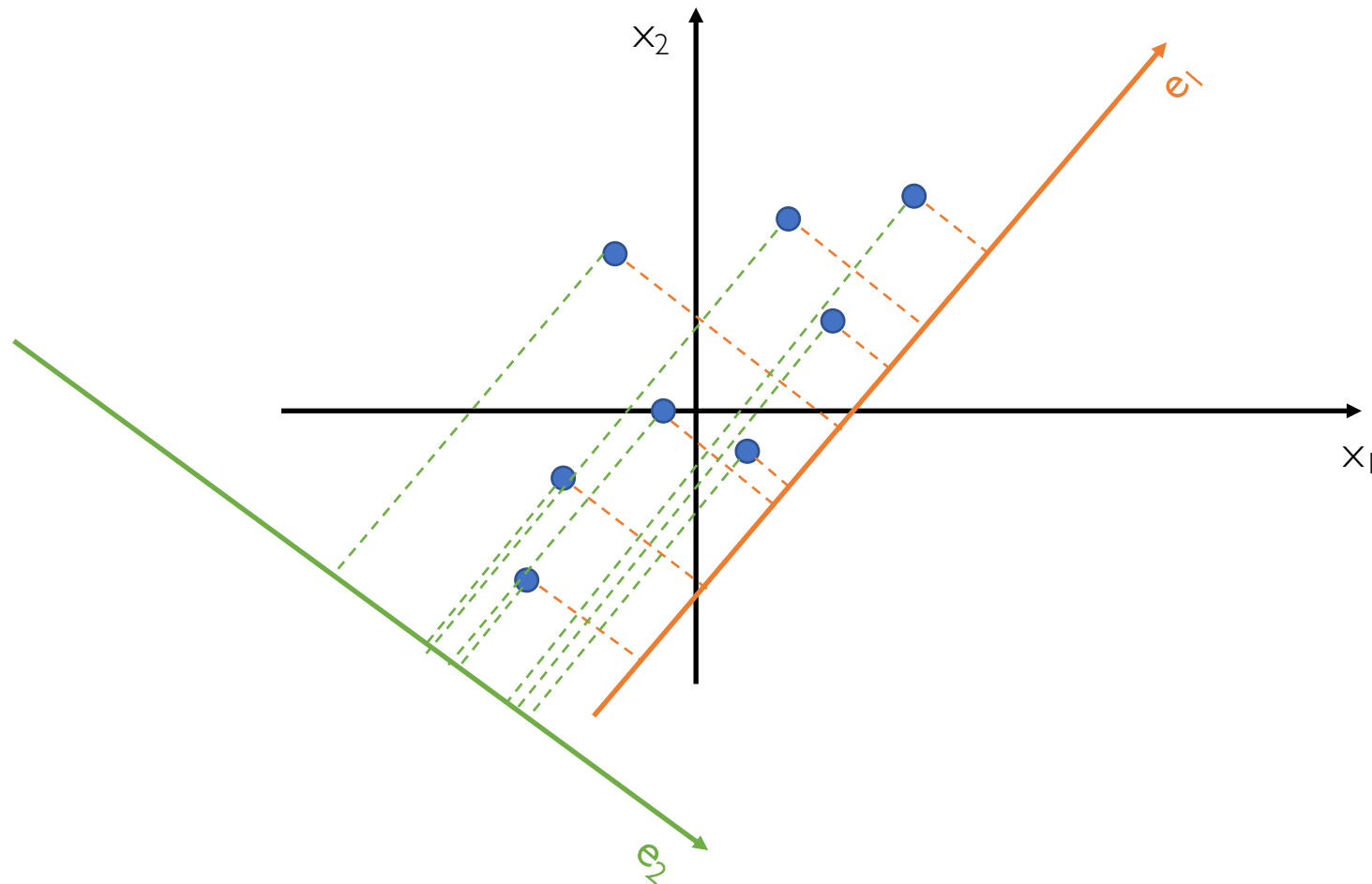
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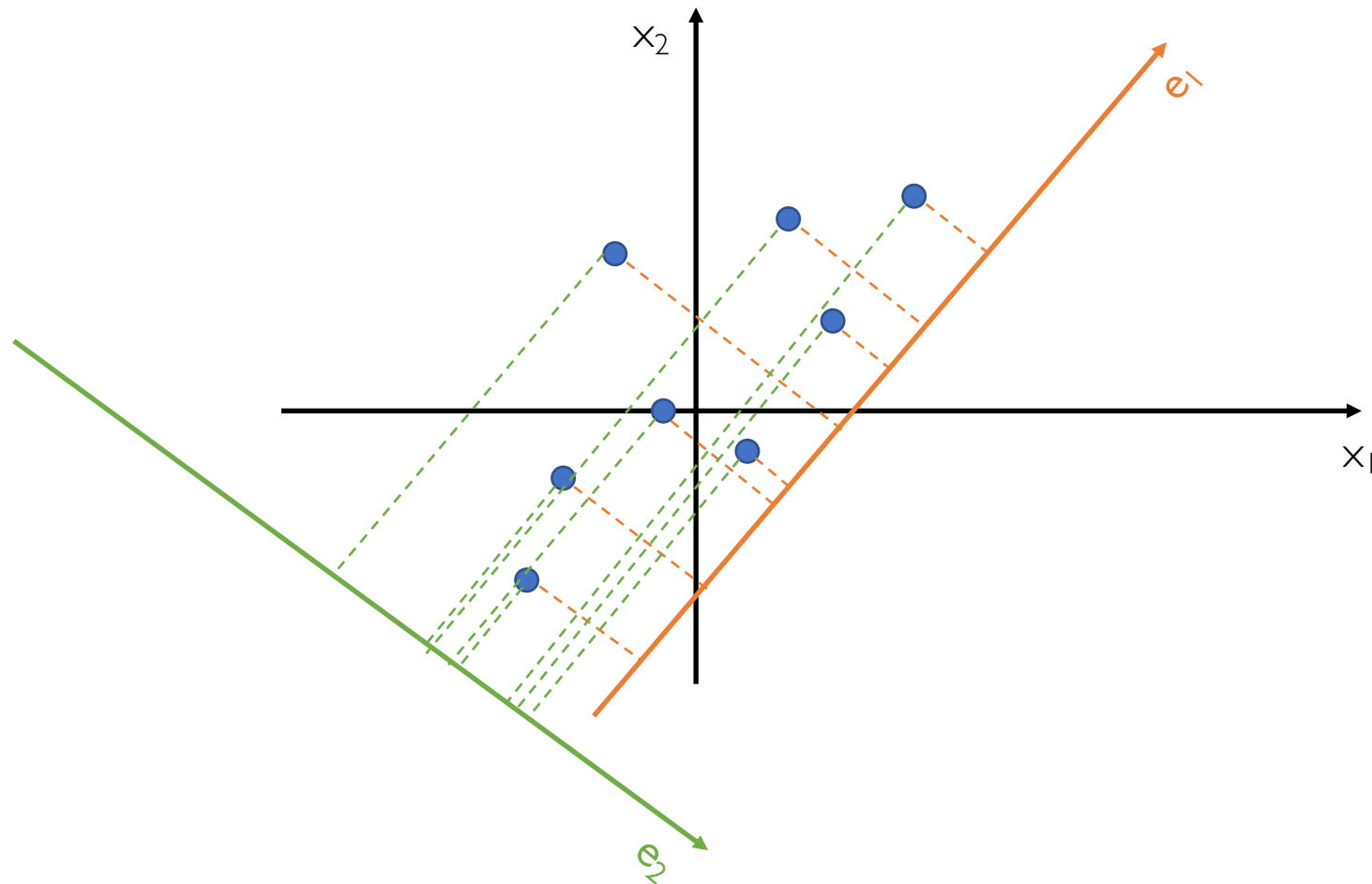
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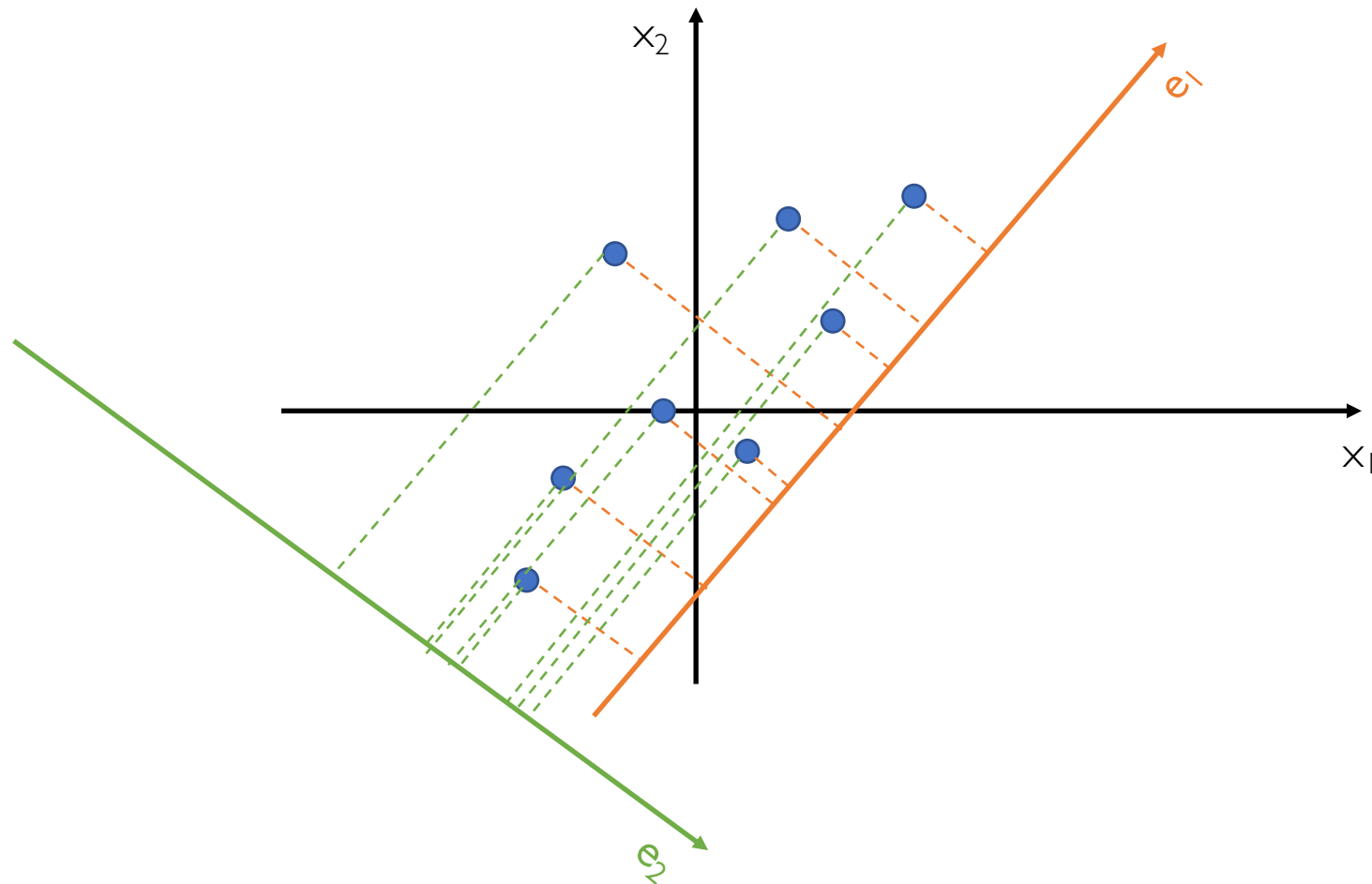
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Which one is better?



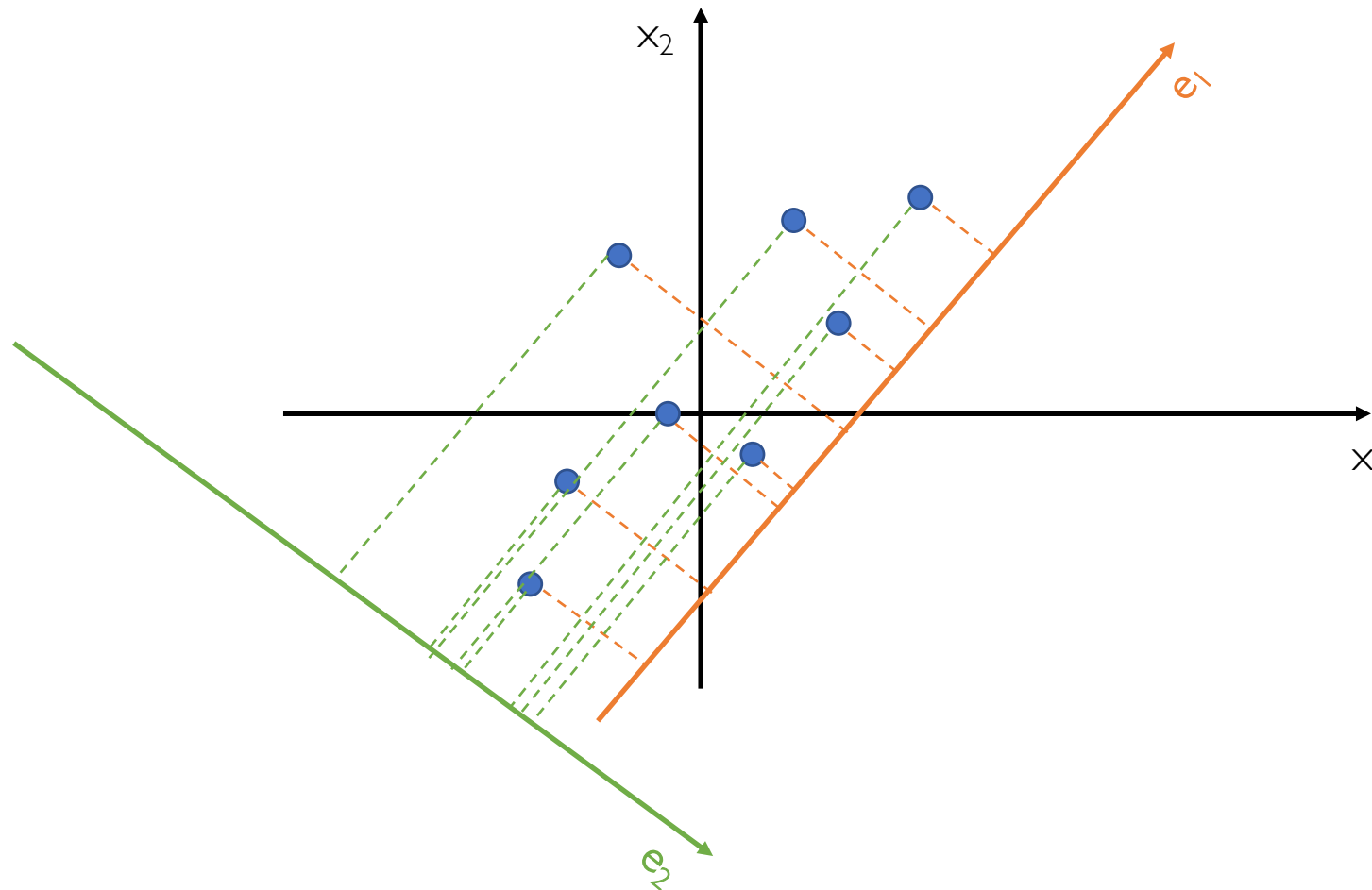
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Points projected onto  $e_1$  look more spread-out than onto  $e_2$



