

Big Data Computing

Master's Degree in Computer Science

2025-2026



SAPIENZA
UNIVERSITÀ DI ROMA

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Recap from Last Lecture(s)

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

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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

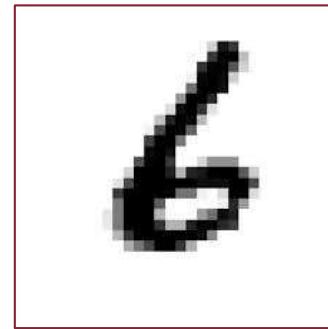
DIMENSIONALITY REDUCTION

Modeled vs. True Dimensionality

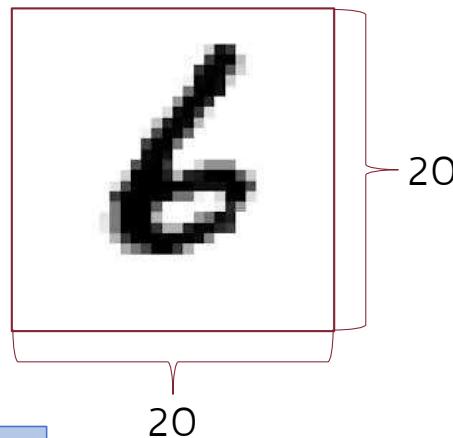
Example
Handwritten digit recognition

0	4	1	9	2	1	3	1	4	3
5	3	6	1	7	2	8	6	9	4
0	9	1	1	2	4	3	2	7	3
8	6	9	0	5	6	0	7	6	1
8	7	9	3	9	8	5	9	3	3
0	7	4	9	8	0	9	4	1	4
4	6	0	4	5	6	1	0	0	1
7	1	6	3	0	2	1	1	1	9
0	2	6	7	8	3	9	0	4	6
7	4	6	8	0	7	8	3	1	5

Modeled vs. True Dimensionality



Modeled vs. True Dimensionality

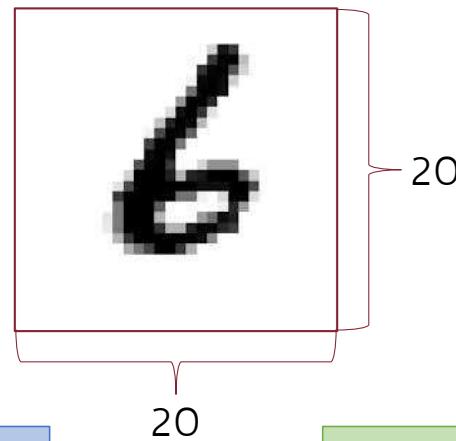


Modeled dimensionality

Each digit represented by 20x20
bitmap

400-dimensional binary vector

Modeled vs. True Dimensionality



Modeled dimensionality

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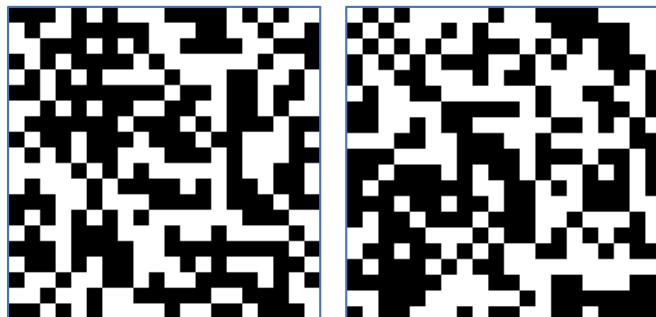
True dimensionality

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

Small variations of the pen-stroke

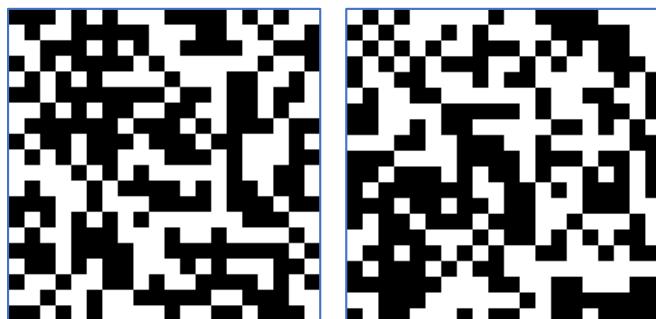
Modeled vs. True Dimensionality

Random samples
from 400-d space

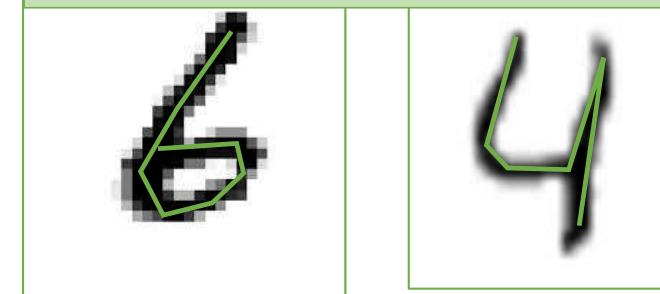


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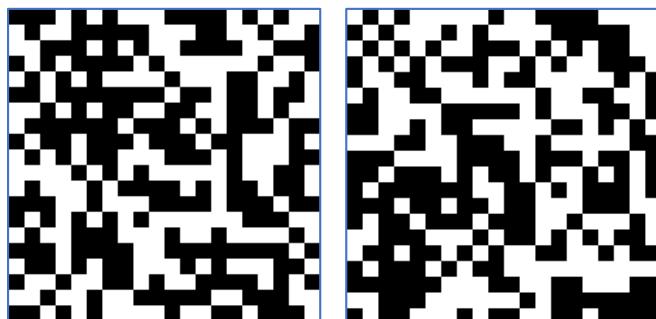


True digits living
in a
400-d space

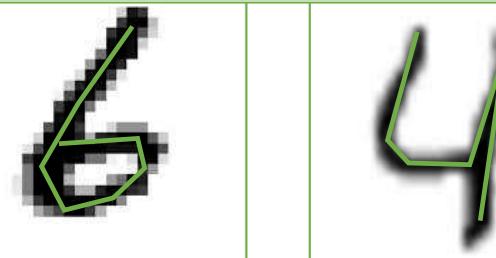


Modeled vs. True Dimensionality

Random samples
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True digits living
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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:

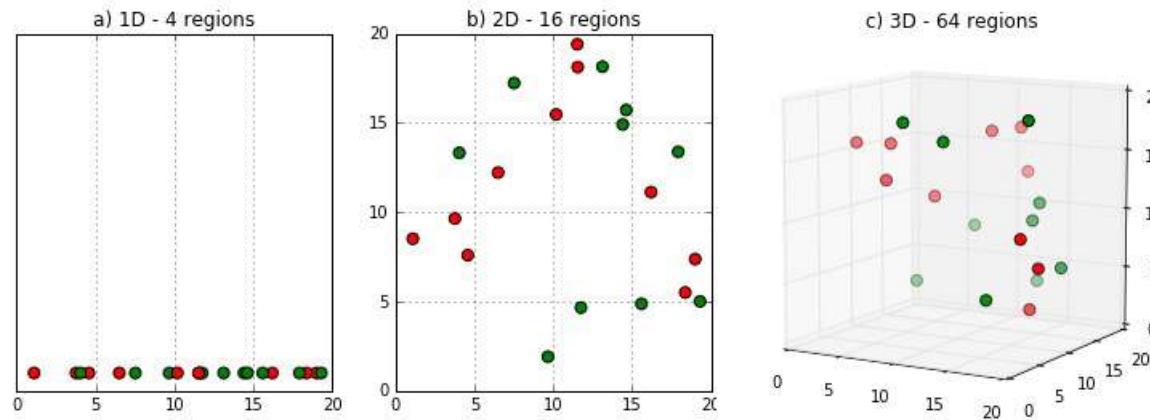
The number of examples must grow exponentially with dimensionality if we want to maintain the same "density"

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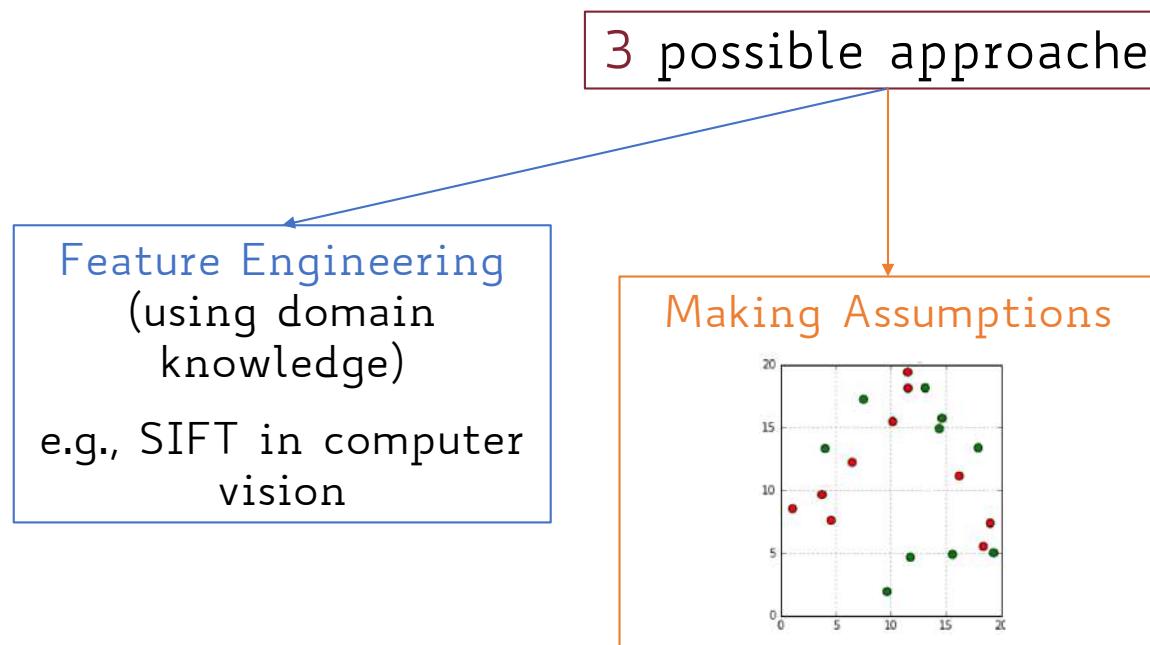


Dealing with High Dimensionality

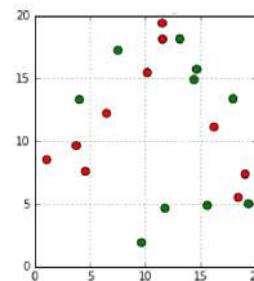
3 possible approaches

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

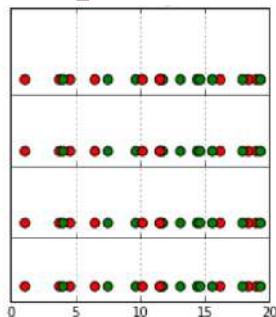
Dealing with High Dimensionality



Dealing with High Dimensionality: Assumptions



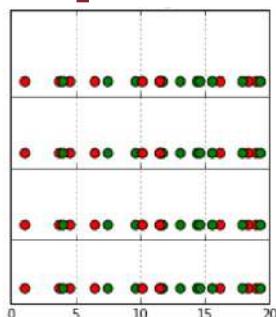
independence



Count along each dimension
separately

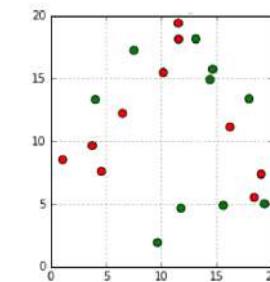
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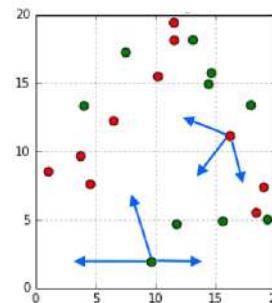


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11/26/2025



smoothness

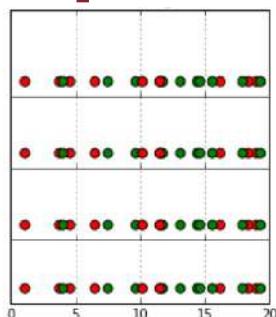


Propagate counts to neighboring regions

20

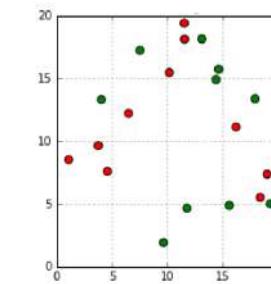
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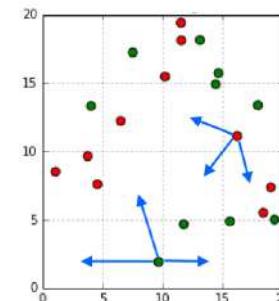


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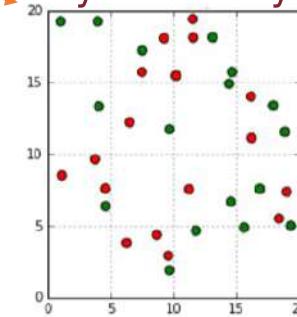


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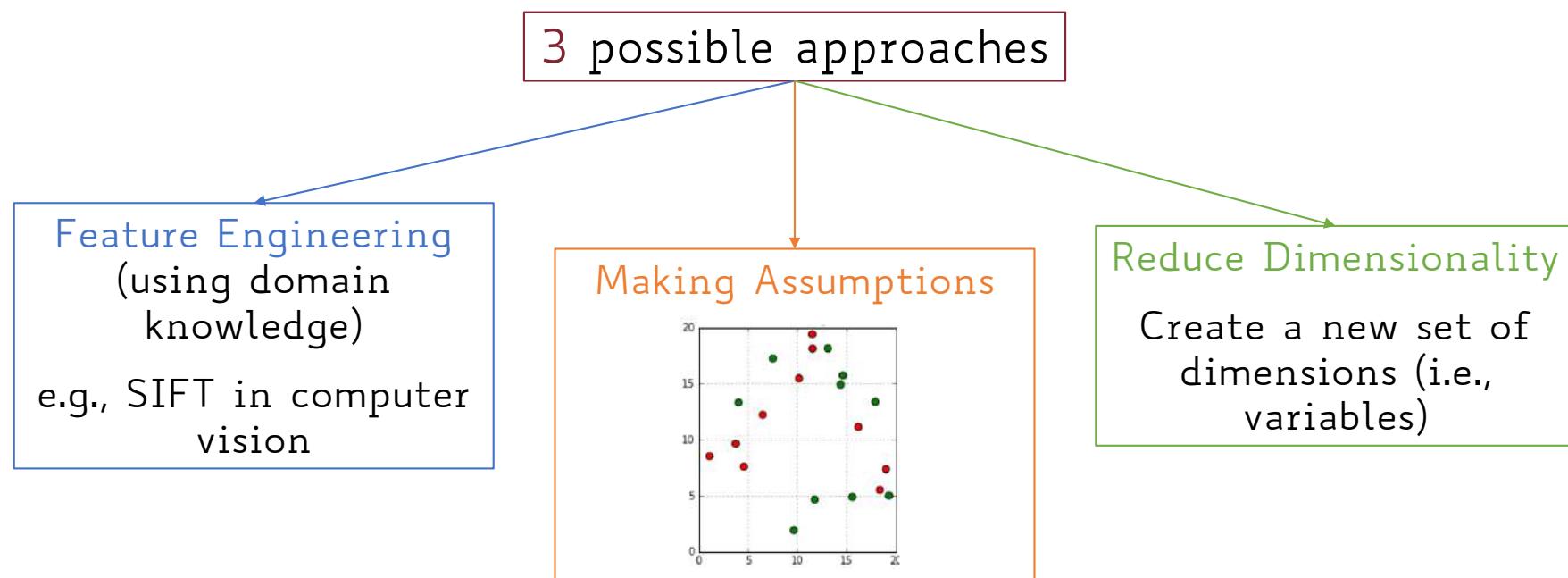
symmetry



Invariance to the order of
dimensions

21

Dealing with High Dimensionality



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)

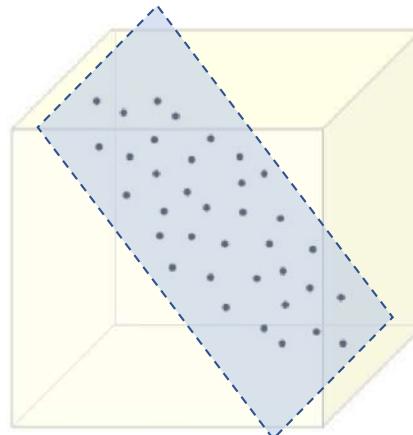
Dimensionality reduction technique based on feature extraction
High-dimensional data is in fact embedded into some lower dimensional space

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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:

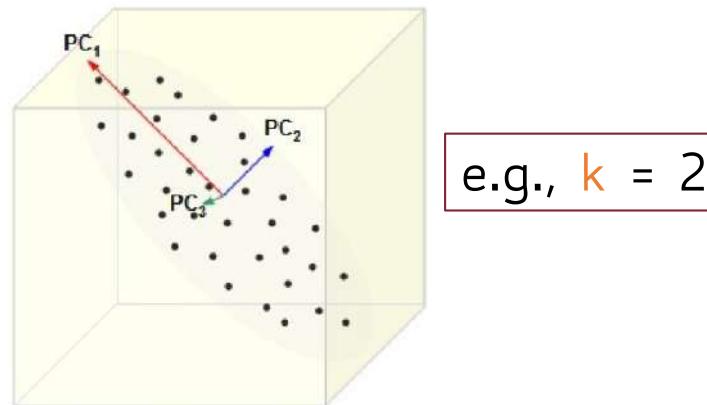
- 1st: direction of the greatest variance of data
- 2nd: perpendicular to 1st and greatest variance of what's left
- ... and so on until d

