CS7015 (Deep Learning) : Lecture 6

Eigen Values, Eigen Vectors, Eigen Value Decomposition, Principal Component Analysis, Singular Value Decomposition

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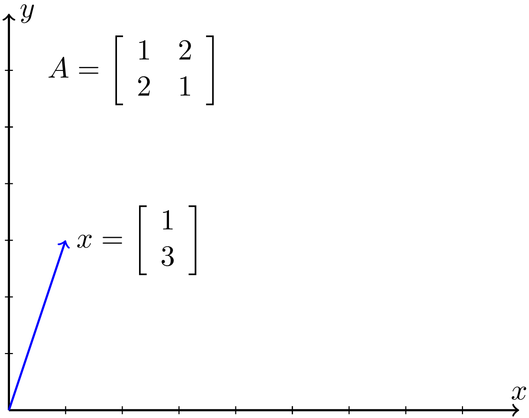
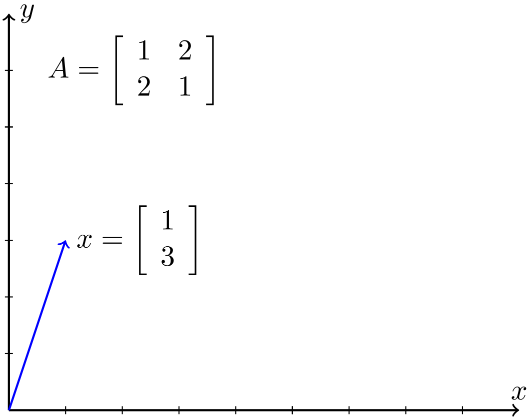
Module 6.1 : Eigenvalues and Eigenvectors



- What happens when a matrix hits a vector?



- What happens when a matrix hits a vector?
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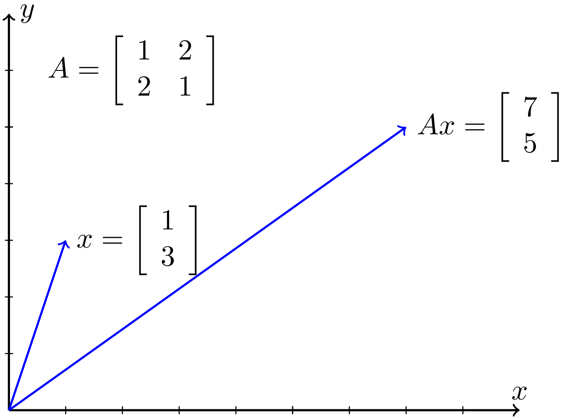

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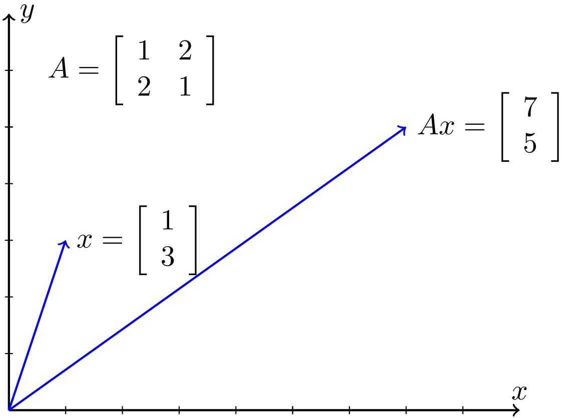
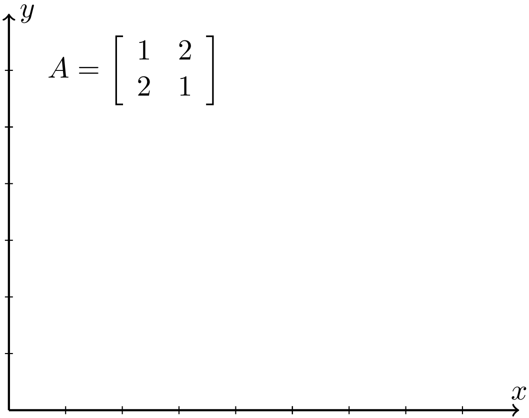
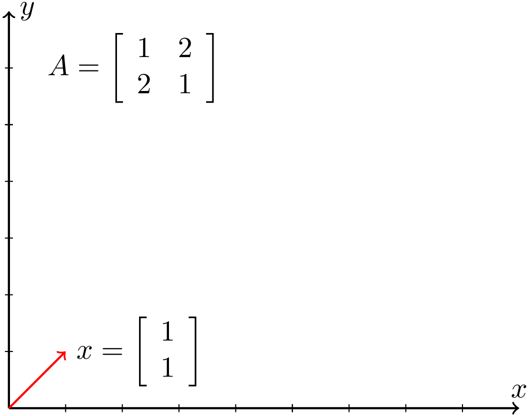


- What happens when a matrix hits a vector?
- The vector gets transformed into a new vector (it strays from its path)
- The vector may also get scaled (elongated or shortened) in the process.

$$A = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$$



- For a given square matrix A, there exist special vectors which refuse to stray from their path.



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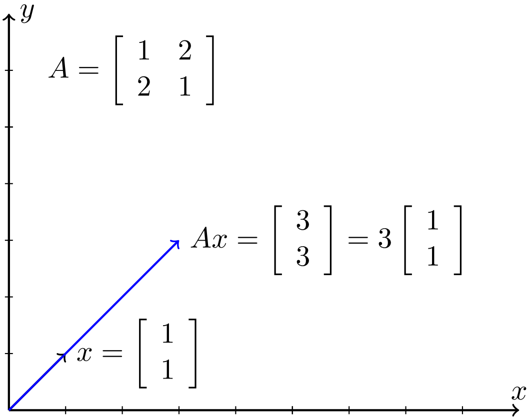

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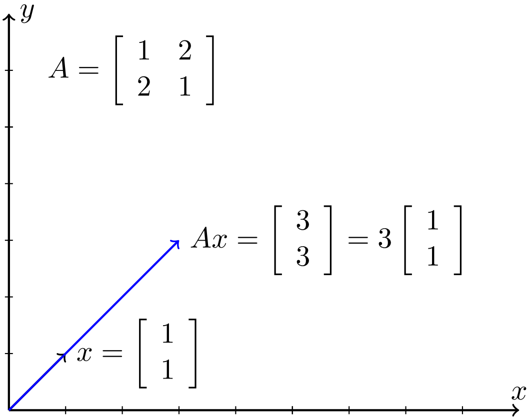

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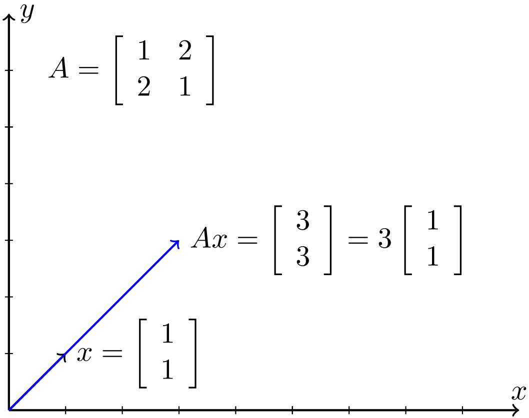
- These vectors are called eigenvectors.



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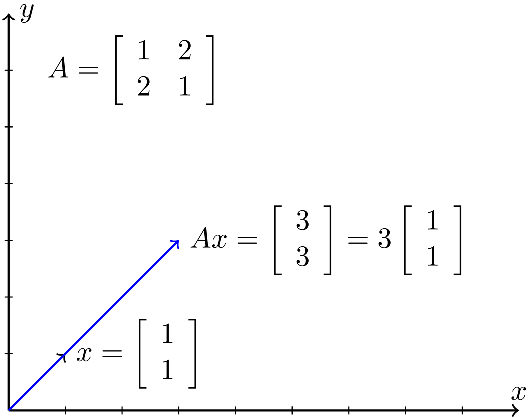
- More formally,

$$Ax = \lambda x \text{ [direction remains the same]}$$



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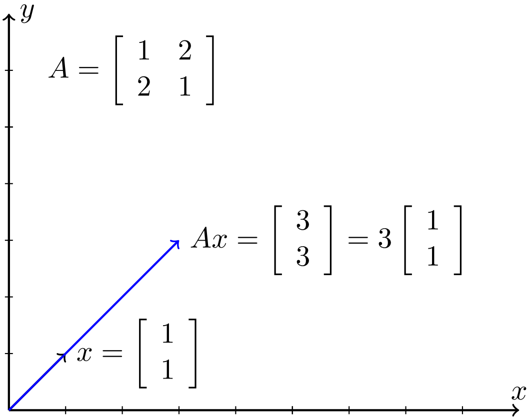
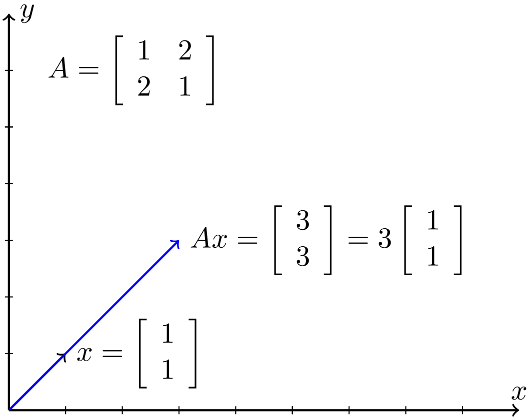
- The vector will only get scaled but will not change its direction.


y
$A = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix}$
$Ax = \begin{bmatrix} 3 \\ 3 \end{bmatrix} = 3 \begin{bmatrix} 1 \\ 1 \end{bmatrix}$
$x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$
x



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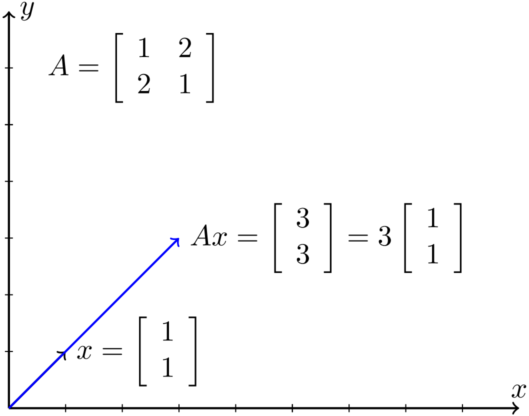

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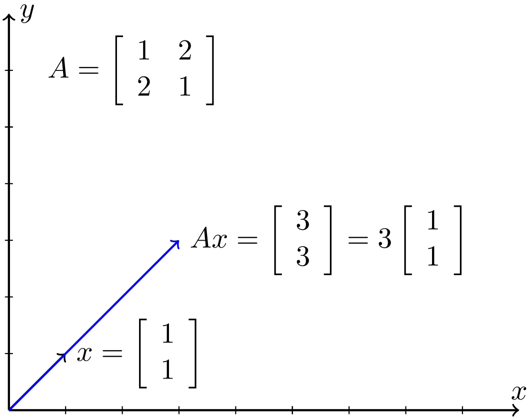
- So what is so special about eigenvectors?
- Why are they always in the limelight?