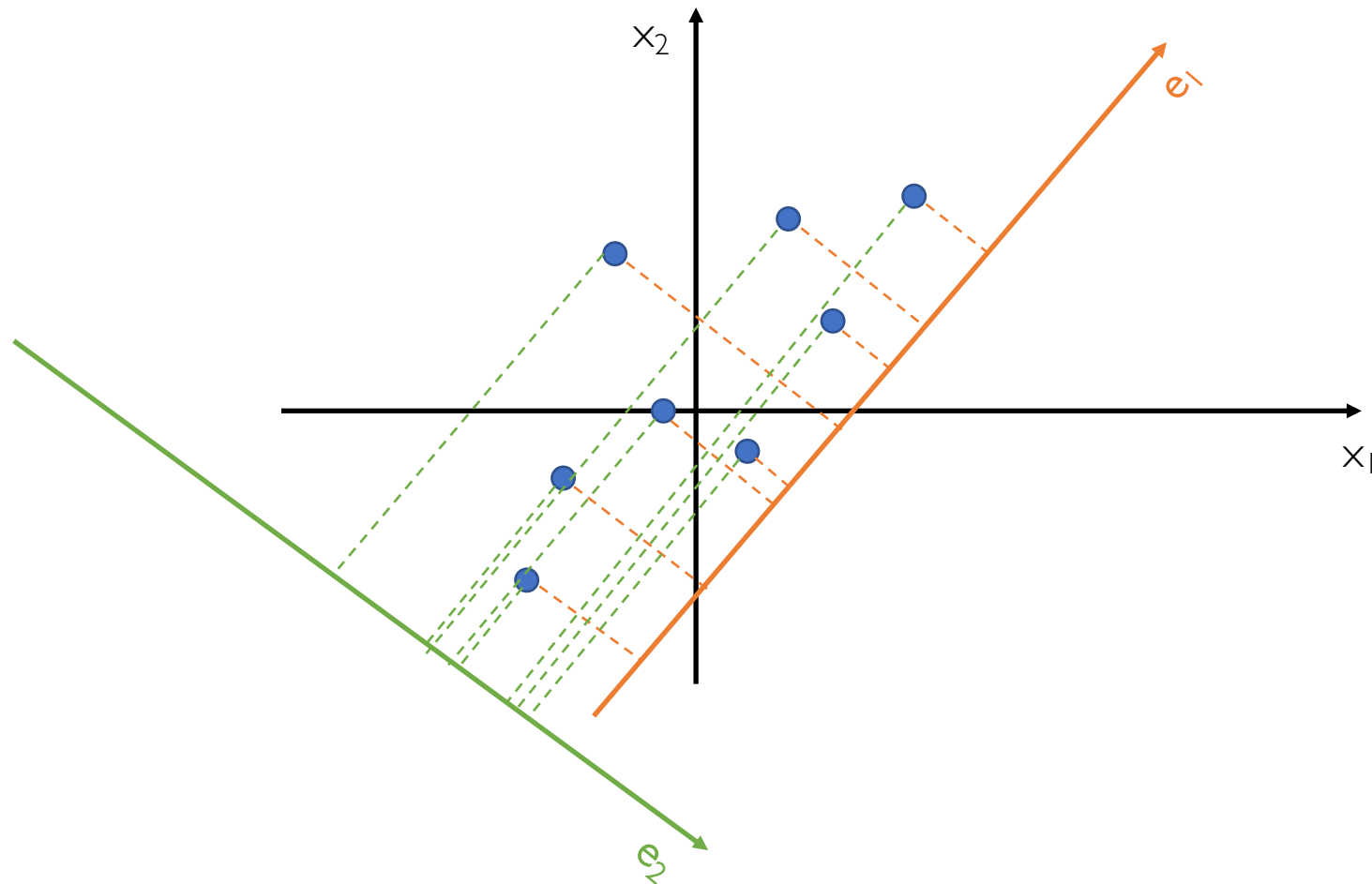
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The **variance** along  $e_1$  is larger than along  $e_2$



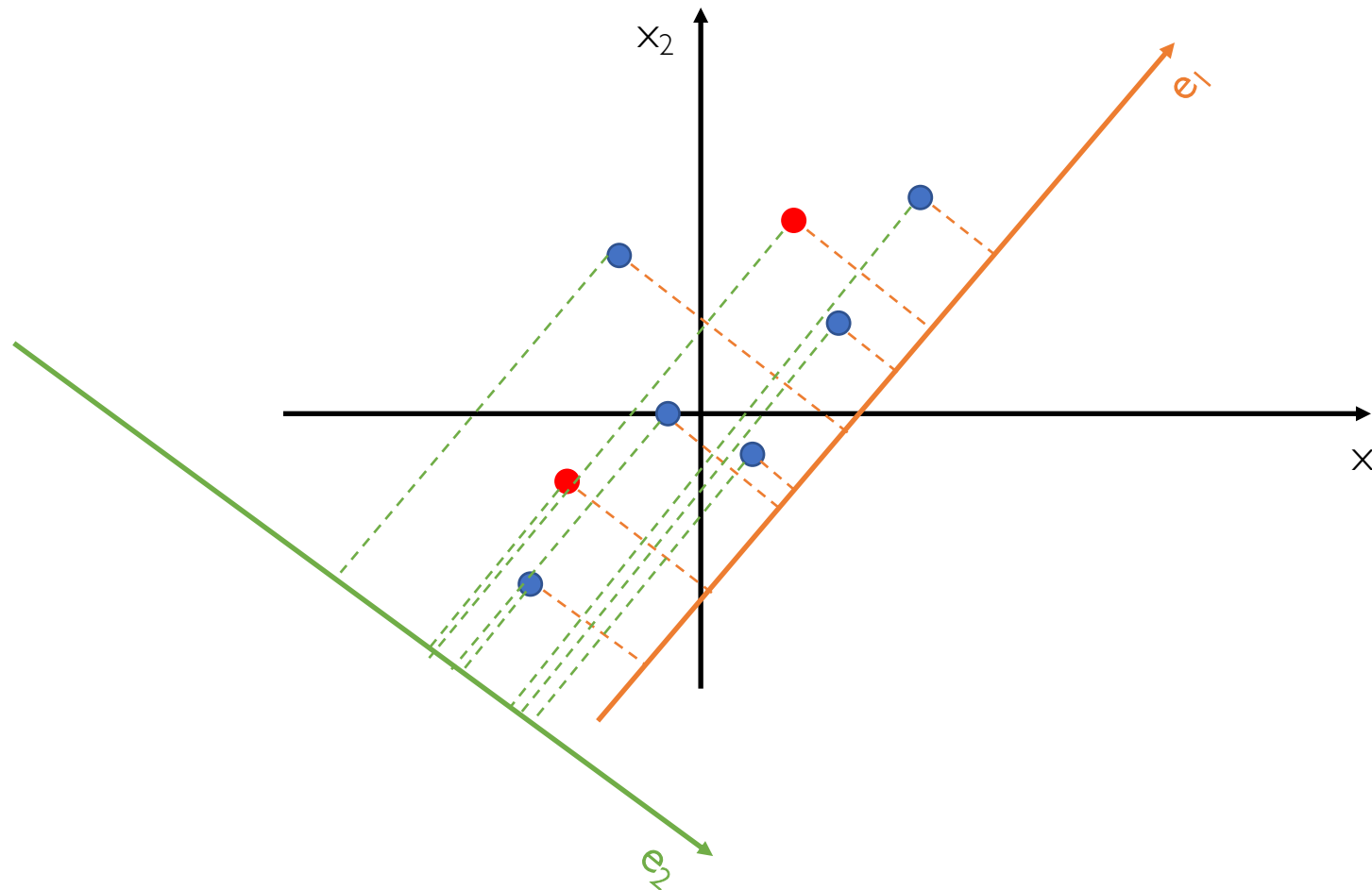
# Why Do We Look for Greatest Variance?

Why is that good?



# Why Do We Look for Greatest Variance?

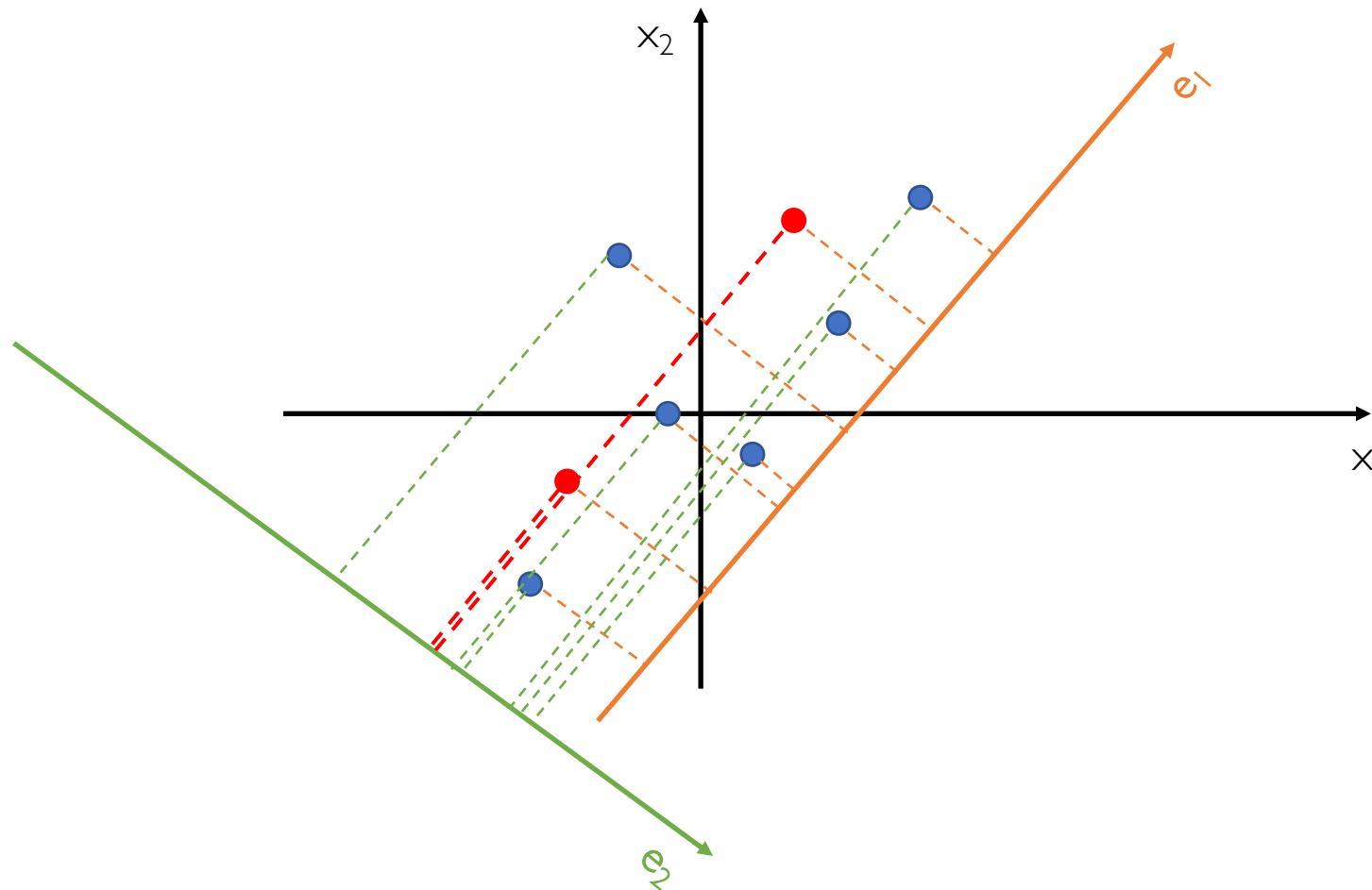
Consider the 2 red points below





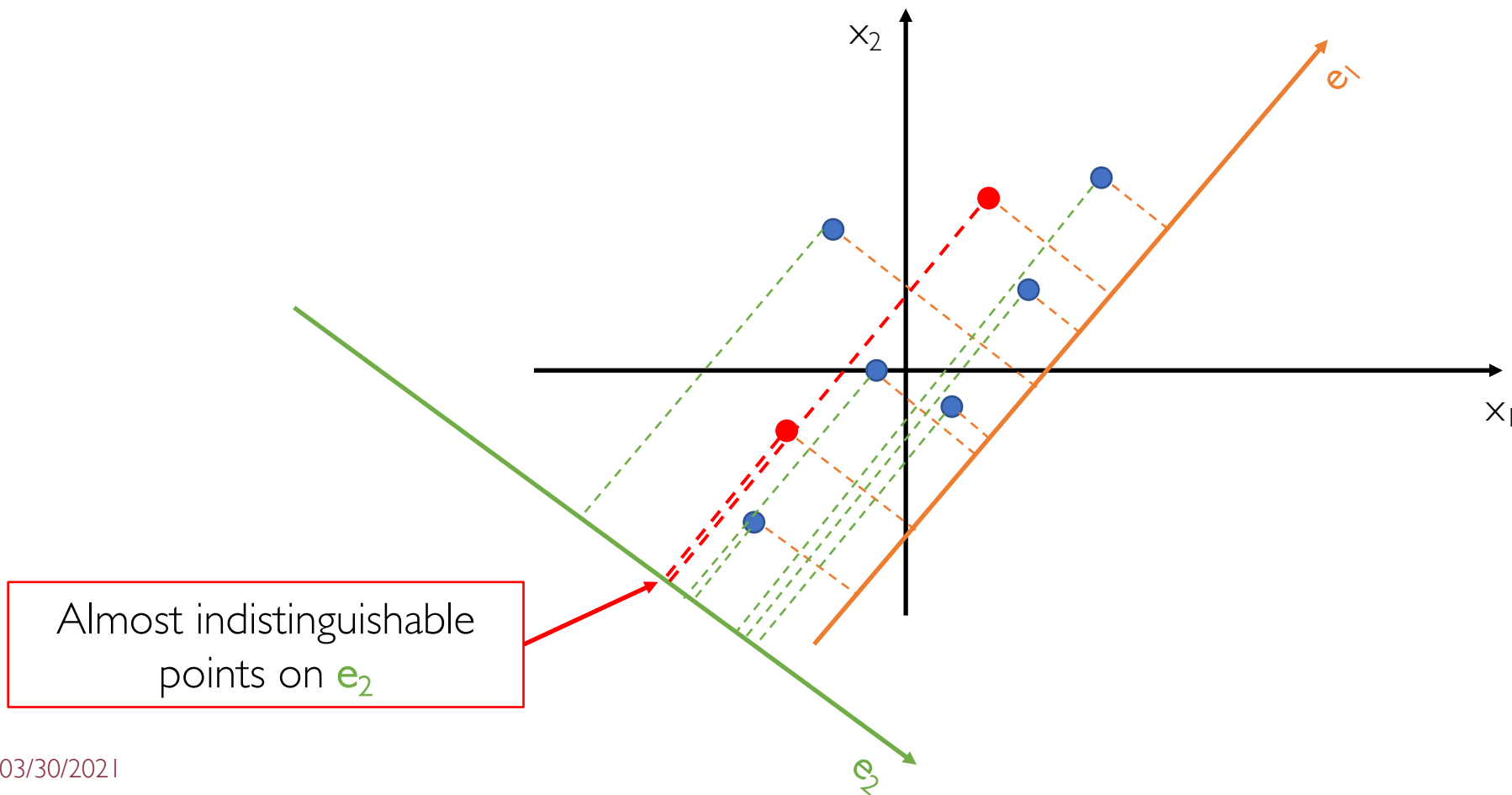
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On  $(x_1, x_2)$  far away from each other, end up close if projected onto  $e_2$



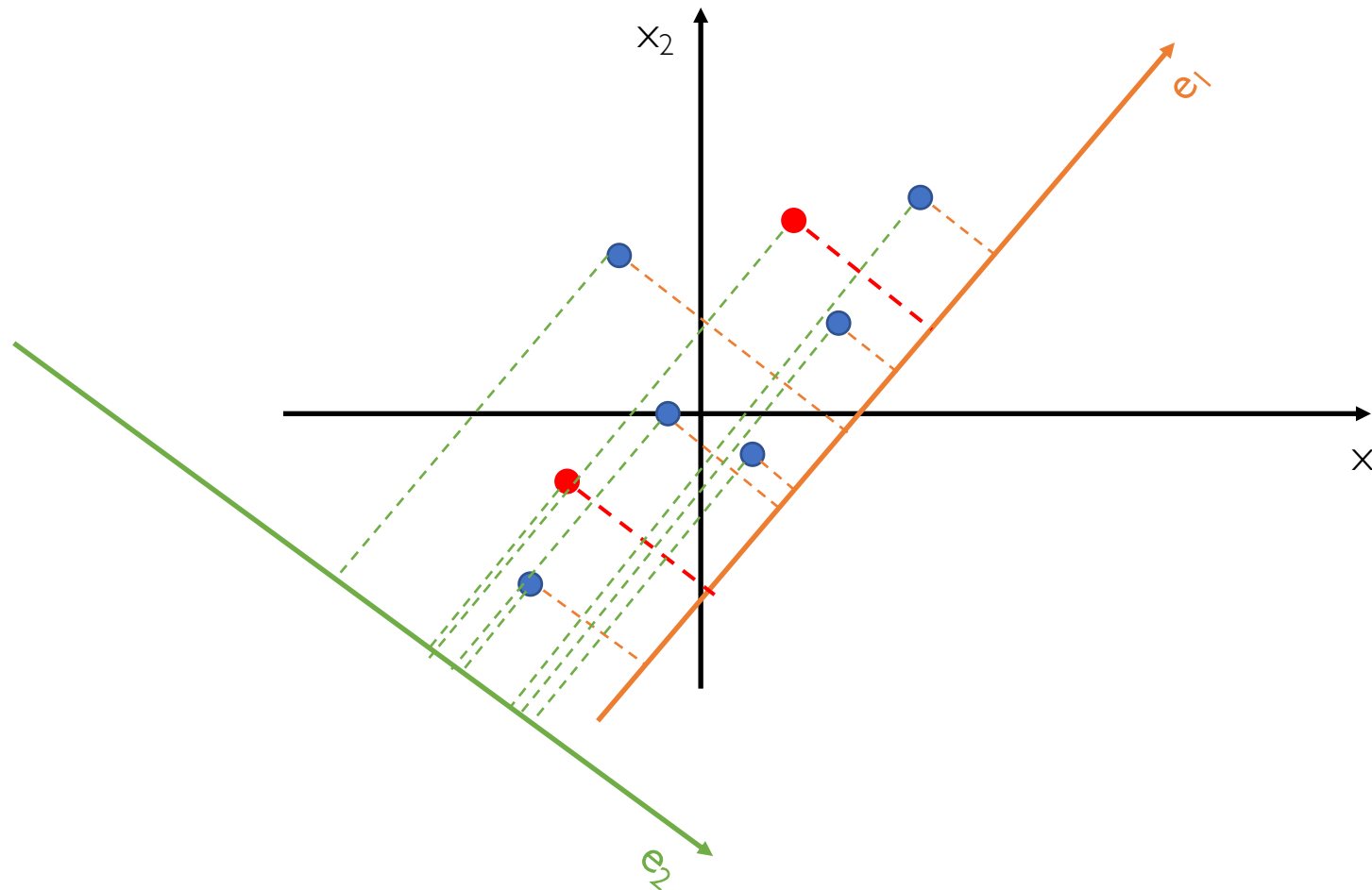
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# Why Do We Look for Greatest Variance?