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The top $k < d$ components become the new dimensions



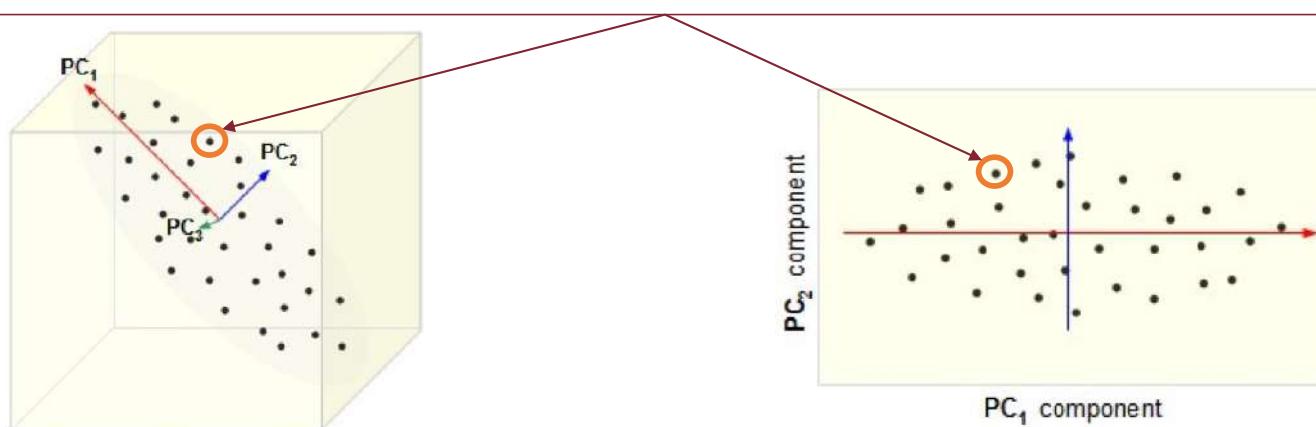
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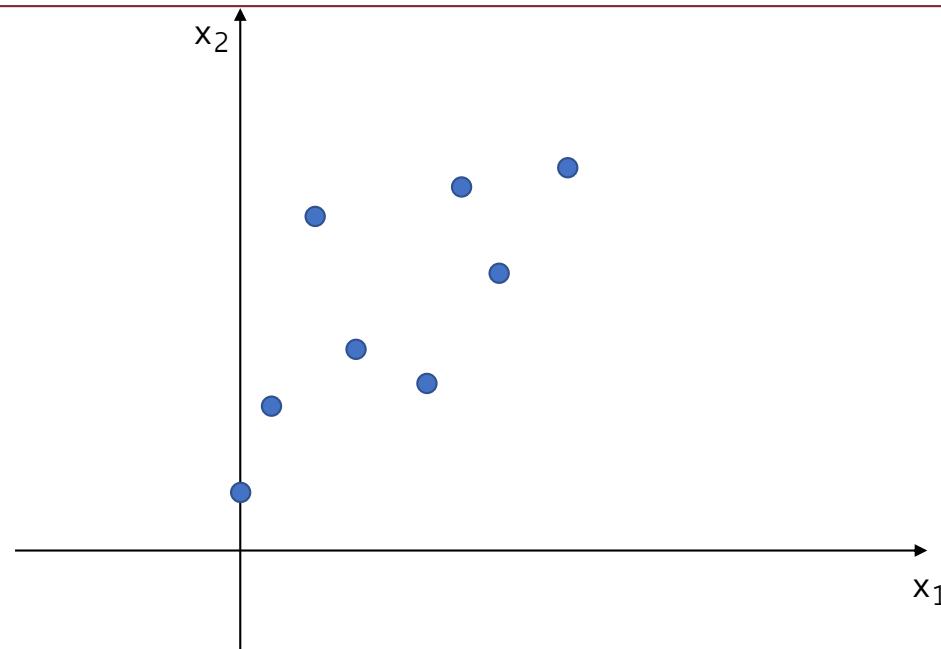
PC_1 and PC_2 are the top-2 principal components

Change the coordinates of every point according to the new dimensions



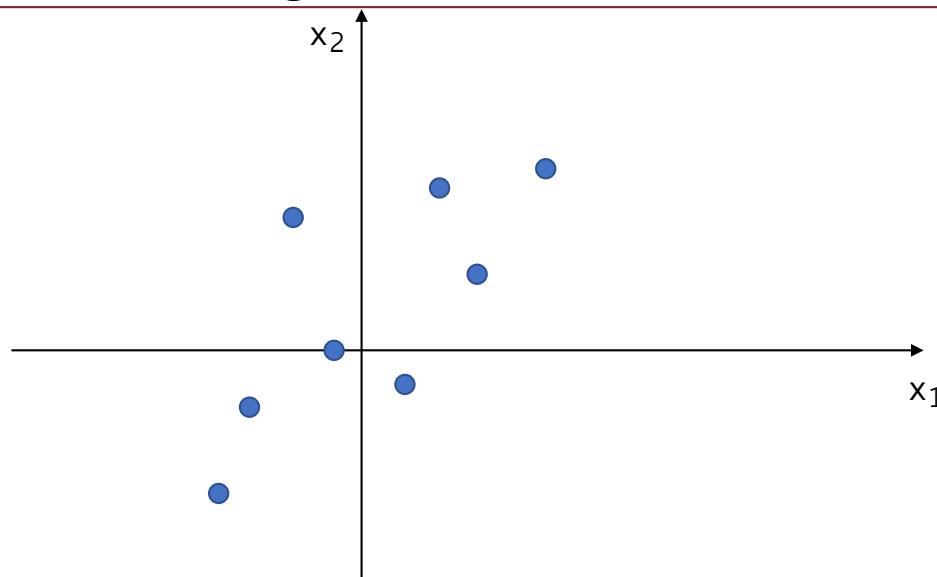
Why Do We Look for Greatest Variance?

Example: Reduce 2-dimensional data
to 1-d



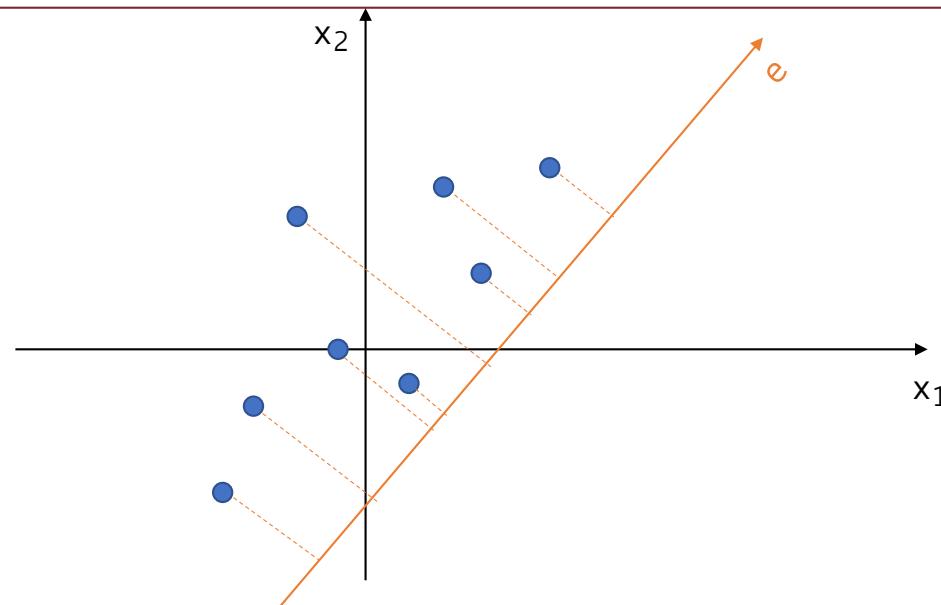
Why Do We Look for Greatest Variance?

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



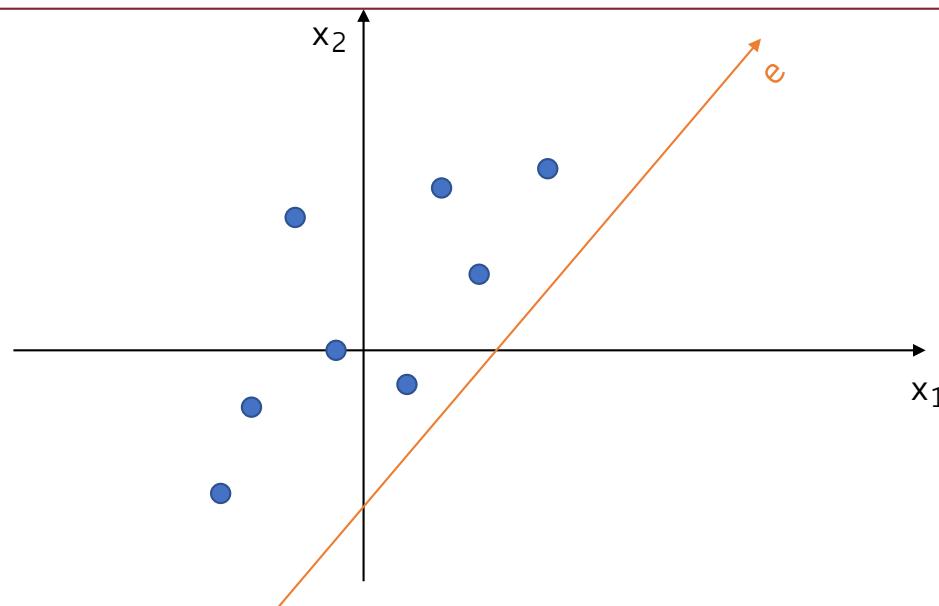
Why Do We Look for Greatest Variance?

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



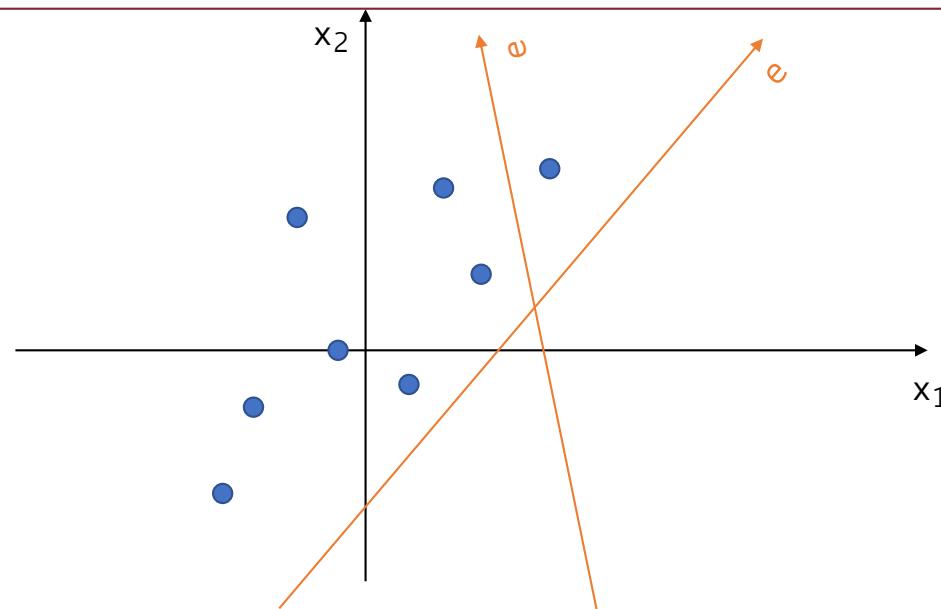
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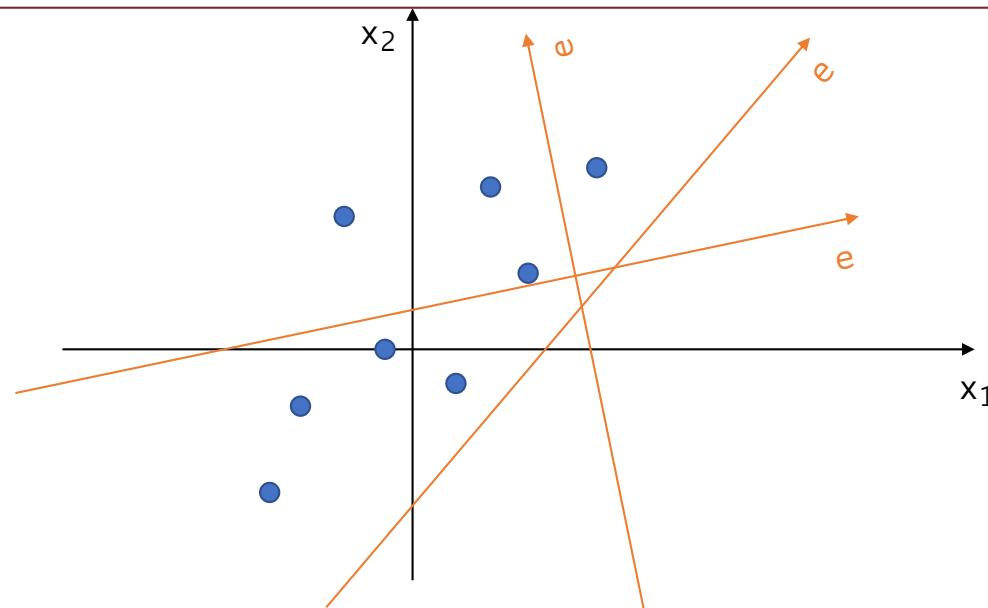
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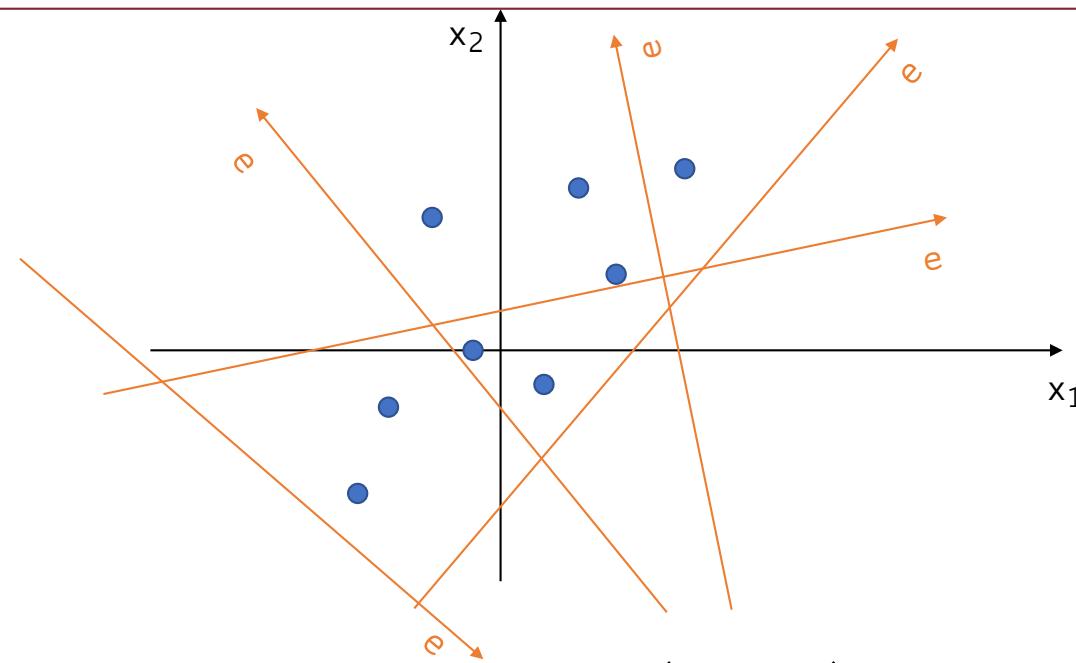
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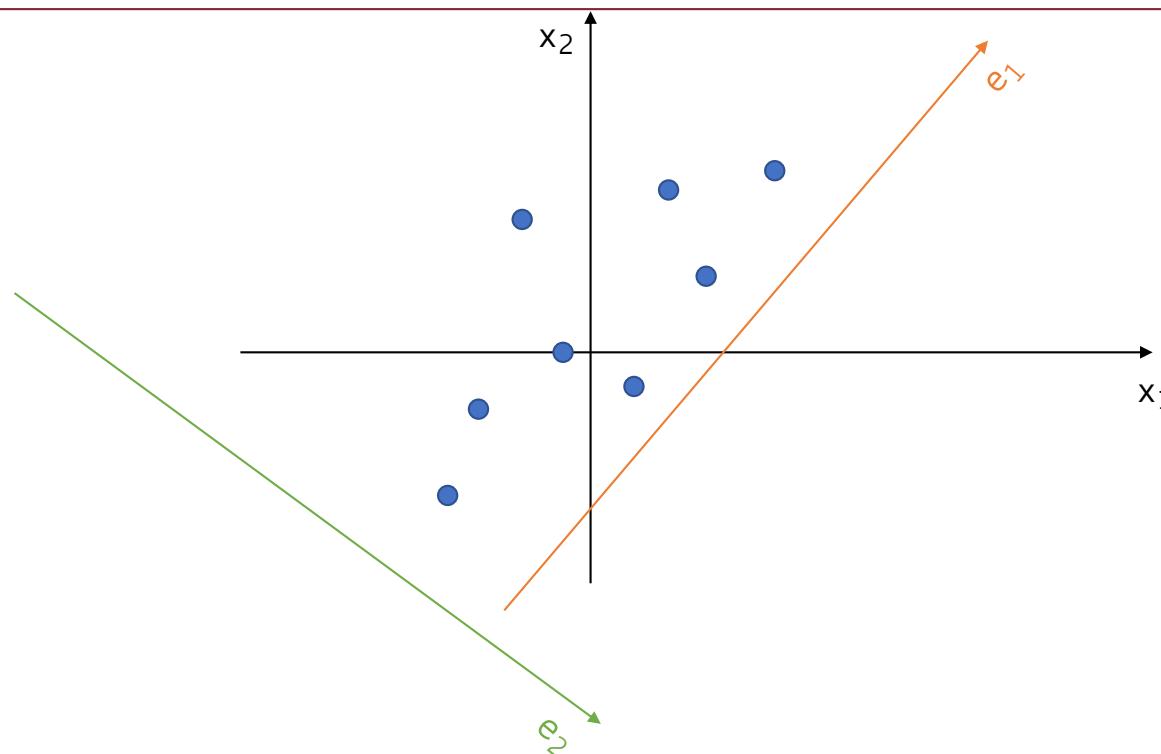
Map, i.e., project (x_1, x_2) to a new single dimension axis e