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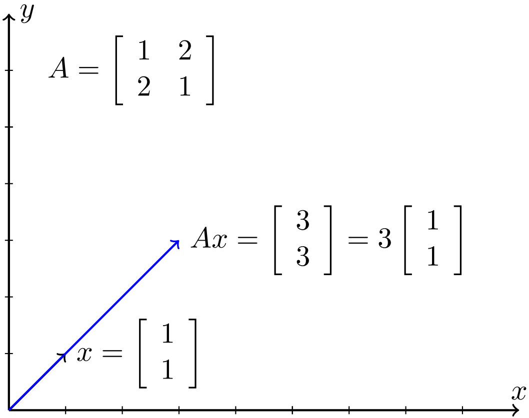
- It turns out that several properties of matrices can be analyzed based on their eigenvalues (for example, see spectral graph theory)



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- Why are they always in the limelight?
- It turns out that several properties of matrices can be analyzed based on their eigenvalues (for example, see spectral graph theory)
- We will now see two cases where eigenvalues/vectors will help us in this course

- Let us assume that on day 0, k_1 students eat Chinese food, and k_2 students eat Mexican food. (Of course, no one eats in the mess!)

Chinese k_1 Mexican k_2

$$v_{(0)} = \begin{bmatrix} k_1 \\ k_2 \end{bmatrix}$$

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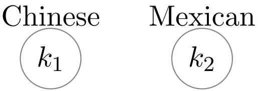

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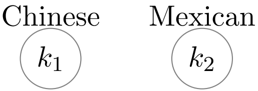

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- Similarly a fraction q of students who ate Mexican food on day $(i-1)$ continue to eat Mexican food on day i, and $(1-q)$ shift to Chinese food.

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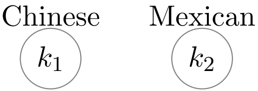

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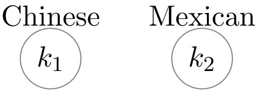

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In general, $v_{(n)} = M^n v_{(0)}$

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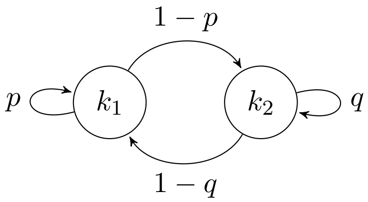
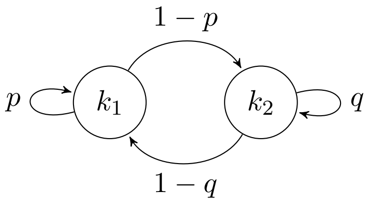
- The number of customers in the two restaurants is thus given by the following series:

$$v_{(0)}, Mv_{(0)}, M^2v_{(0)}, M^3v_{(0)}, \ldots$$

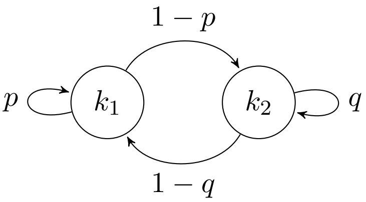


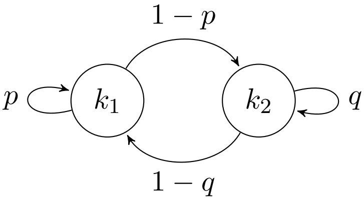
$1-p$
p
k_1
k_2
q
$1-q$

- This is a problem for the two restaurant owners.

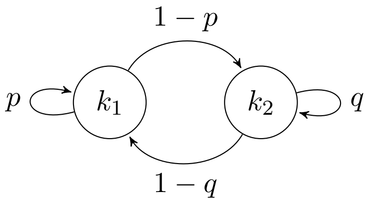


- This is a problem for the two restaurant owners.
- The number of patrons is changing constantly.





- This is a problem for the two restaurant owners.
- The number of patrons is changing constantly.
- Or is it? Will the system eventually reach a steady state? (i.e. will the number of customers in the two restaurants become constant over time?)



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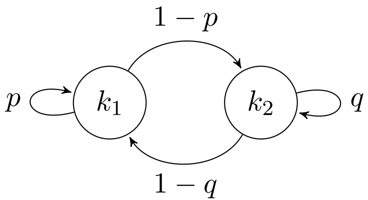

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- Let's see how?

Definition

Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvectors of an $n \times n$ matrix A. λ_1 is called the dominant eigen value of A if

$$|\lambda_1| \geq |\lambda_i| \; i = 2, \ldots, n$$

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A matrix M is called a stochastic matrix if all the entries are positive and the sum of the elements in each column is equal to 1.
(Note that the matrix in our example is a stochastic matrix)

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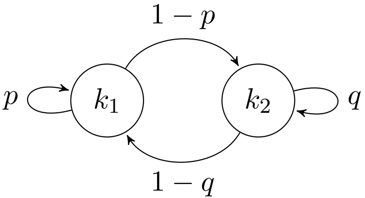
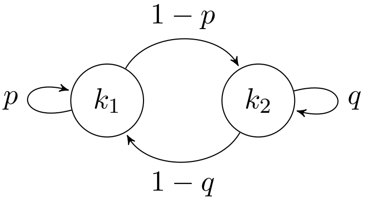
Theorem

If A is a $n \times n$ square matrix with a dominant eigenvalue, then the sequence of vectors given by $Av_0, A^2v_0, \ldots, A^nv_0, \ldots$ approaches a multiple of the dominant eigenvector of A.
(the theorem is slightly misstated here for ease of explanation)

- Let e_d be the dominant eigenvector of M and $\lambda_d = 1$ the corresponding dominant eigenvalue



- Let e_d be the dominant eigenvector of M and $\lambda_d = 1$ the corresponding dominant eigenvalue
- Given the previous definitions and theorems, what can you say about the sequence $Mv_{(0)}, M^2v_{(0)}, M^3v_{(0)}, \ldots$?



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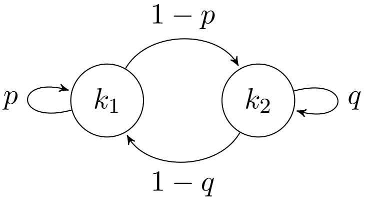
- There exists an n such that

$$v_{(n)} = M^n v_{(0)} = ke_d \text{ (some multiple of } e_d)$$



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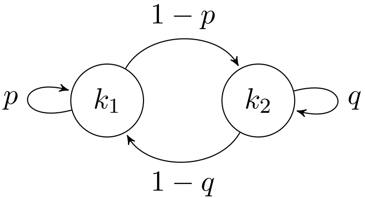
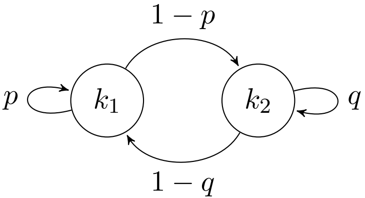
- Now what happens at time step $(n+1)$?

$$v_{(n+1)} = Mv_{(n)} = M(ke_d) = k(Me_d) = k(\lambda_d e_d) = ke_d$$





- Let e_d be the dominant eigenvector of M and $\lambda_d = 1$ the corresponding dominant eigenvalue
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- The population in the two restaurants becomes constant after time step n.
  See Proof Here

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$$A^{p+1} x_0 = A(A^p x_0) = k A e_d = k \lambda_d e_d$$

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- In general, if λ_d is the dominant eigenvalue of a matrix A, what would happen to the sequence $x_0, Ax_0, A^2x_0, \ldots$ if
  - $|\lambda_d| > 1$

- Now instead of a stochastic matrix let us consider any square matrix A
- Let p be the time step at which the sequence $x_0, Ax_0, A^2x_0, \ldots$ approaches a multiple of e_d (the dominant eigenvector of A)

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\begin{aligned}
A^p x_0 &= k e_d \\
A^{p+1} x_0 &= A(A^p x_0) = kAe_d = k\lambda_d e_d \\
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- In general, if λ_d is the dominant eigenvalue of a matrix A, what would happen to the sequence $x_0, Ax_0, A^2x_0, \ldots$ if
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  - $|\lambda_d| > 1$ (will explode)
  - $|\lambda_d| < 1$ (will vanish)
  - $|\lambda_d| = 1$ (will reach a steady state)
- (We will use this in the course at some point)

Module 6.2 : Linear Algebra - Basic Definitions

- We will see some more examples where eigenvectors are important, but before that let's revisit some basic definitions from linear algebra.

Basis

A set of vectors $\in \mathbb{R}^n$ is called a basis, if they are linearly independent and every vector $\in \mathbb{R}^n$ can be expressed as a linear combination of these vectors.