If projected onto  $e_1$  they better preserve their distance



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- Intuitively, we want to minimize the chance that 2 points that are far in the original space end up close in the lower dimensional space
- Minimize distances between points as measured on  $(x_1, x_2)$  space and those measured on **e**



## 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

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

where  $\mu = E[X]$



# 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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  - Do  $X$  and  $Y$  increase/decrease together, or when one increases/decreases the other decreases/increases?
- Formally, it is the expected value of the product of their deviations from their individual means

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

where  $\mu_X = E[X]$  and  $\mu_Y = E[Y]$

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

# Covariance Matrix

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

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- Given a random vector  $\mathbf{X} = (X_1, \dots, X_d)$  its covariance matrix  $K$  is a  $d \times d$  square matrix with the covariance between each pair of elements
- In the matrix diagonal there are variances, i.e., the covariance of each element with itself

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

# Covariance Matrix of Original Dimensions

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

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- 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:  $\mathbf{x}_1, \dots, \mathbf{x}_n$   
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:

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

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

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

# 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:

$$x'_{i,1} = x_{i,1} - \mu_1; x'_{i,2} = x_{i,2} - \mu_2$$

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

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

# Covariance Matrix of Original Dimensions

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

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0-mean

# Covariance Matrix of Original Dimensions

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

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

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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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$$\text{Cov}(X_1, X_2) = \frac{1}{n} \sum_{i=1}^n x'_{i,1} * x'_{i,2}$$

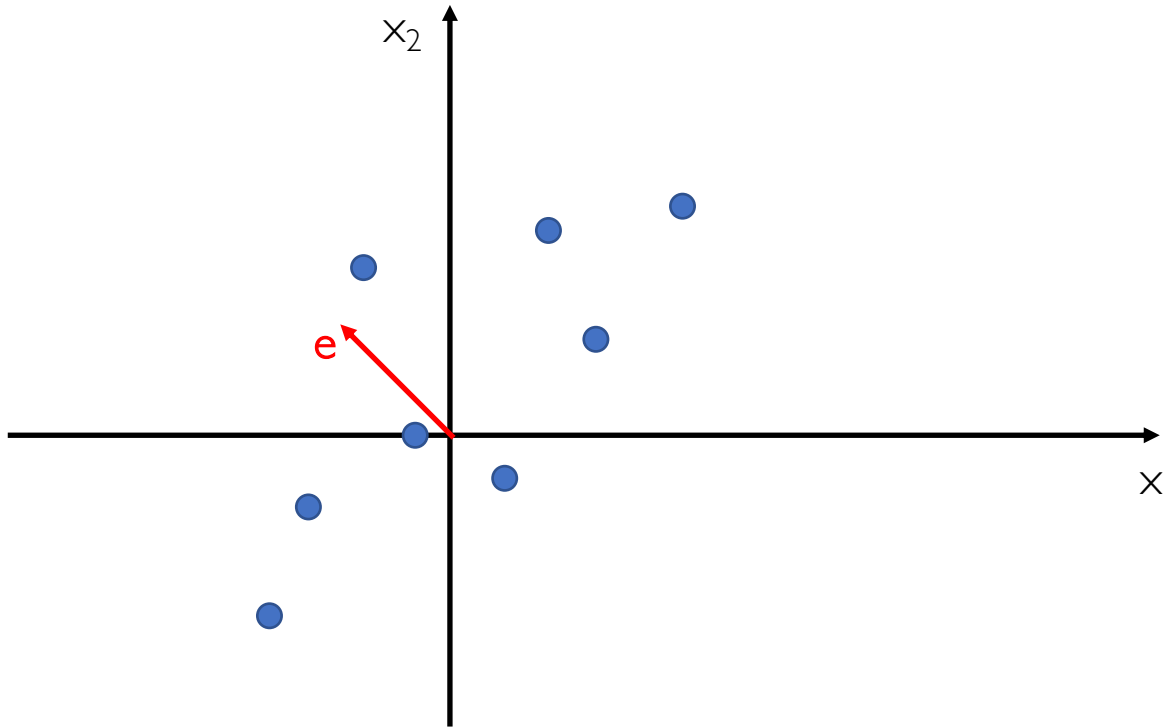
# Covariance Matrix of Original Dimensions

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

$$\begin{matrix} & \begin{matrix} x_1 & x_2 \end{matrix} \\ \begin{matrix} x_1 \\ x_2 \end{matrix} & \begin{bmatrix} 2 & 4/5 \\ 4/5 & 3/5 \end{bmatrix} \end{matrix}$$
$$\text{Cov}(X_1, X_2) = \frac{1}{n} \sum_{i=1}^n x'_{i,1} * x'_{i,2}$$
$$\text{Cov}(X_2, X_2) = \text{Var}(X_2) = \frac{1}{n} \sum_{i=1}^n (x'_{i,2})^2$$



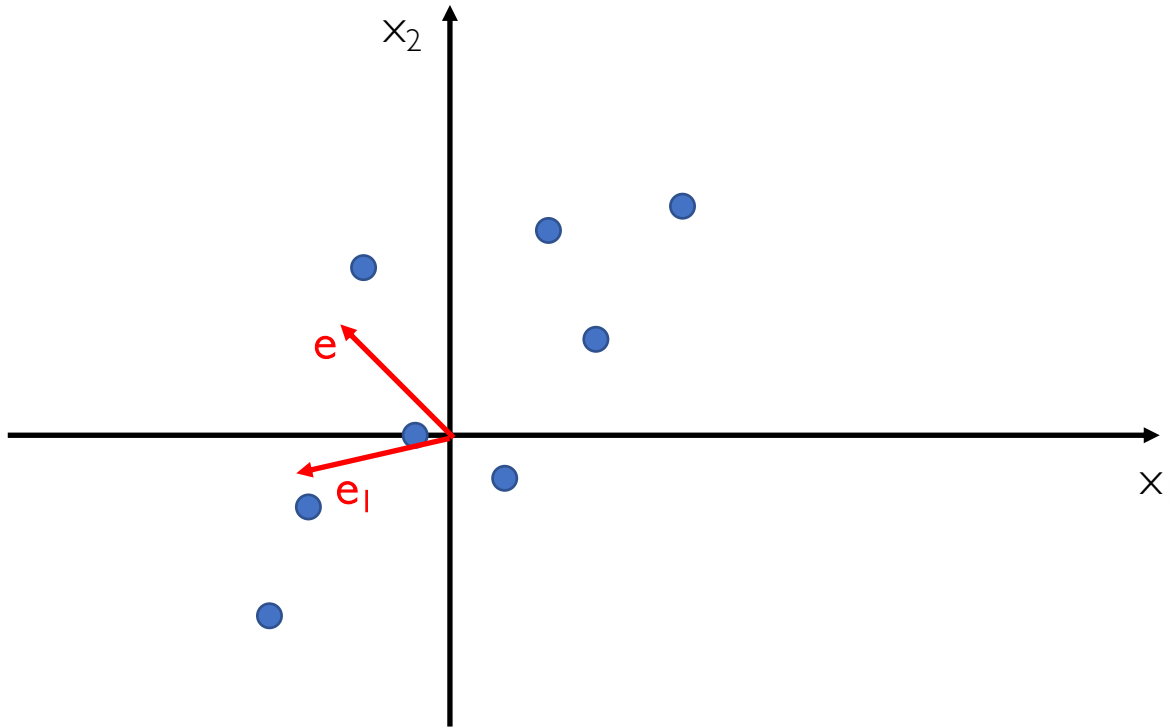
# Covariance Matrix of Original Dimensions



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

$$\underbrace{\begin{bmatrix} 2 & 4/5 \\ 4/5 & 3/5 \end{bmatrix}}_K \underbrace{\begin{bmatrix} -1 \\ 1 \end{bmatrix}}_e =$$

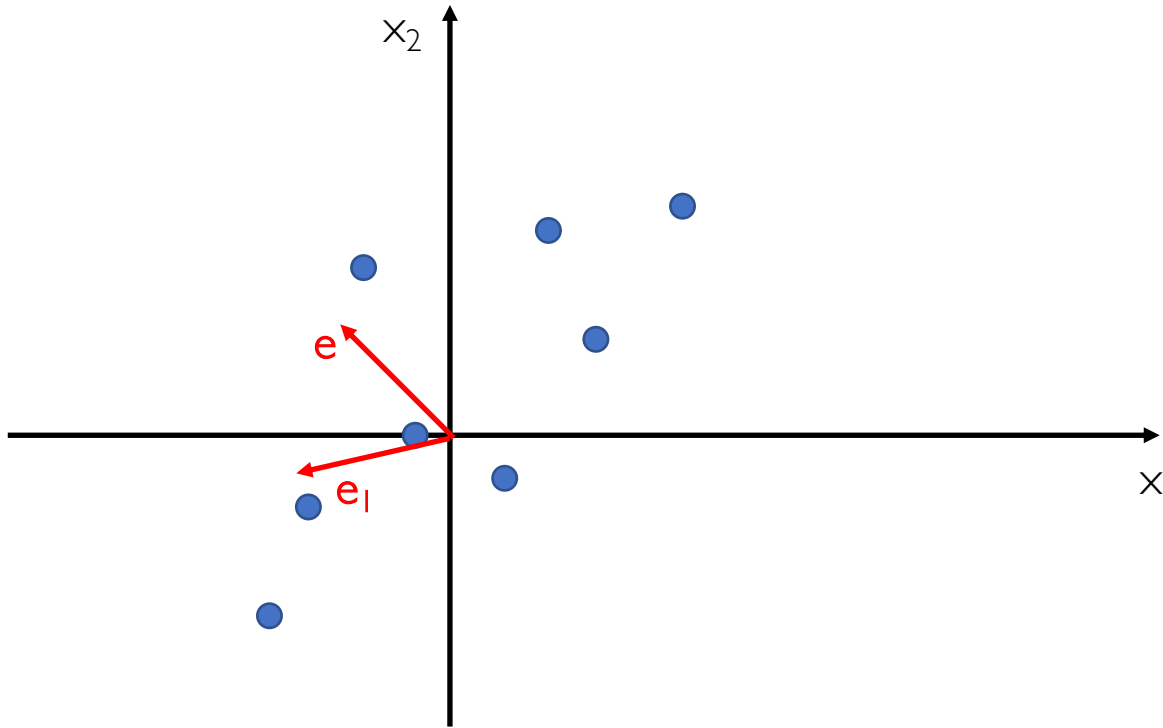
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# Covariance Matrix of Original Dimensions

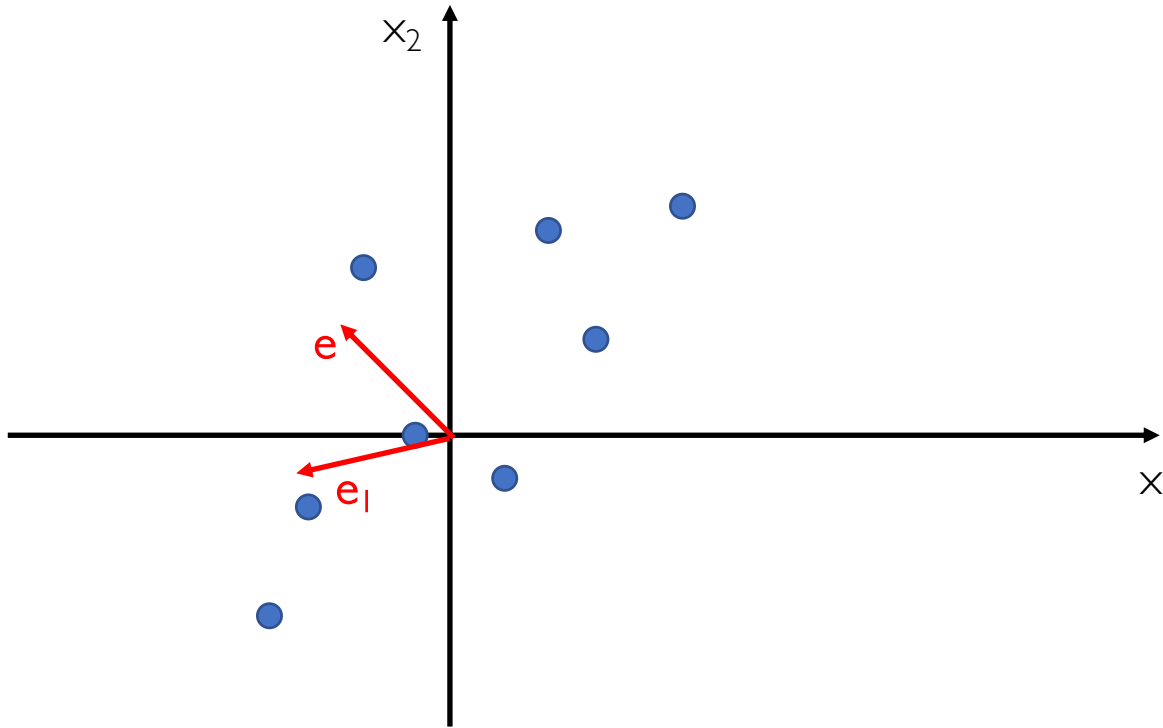


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slope =  $1/-1 = -1$

# Covariance Matrix of Original Dimensions



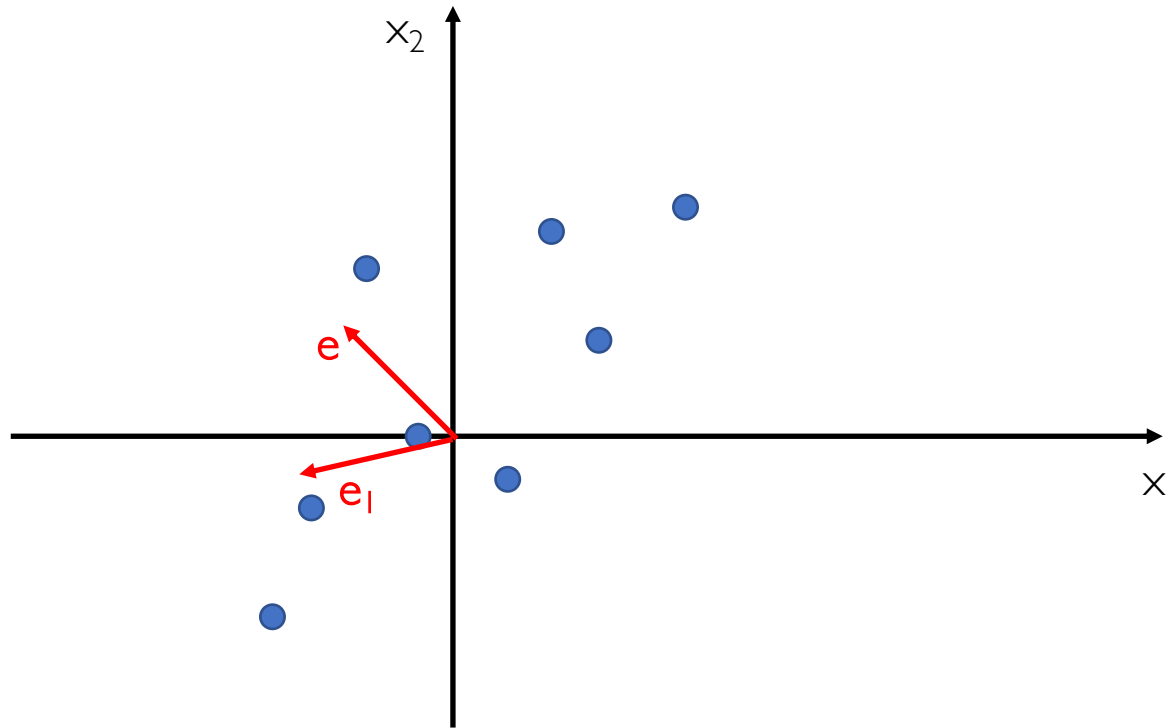
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new slope =  $-(1/5)/-(6/5) = 1/6$