infinitely many mappings from (x_1, x_2) to a new axis e_{40}

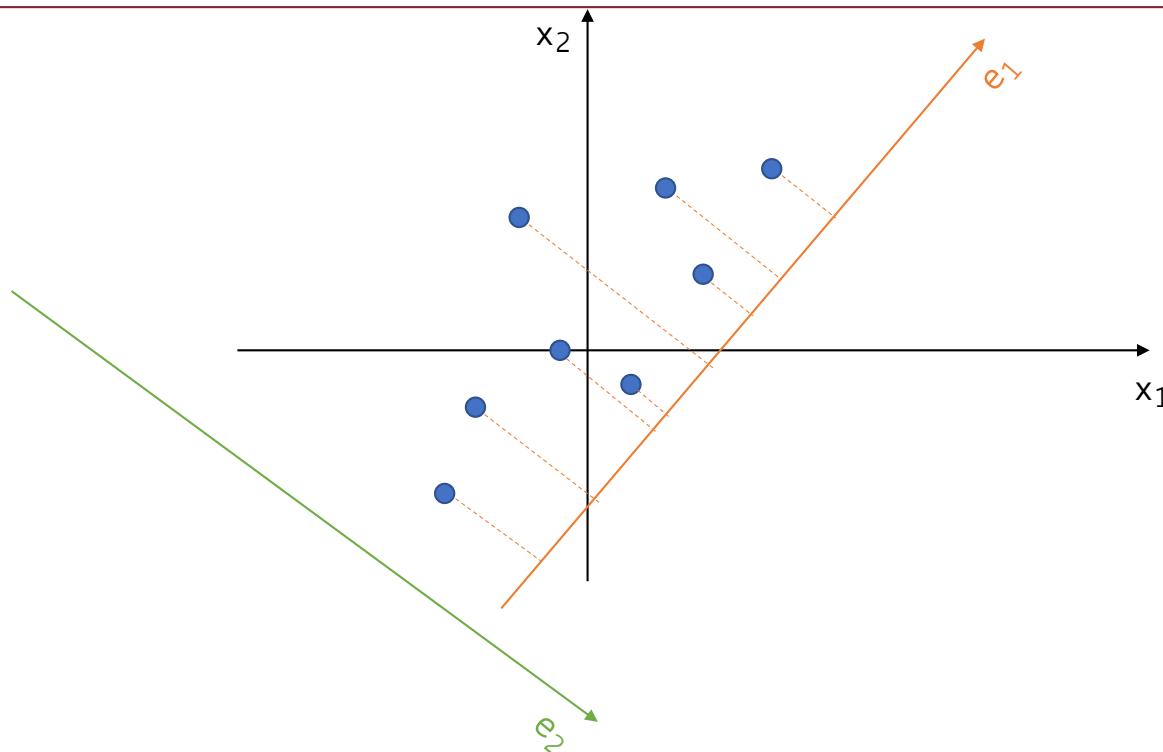
Why Do We Look for Greatest Variance?

Let's consider 2 different mappings e_1 and e_2



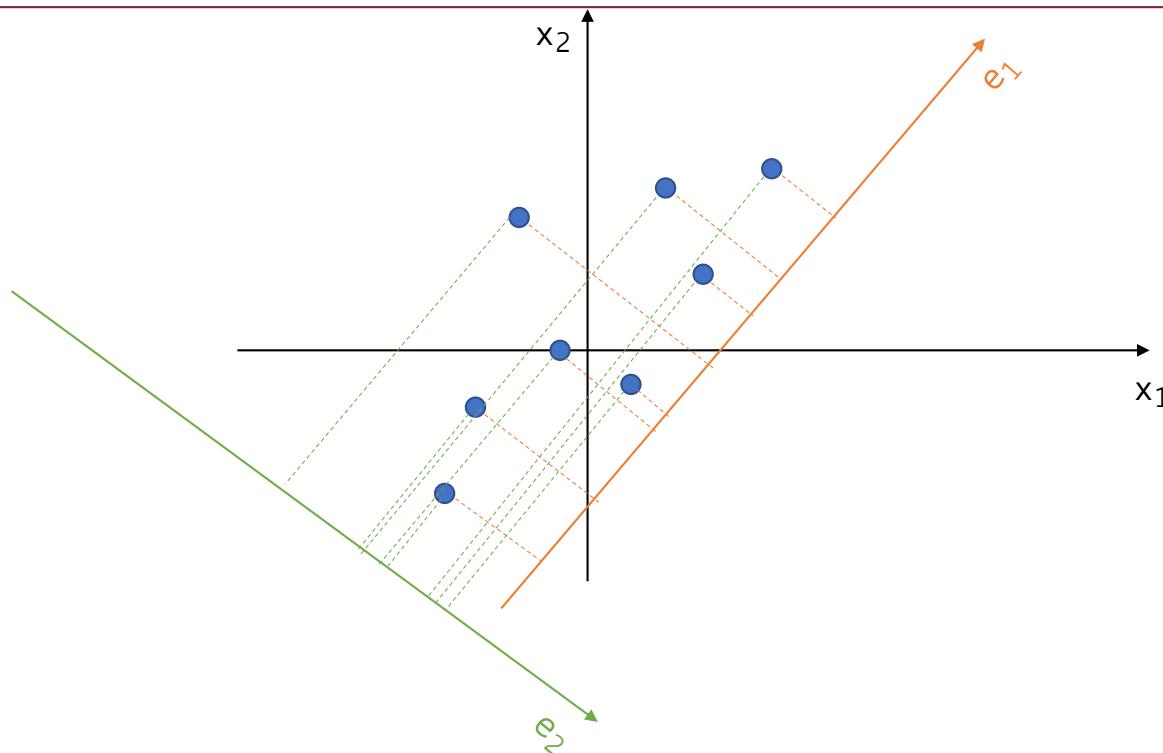
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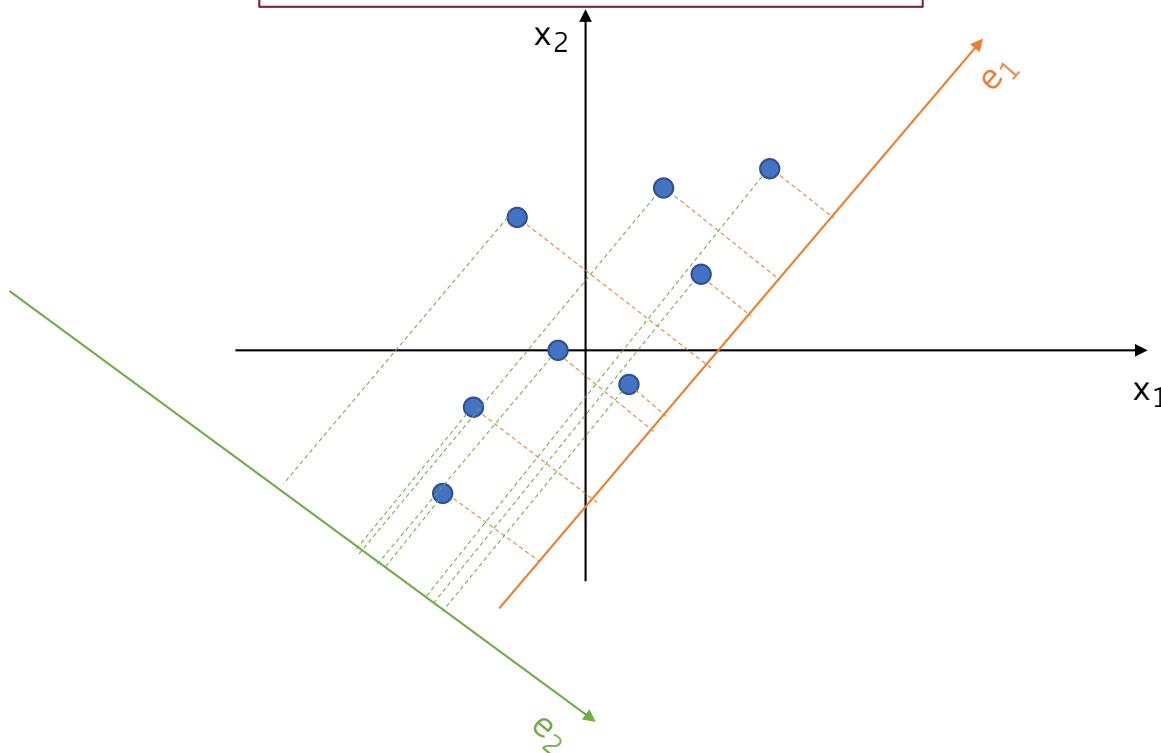
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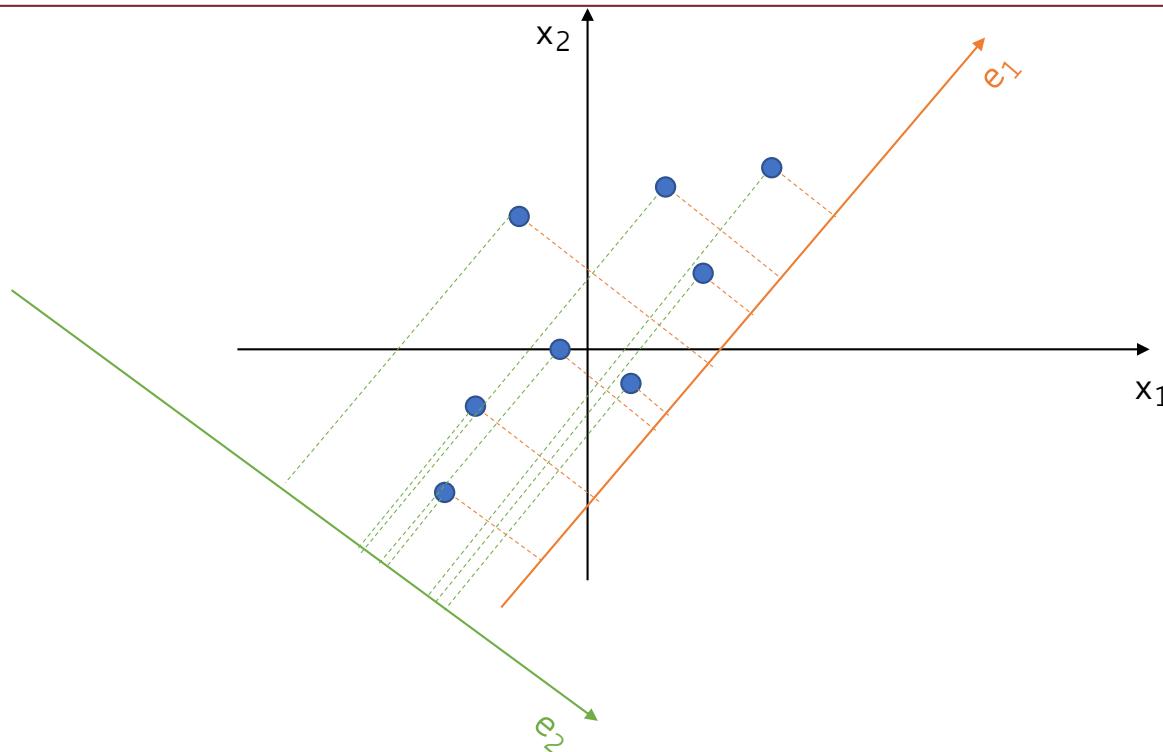
Why Do We Look for Greatest Variance?

Which one is better?



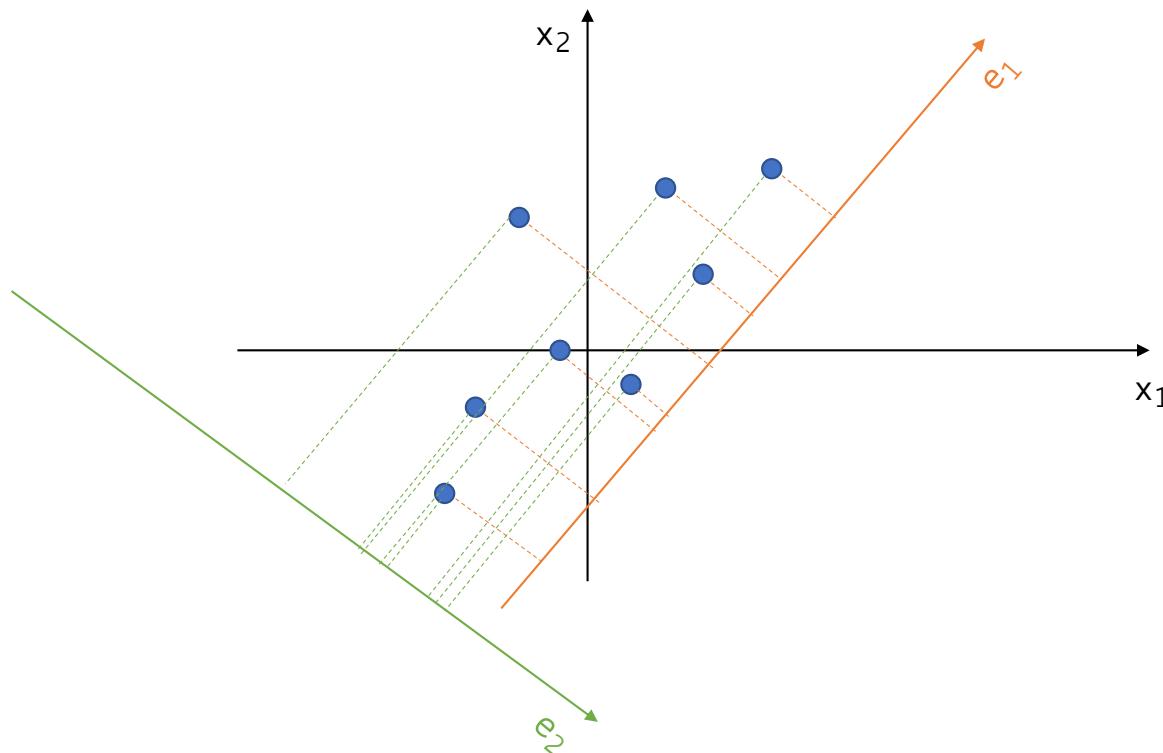
Why Do We Look for Greatest Variance?

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



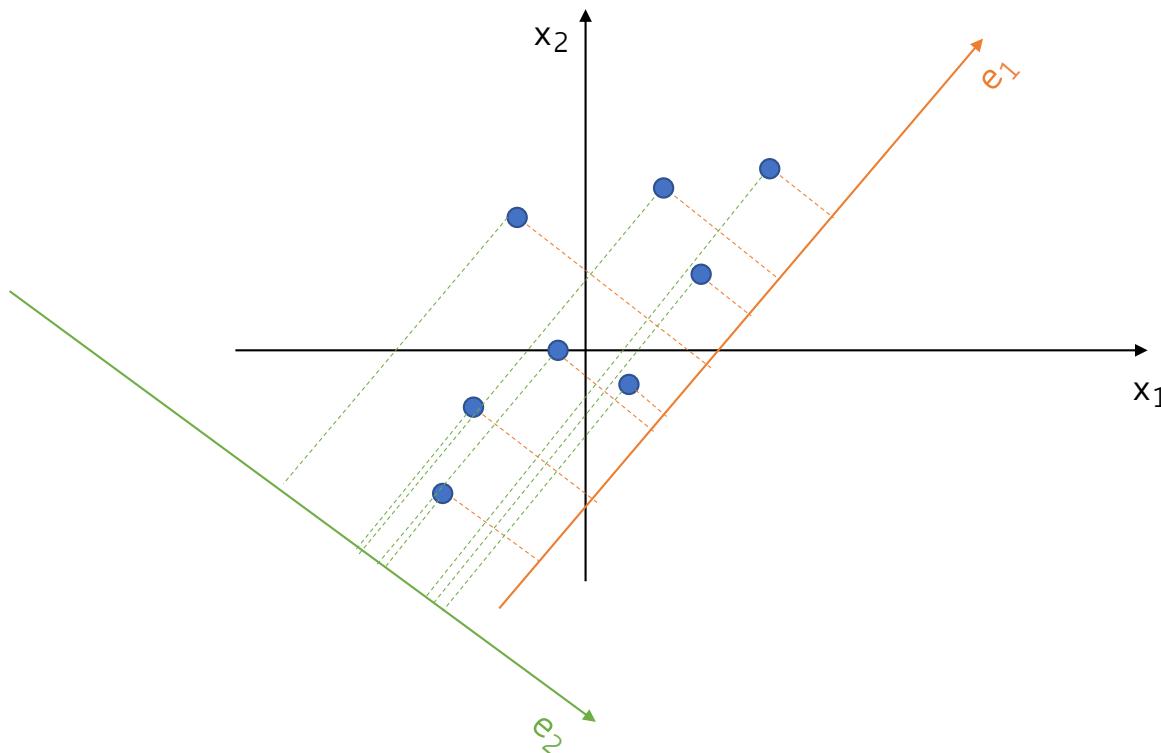
Why Do We Look for Greatest Variance?

