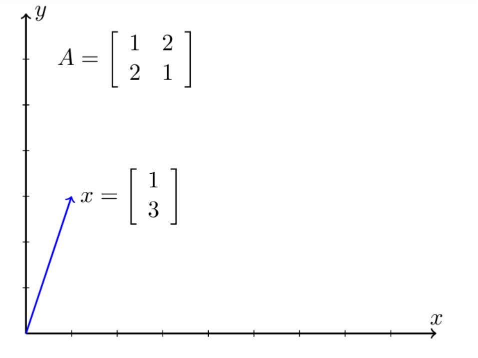
Principal Component Analysis

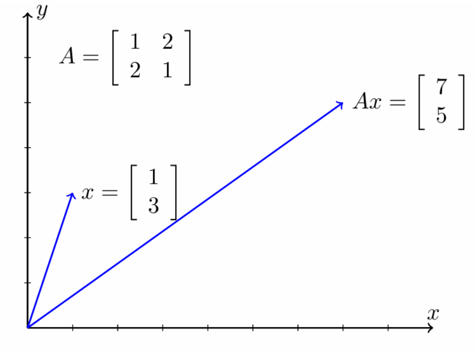
Ananda Biswas

Contents

- Eigenvalues and Eigenvectors



- What happens when a matrix hits a vector?



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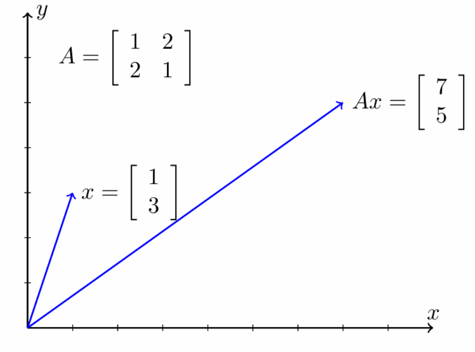
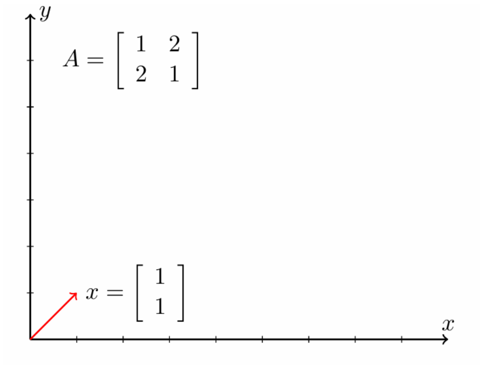
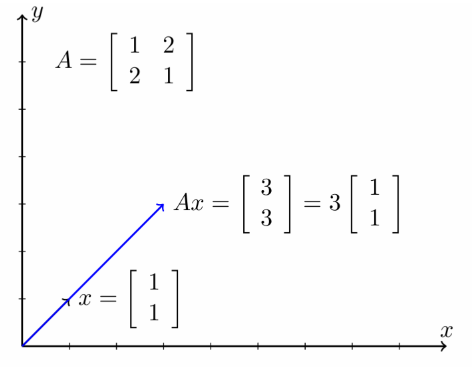


- What happens when a matrix hits a vector?
- The vector gets transformed into a new vector (it strays from its path)
- The vector may also get scaled (elongated or shortened) in the process.



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



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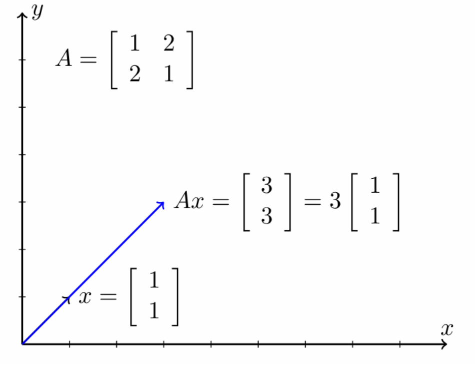
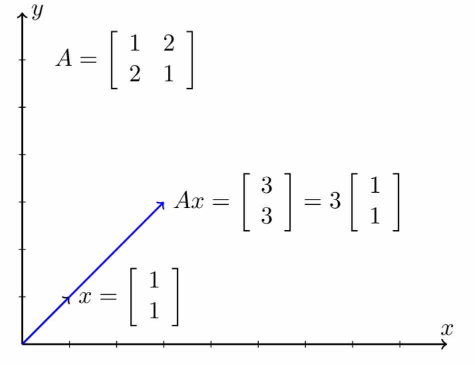


- For a given square matrix A, there exists special vectors which refuse to stray from their path.
- These vectors are called <u>eigenvectors</u>.



- For a given square matrix A, there exists special vectors which refuse to stray from their path.
- These vectors are called eigenvectors.
- The relative change in magnitude are the corresponding eigenvalues.