# Covariance Matrix of Original Dimensions



Turns towards the direction of the greatest variance

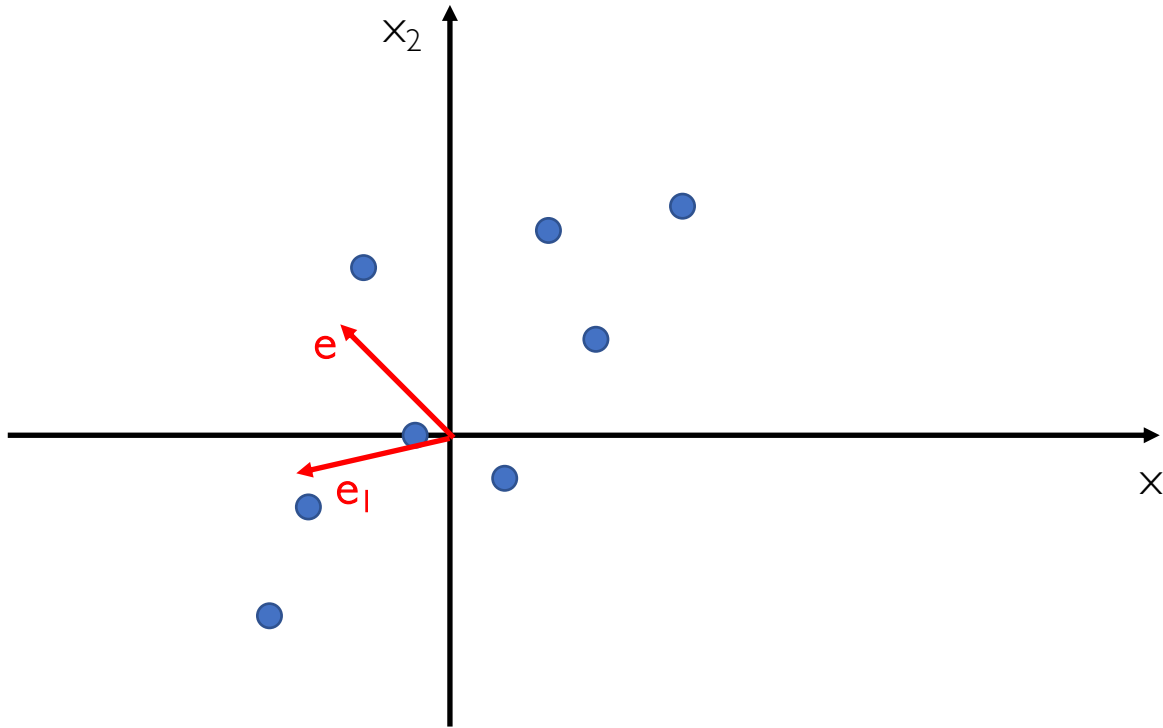
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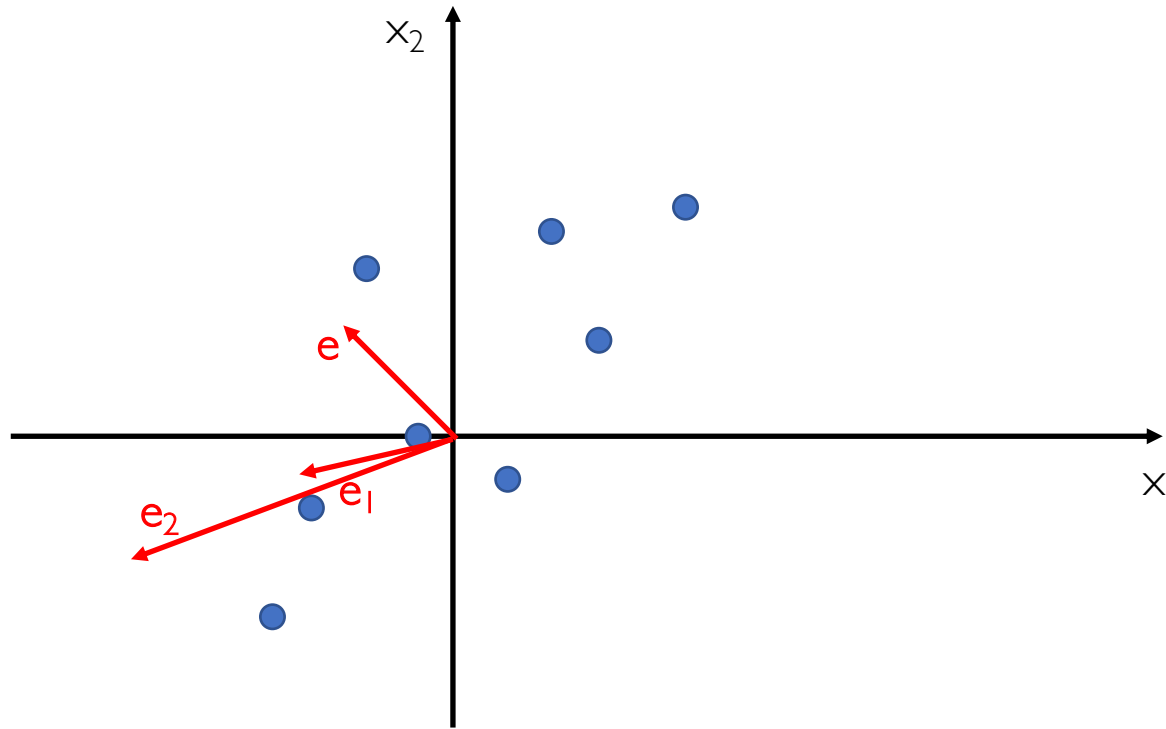
# Covariance Matrix of Original Dimensions



Let's repeat the previous step multiplying the covariance matrix  $K$  by  $e_1 = (-6/5, -1/5)$

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

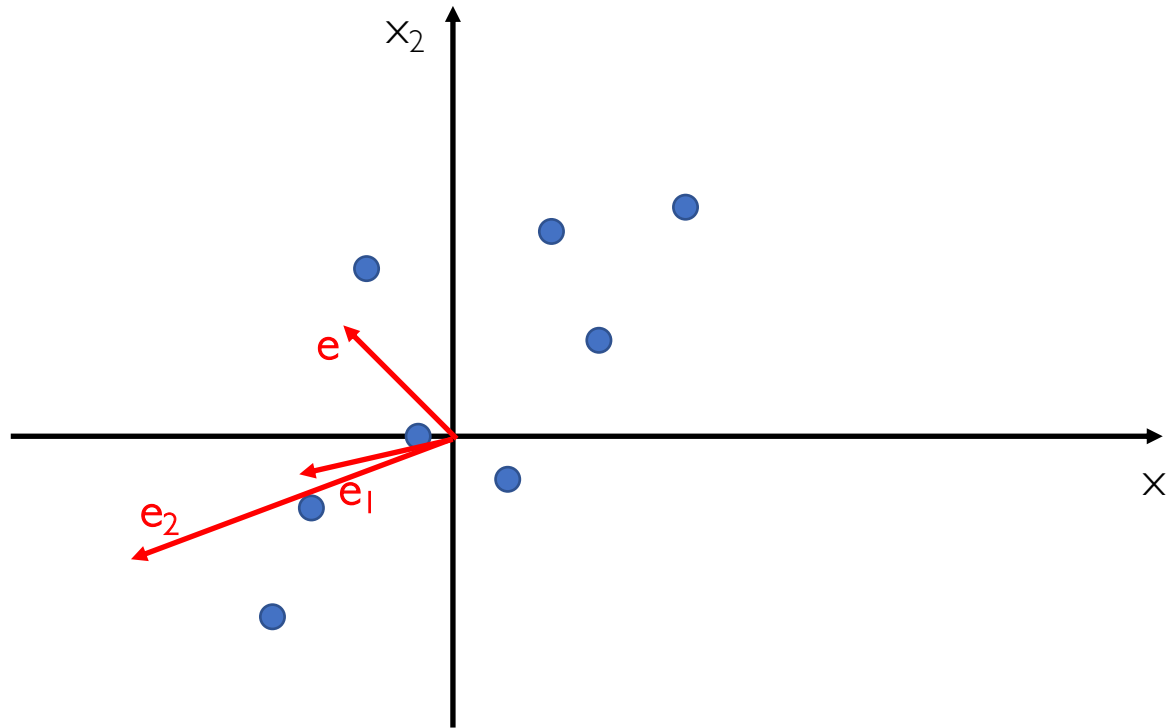
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slope = 1/6

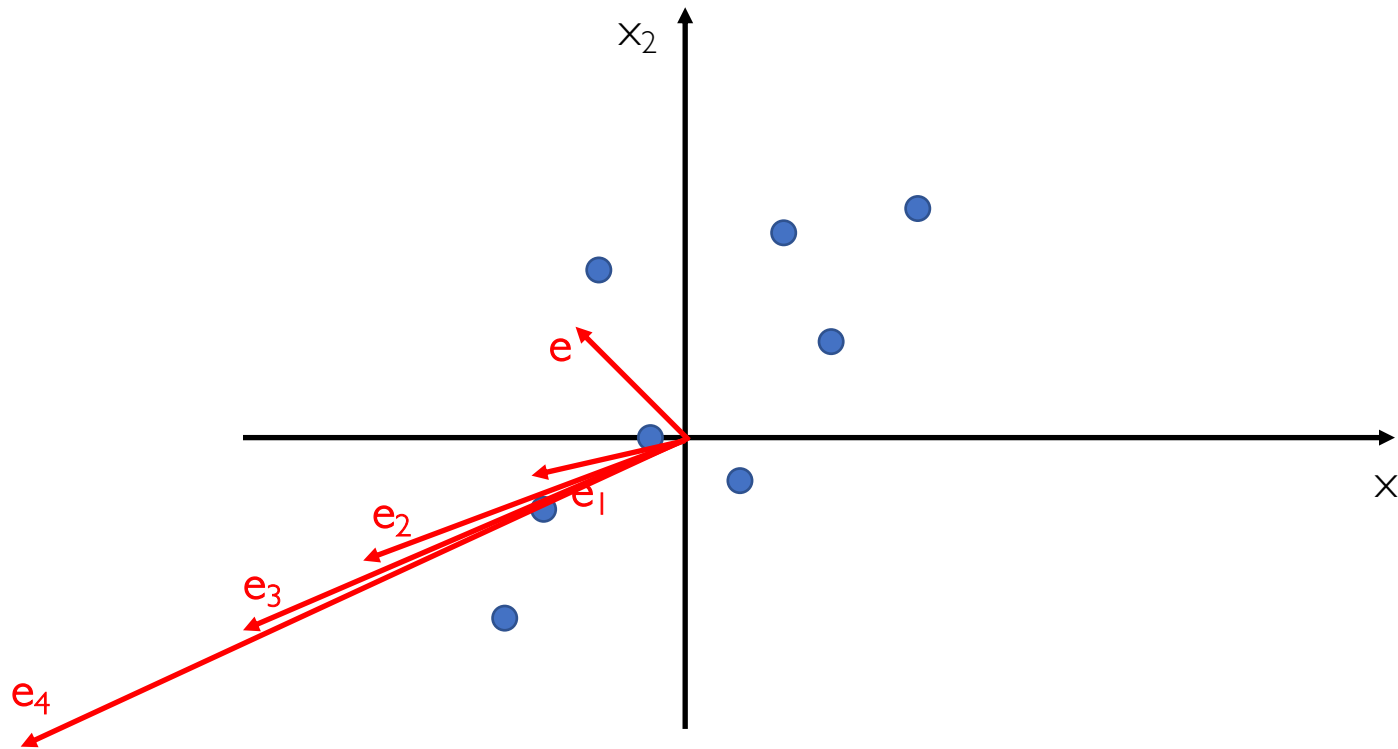
Turns towards the direction of the greatest variance

new slope = 27/64



# Covariance Matrix of Original Dimensions

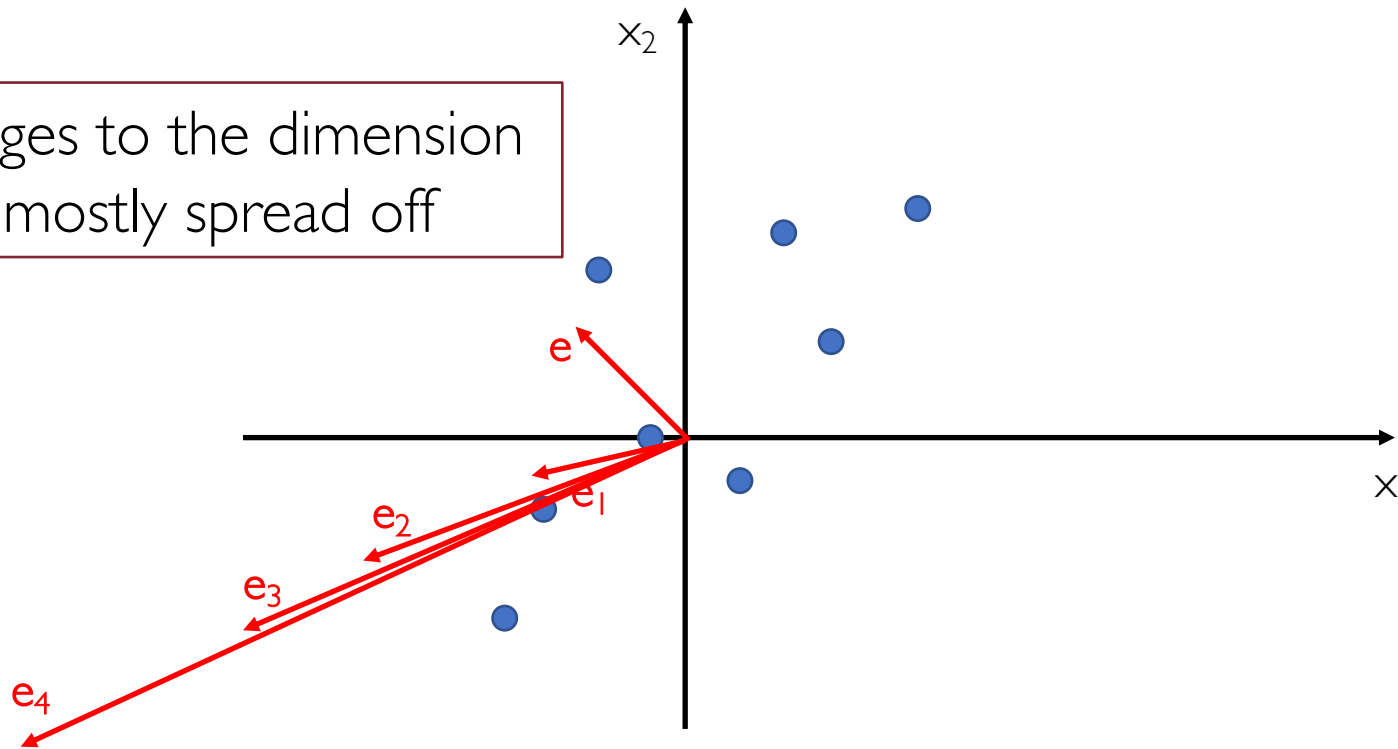
If we keep doing this the resulting vector is getting **longer** and **turns** towards the direction of the **largest variance**