The variance along e_1 is larger than along e_2



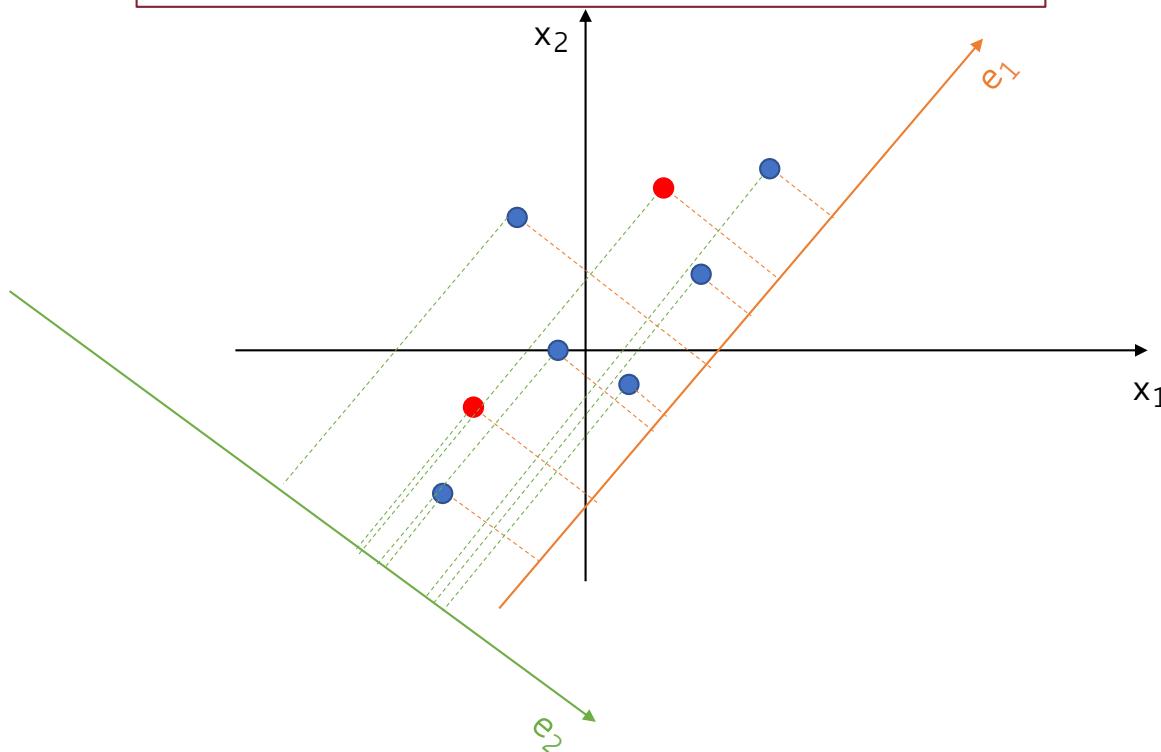
Why Do We Look for Greatest Variance?

Why is that good?



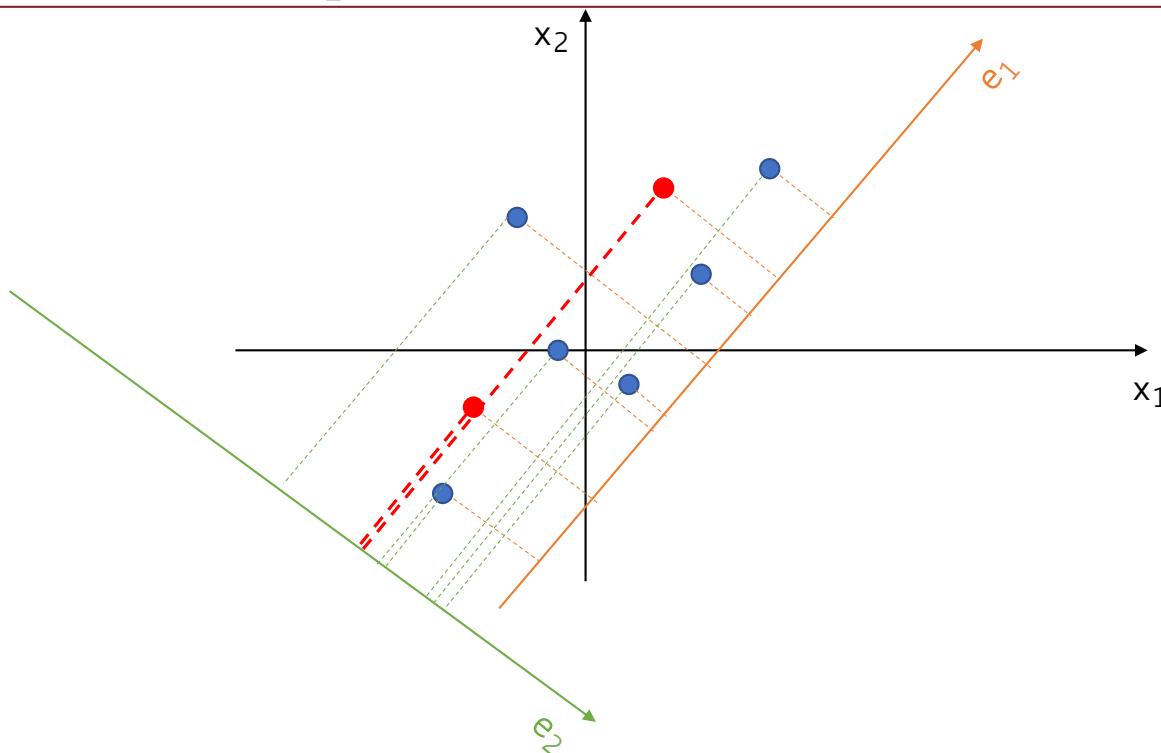
Why Do We Look for Greatest Variance?

Consider the 2 red points below



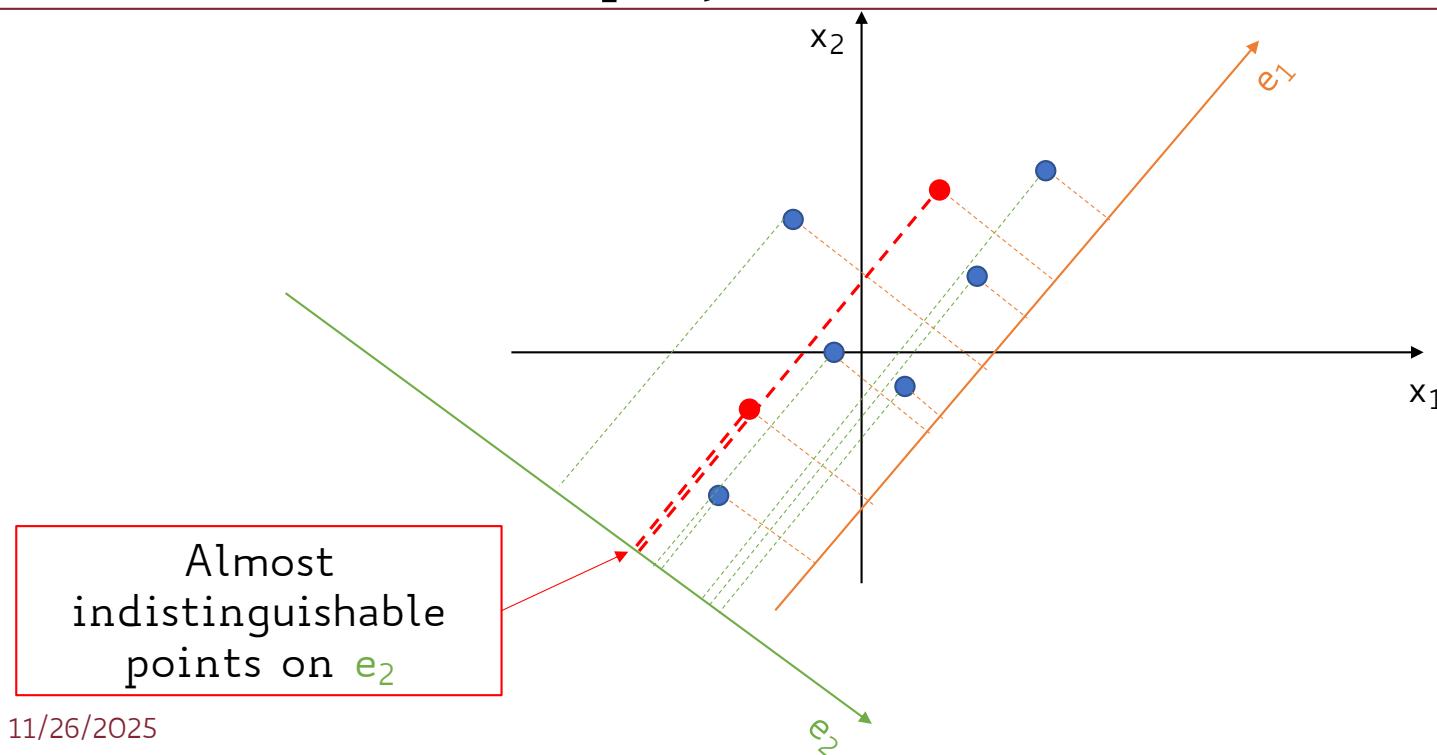
Why Do We Look for Greatest Variance?

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



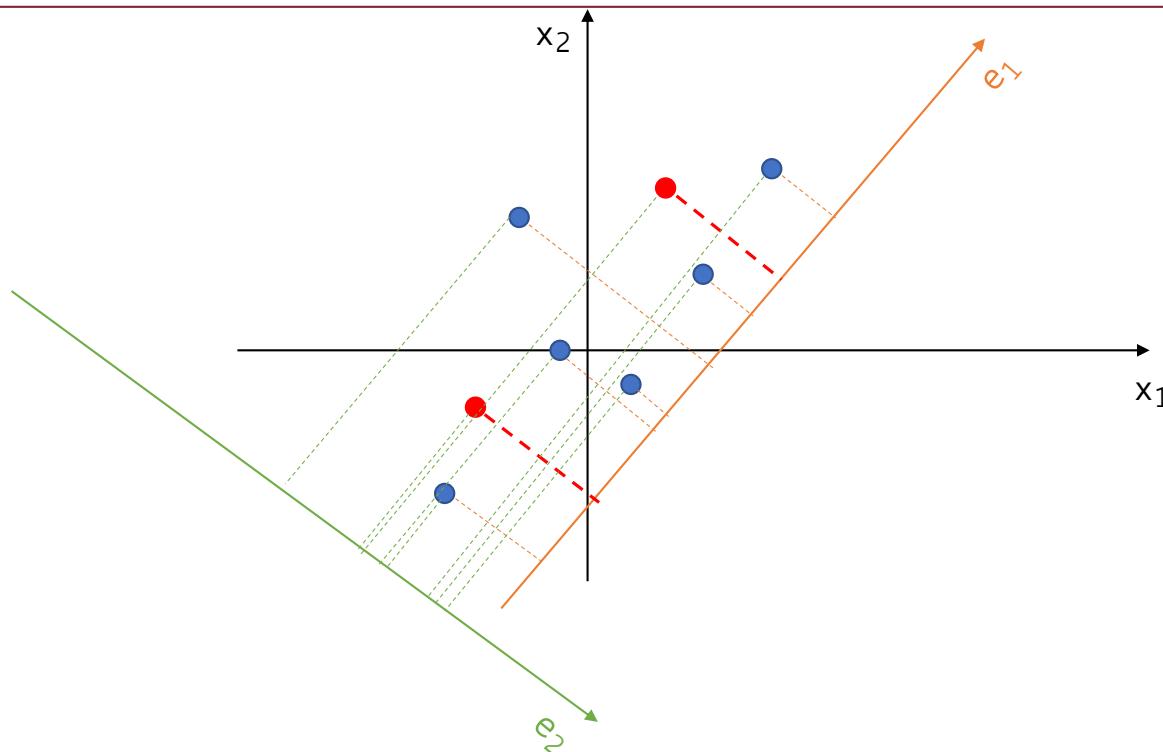
Why Do We Look for Greatest Variance?

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



Why Do We Look for Greatest Variance?

If projected onto e_1 they better preserve their distance



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- 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

- The variance of a random variable X measures how far a set of (random) numbers are spread out from their mean value

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

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

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

Covariance Matrix

- Given a random vector $X = (X_1, \dots, X_d)$ 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 $X = (X_1, \dots, X_d)$ 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 $X = (X_1, \dots, X_d)$

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- The original set of dimensions is a random vector $X = (X_1, \dots, X_d)$
- In our example, $d = 2$ and $X = (X_1, X_2)$
- 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

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

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

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

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

Covariance Matrix of Original Dimensions

Let us rewrite each data point \mathbf{x}_i as follows:

$$\mathbf{x}_i = (x'_{i,1}, x'_{i,2}) \text{ where:}$$

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Covariance Matrix of Original Dimensions

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

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

Covariance Matrix of Original Dimensions

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

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

O-mean

Covariance Matrix of Original Dimensions

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

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

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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

$$\begin{matrix} & \begin{matrix} x_1 & x_2 \end{matrix} \\ \begin{matrix} x_1 \\ x_2 \end{matrix} & \begin{bmatrix} 2 & 4/5 \\ 4/5 & 3/5 \end{bmatrix} \end{matrix}$$

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Covariance Matrix of Original Dimensions

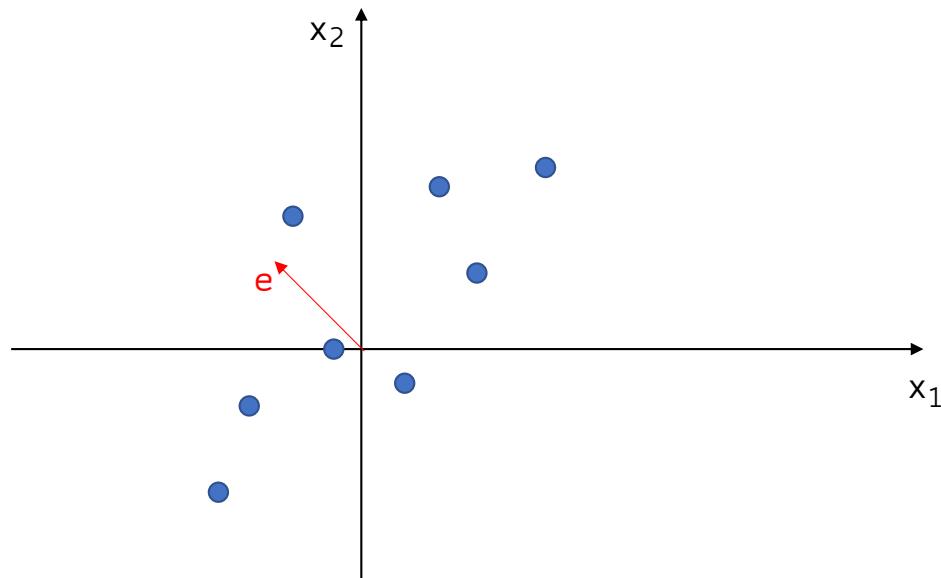
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$$\text{Cov}(X_2, X_2) = \text{Var}(X_2) = \frac{1}{n} \sum_{i=1}^n (x'_{i,2})^2$$

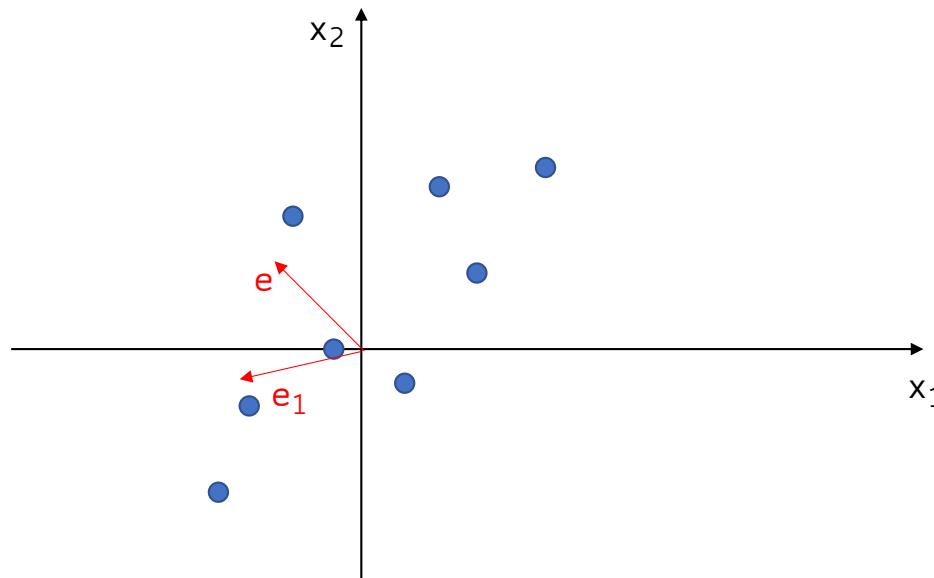
Covariance Matrix of Original Dimensions