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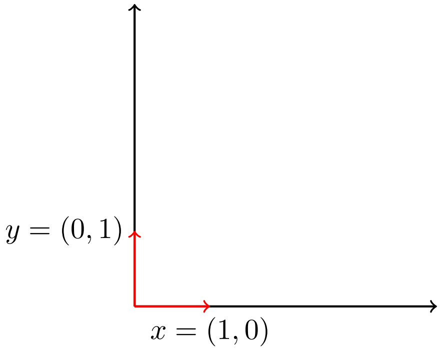
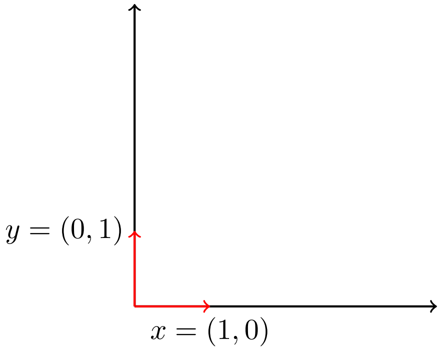
Linearly independent vectors

A set of n vectors $v_1, v_2, \ldots, v_n$ is linearly independent if no vector in the set can be expressed as a linear combination of the remaining $n-1$ vectors.
In other words, the only solution to

$$c_1 v_1 + c_2 v_2 + \ldots c_n v_n = 0 \text{ is } c_1 = c_2 = \cdots = c_n = 0 (c_i\text{'s } are\ scalars)$$

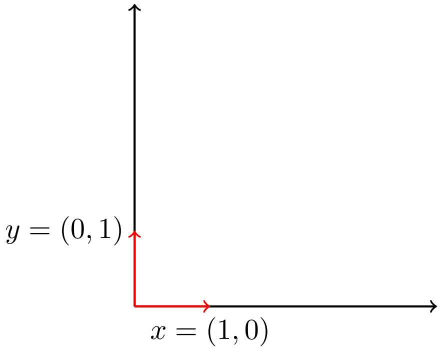


- For example consider the space $\mathbb{R}^2$



- For example consider the space $\mathbb{R}^2$
- Now consider the vectors

$$x = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \text{ and } y = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$



- For example consider the space $\mathbb{R}^2$
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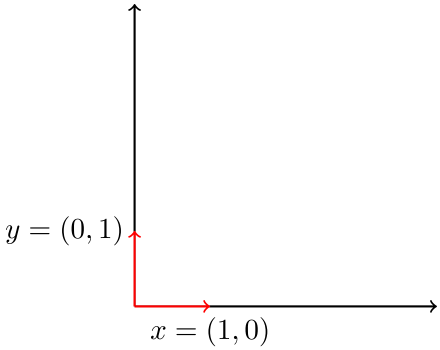
$$x = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \text{ and } y = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

- Any vector $\begin{bmatrix} a \\ b \end{bmatrix} \in \mathbb{R}^2$, can be expressed as a linear combination of these two vectors i.e

$$\begin{bmatrix} a \\ b \end{bmatrix} = a \begin{bmatrix} 1 \\ 0 \end{bmatrix} + b \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$



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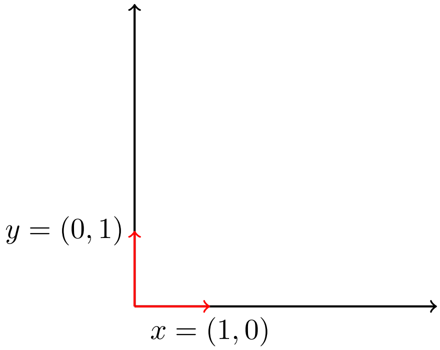
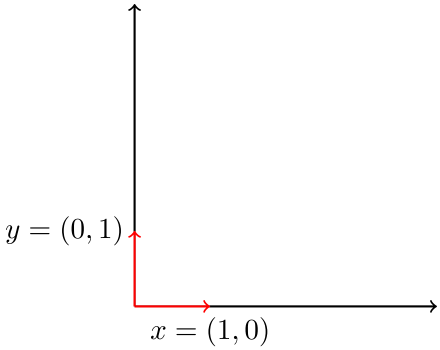
$$\begin{bmatrix} a \\ b \end{bmatrix} = a \begin{bmatrix} 1 \\ 0 \end{bmatrix} + b \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

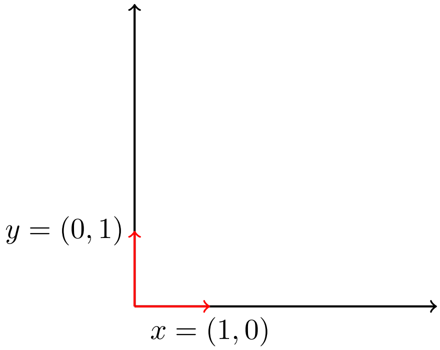
- Further, x and y are linearly independent. (the only solution to $c_1 x + c_2 y = 0$ is $c_1 = c_2 = 0$)



- In fact, turns out that x and y are unit vectors in the direction of the co-ordinate axes.



- In fact, turns out that x and y are unit vectors in the direction of the co-ordinate axes.
- And indeed we are used to representing all vectors in $\mathbb{R}^2$ as a linear combination of these two vectors.



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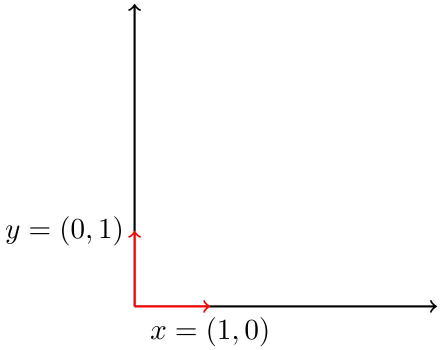
- But there is nothing sacrosanct about the particular choice of x and y.



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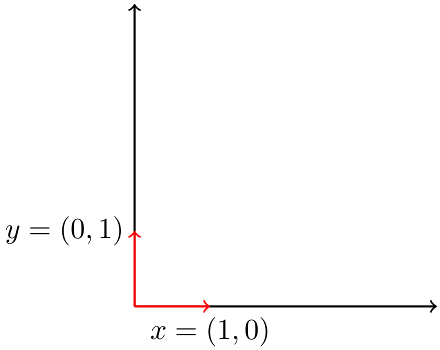
- We could have chosen any 2 linearly independent vectors in $\mathbb{R}^2$ as the basis vectors.



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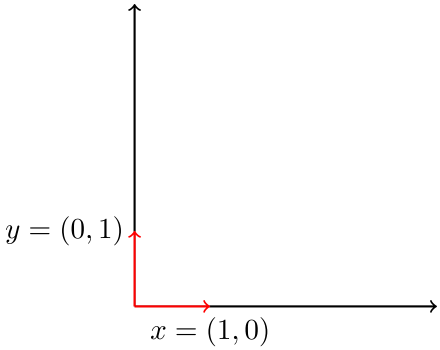
- For example, consider the linearly independent vectors, $[2, 3]^T$ and $[5, 7]^T$. See how any vector $[a, b]^T \in \mathbb{R}^2$ can be expressed as a linear combination of these two vectors.



$$\begin{bmatrix} a \\ b \end{bmatrix} = x_1 \begin{bmatrix} 2 \\ 3 \end{bmatrix} + x_2 \begin{bmatrix} 5 \\ 7 \end{bmatrix}$$

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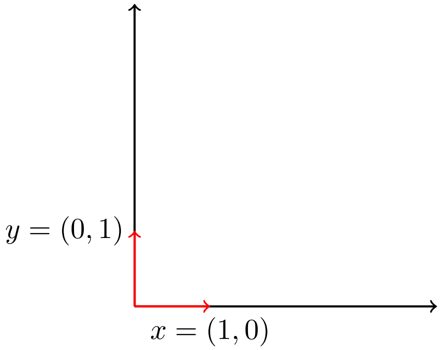

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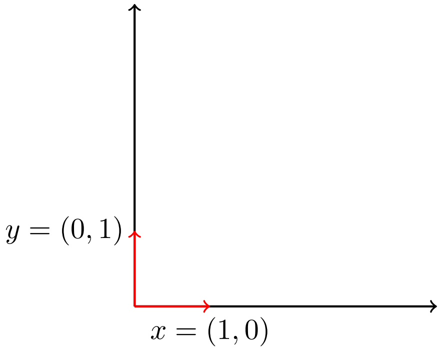
- For example, consider the linearly independent vectors, $[2, 3]^T$ and $[5, 7]^T$. See how any vector $[a, b]^T \in \mathbb{R}^2$ can be expressed as a linear combination of these two vectors.
- We can find x_1 and x_2 by solving a system of linear equations.



$$a = 2x_1 + 5x_2$$
$$b = 3x_1 + 7x_2$$

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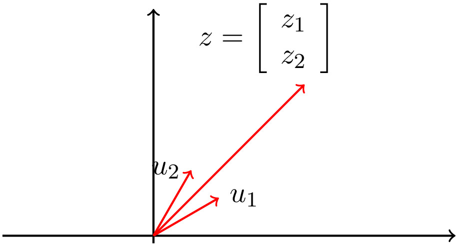
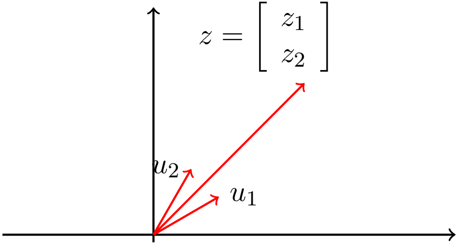


- In general, given a set of linearly independent vectors $u_1, u_2, \ldots u_n \in \mathbb{R}^n$, we can express any vector $z \in \mathbb{R}^n$ as a linear combination of these vectors.