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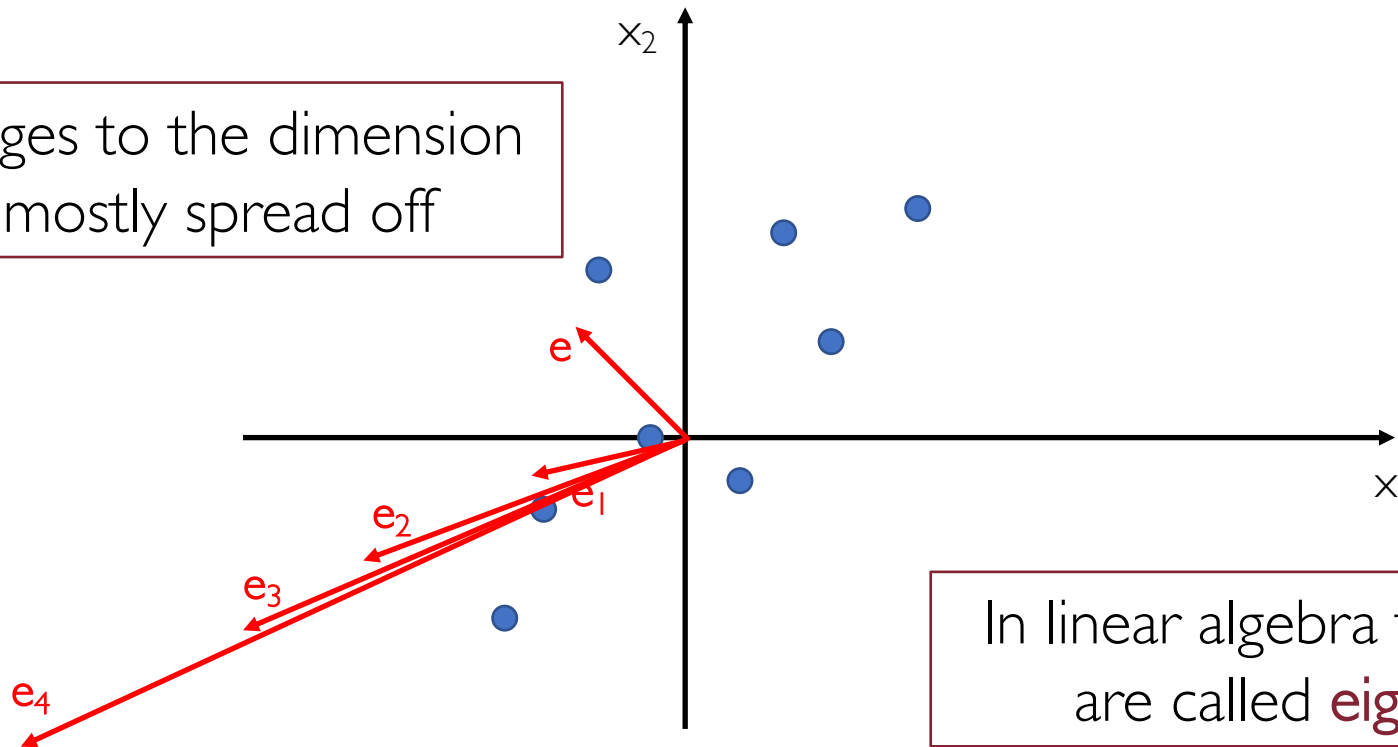
The slope converges to the dimension where data is mostly spread off



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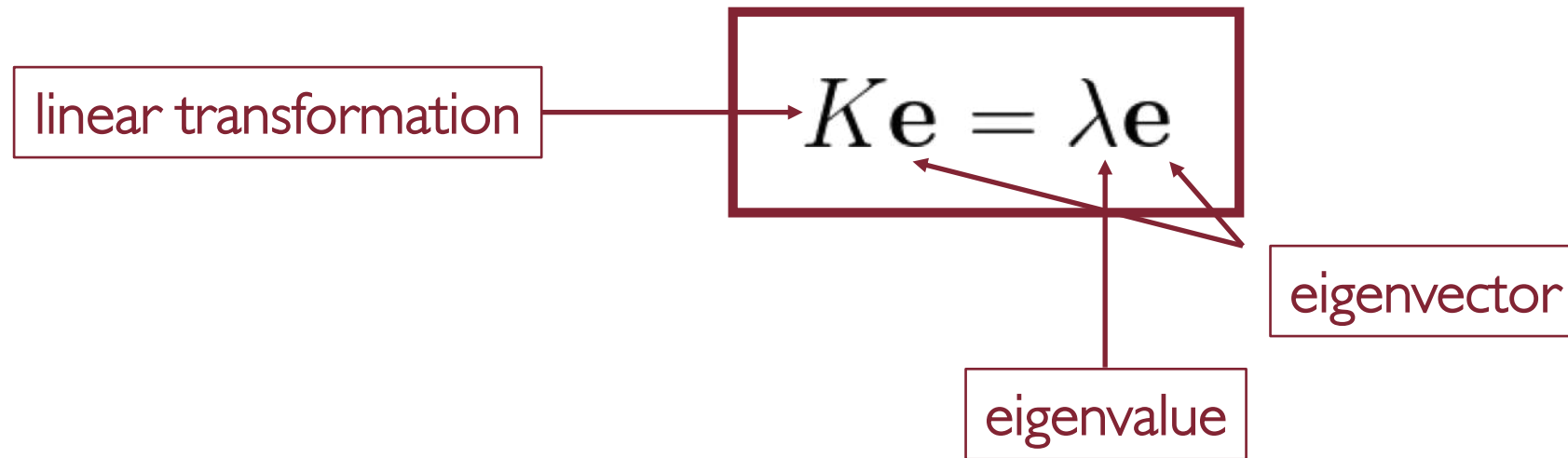


In linear algebra those vectors are called **eigenvectors**

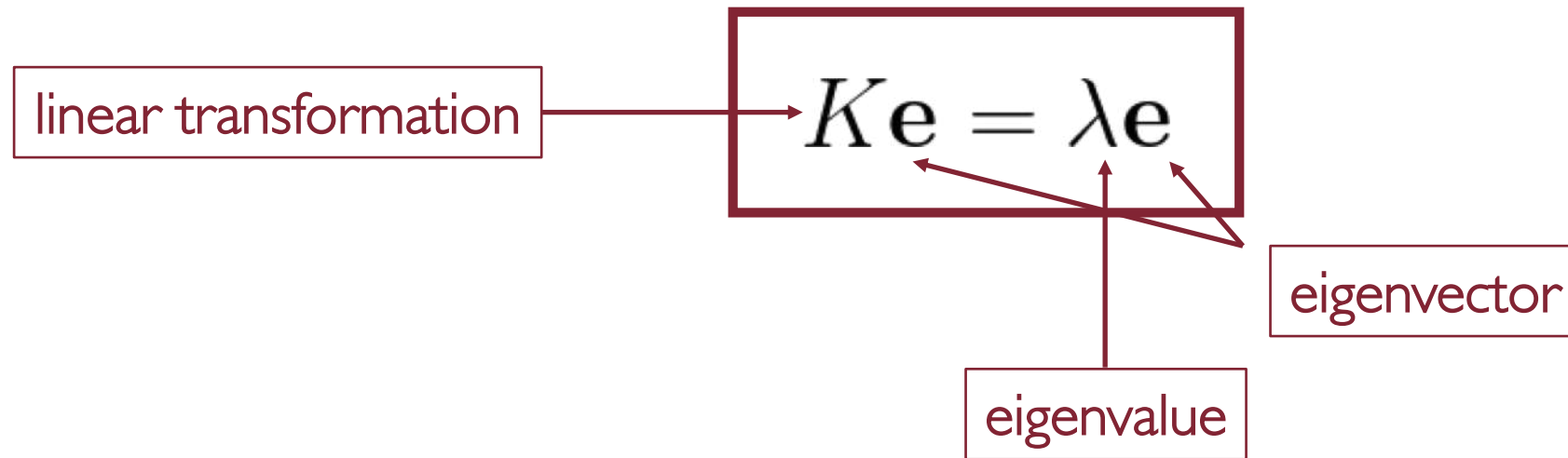
# Eigenvectors of the Covariance Matrix

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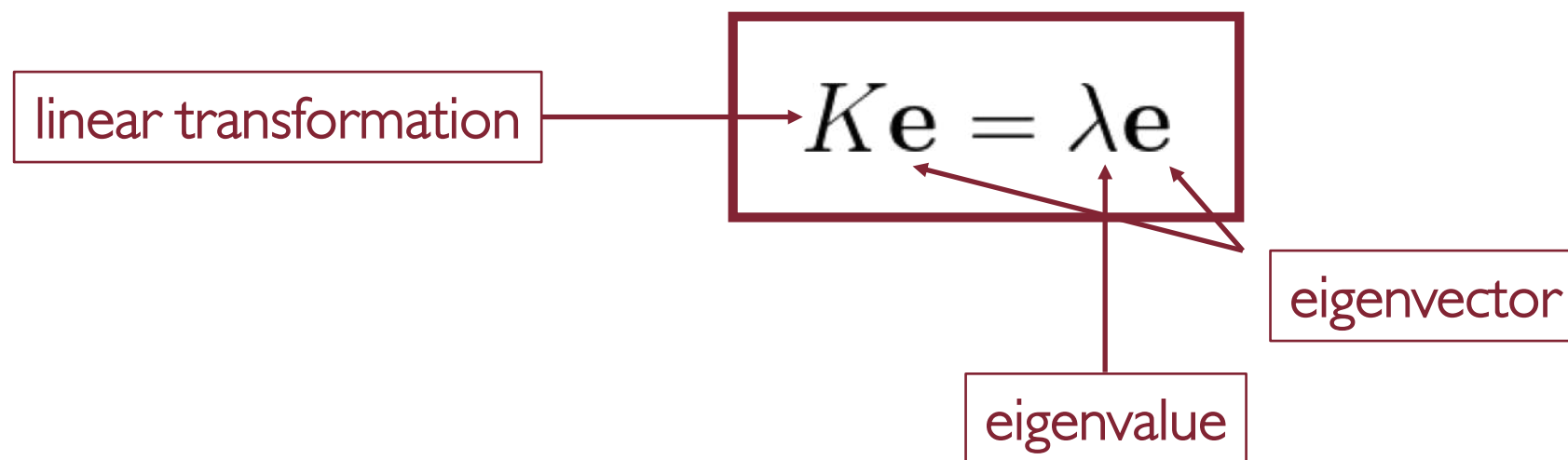


# Eigenvectors of the Covariance Matrix



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

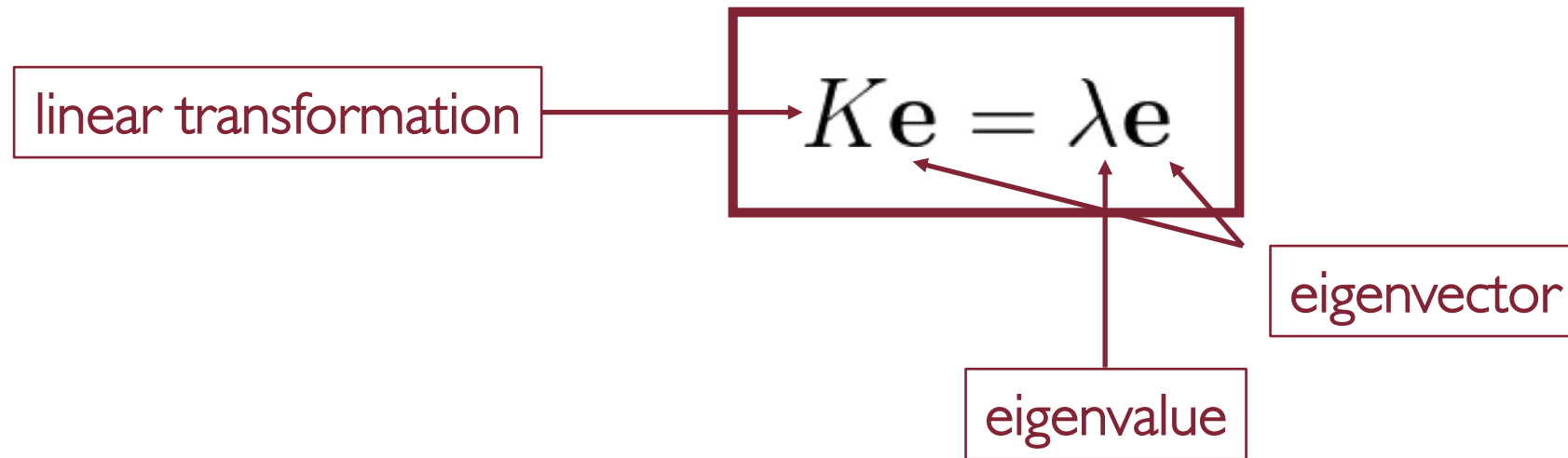
# Eigenvectors of the Covariance Matrix



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

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



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  $\lambda$  (**eigenvalue**)

## Principal Components

eigenvectors of the covariance matrix with the **largest** eigenvalues



# How Do We Compute Eigenvectors?

Remember that we want to solve for  $\mathbf{e}$  the following:

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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

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The only way for the homogeneous system above to have a **non-trivial** solution is for its matrix  $(K - \lambda I)$  to be **non-invertible**, otherwise:

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

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The corresponding homogeneous system will have a **non-trivial** solution



# How Do We Compute Eigenvectors?

I. Find the eigenvalues by solving for  $\lambda$ :  $\det(K - \lambda I) = 0$

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

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characteristic equation of  $K$

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characteristic equation of K

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

# 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  $\lambda_1$

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

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

# How Do We Compute Eigenvectors?

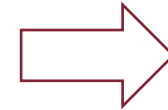
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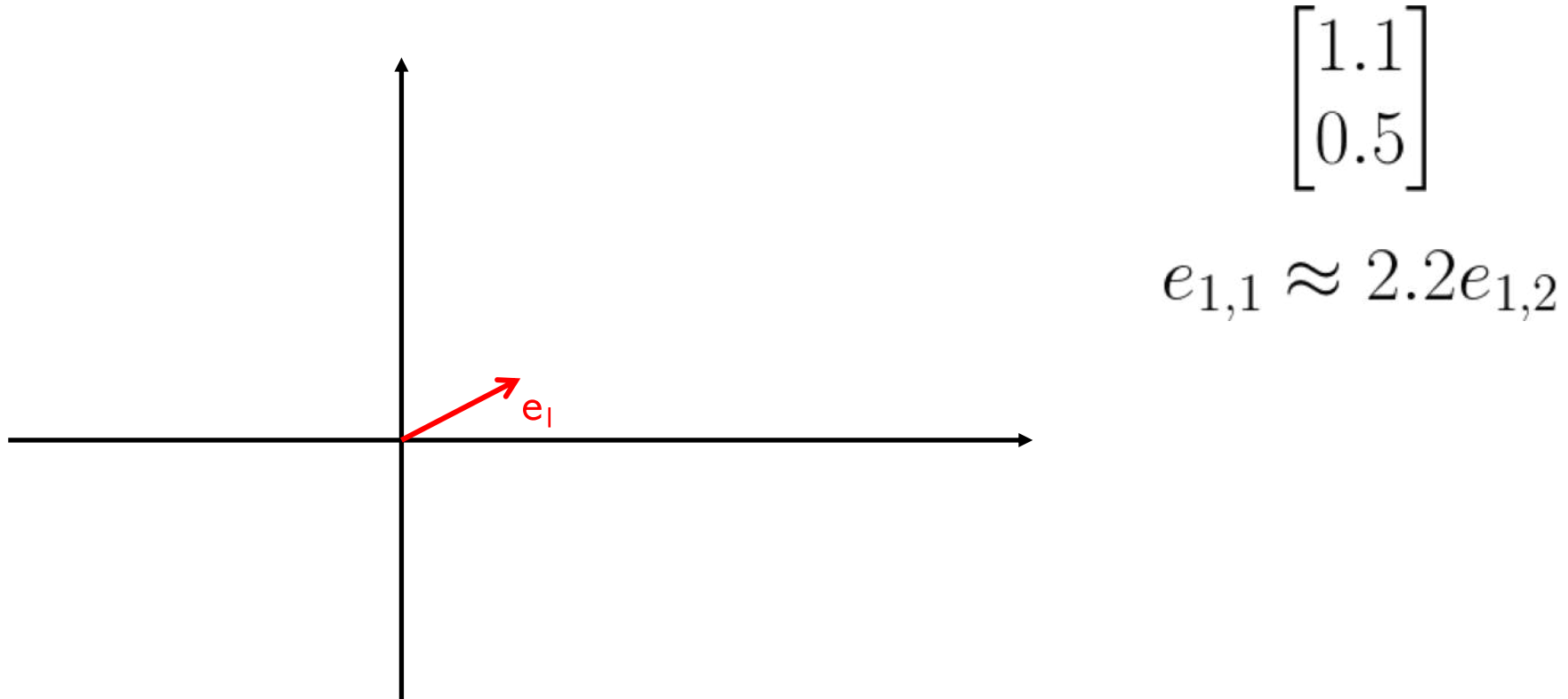