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

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

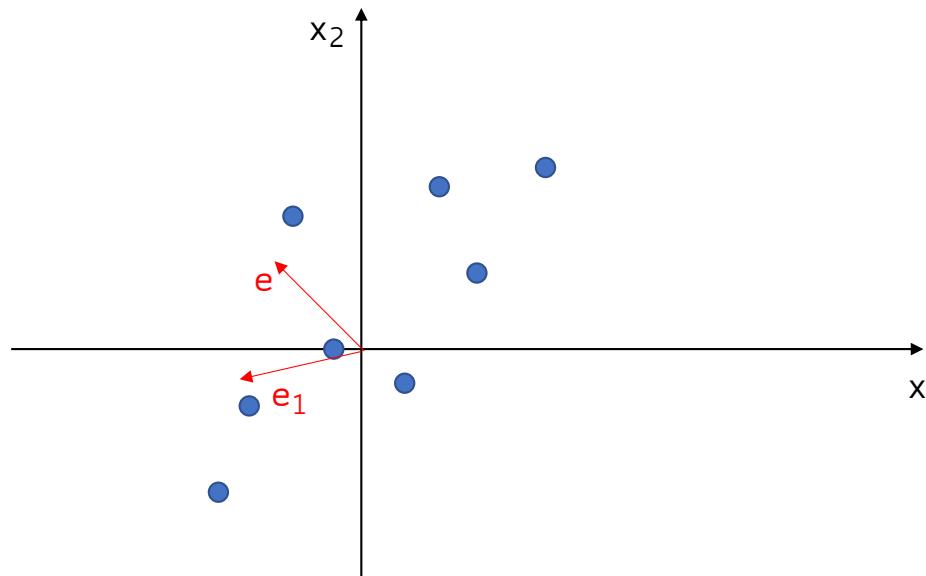
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Covariance Matrix of Original Dimensions

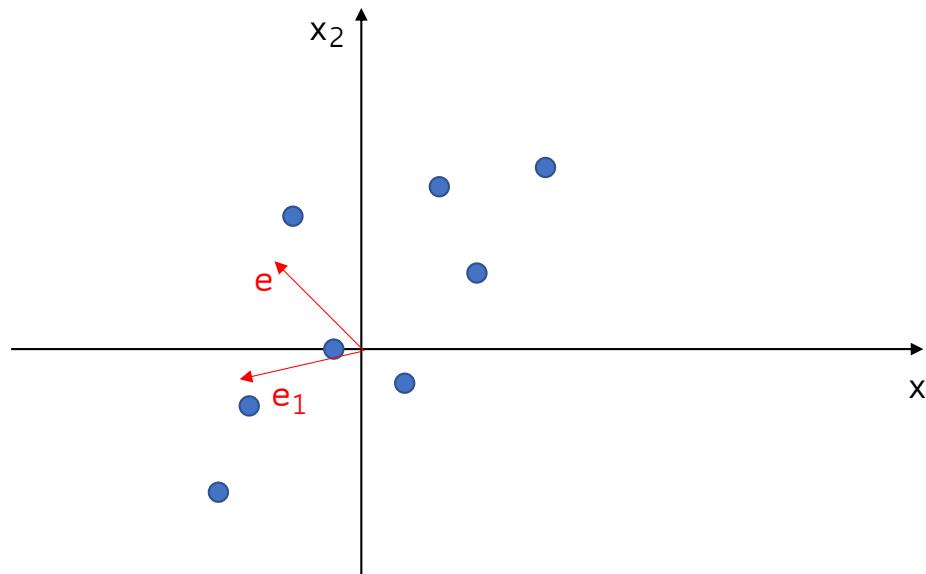


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$\boxed{\text{slope} = 1/-1 = -1}$

Covariance Matrix of Original Dimensions



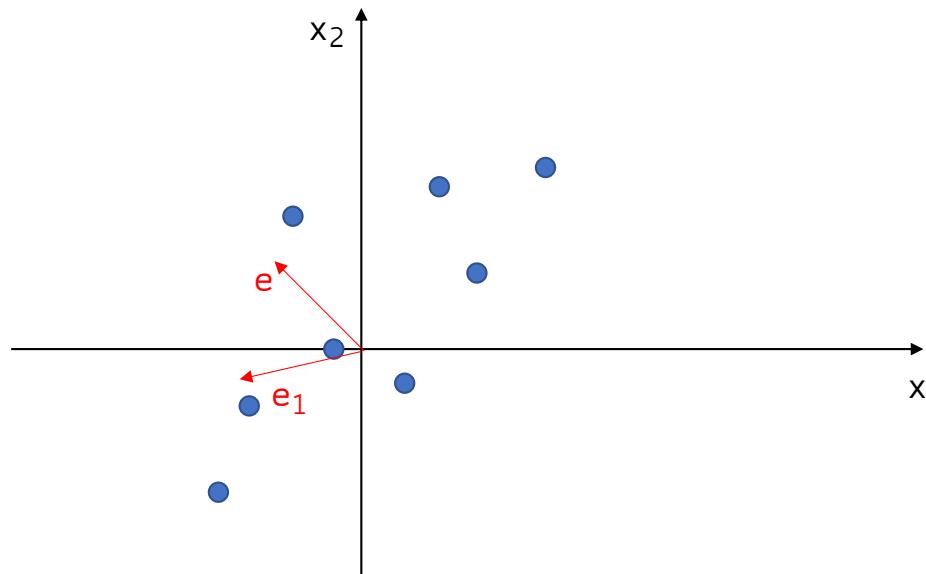
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Covariance Matrix of Original Dimensions



Turns towards the direction of the greatest variance

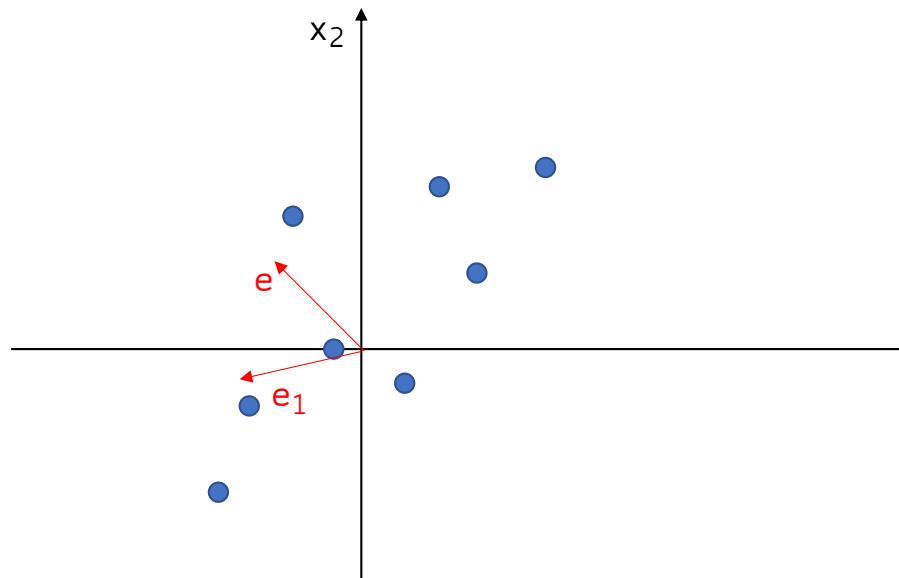
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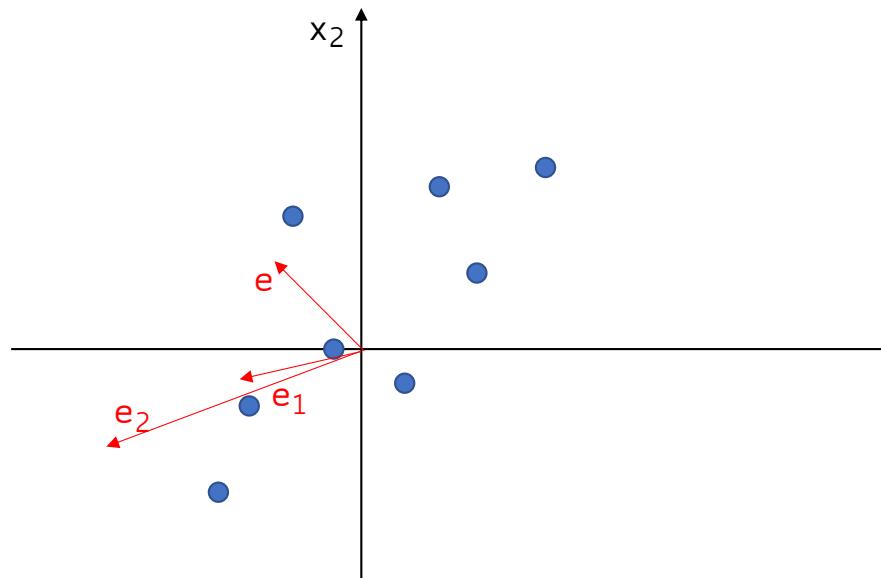
Covariance Matrix of Original Dimensions



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

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

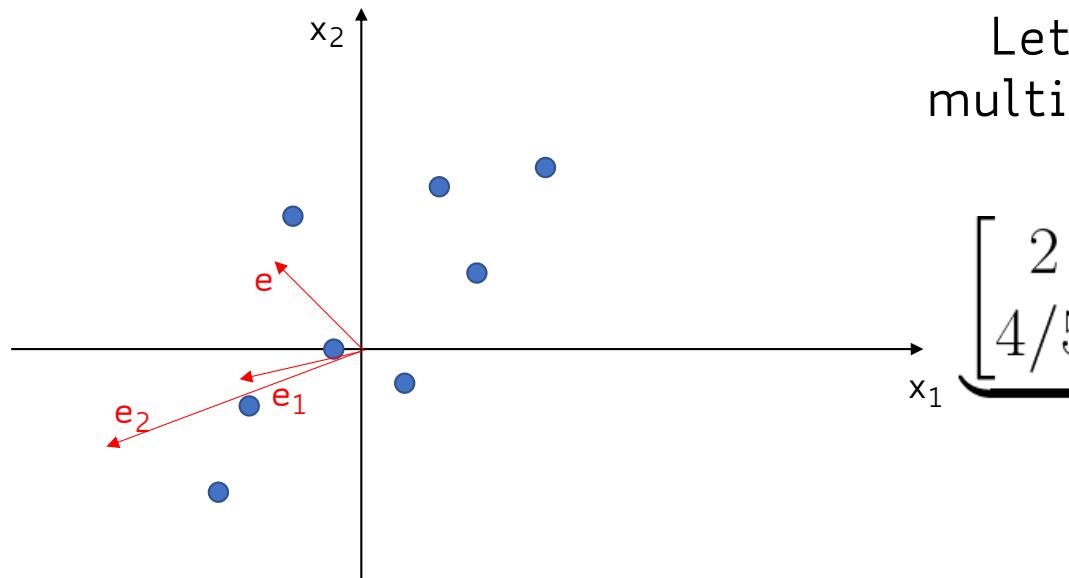
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Covariance Matrix of Original Dimensions



Turns towards the direction of the greatest variance

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

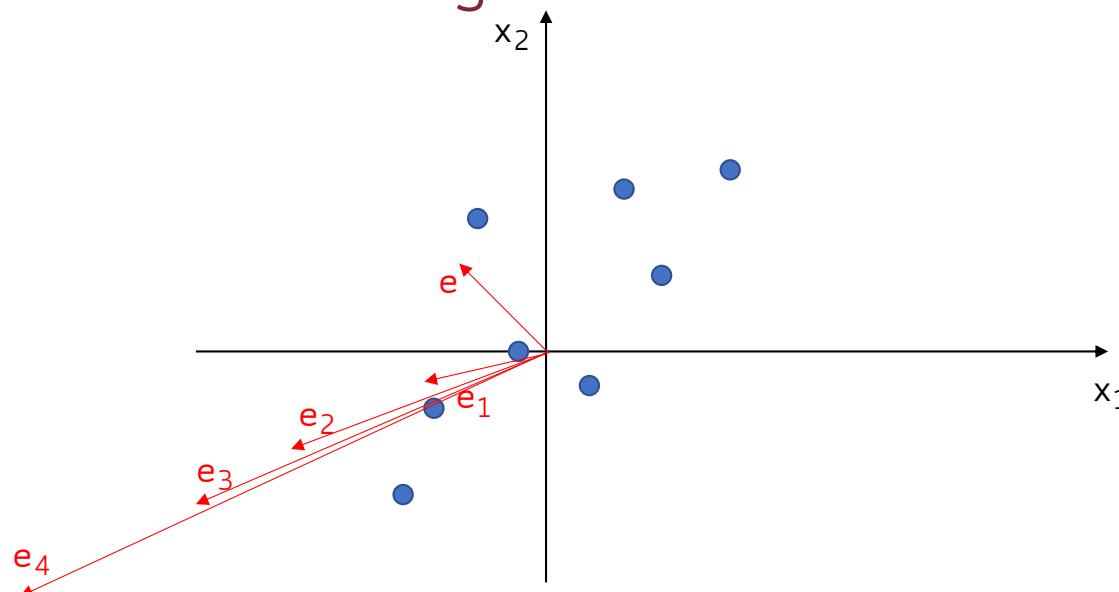
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slope = $1/6$

new slope = $27/64$

Covariance Matrix of Original Dimensions

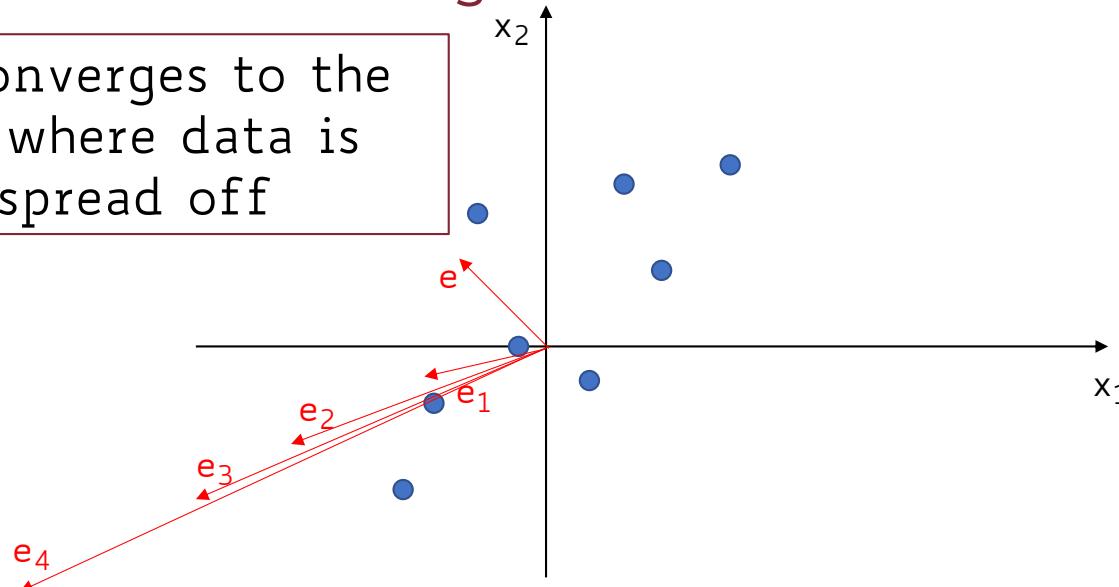
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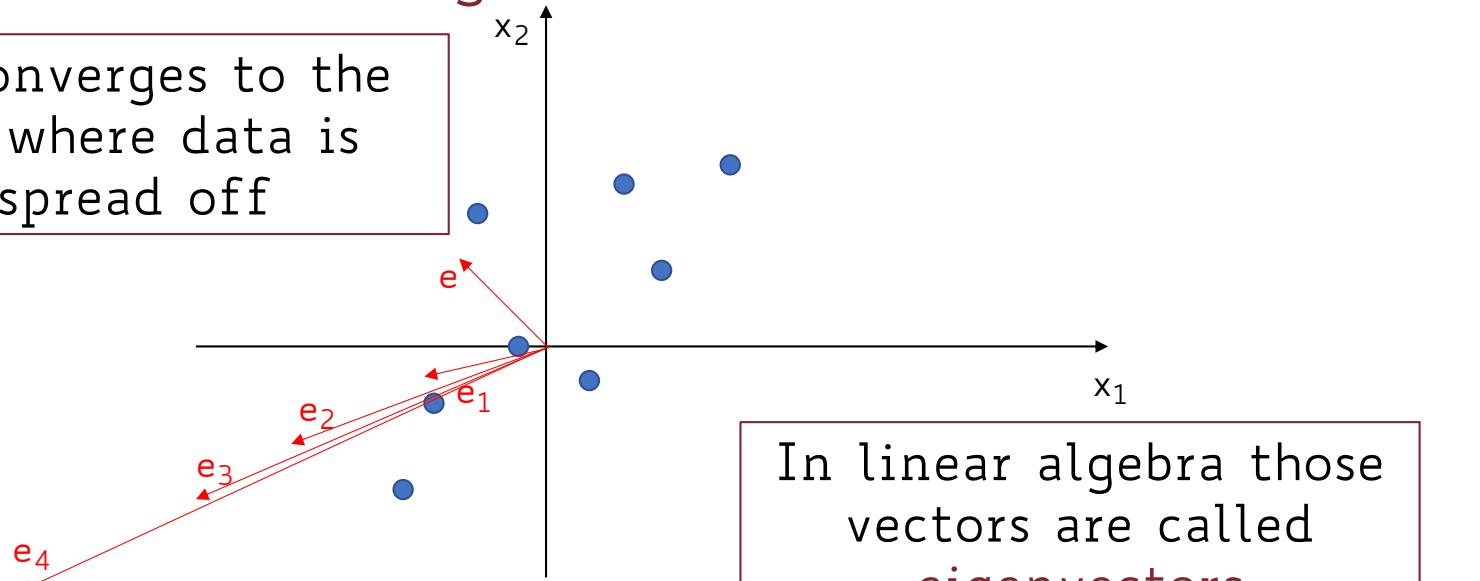
The slope converges to the dimension where data is mostly spread off