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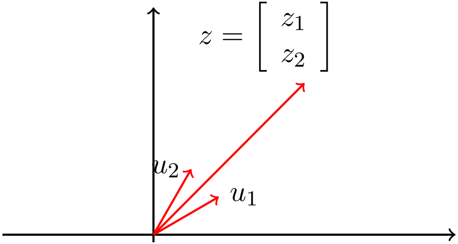

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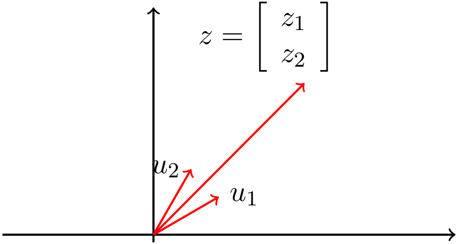

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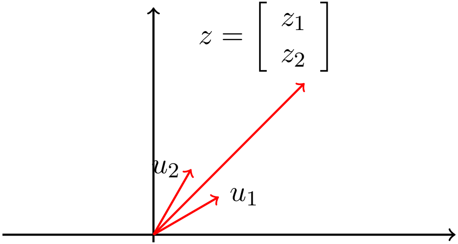
(Basically rewriting in matrix form)



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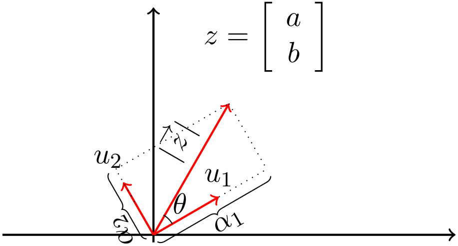
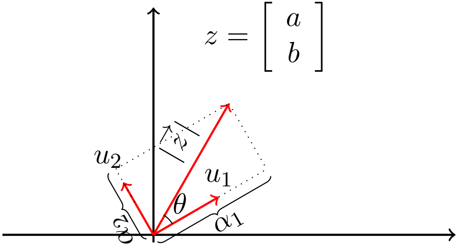
- We can now find the α_is using Gaussian Elimination (Time Complexity: $O(n^3)$)



- Now let us see if we have orthonormal basis.



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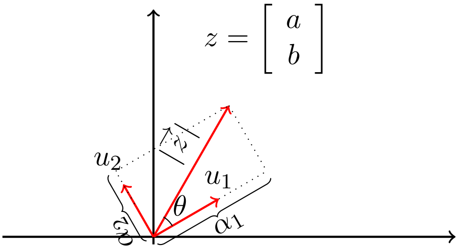
- $u_i^T u_j = 0 \ \forall i \neq j$ and $u_i^T u_i = \|u_i\|^2 = 1$



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- Again we have:

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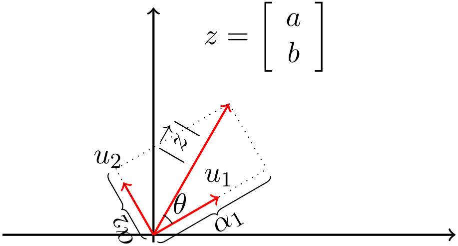

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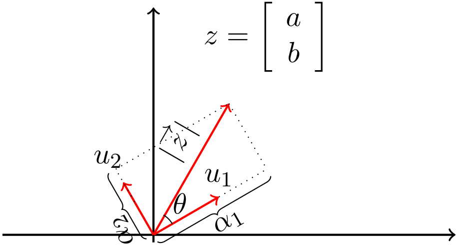

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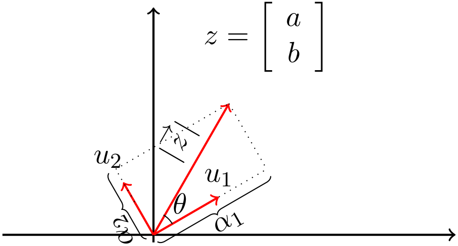

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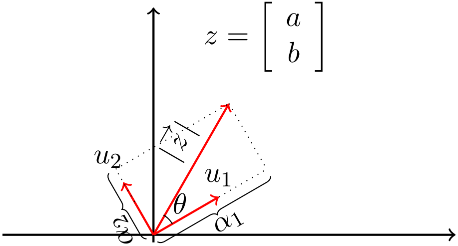
- We can directly find each α_i using a dot product between z and u_i (time complexity $O(N)$)



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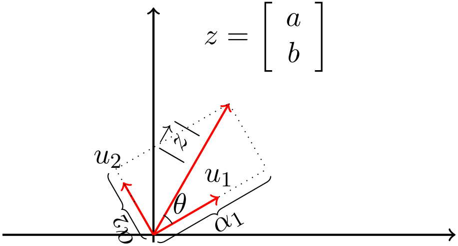
- The total complexity will be $O(N^2)$



$$\alpha_1 = |\vec{z}|cos\theta = |\vec{z}|\frac{z^T u_1}{|\vec{z}||u_1|} = z^T u_1$$

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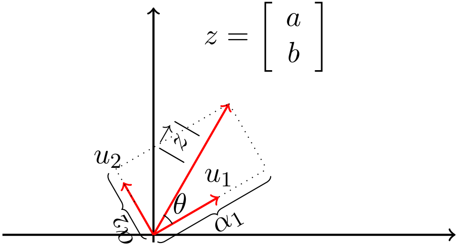
- The total complexity will be $O(N^2)$



$$\alpha_1 = |\vec{z}|cos\theta = |\vec{z}|\frac{z^T u_1}{|\vec{z}||u_1|} = z^T u_1$$

Similarly, $\alpha_2 = z^T u_2$.

- Now let us see if we have orthonormal basis.
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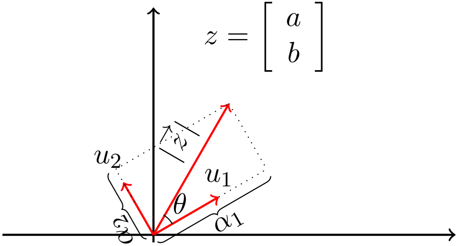

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When u_1 and u_2 are unit vectors along the co-ordinate axes

$$z = \begin{bmatrix} a \\ b \end{bmatrix} = a\begin{bmatrix} 1 \\ 0 \end{bmatrix} + b\begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

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Remember

An orthogonal basis is the most convenient basis that one can hope for.

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The eigenvectors of a matrix $A \in \mathbb{R}^{n \times n}$ having distinct eigenvalues are linearly independent.

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- Why would we want to use the eigenvectors as a basis instead of the more natural co-ordinate axes?
- We will answer this question soon.

Module 6.3 : Eigenvalue Decomposition

Before proceeding let's do a quick recap of eigenvalue decomposition.

- Let $u_1, u_2, \ldots, u_n$ be the eigenvectors of a matrix A and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the corresponding eigenvalues.

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- where Λ is a diagonal matrix whose diagonal elements are the eigenvalues of A.

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$$A = U\Lambda U^{-1} \qquad \text{[eigenvalue decomposition]}$$
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  - *i.e.* if A has n distinct eigenvalues [**sufficient condition, proof : Slide 19 Theorem 1**]

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$$\begin{aligned} Q_{ij} = u_i^T u_j \quad &= 0 \text{ if } i \neq j \\ &= 1 \text{ if } i = j \end{aligned}$$

$$\therefore U^T U = \mathbb{I} \text{ (the identity matrix)}$$

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- U^T is the inverse of U (very convenient to calculate)

Something to think about

- Given the EVD, $A = U\Sigma U^T$,
  what can you say about the sequence $x_0, Ax_0, A^2x_0, \ldots$ in terms of the eigen values of A.
  (Hint: You should arrive at the same conclusion we saw earlier)

Theorem (one more important property of eigenvectors)

If A is a square symmetric $N \times N$ matrix, then the solution to the following optimization problem is given by the eigenvector corresponding to the largest eigenvalue of A.

$$\max_x \; x^T A x$$

$$\text{s.t } \|x\| = 1$$

and the solution to

$$\min_x \; x^T A x$$

$$\text{s.t } \|x\| = 1$$

is given by the eigenvector corresponding to the smallest eigenvalue of A.

Proof: Next slide.

- This is a constrained optimization problem that can be solved using Lagrange Multipliers:

$$L = x^T A x - \lambda(x^T x - 1)$$

$$\frac{\partial L}{\partial x} = 2Ax - \lambda(2x) = 0 => Ax = \lambda x$$

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- Therefore, the critical points of this constrained problem are the eigenvalues of A.
- The maximum value is the largest eigenvalue, while the minimum value is the smallest eigenvalue.

The story so far...

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- The eigenvectors corresponding to different eigenvalues are linearly independent.

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- The eigenvectors of a square symmetric matrix are orthogonal.
- The eigenvectors of a square symmetric matrix can thus form a convenient basis.
- We will put all of this to use.

Module 6.4 : Principal Component Analysis and its Interpretations

The story ahead...