$$e_{1,1} \approx 2.2e_{1,2}$$

The system has infinitely many solutions

# How Do We Compute Eigenvectors?

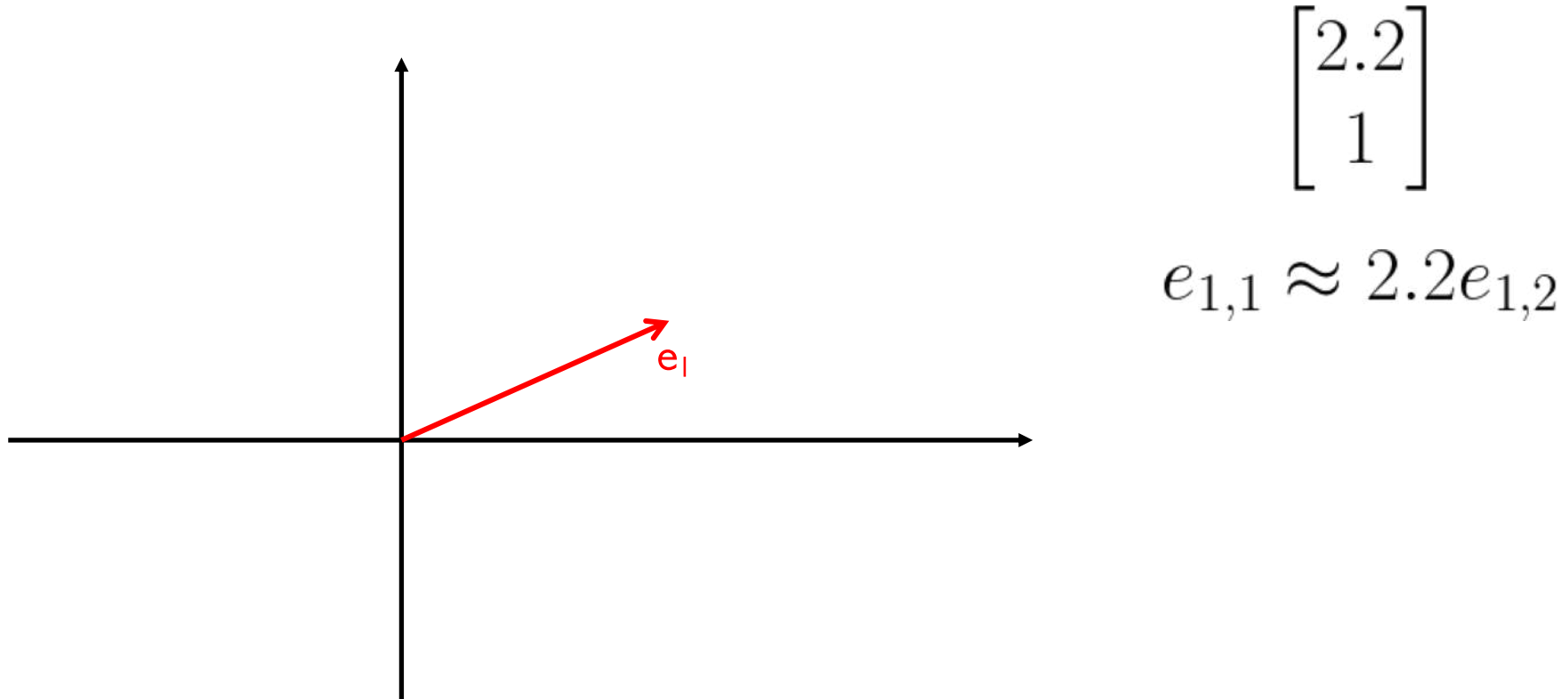
Any vector which satisfies the relationship above works!





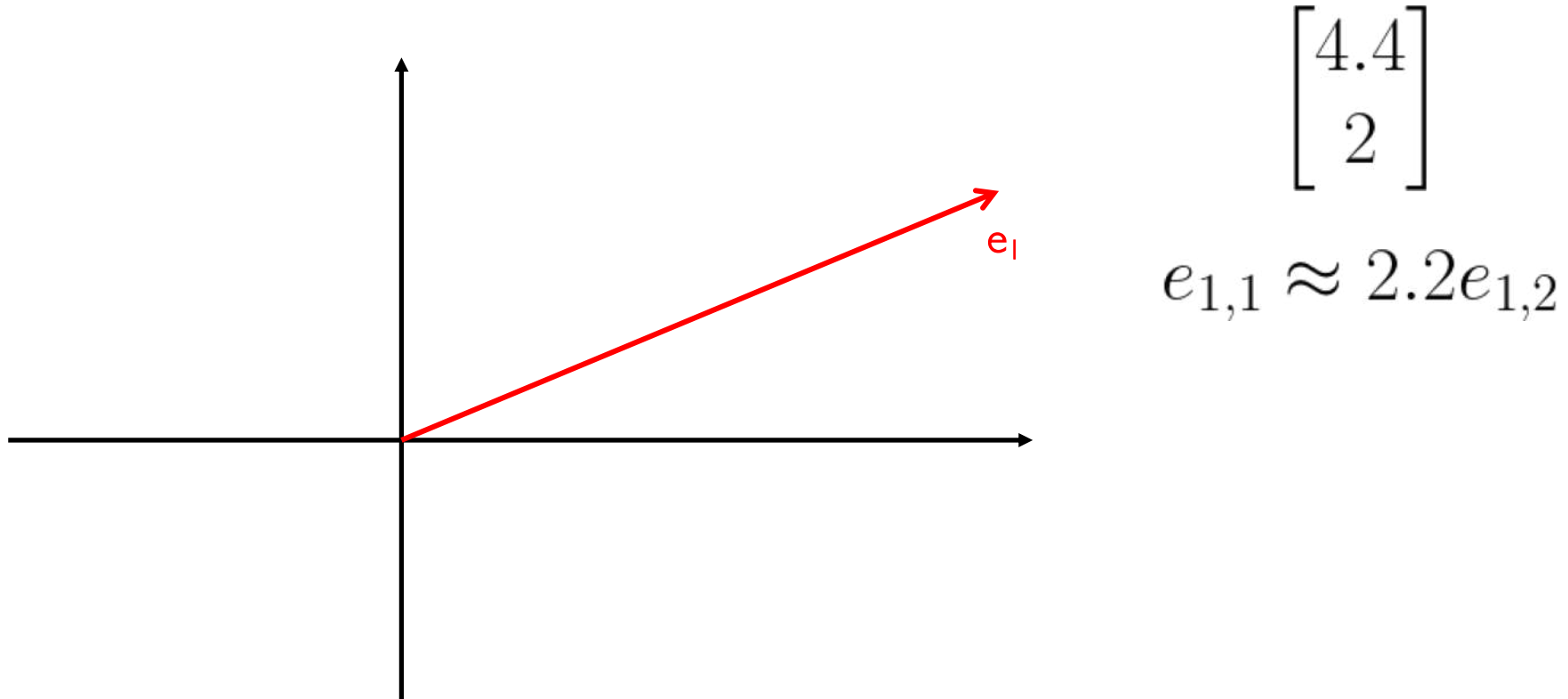
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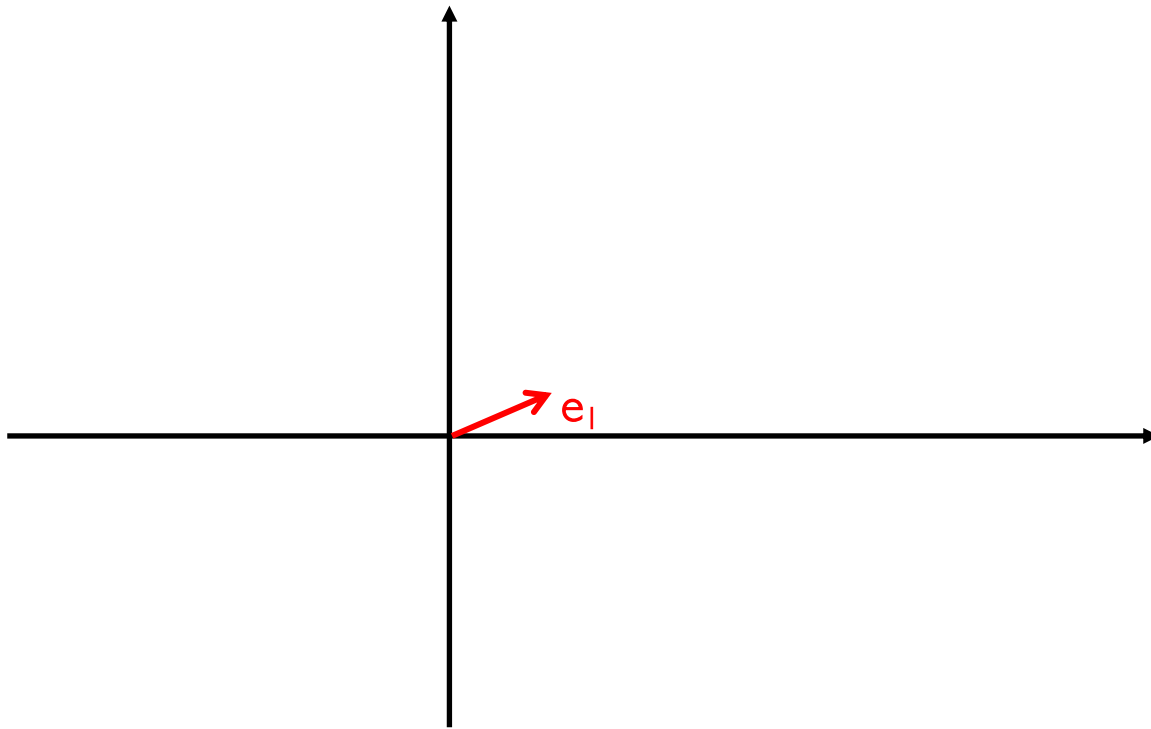
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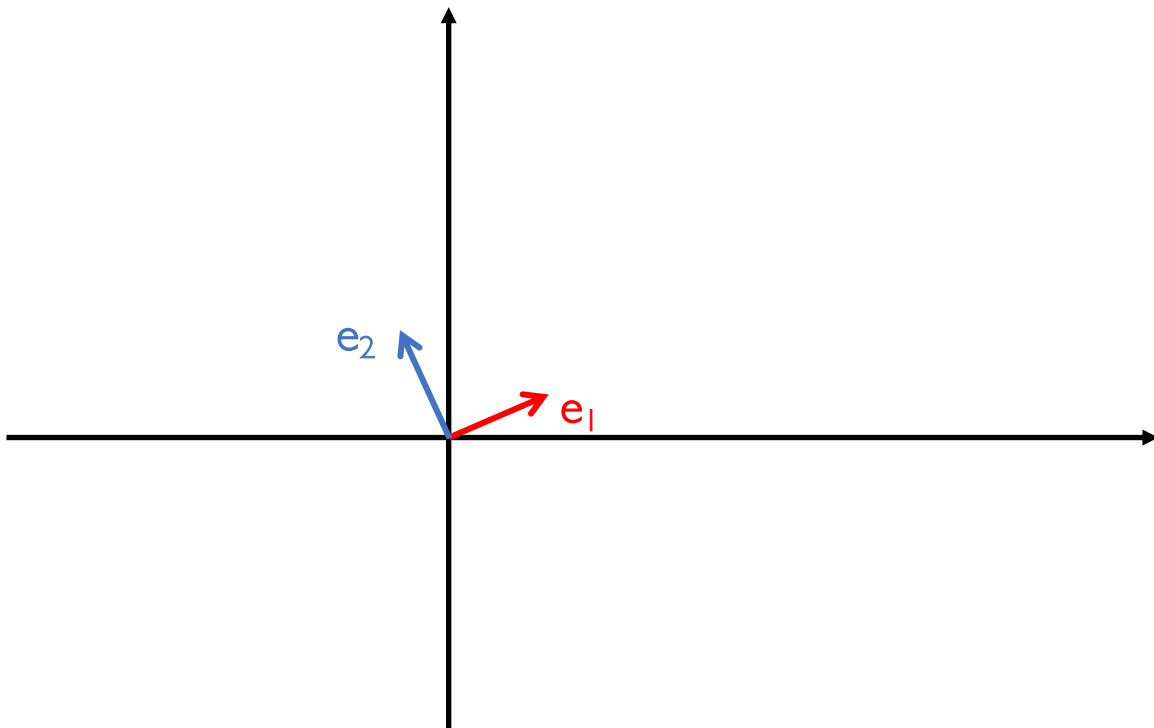
By convention, we restrict to  $\|\mathbf{e}_i\| = 1$



$$\begin{bmatrix} 0.91 \\ 0.41 \end{bmatrix}$$
$$e_{1,1} \approx 2.2e_{1,2}$$

# How Do We Compute Eigenvectors?

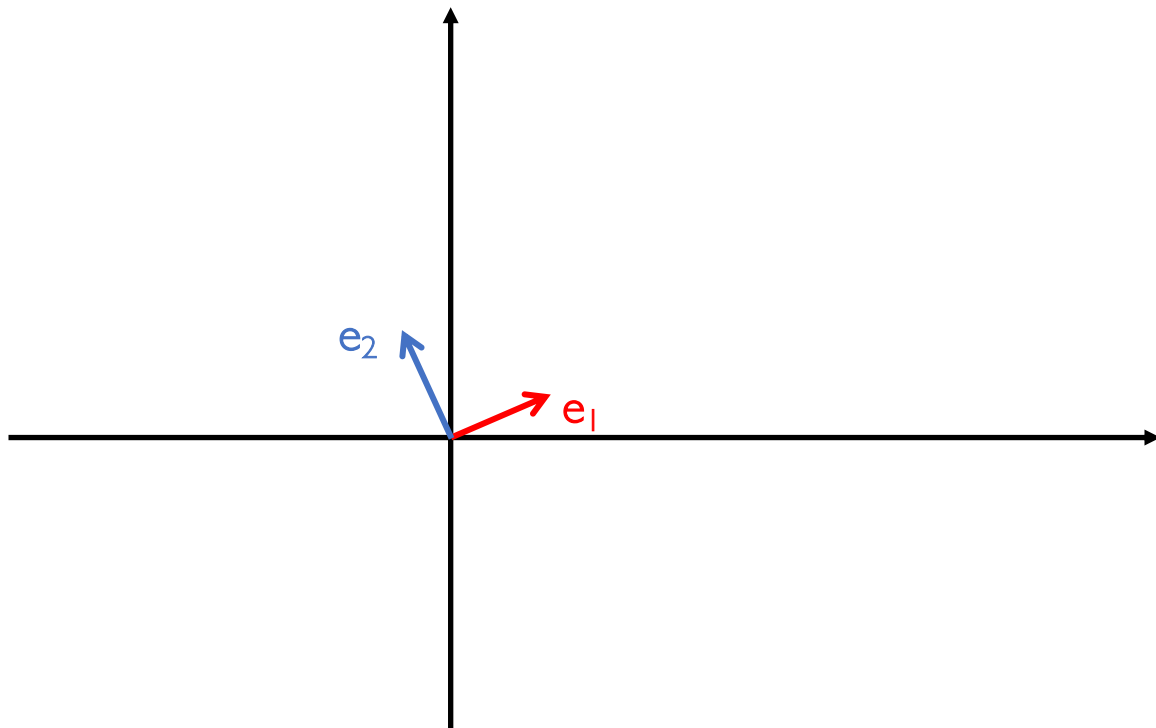
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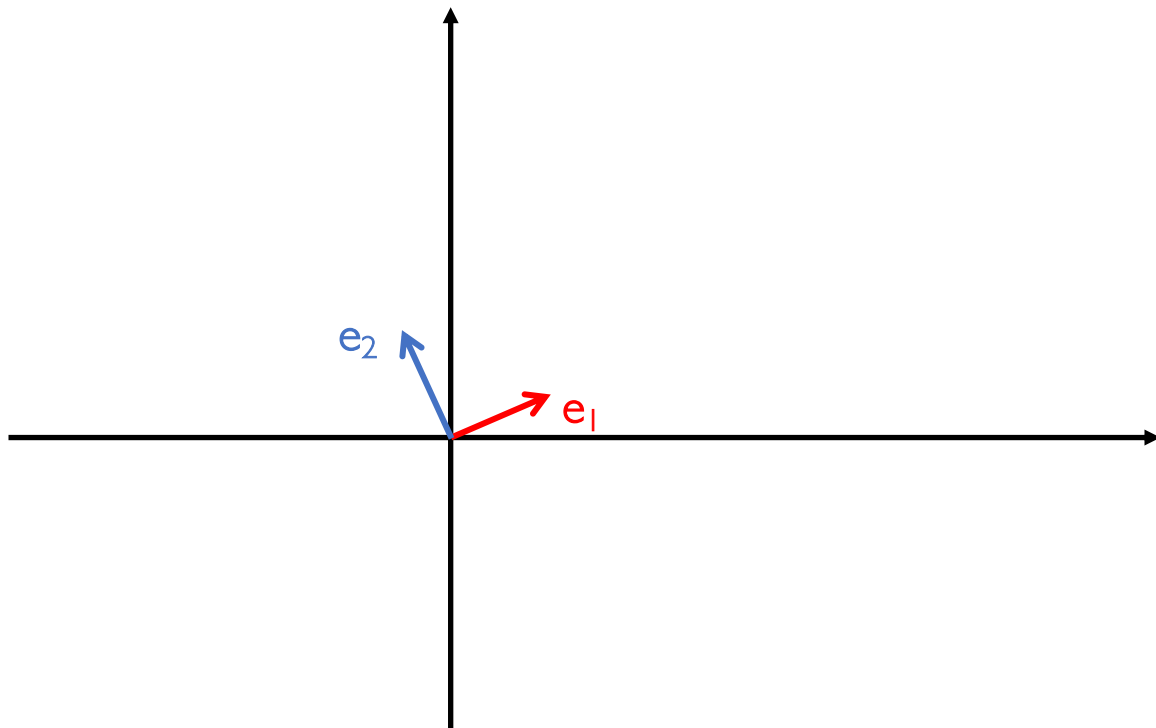
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This is just orthogonal to the previously found  $\mathbf{e}_1$