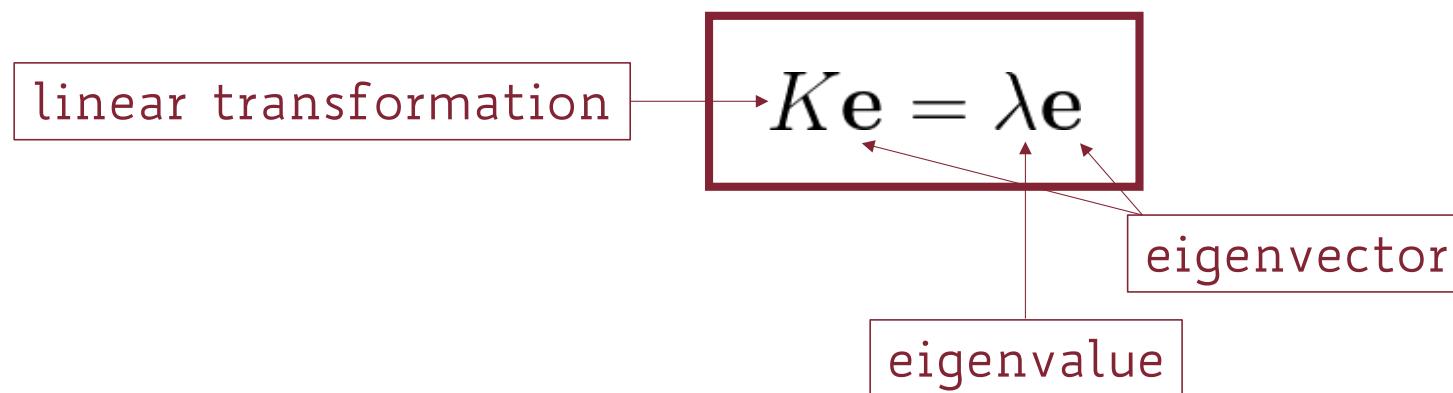
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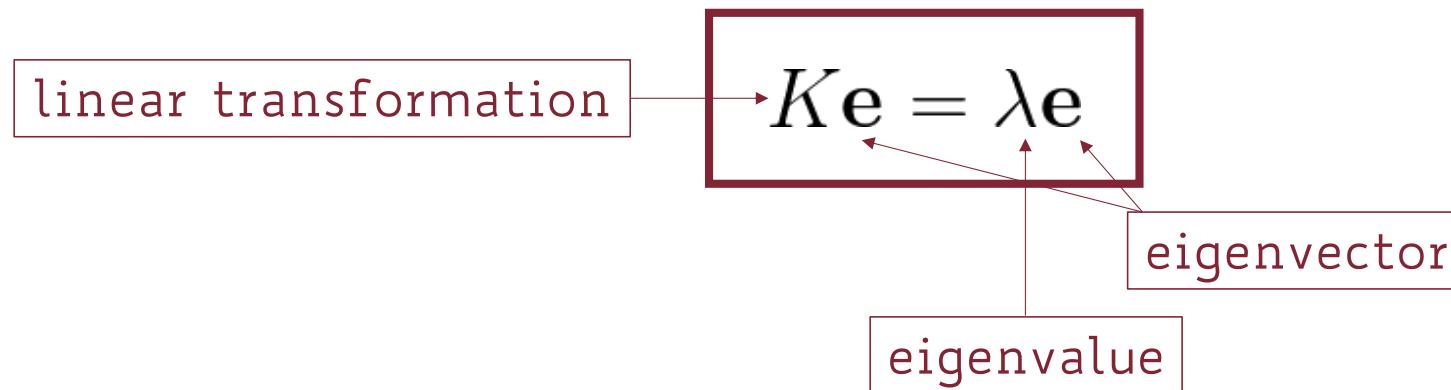
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Eigenvectors of the Covariance Matrix

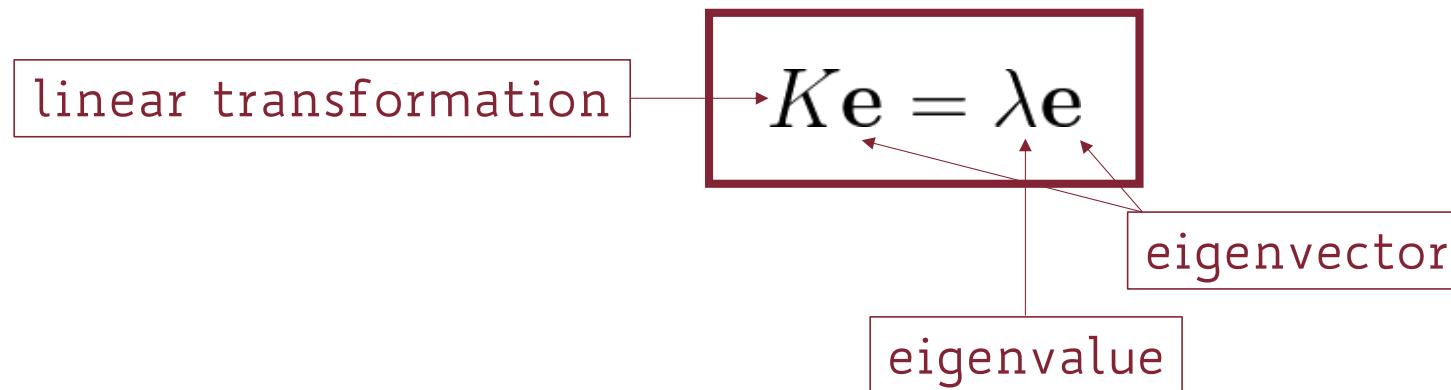


Eigenvectors of the Covariance Matrix



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 λ (**eigenvalue**)

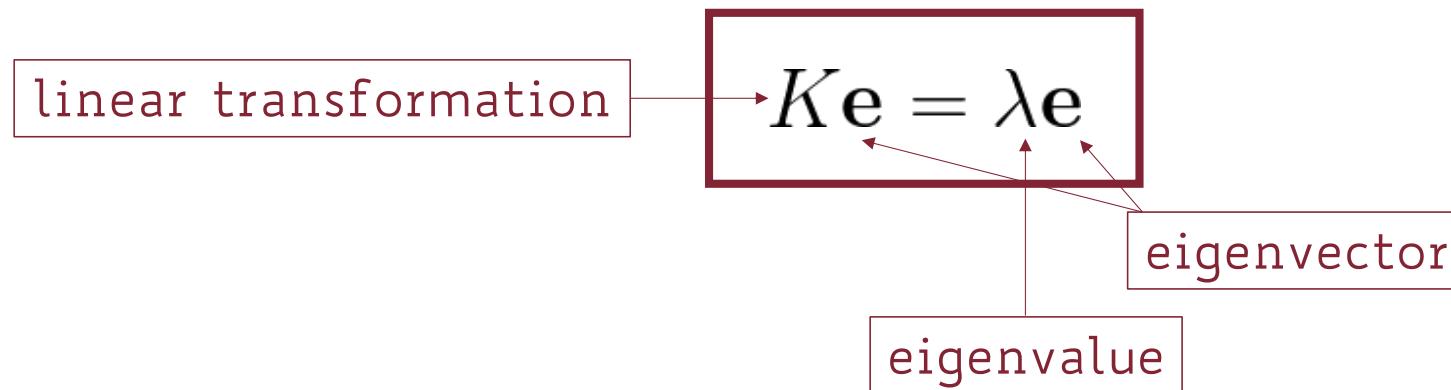
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In other words, eigenvectors encapsulate all the relevant information to describe a linear transformation (in our case, represented by the covariance matrix K)

Eigenvectors of the Covariance Matrix



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 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:

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

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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

How Do We Compute Eigenvectors?

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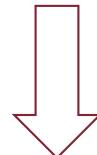
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The corresponding homogeneous system will have a **non-trivial** solution

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

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

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 characteristic equation of K

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

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?

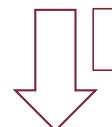
Let's see what happens for λ_1

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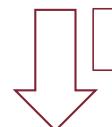
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$$\begin{cases} 2e_{1,1} + 0.8e_{1,2} = 2.36e_{1,1} \\ 0.8e_{1,1} + 0.6e_{1,2} = 2.36e_{1,2} \end{cases}$$

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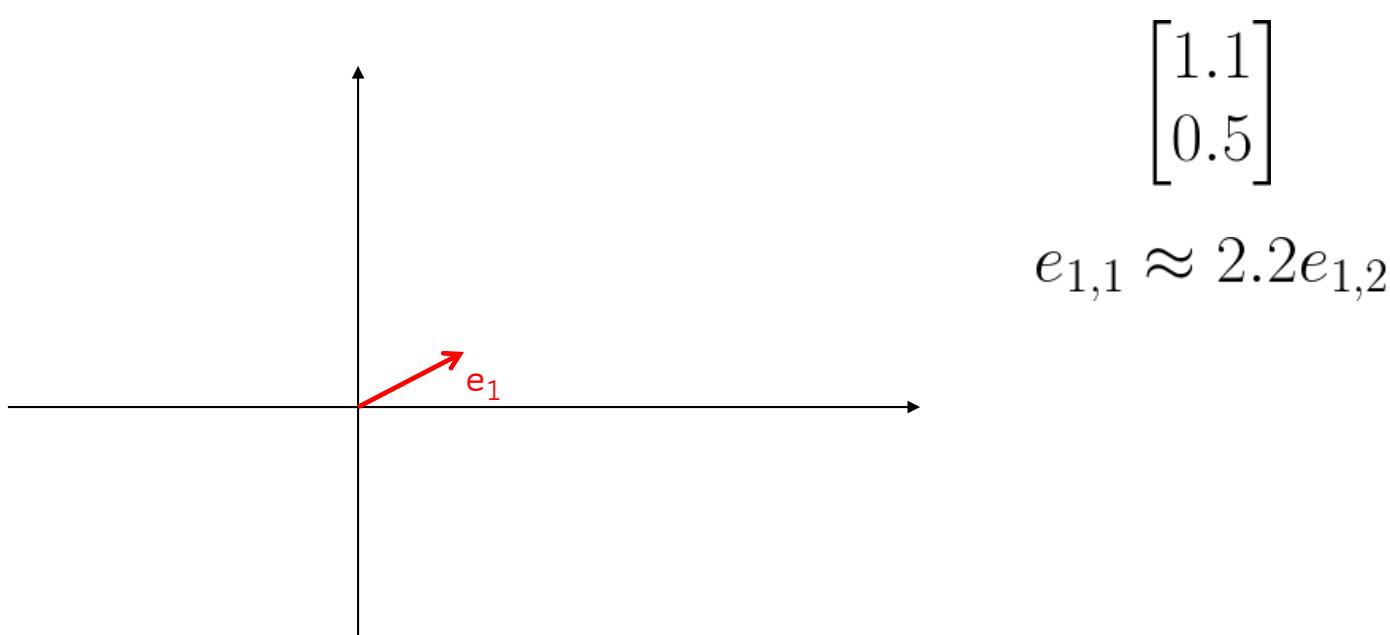
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$$e_{1,1} \approx 2.2e_{1,2}$$

The system has infinitely many solutions

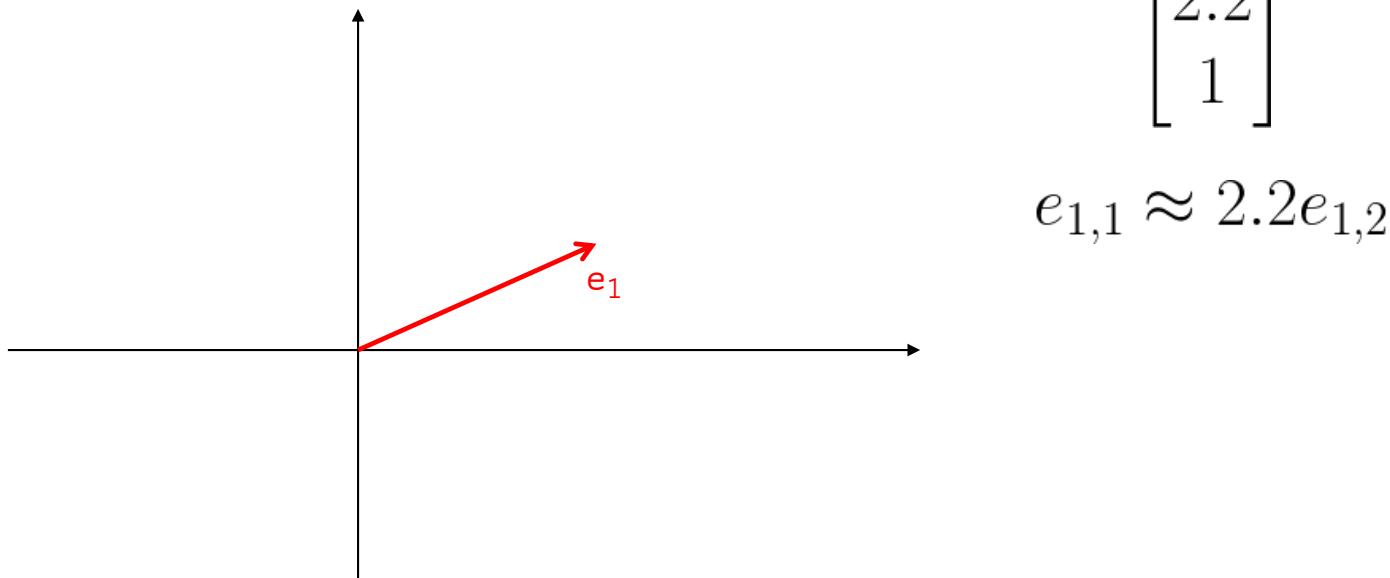
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Any vector which satisfies the relationship above works!