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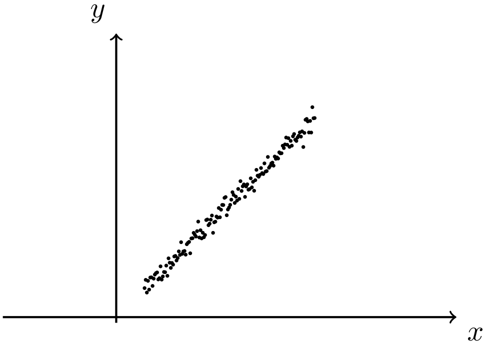
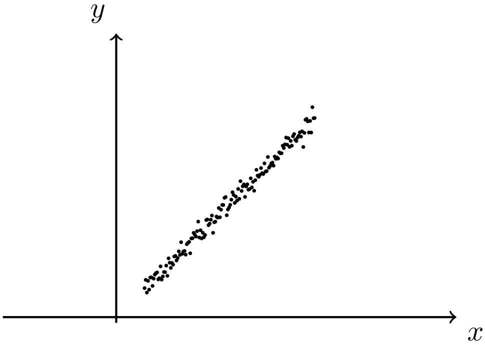
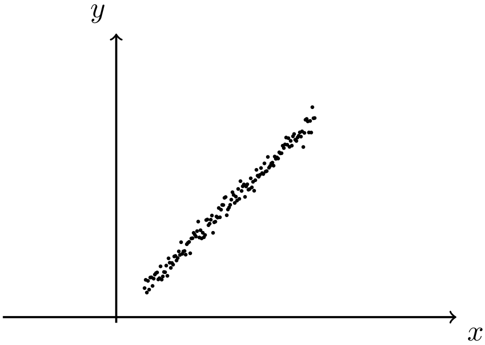
- Over the next few slides we will introduce Principal Component Analysis and see three different interpretations of it



- Consider the following data



- Consider the following data
- Each point (vector) here is represented using a linear combination of the x and y axes (i.e. using the point's x and y co-ordinates)



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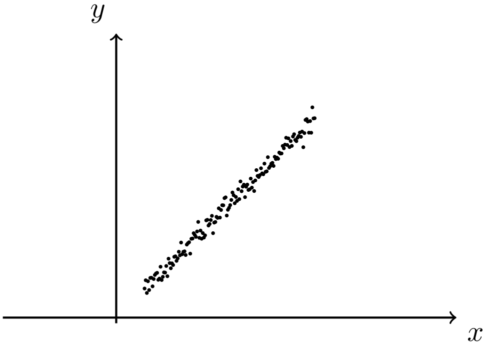

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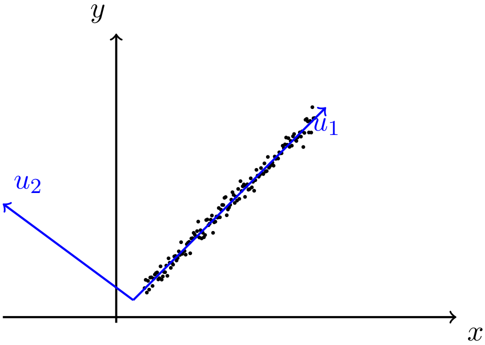
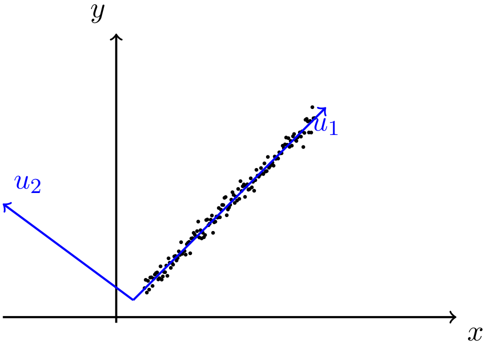
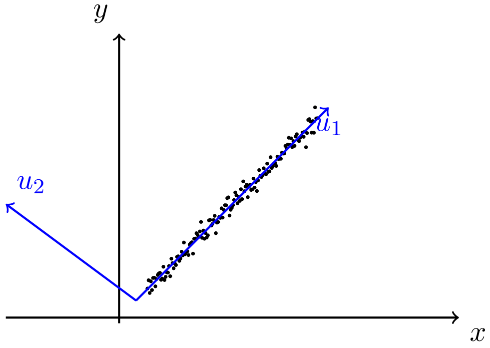
- Each point (vector) here is represented using a linear combination of the x and y axes (i.e. using the point's x and y co-ordinates)
- In other words we are using x and y as the basis
- What if we choose a different basis?



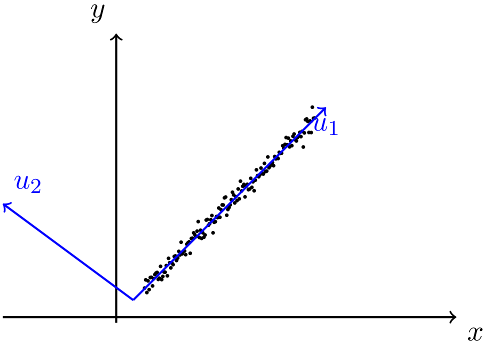
- For example, what if we use u_1 and u_2 as a basis instead of x and y.



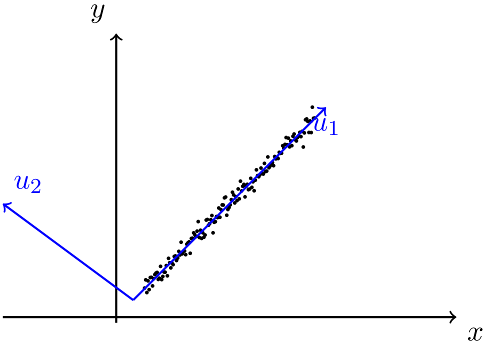
- For example, what if we use u_1 and u_2 as a basis instead of x and y.
- We observe that all the points have a very small component in the direction of u_2 (almost noise)



- For example, what if we use u_1 and u_2 as a basis instead of x and y.
- We observe that all the points have a very small component in the direction of u_2 (almost noise)
- It seems that the same data which was originally in $\mathbb{R}^2(x, y)$ can now be represented in $\mathbb{R}^1(u_1)$ by making a smarter choice for the basis



- Let's try stating this more formally



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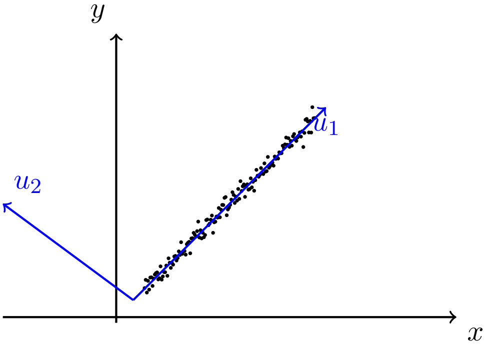
- Why do we not care about u_2?



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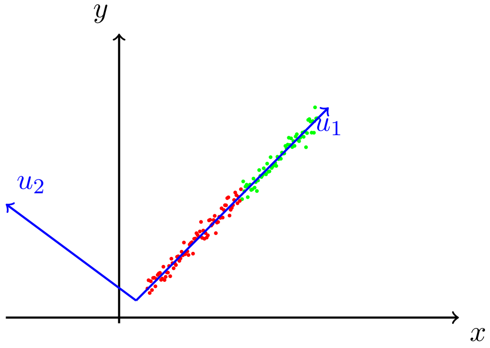
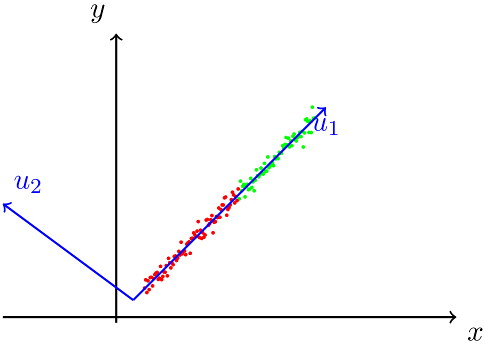
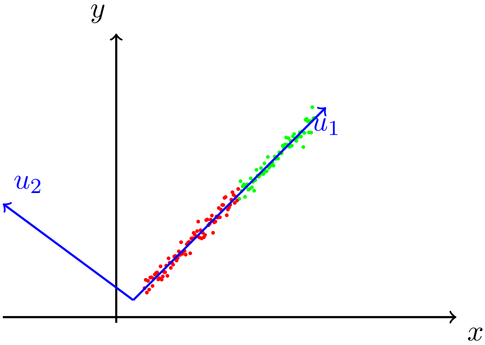
- Why do we not care about u_2?
- Because the variance in the data in this direction is very small (all data points have almost the same value in the u_2 direction)



- Let's try stating this more formally
- Why do we not care about u_2?
- Because the variance in the data in this direction is very small (all data points have almost the same value in the u_2 direction)
- If we were to build a classifier on top of this data then u_2 would not contribute to the classifier as the points are not distinguishable along this direction



- In general, we are interested in representing the data using fewer dimensions such that



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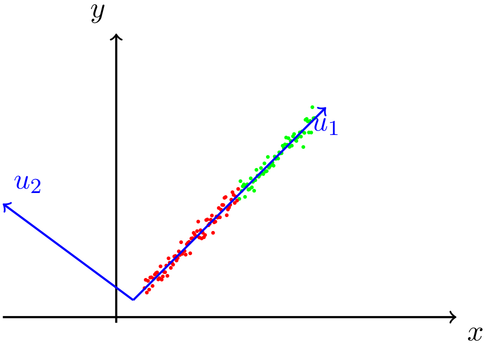

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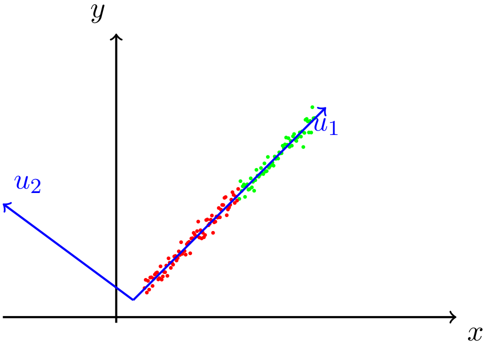
- Is that all?



- In general, we are interested in representing the data using fewer dimensions such that the data has high variance along these dimensions
- Is that all?
- No, there is something else that we desire. Let's see what.

x	**y**	**z**
1	1	1
0.5	0	0
0.25	1	1
0.35	1.5	1.5
0.45	1	1
0.57	2	2.1
0.62	1.1	1
0.73	0.75	0.76
0.72	0.86	0.87

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- Consider the following data
- Is z adding any new information beyond what is already contained in y?