$\mathbf{e}_1$  and  $\mathbf{e}_2$  are the new coordinate system replacing the original  $x_1$  and  $x_2$

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

# Principal Components

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

$\mathbf{e}_1$  is the 1st principal component as it is the eigenvector corresponding to the **largest** eigenvalue

$\mathbf{e}_2$  is the 2nd principal component as it is the eigenvector corresponding to the **smallest** eigenvalue

# Projecting to New Dimensions: 2-d Case

- $\mathbf{e}_1$  and  $\mathbf{e}_2$  identify our new coordinate system (principal components)



# Projecting to New Dimensions: 2-d Case

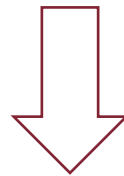
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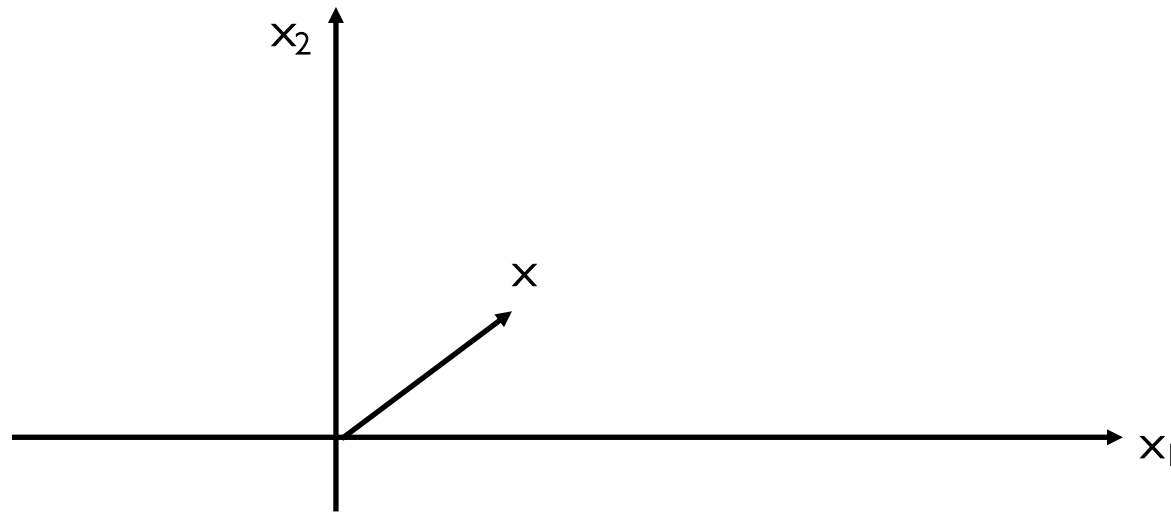
## Goal

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

# Projecting to New Dimensions: 2-d Case

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

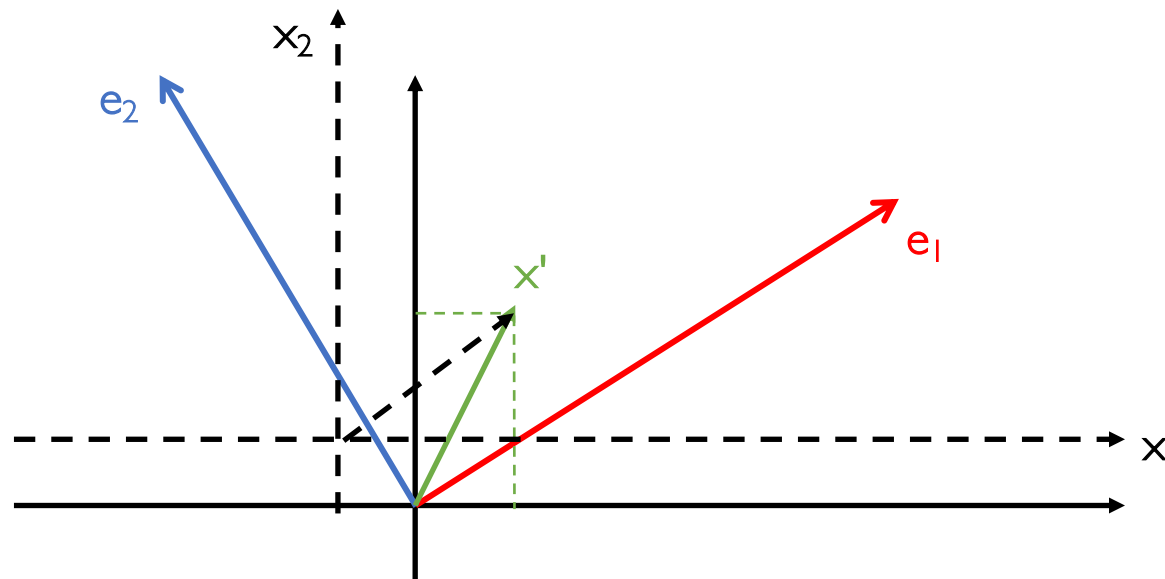
$$\mathbf{x}' = \mathbf{x} - \boldsymbol{\mu} = (x_1 - \mu_1, x_2 - \mu_2)$$



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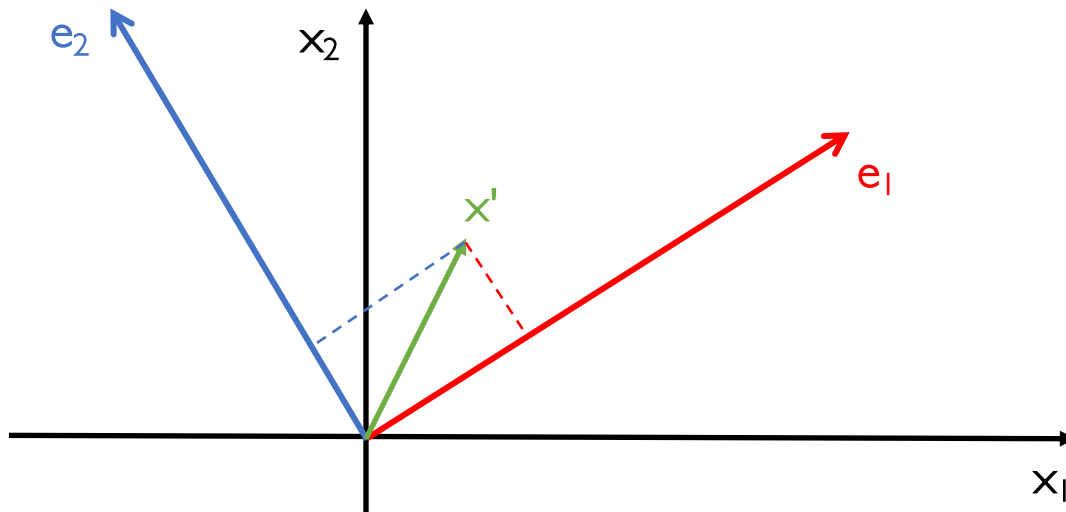
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# Projecting to New Dimensions: 2-d Case

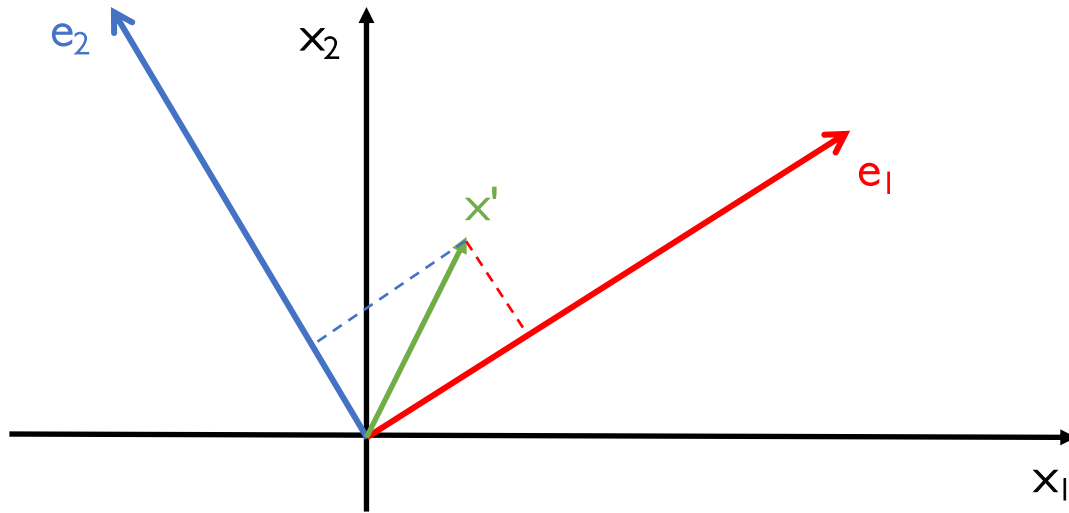
2. Project  $\mathbf{x}'$  on each dimension  $\mathbf{e}_1$  and  $\mathbf{e}_2$

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



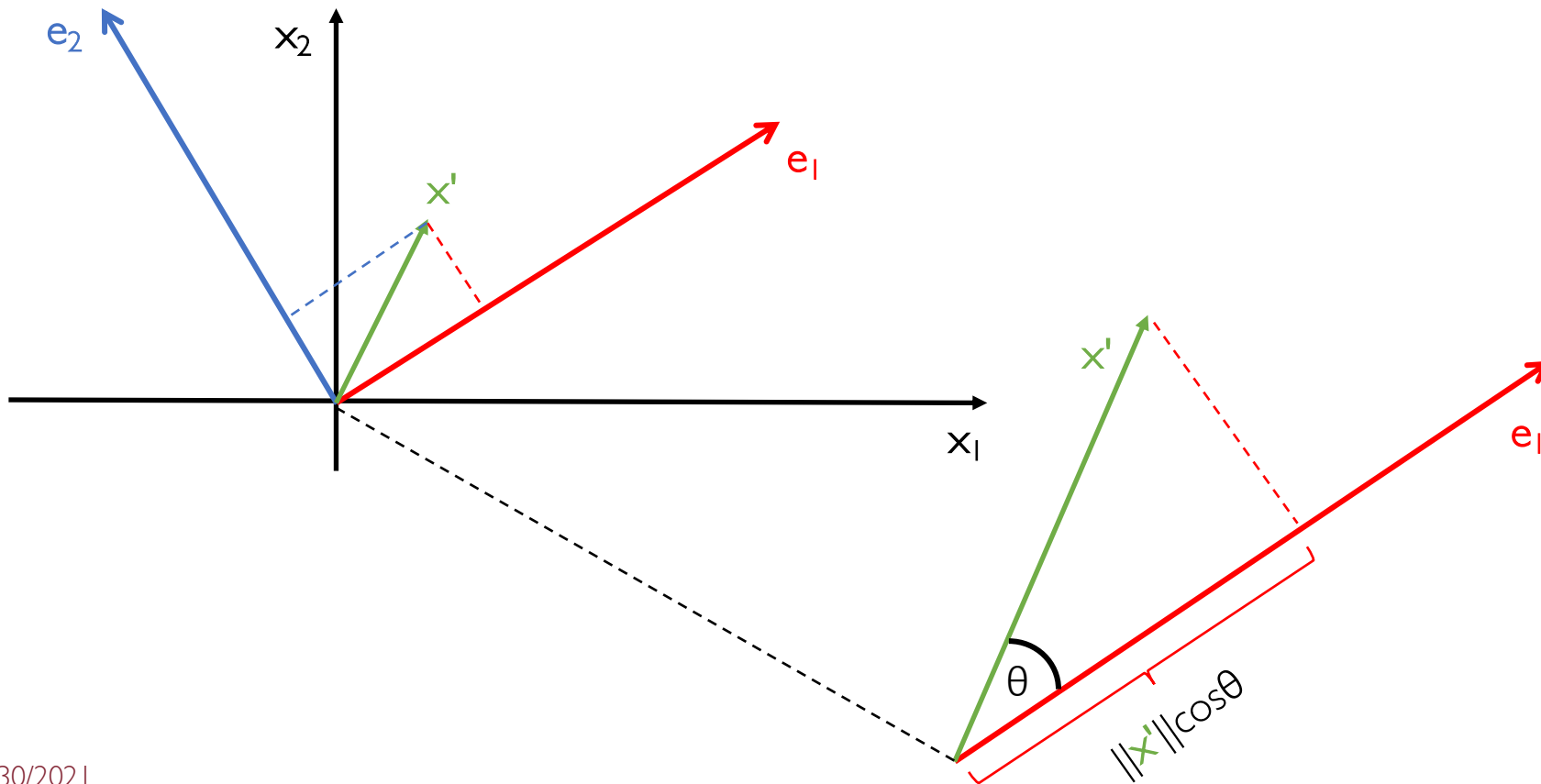
# Projecting to New Dimensions: 2-d Case

Why the dot product?



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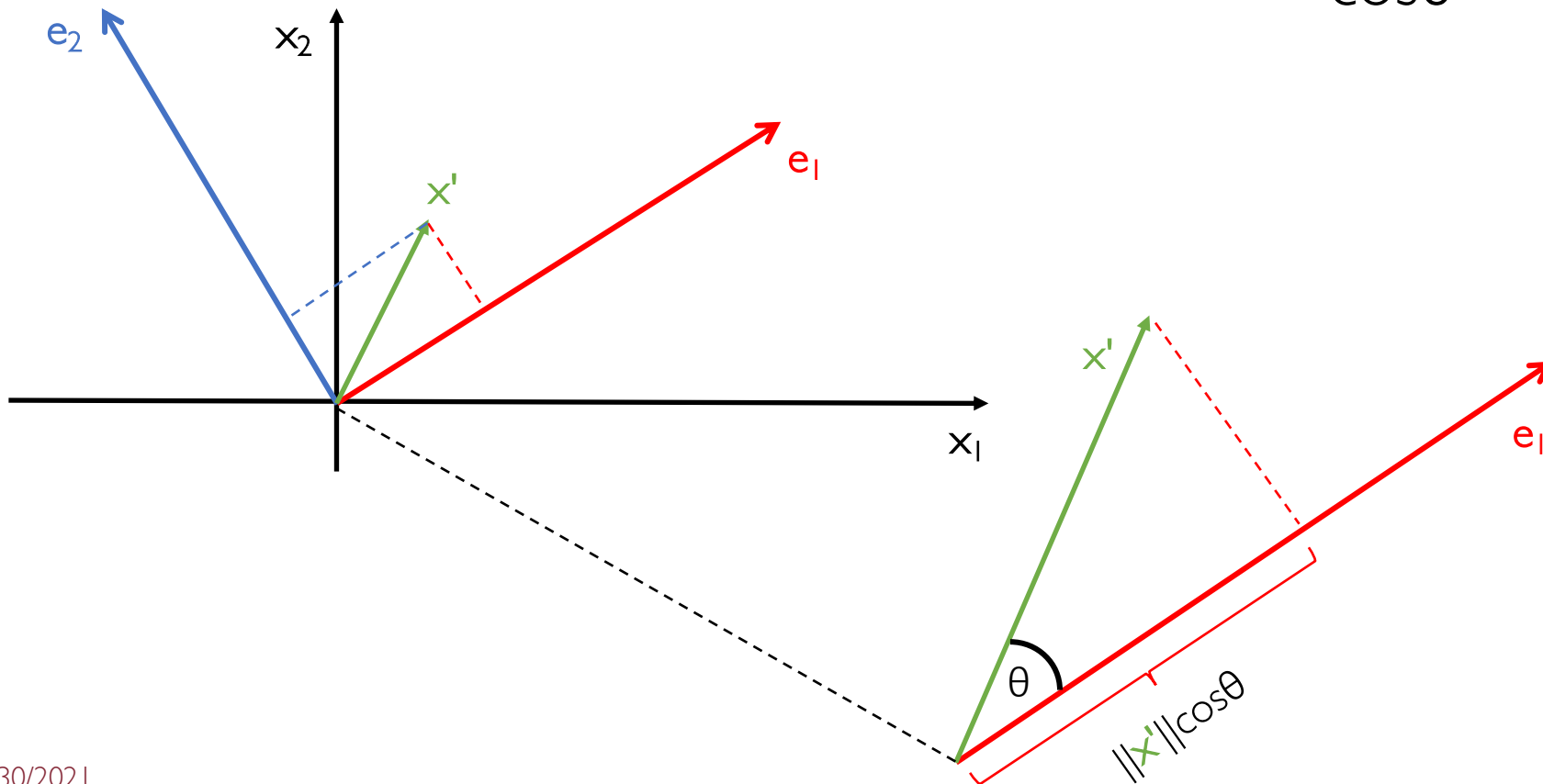