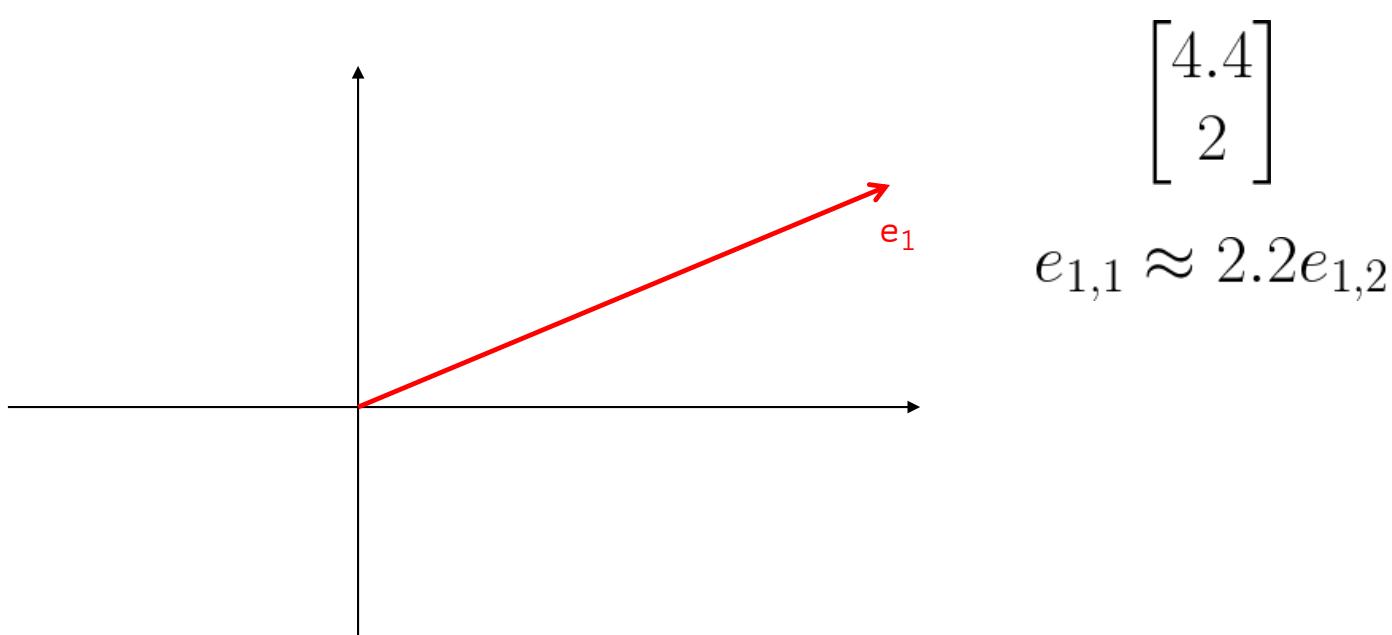
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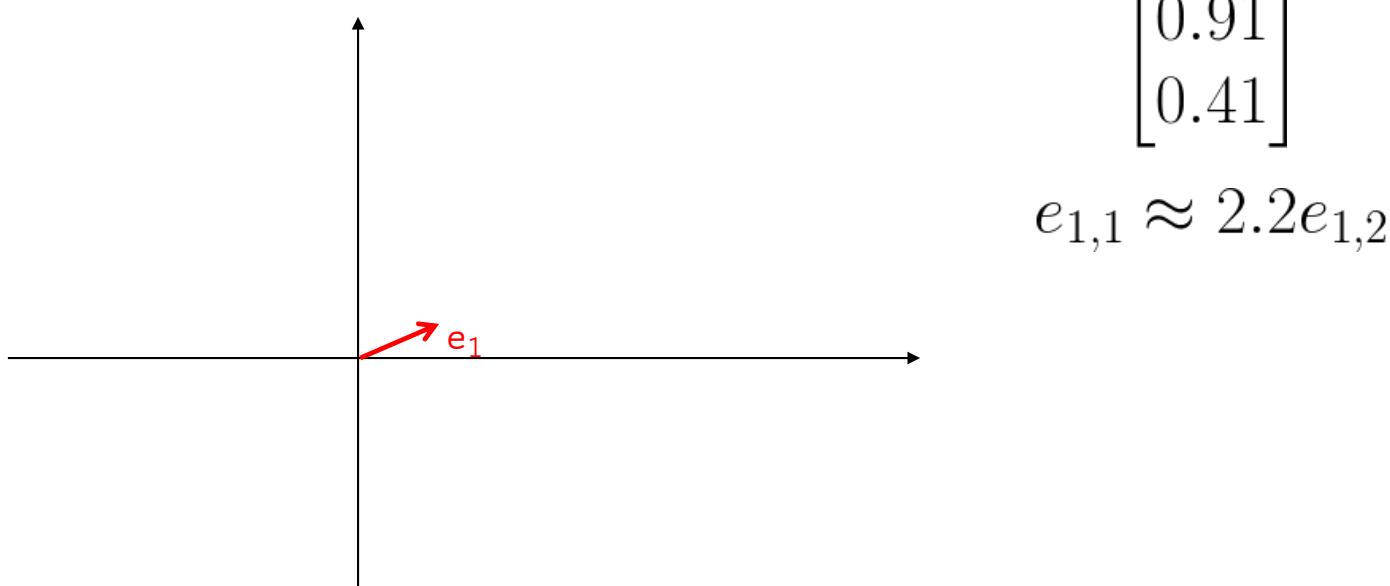
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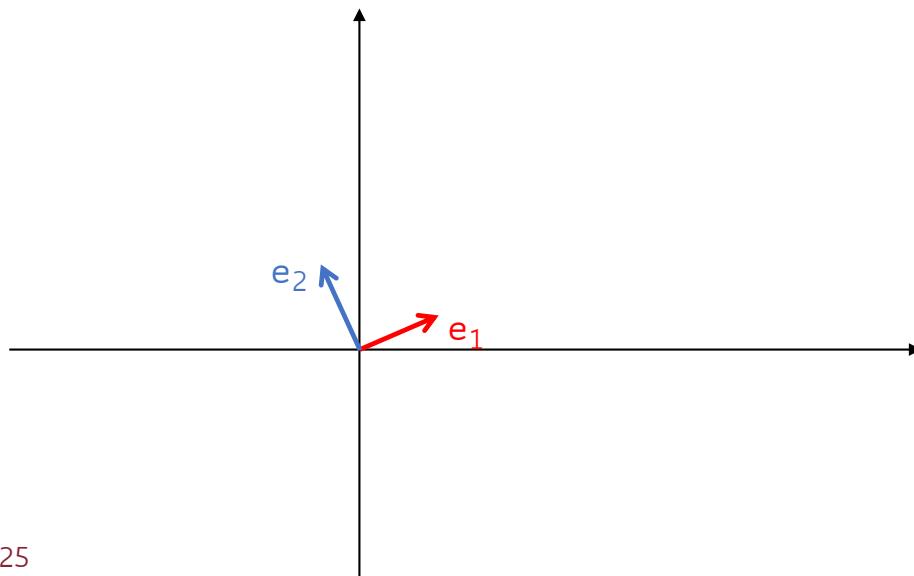
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By convention, we restrict to $\|\mathbf{e}_1\| = 1$



How Do We Compute Eigenvectors?

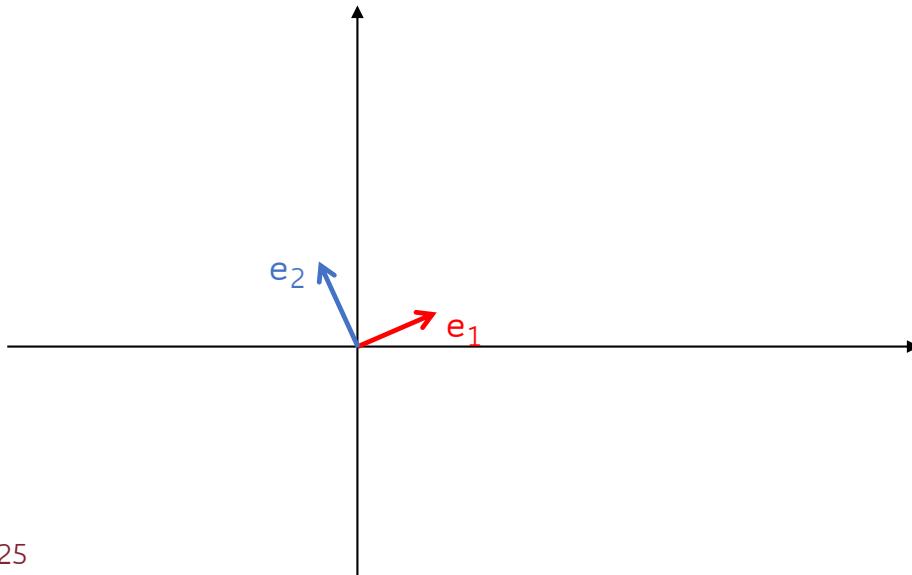
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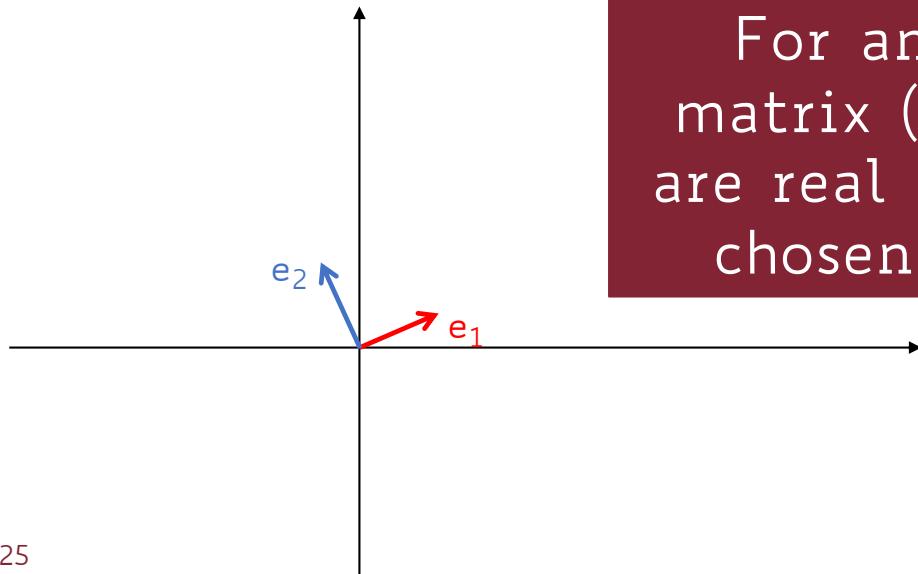
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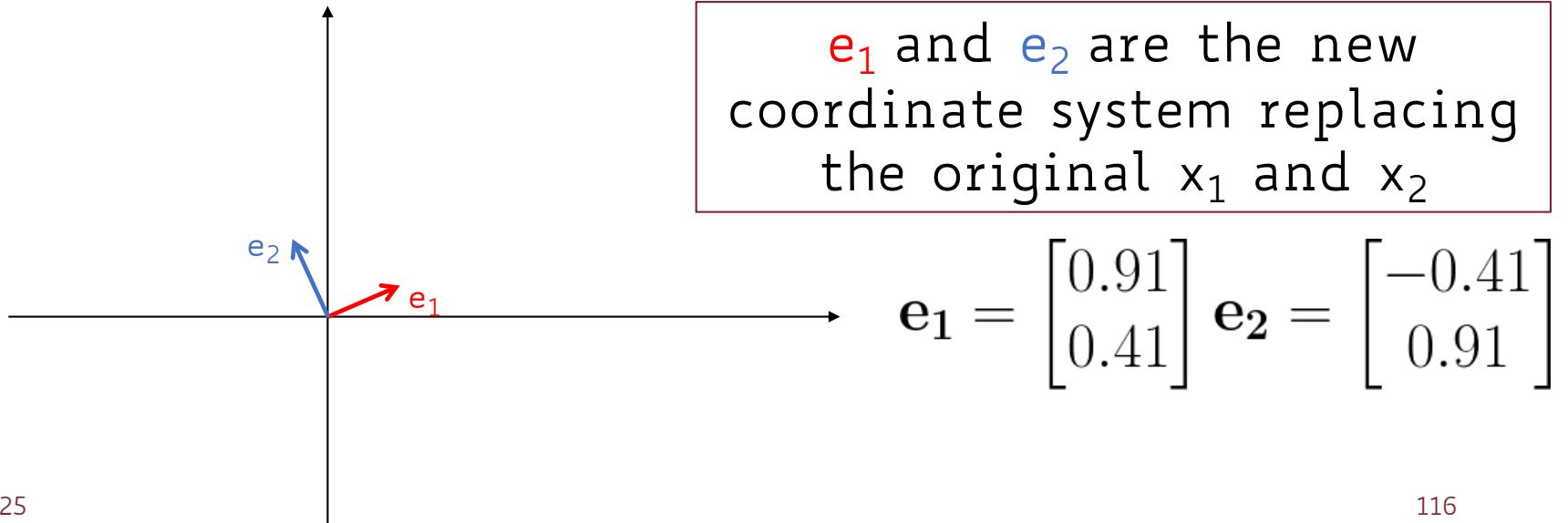


For any $d \times d$ real symmetric matrix (like K), the eigenvalues are real and eigenvectors can be chosen real and orthonormal

How Do We Compute Eigenvectors?

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

This is just orthogonal to the previously found e_1



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

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

Projecting to New Dimensions: 2-d Case

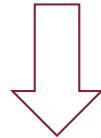
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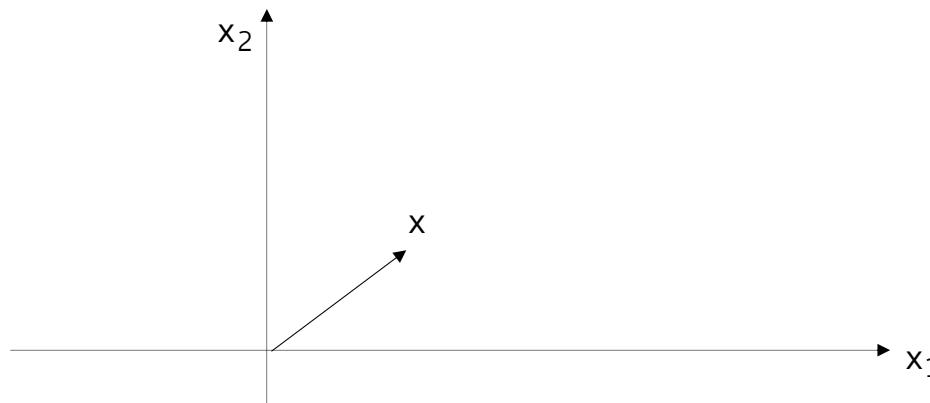
Goal

We want to represent x in the new (e_1, e_2) -coordinate system

Projecting to New Dimensions: 2-d Case

1. Center x around the mean of each dimension

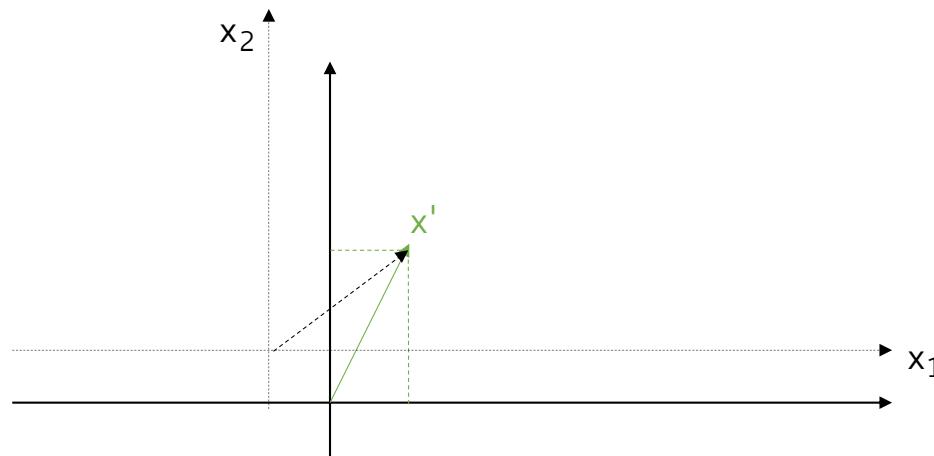
$$\mathbf{x}' = \mathbf{x} - \boldsymbol{\mu} = (x_1 - \mu_1, x_2 - \mu_2)$$



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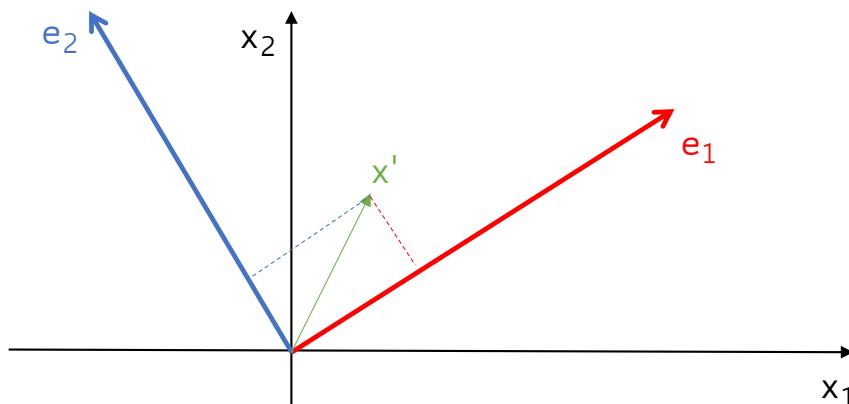
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Projecting to New Dimensions: 2-d Case

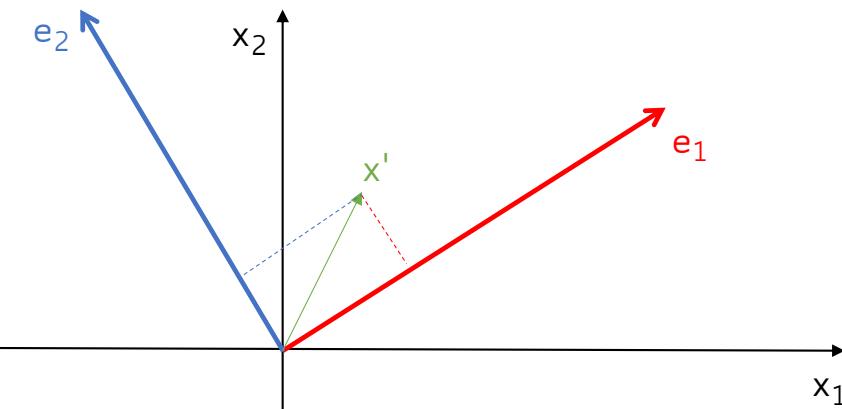
2. Project \mathbf{x}' on each dimension \mathbf{e}_1 and \mathbf{e}_2

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



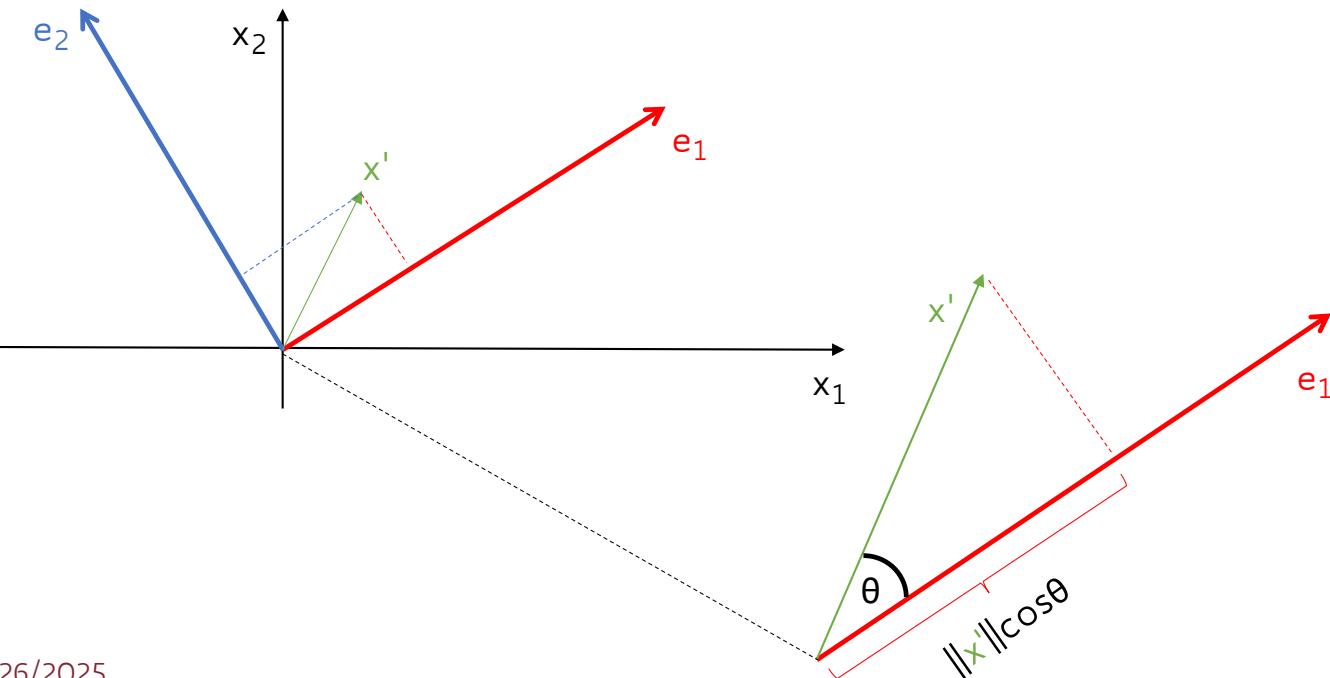
Projecting to New Dimensions: 2-d Case

Why the dot product?