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$$\rho_{yz} = \frac{\sum_{i=1}^{n}(y_i - \overline{y})(z_i - \overline{z})}{\sqrt{\sum_{i=1}^{n}(y_i - \overline{y})^2}\sqrt{\sum_{i=1}^{n}(z_i - \overline{z})^2}}$$

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- Consider the following data
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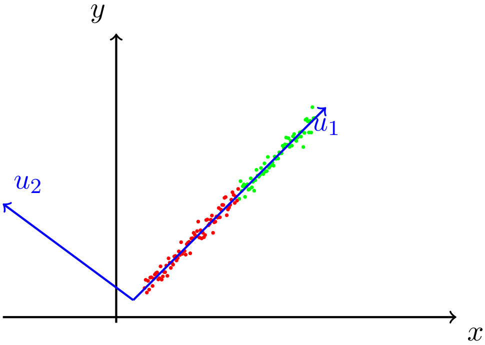
- In other words the column z is redundant since it is linearly dependent on y.



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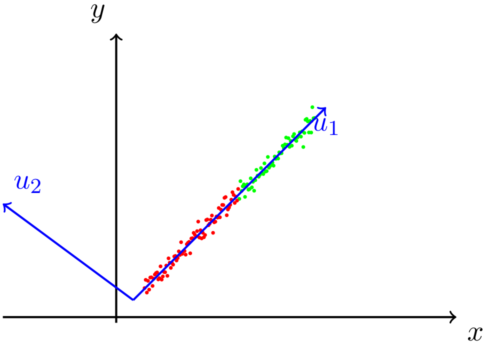

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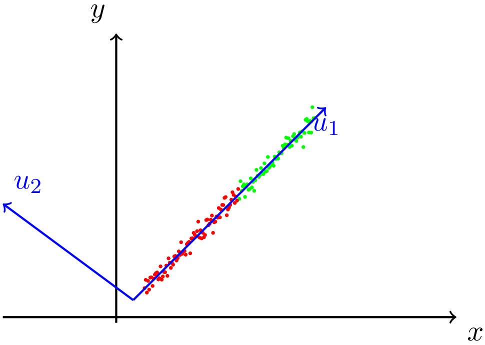

In general, we are interested in representing the data using fewer dimensions such that

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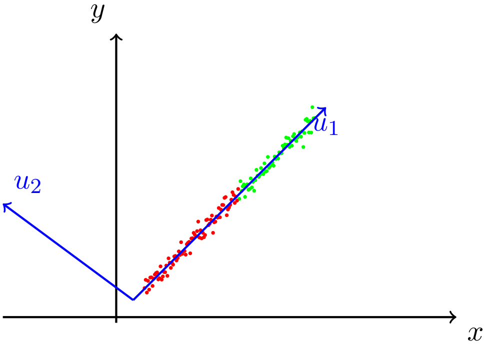

In general, we are interested in representing the data using fewer dimensions such that

- the data has high variance along these dimensions
- the dimensions are linearly independent (uncorrelated)
- (even better if they are orthogonal because that is a very convenient basis)

Let $p_1, p_2, \cdots, p_n$ be a set of such n linearly independent orthonormal vectors. Let P be a $n \times n$ matrix such that $p_1, p_2, \cdots, p_n$ are the columns of P.

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Let $x_1, x_2, \cdots, x_m \in \mathbb{R}^n$ be m data points and let X be a matrix such that $x_1, x_2, \cdots, x_m$ are the rows of this matrix. Further let us assume that the data is 0-mean and unit variance.

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We want to represent each x_i using this new basis P.

$$x_i = \alpha_{i1}p_1 + \alpha_{i2}p_2 + \alpha_{i3}p_3 + \cdots + \alpha_{in}p_n$$

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For an orthonormal basis we know that we can find these $\alpha_i's$ using

$$\alpha_{ij} = x_i^T p_j = \begin{bmatrix} \leftarrow & x_i & \rightarrow \end{bmatrix}^T \begin{bmatrix} \uparrow \\ p_j \\ \downarrow \end{bmatrix}$$

In general, the transformed data $\hat{x}_i$ is given by

$$\hat{x}_i = \begin{bmatrix} \leftarrow & x_i^T & \rightarrow \end{bmatrix} \begin{bmatrix} \uparrow & & \uparrow \\ p_1 & \cdots & p_n \\ \downarrow & & \downarrow \end{bmatrix} = x_i^T P$$

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and

$$\hat{X} = XP \qquad (\hat{X} \text{ is the matrix of transformed points})$$

Theorem:
If X is a matrix such that its columns have zero mean and if $\hat{X} = XP$ then the columns of $\hat{X}$ will also have zero mean.

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$$\mathbf{1}^T \hat{X} = \mathbf{1}^T XP = (\mathbf{1}^T X)P$$

But $\mathbf{1}^T X$ is the row vector containing the sums of the columns of X. Thus $\mathbf{1}^T X = 0$. Therefore, $\mathbf{1}^T \hat{X} = 0$.

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Theorem:

$X^T X$ is a symmetric matrix.

Proof: We can write $(X^T X)^T = X^T (X^T)^T = X^T X$

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If X is a matrix whose columns are zero mean then $\Sigma = \frac{1}{m}X^TX$ is the covariance matrix. In other words each entry Σ_{ij} stores the covariance between columns i and j of X.

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Explanation: Let C be the covariance matrix of X. Let μ_i, μ_j denote the means of the i^{th} and j^{th} column of X respectively. Then by definition of covariance, we can write :

$$
\begin{aligned}
C_{ij} &= \frac{1}{m}\sum_{k=1}^{m}(X_{ki} - \mu_i)(X_{kj} - \mu_j) \\
&= \frac{1}{m}\sum_{k=1}^{m} X_{ki}X_{kj} \qquad\qquad (\because \mu_i = \mu_j = 0) \\
&= \frac{1}{m}X_i^TX_j = \frac{1}{m}(X^TX)_{ij}
\end{aligned}
$$

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- Ideally we want,

$$\begin{aligned}
\left(\frac{1}{m}\hat{X}^T\hat{X}\right)_{ij} &= 0 & \qquad & i \neq j \text{ (covariance} = 0) \\
\left(\frac{1}{m}\hat{X}^T\hat{X}\right)_{ij} &\neq 0 & \qquad & i = j \text{ (variance} \neq 0)
\end{aligned}$$

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In other words, we want

$$\frac{1}{m}\hat{X}^T\hat{X} = P^T\Sigma P = D \qquad \text{[where D is a diagonal matrix]}$$

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- **Answer:** A matrix P whose columns are the eigen vectors of $\Sigma = X^T X$ [By Eigen Value Decomposition]
- Thus, the new basis P used to transform X is the basis consisting of the eigen vectors of $X^T X$

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- This method is called Principal Component Analysis for transforming the data to a new basis where the dimensions are non-redundant (low covariance) & not noisy (high variance)
- In practice, we select only the top-k dimensions along which the variance is high (this will become more clear when we look at an alternalte interpretation of PCA)

Module 6.5 : PCA : Interpretation 2

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$$\hat{x}_i = \sum_{j=1}^{k} \alpha_{ik} p_k$$

We want to select $p'_i s$ such that we minimise the reconstructed error

$$e = \sum_{i=1}^{m} (x_i - \hat{x}_i)^T (x_i - \hat{x}_i)$$

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\begin{aligned}
e &= \sum_{i=1}^{m} (x_i - \hat{x}_i)^T (x_i - \hat{x}_i) \\
&= \sum_{i=1}^{m} \left(\sum_{j=1}^{n} \alpha_{ij} p_j - \sum_{j=1}^{k} \alpha_{ij} p_j \right)^2
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&= \sum_{i=1}^{m} \left(\alpha_{i,k+1} p_{k+1} + \alpha_{i,k+2} p_{k+2} + \ldots + \alpha_{i,n} p_n \right)^T \left(\alpha_{i,k+1} p_{k+1} + \alpha_{i,k+2} p_{k+2} + \ldots + \alpha_{i,n} p_n \right)
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&= \sum_{i=1}^{m}\left(\alpha_{i,k+1}p_{k+1} + \alpha_{i,k+2}p_{k+2} + \ldots + \alpha_{i,n}p_n\right)^T\left(\alpha_{i,k+1}p_{k+1} + \alpha_{i,k+2}p_{k+2} + \ldots + \alpha_{i,n}p_n\right) \\
&= \sum_{i=1}^{m}\sum_{j=k+1}^{n}\alpha_{ij}p_j^T p_j \alpha_{ij} + \sum_{i=1}^{m}\sum_{j=k+1}^{n}\sum_{L=k+1, L\neq k}^{n}\alpha_{ij}p_j^T p_L \alpha_{iL}
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&= \sum_{i=1}^{m} \sum_{j=k+1}^{n} \alpha_{ij}^2 \qquad\qquad (\because p_j^T p_j = 1, p_i^T p_j = 0 \quad \forall i \neq j)
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&= \sum_{i=1}^{m} (\alpha_{i,k+1} p_{k+1} + \alpha_{i,k+2} p_{k+2} + \ldots + \alpha_{i,n} p_n)^T (\alpha_{i,k+1} p_{k+1} + \alpha_{i,k+2} p_{k+2} + \ldots + \alpha_{i,n} p_n) \\
&= \sum_{i=1}^{m} \sum_{j=k+1}^{n} \alpha_{ij} p_j^T p_j \alpha_{ij} + \sum_{i=1}^{m} \sum_{j=k+1}^{n} \sum_{L=k+1, L \neq k}^{n} \alpha_{ij} p_j^T p_L \alpha_{iL} \\
&= \sum_{i=1}^{m} \sum_{j=k+1}^{n} \alpha_{ij}^2 \qquad\qquad (\because p_j^T p_j = 1, p_i^T p_j = 0 \quad \forall i \neq j) \\
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$$= \sum_{i=1}^{m} \left(\sum_{j=1}^{n} \alpha_{ij} p_j - \sum_{j=1}^{k} \alpha_{ij} p_j \right)^2$$

$$= \sum_{i=1}^{m} \left(\sum_{j=k+1}^{n} \alpha_{ij} p_j \right)^2 = \sum_{i=1}^{m} \left(\sum_{j=k+1}^{n} \alpha_{ij} p_j \right)^T \left(\sum_{j=k+1}^{n} \alpha_{ij} p_j \right)$$