# Projecting to New Dimensions: 2-d Case

Why the dot product?

$$\cos\theta = (\mathbf{x}'\mathbf{e}_1)/\|\mathbf{x}'\|\|\mathbf{e}_1\|$$

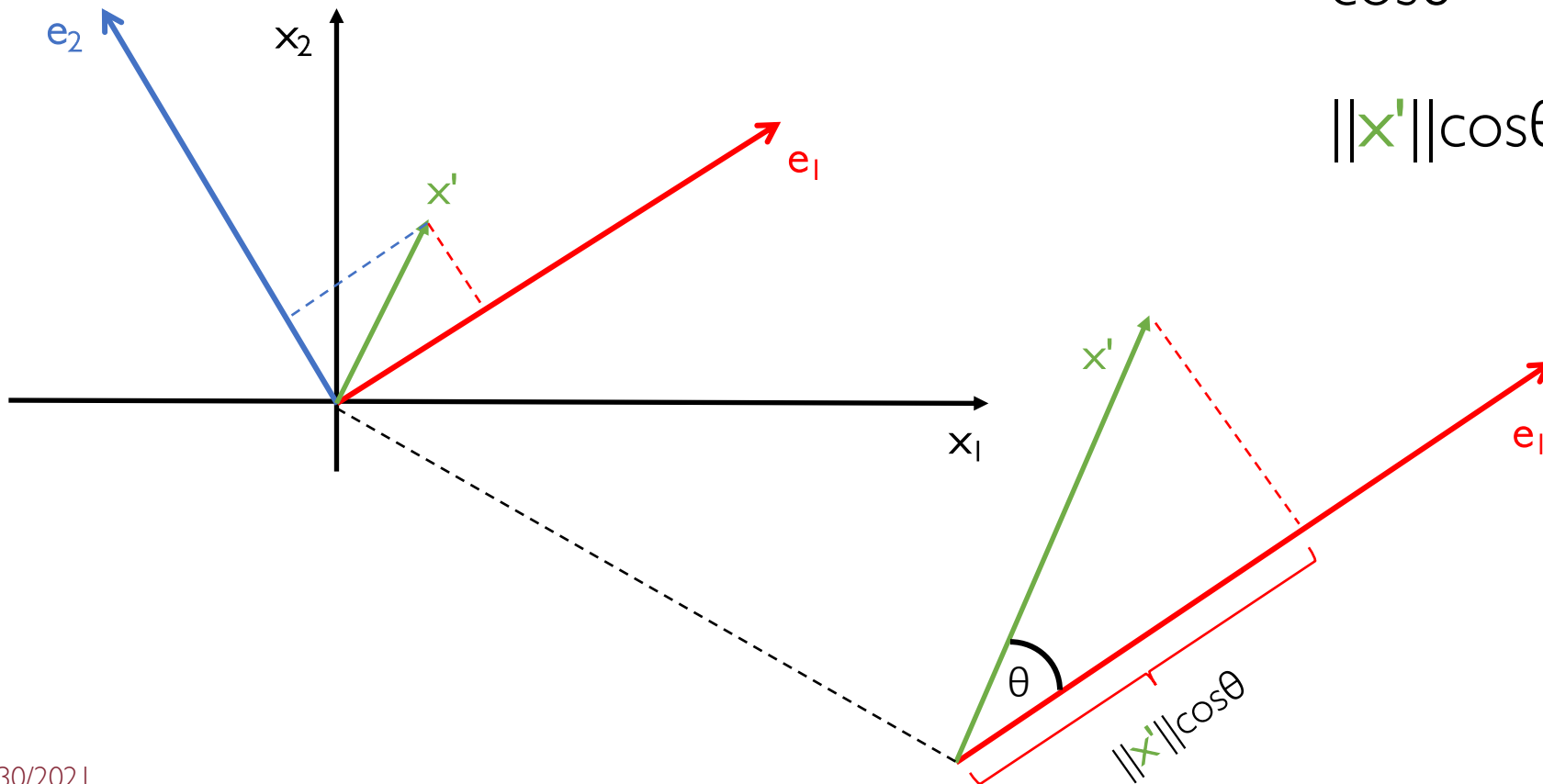


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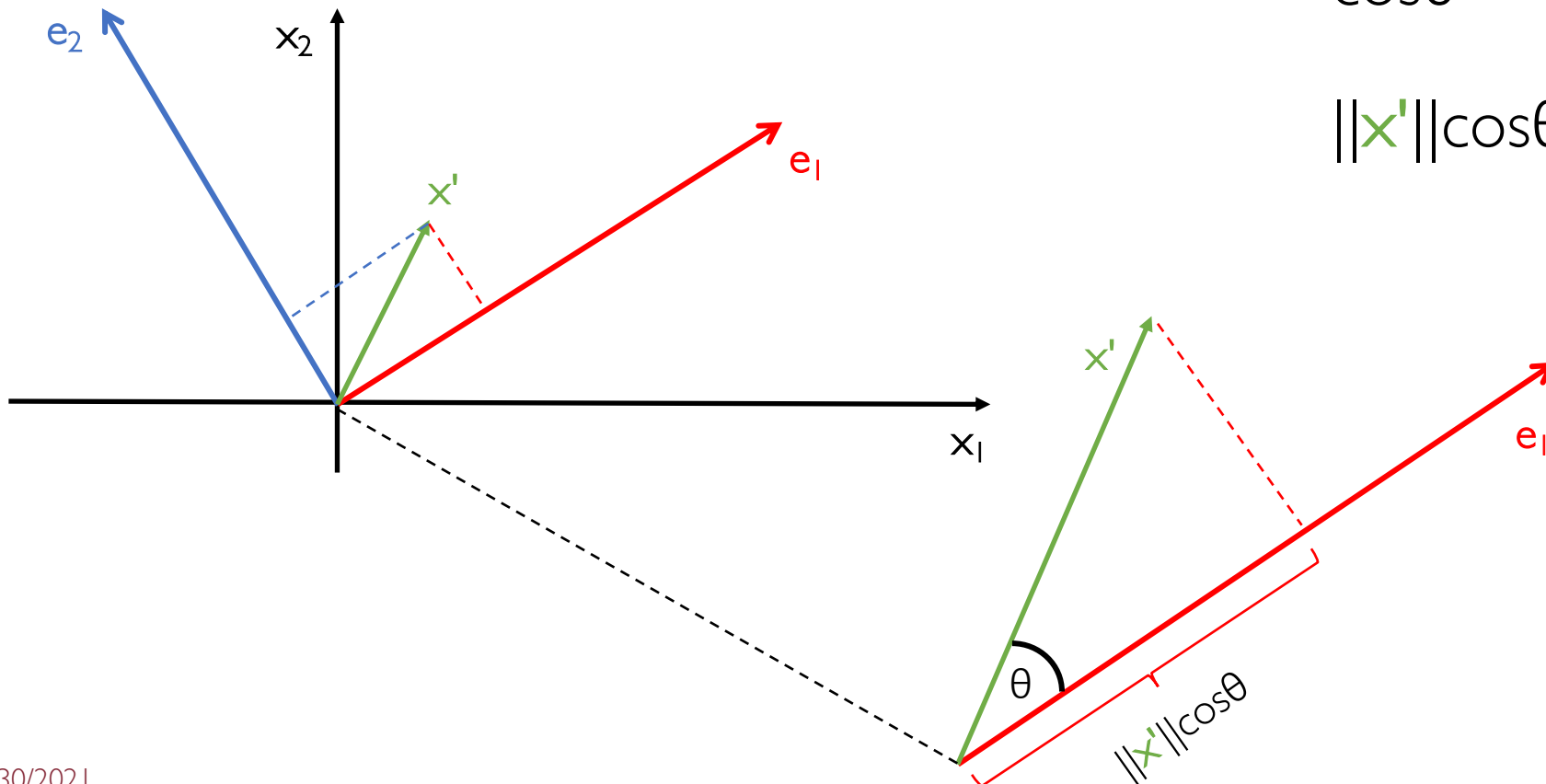
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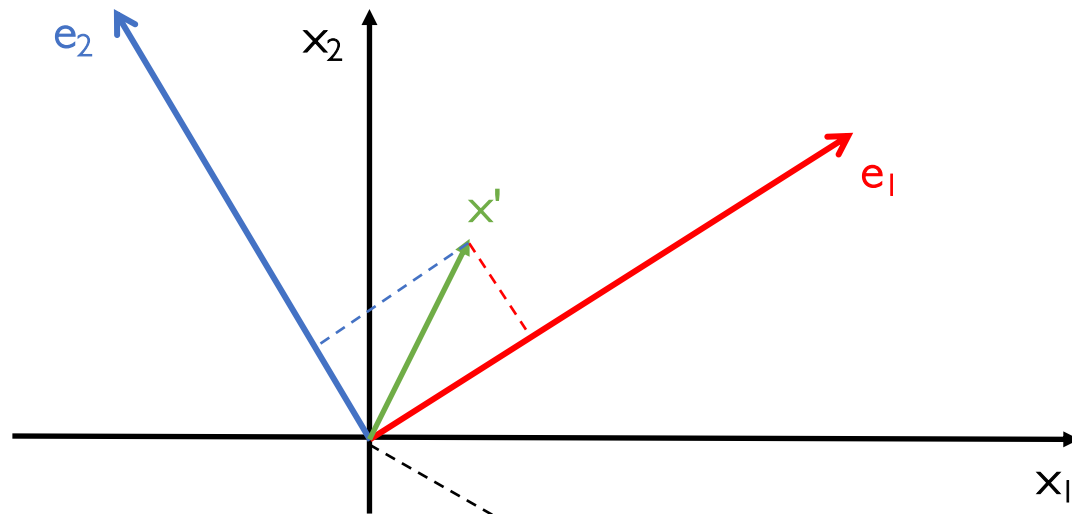
$$\|\mathbf{x}'\|\cos\theta = \mathbf{x}'\mathbf{e}_1/\|\mathbf{e}_1\|$$

$$\|\mathbf{e}_1\| = 1$$



# Projecting to New Dimensions: 2-d Case

Why the dot product?



$$\cos\theta = (\mathbf{x}'\mathbf{e}_1)/\|\mathbf{x}'\|\|\mathbf{e}_1\|$$

$$\|\mathbf{x}'\|\cos\theta = \mathbf{x}'\mathbf{e}_1/\|\mathbf{e}_1\|$$

$$\|\mathbf{x}'\|\cos\theta = \mathbf{x}'\mathbf{e}_1$$

$$\|\mathbf{e}_1\| = 1$$

# Projecting to New Dimensions: 2-d Case

The new coordinates of the original data point  $\mathbf{x}$  according to the eigenvectors  $\mathbf{e}_1$  and  $\mathbf{e}_2$  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

# Projecting to New Dimensions: $d$ -dimensions

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I. Mean centering

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



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## 2. Projection to principal components

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

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More details available here:

[https://github.com/gtolomei/big-data-computing/raw/master/extra/Notes\\_on\\_Principal\\_Component\\_Analysis.pdf](https://github.com/gtolomei/big-data-computing/raw/master/extra/Notes_on_Principal_Component_Analysis.pdf)

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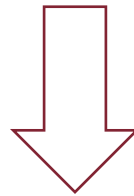
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Pick the subset of  $k$  eigenvectors that "explain" the most variance

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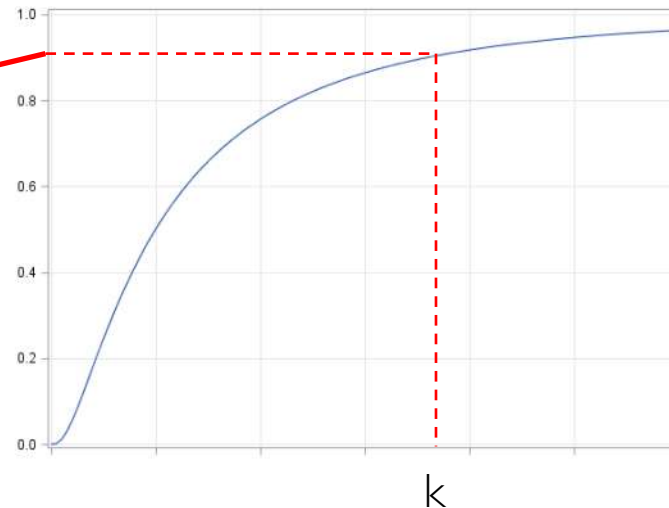
1. Sort eigenvectors by eigenvalues such that  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_d$



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

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

e.g.,  $x = 90\div 95\%$



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## Solution

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

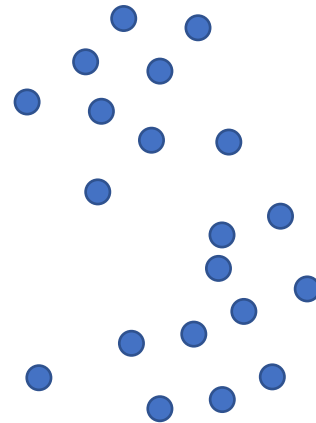
$$z = \frac{x - \mu}{\sigma}$$

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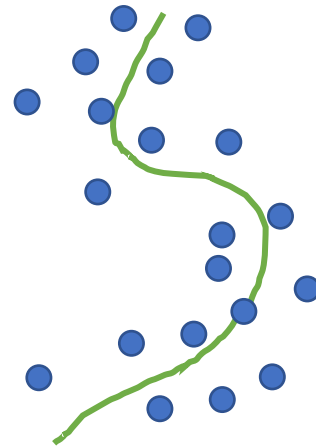
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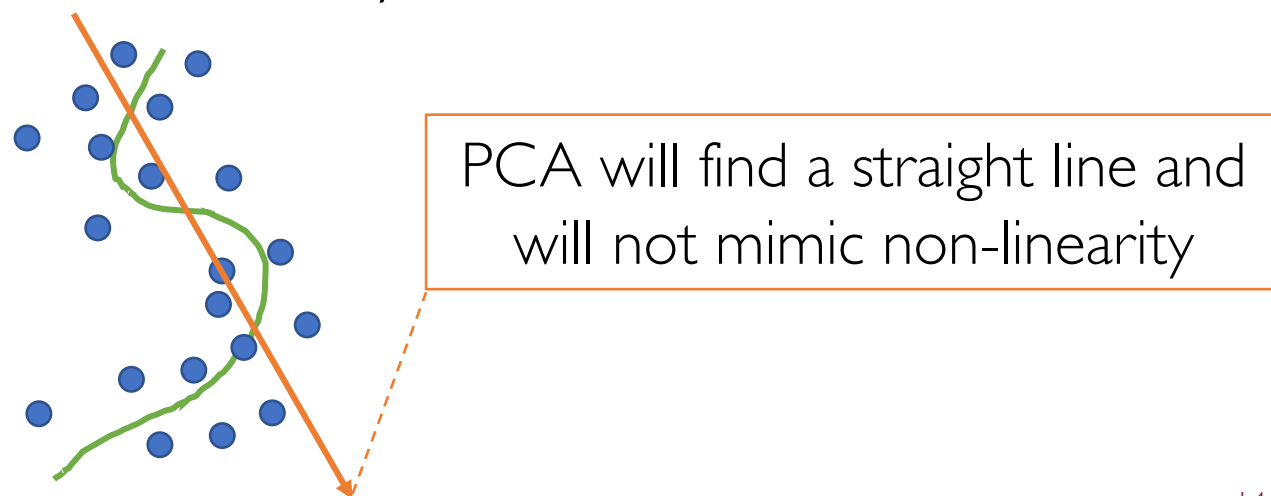
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