Projecting to New Dimensions: 2-d Case

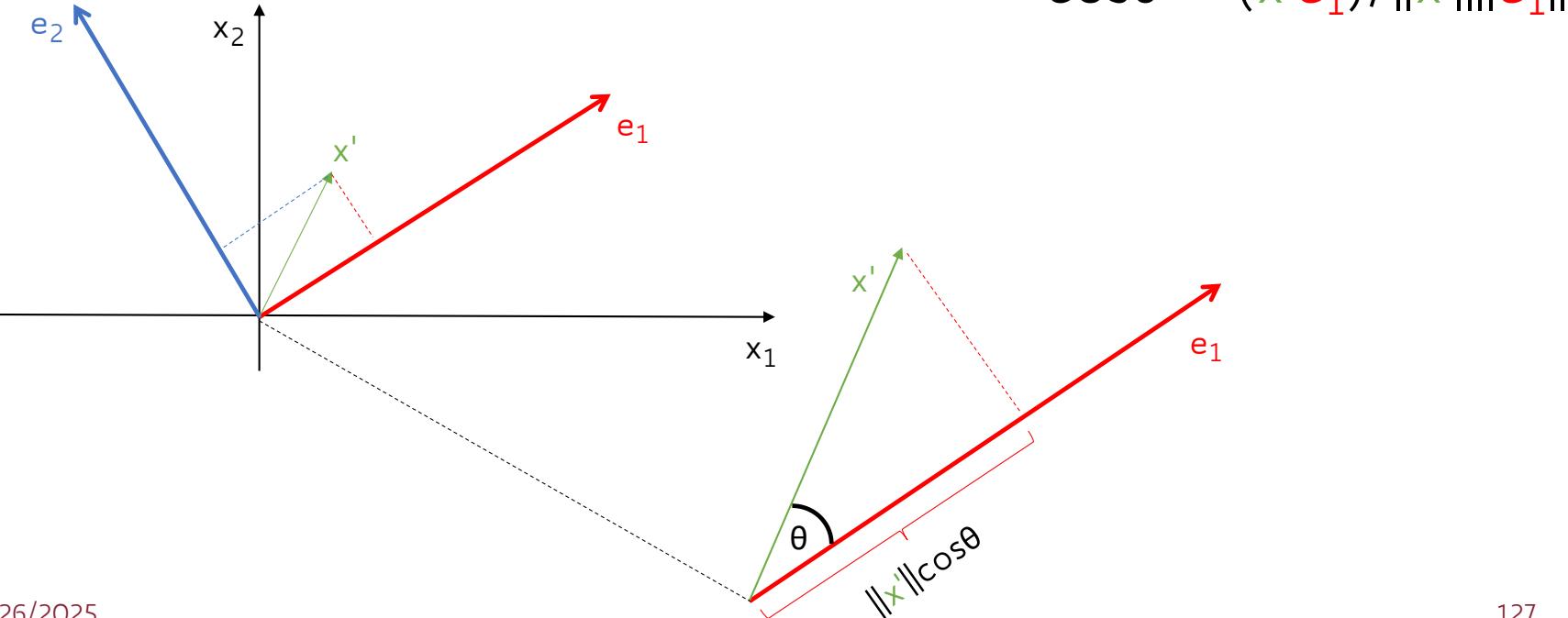
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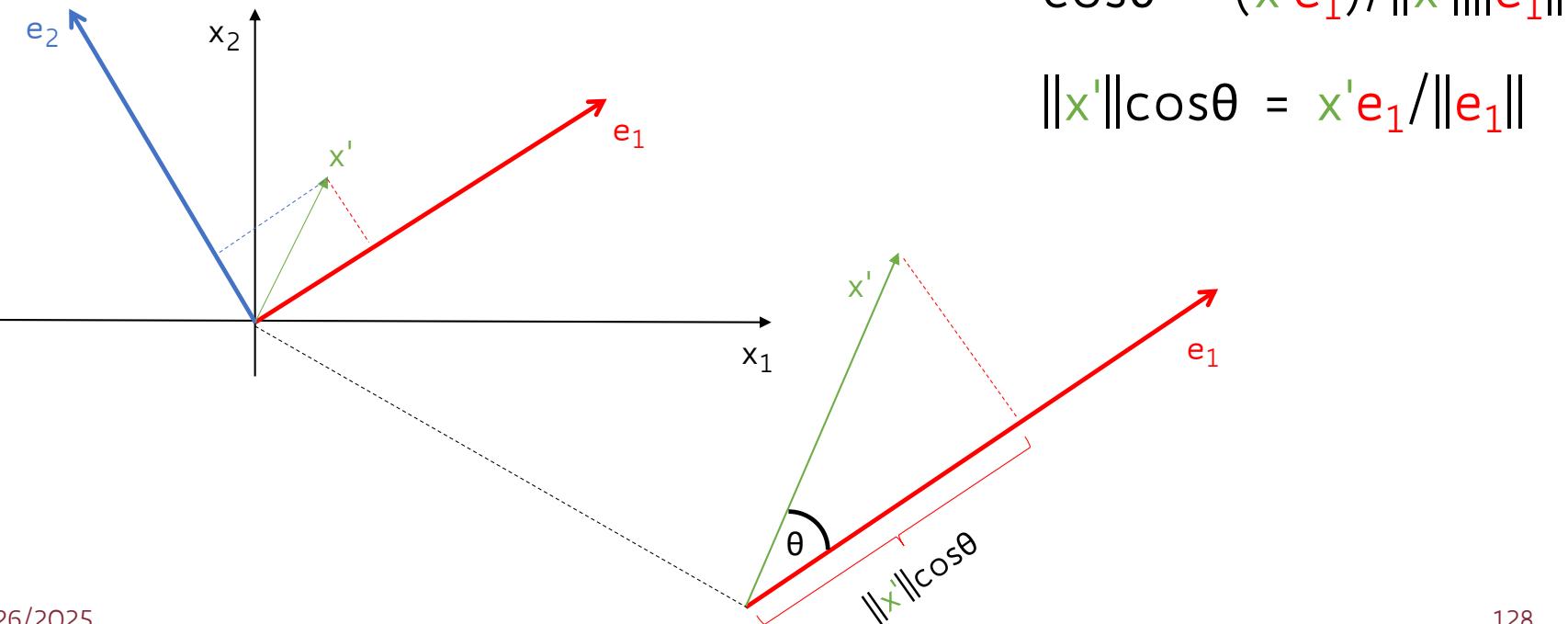
Why the dot product?

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



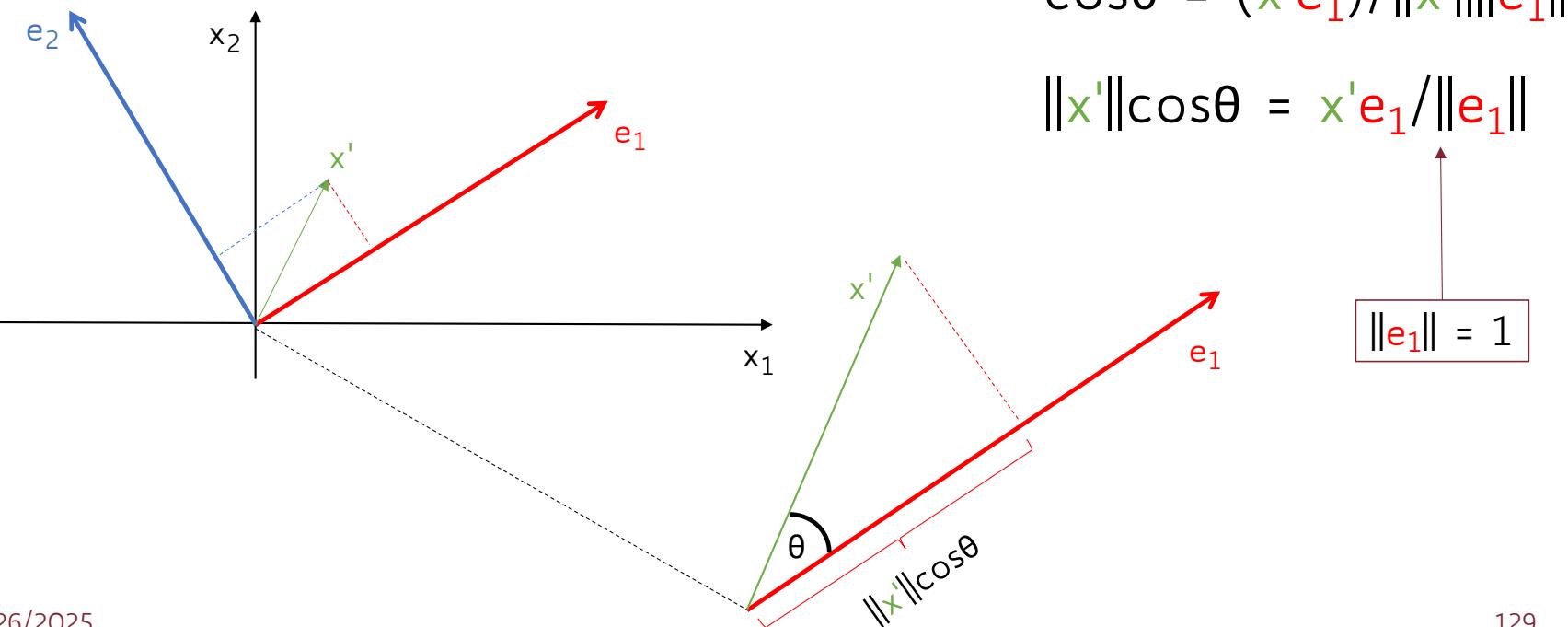
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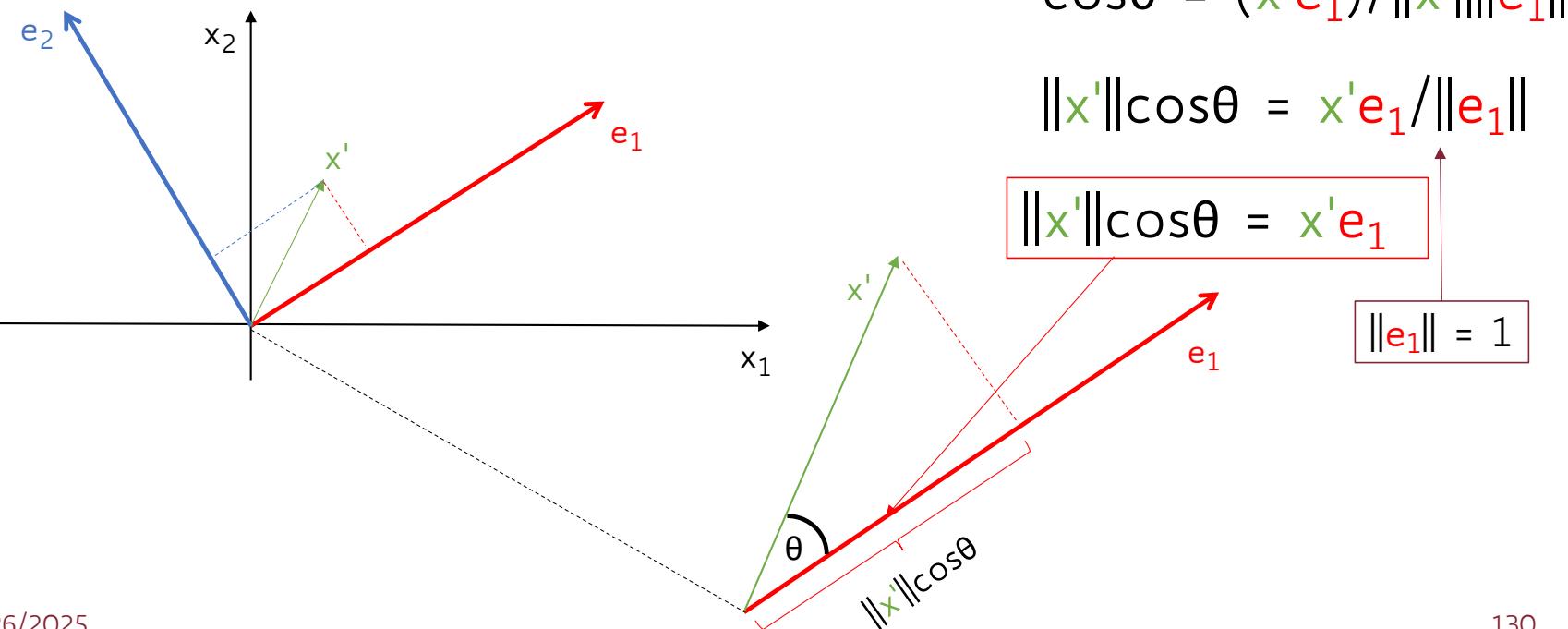
Projecting to New Dimensions: 2-d Case

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Projecting to New Dimensions: 2-d Case

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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

Projecting to New Dimensions: d -dimensions

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

Original d -dimensional data point

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

$k \ll d$
principal components

Projecting to New Dimensions: d -dimensions

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$k \ll d$, $\mathbf{e}_i \in \mathbb{R}^d$

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

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

Original d -dimensional data point

$$\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_k$$

$k \ll d$, $\mathbf{e}_i \in \mathbb{R}^d$

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/qtolomei/big-data-computing/raw/master/extras/Notes_on_Principal_Component_Analysis.pdf

How Many Dimensions?

- In a d -dimensional space we may have e_1, \dots, e_d length-1 eigenvectors

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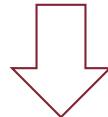
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Pick the subset of k eigenvectors that "explain" the most variance

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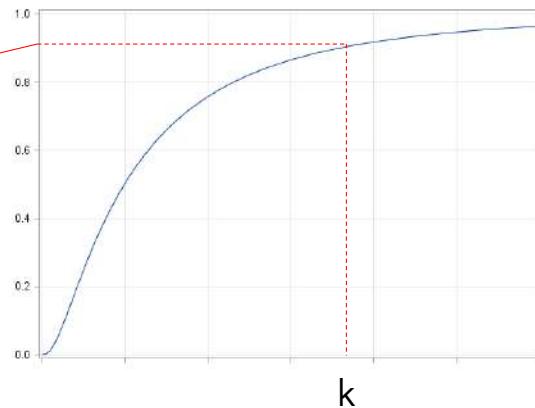
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2. Pick the first k eigenvectors that explain $x\%$ of the total variance

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

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



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Solution

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

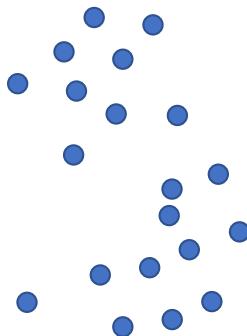
$$z = \frac{x - \mu}{\sigma}$$

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- PCA assumes the projection subspace is linear, i.e., an hyperplane:
 - 1-d \rightarrow straight line, 2-d \rightarrow flat surface, ...

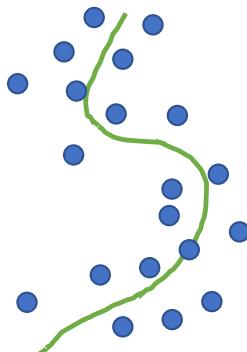
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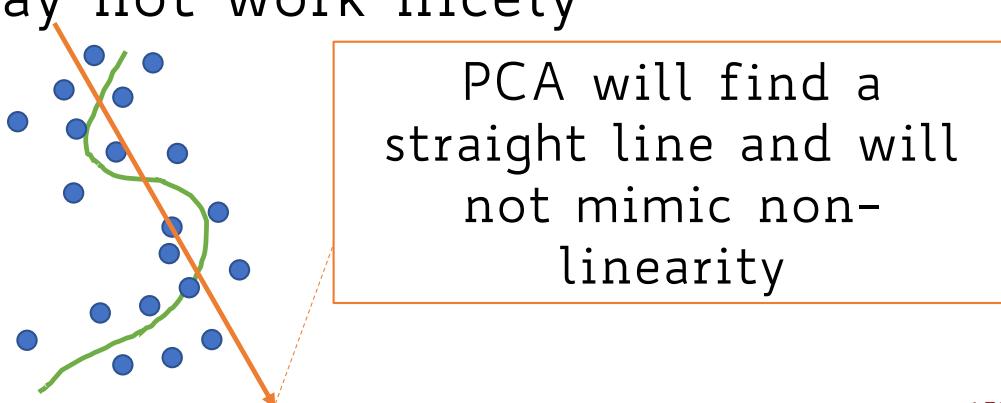
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- Suggested video: <https://www.youtube.com/watch?v=PFDu9oVAE-g>