$$= \sum_{i=1}^{m} (\alpha_{i,k+1} p_{k+1} + \alpha_{i,k+2} p_{k+2} + \ldots + \alpha_{i,n} p_n)^T (\alpha_{i,k+1} p_{k+1} + \alpha_{i,k+2} p_{k+2} + \ldots + \alpha_{i,n} p_n)$$

$$= \sum_{i=1}^{m} \sum_{j=k+1}^{n} \alpha_{ij} p_j^T p_j \alpha_{ij} + \sum_{i=1}^{m} \sum_{j=k+1}^{n} \sum_{L=k+1, L \neq k}^{n} \alpha_{ij} p_j^T p_L \alpha_{iL}$$

$$= \sum_{i=1}^{m} \sum_{j=k+1}^{n} \alpha_{ij}^2 \qquad (\because p_j^T p_j = 1, p_i^T p_j = 0 \quad \forall i \neq j)$$

$$= \sum_{i=1}^{m} \sum_{j=k+1}^{n} (x_i^T p_j)^2$$

$$= \sum_{i=1}^{m} \sum_{j=k+1}^{n} (p_j^T x_i)(x_i^T p_j)$$

$$
\begin{aligned}
e &= \sum_{i=1}^{m} (x_i - \hat{x}_i)^T (x_i - \hat{x}_i) \\
&= \sum_{i=1}^{m} \left(\sum_{j=1}^{n} \alpha_{ij} p_j - \sum_{j=1}^{k} \alpha_{ij} p_j \right)^2 \\
&= \sum_{i=1}^{m} \left(\sum_{j=k+1}^{n} \alpha_{ij} p_j \right)^2 = \sum_{i=1}^{m} \left(\sum_{j=k+1}^{n} \alpha_{ij} p_j \right)^T \left(\sum_{j=k+1}^{n} \alpha_{ij} p_j \right) \\
&= \sum_{i=1}^{m} \left(\alpha_{i,k+1} p_{k+1} + \alpha_{i,k+2} p_{k+2} + \ldots + \alpha_{i,n} p_n \right)^T \left(\alpha_{i,k+1} p_{k+1} + \alpha_{i,k+2} p_{k+2} + \ldots + \alpha_{i,n} p_n \right) \\
&= \sum_{i=1}^{m} \sum_{j=k+1}^{n} \alpha_{ij} p_j^T p_j \alpha_{ij} + \sum_{i=1}^{m} \sum_{j=k+1}^{n} \sum_{L=k+1, L \neq k}^{n} \alpha_{ij} p_j^T p_L \alpha_{iL} \\
&= \sum_{i=1}^{m} \sum_{j=k+1}^{n} \alpha_{ij}^2 \qquad (\because p_j^T p_j = 1, p_i^T p_j = 0 \quad \forall i \neq j) \\
&= \sum_{i=1}^{m} \sum_{j=k+1}^{n} \left(x_i^T p_j \right)^2
\end{aligned}
$$

$$
\begin{aligned}
&= \sum_{i=1}^{m} \sum_{j=k+1}^{n} \left(p_j^T x_i \right) \left(x_i^T p_j \right) \\
&= \sum_{j=k+1}^{n} p_j^T \left(\sum_{i=1}^{m} x_i x_i^T \right) p_j
\end{aligned}
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e &= \sum_{i=1}^{m} (x_i - \hat{x}_i)^T (x_i - \hat{x}_i) \\
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&= \sum_{i=1}^{m} \sum_{j=k+1}^{n} \alpha_{ij} p_j^T p_j \alpha_{ij} + \sum_{i=1}^{m} \sum_{j=k+1}^{n} \sum_{L=k+1, L \neq k}^{n} \alpha_{ij} p_j^T p_L \alpha_{iL} \\
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\begin{aligned}
&= \sum_{i=1}^{m} \sum_{j=k+1}^{n} \left(p_j^T x_i \right) \left(x_i^T p_j \right) \\
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&= \sum_{j=k+1}^{n} p_j^T m C p_j \qquad \left[\because \frac{1}{m} \sum_{i=1}^{m} x_i x_i^T = \frac{X^T X}{m} = C \right]
\end{aligned}
$$

We want to minimize e

$$\min_{p_{k+1}, p_{k+2}, \cdots, p_n} \sum_{j=k+1}^{n} p_j^T mC p_j \qquad s.t. \quad p_j^T p_j = 1 \quad \forall j = k+1, k+2, \cdots, n$$

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The solution to the above problem is given by the eigen vectors corresponding to the smallest eigen values of C (**Proof : refer Slide 26**).

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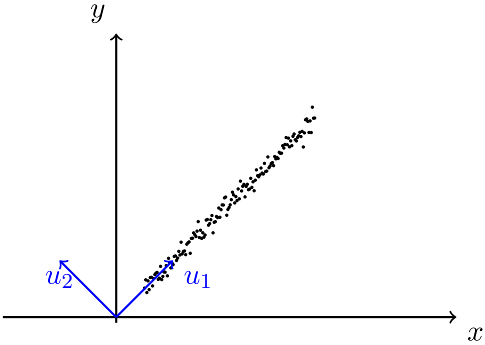
The solution to the above problem is given by the eigen vectors corresponding to the smallest eigen values of C (**Proof : refer Slide 26**).

Thus we select $P = p_1, p_2, \cdots, p_n$ as eigen vectors of C and retain only top-k eigen vectors to express the data [or discard the eigen vectors $k+1, \cdots, n$]

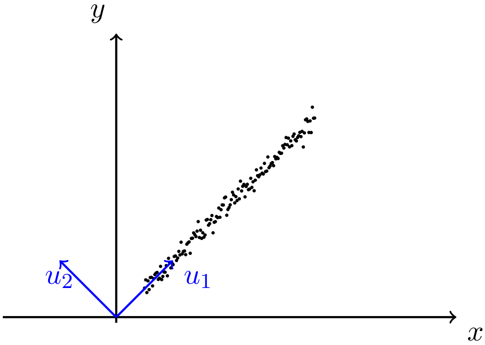
Key Idea

Minimize the error in reconstructing x_i after projecting the data on to a new basis.

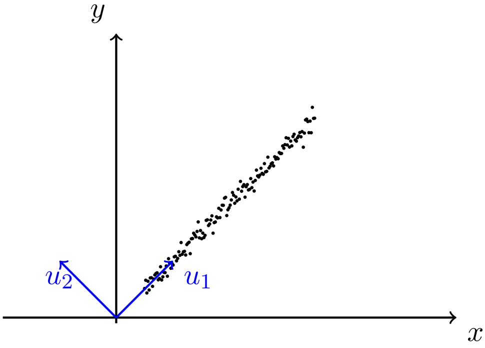
Let's look at the ***'Reconstruction Error'*** *in the context of our toy example*



- $u_1 = [1,1]$ and $u_2 = [-1,1]$ are the new basis vectors



- $u_1 = [1, 1]$ and $u_2 = [-1, 1]$ are the new basis vectors
- Let us convert them to unit vectors $u_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$ & $u_2 = \begin{bmatrix} \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$



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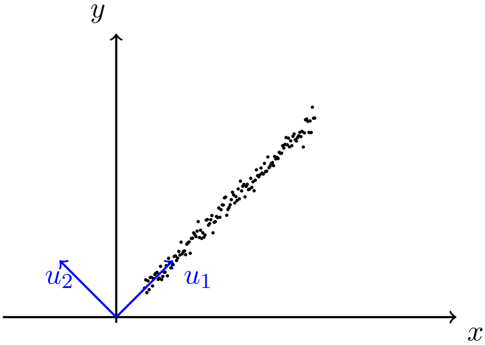
- Consider the point $x = [3.3, 3]$ in the original data



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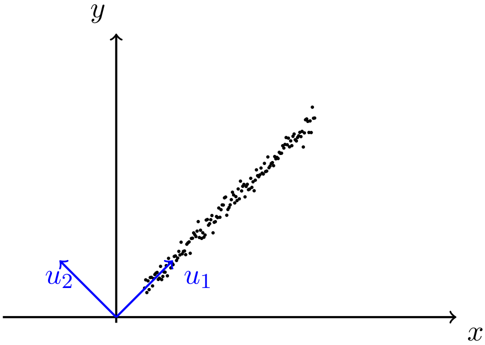

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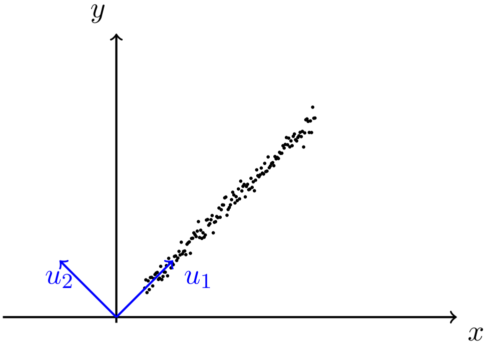

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$$x = \alpha_1 u_1 + \alpha_2 u_2 = \begin{bmatrix} 3.3 & 3 \end{bmatrix}$$

- But we are going to reconstruct it using fewer (only $k = 1 < n$ dimensions, ignoring the low variance u_2 dimension)

$$\hat{x} = \alpha_1 u_1 = \begin{bmatrix} 3.15 & 3.15 \end{bmatrix}$$

(reconstruction with minimum error)

Recap

- The eigen vectors of a matrix with distinct eigenvalues are linearly independent

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- PCA exploits this fact by representing the data using a new basis comprising only the top-k eigen vectors
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- **These are also the directions along which the variance is minimum**

Module 6.6 : PCA : Interpretation 3

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- So far we have paid a lot of attention to the covariance
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- But what about variance? Have we achieved our stated goal of high variance along dimensions?
- To answer this question we will see yet another interpretation of PCA

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$$\hat{X}_i = Xp_i$$

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$$\begin{aligned}\frac{\hat{X}_i^T \hat{X}_i}{m} &= \frac{1}{m} p_i^T \underbrace{X^T X p_i} \\ &= \frac{1}{m} p_i^T \lambda_i p_i \qquad\qquad [\because p_i \text{ is the eigen vector of } X^T X]\end{aligned}$$

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&= \frac{1}{m} \lambda_i \underbrace{p_i^T p_i}_{=1}
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- Thus the variance along the i^{th} dimension (i^{th} eigen vector of $X^T X$) is given by the corresponding (scaled) eigen value.
- Hence, we did the right thing by discarding the dimensions (eigenvectors) corresponding to lower eigen values!

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- It ensures that the data can be represented using less number of dimensions

Module 6.7 : PCA : Practical Example

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- Let's see what we get
- What we have plotted here are the first 16 eigen vectors of X^TX (basically, treating each 10K dimensional eigen vector as a 100×100 dimensional image)

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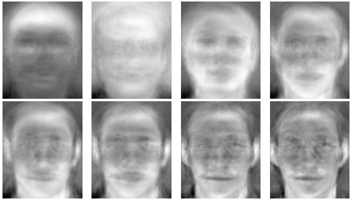
$$\sum_{i=1}^{4} \alpha_{1i} p_i$$



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$$\sum_{i=1}^{8} \alpha_{1i} p_i$$

$$\sum_{i=1}^{12} \alpha_{1i} p_i$$

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- Then for each image i we just need to store the scalar values $\alpha_{i1}, \alpha_{i2}, \cdots, \alpha_{ik}$
- This significantly reduces the storage cost without much loss in image quality

Module 6.8 : Singular Value Decomposition

Let us get some more perspective on eigen vectors before moving ahead

- Let $v_1, v_2, \cdots, v_n$ be the eigen vectors of A and let $\lambda_1, \lambda_2, \cdots, \lambda_n$ be corresponding eigen values

$$Av_1 = \lambda_1 v_1, Av_2 = \lambda_2 v_2, \cdots, Av_n = \lambda_n v_n$$

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- Let $v_1, v_2, \cdots, v_n$ be the eigen vectors of A and let $\lambda_1, \lambda_2, \cdots, \lambda_n$ be corresponding eigen values

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- The matrix multiplication reduces to a scalar multiplication if the eigen vectors of A are used as a basis.

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- We will see the answer to this question over the next few slides

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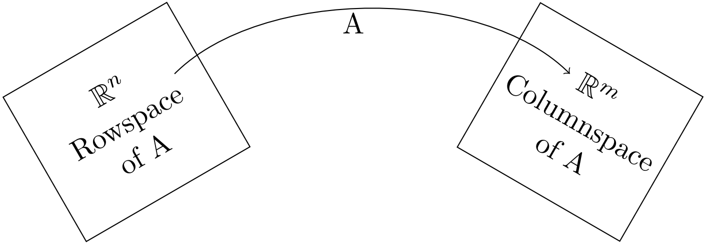
Let's look at a geometric interpretation of this



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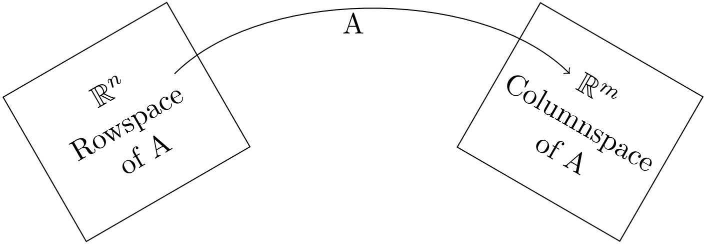

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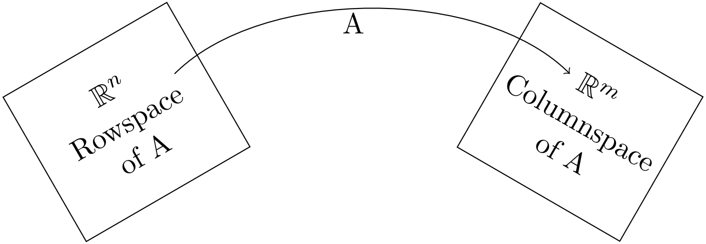

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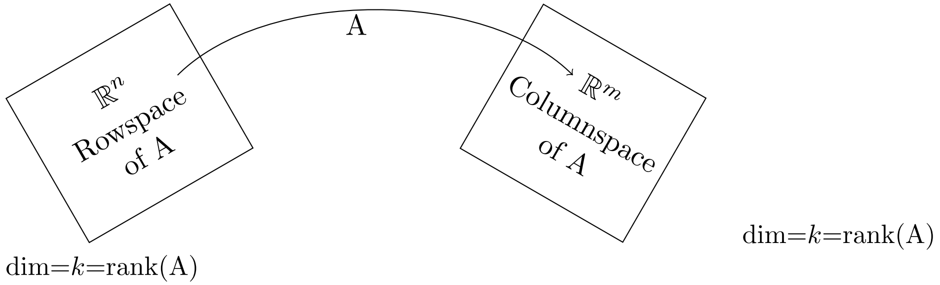

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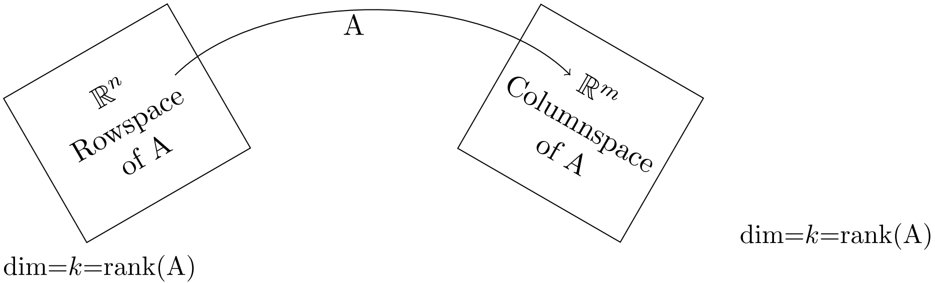

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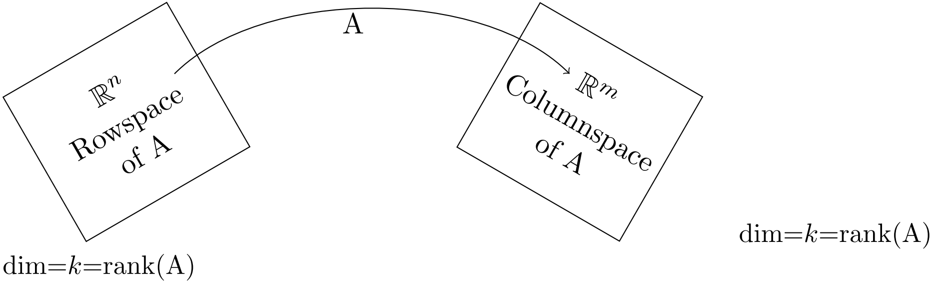

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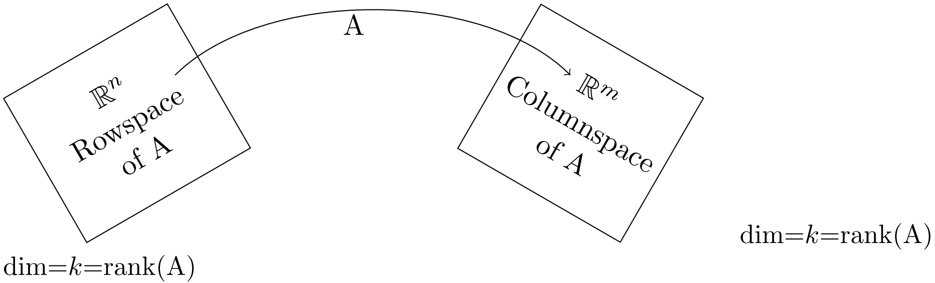

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- We are interested in finding a basis U, V such that
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- such that if the inputs and outputs are represented using this basis then the operation Ax reduces to a scalar operation

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- Hence we need only k dimensions to represent x

$$x = \sum_{i=1}^{k} \alpha_i v_i$$

- Let's look at a way of writing this as a matrix operation

$$Av_1 = \sigma_1 u_1, Av_2 = \sigma_2 u_2, \cdots, Av_k = \sigma_k u_k$$

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- If we have k orthogonal vectors ($V_{n\times k}$) then using Gram Schmidt orthogonalization, we can find $n-k$ more orthogonal vectors to complete the basis for $\mathbb{R}^n$ [We can do the same for U]

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- What does this look like?

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- Suppose V, U and Σ exist, then

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- Thus U and V are the eigen vectors of AA^T and A^TA respectively and $\Sigma^2 = \Lambda$ where Λ is the diagonal matrix containing eigen values of A^TA

$$
\begin{bmatrix} & & \\ & A & \\ & & \end{bmatrix}_{m\times n} = \begin{bmatrix} \uparrow & \cdots & \uparrow \\ & & \\ u_1 & \cdots & u_k \\ \downarrow & \cdots & \downarrow \end{bmatrix}_{m\times k} \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_k \end{bmatrix}_{k\times k} \begin{bmatrix} \leftarrow & v_1 & \rightarrow \\ & \vdots & \\ \leftarrow & v_k & \rightarrow \end{bmatrix}_{k\times n}
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$$
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Theorem:

$\sigma_1 u_1 v_1^T$ is the best rank-1 approximation of the matrix A. $\sum_{i=1}^{2} \sigma_i u_i v_i^T$ is the best rank-2 approximation of matrix A. In general, $\sum_{i=1}^{k} \sigma_i u_i v_i^T$ is the best rank-k approximation of matrix A. In other words, the solution to

$$\min \|A - B\|_F^2 \quad \text{is given by :}$$

$$B = U_{.,k} \Sigma_{k,k} V_{k,.}^T \quad \text{(minimizes reconstruction error of A)}$$

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