Theorem

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.

$$\max_{\underset{\sim}{x}} \ \underset{\sim}{x}^T A \underset{\sim}{x}$$

$$\text{s.t. } \|\underset{\sim}{x}\| = 1, \ \underset{\sim}{x} \in \mathbb{R}^n$$

and the solution to

$$\min_{\underset{\sim}{x}} \ \underset{\sim}{x}^T A \underset{\sim}{x}$$

$$\text{s.t. } \|\underset{\sim}{x}\| = 1, \ \underset{\sim}{x} \in \mathbb{R}^n$$

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

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

$$L = \underset{\sim}{x}^T A \underset{\sim}{x} - \lambda(\underset{\sim}{x}^T \underset{\sim}{x} - 1)$$

$$\frac{\partial L}{\partial \underset{\sim}{x}} = 2A\underset{\sim}{x} - \lambda(2\underset{\sim}{x}) = 0 \Rightarrow A\underset{\sim}{x} = \lambda \underset{\sim}{x}$$

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- Multiplying by $\underset{\sim}{x}^T$:

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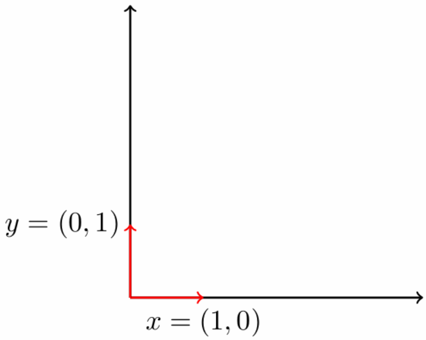
- Therefore, the critical points of this constrained problem are the eigenvalues of A.
- The maximum value is the largest eigenvalue, while the minimum value is the smallest eigenvalue.

Linearly Independent Vectors

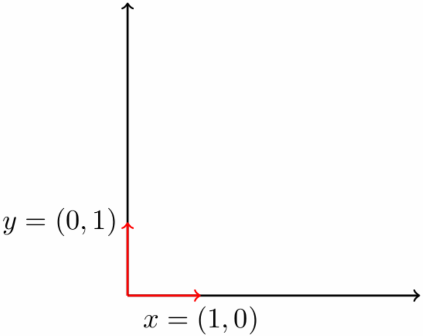
A set of n vectors $v_1, v_2, \dots, v_n$ is called **linearly independent** if and only if no vector in the set can be expressed as a linear combination of the remaining $n-1$ vectors.

Basis

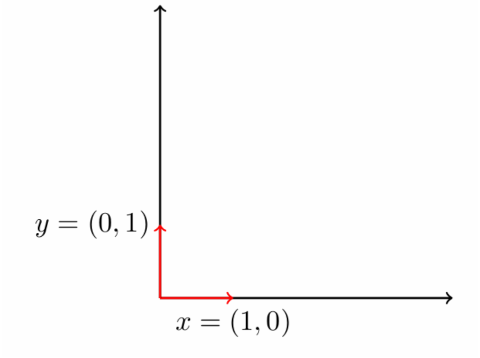
A set of vectors $\in \mathbb{R}^n$ is called a **basis**, if they are linearly independent and every vector $\in \mathbb{R}^n$ can be expressed as a linear combination of these vectors.



- Consider the space $\mathbb{R}^2$.

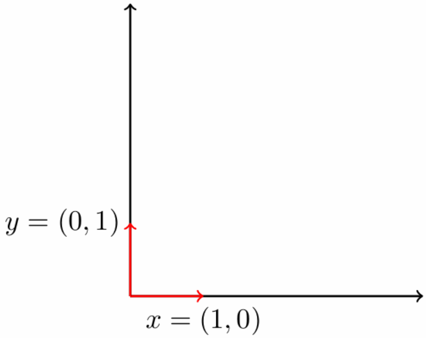


- Consider the space $\mathbb{R}^2$.
- Consider two vectors $\underset{\sim}{x} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\underset{\sim}{y} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$.

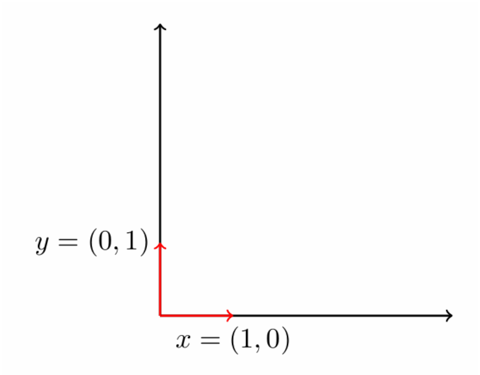


- Consider the space $\mathbb{R}^2$.
- Consider two vectors $\underset{\sim}{x} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\underset{\sim}{y} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$.
- Any vector $\begin{bmatrix} a \\ b \end{bmatrix}$ can be expressed as a linear combination of these two vectors *i.e.*

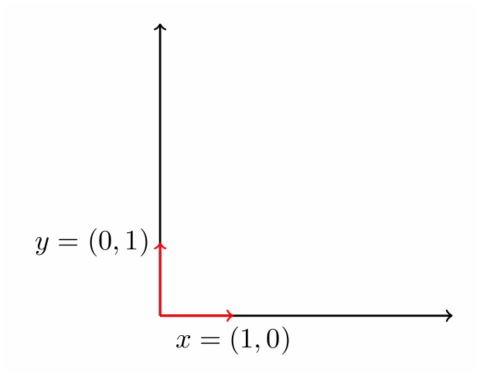
$$\begin{bmatrix} a \\ b \end{bmatrix} = a \begin{bmatrix} 1 \\ 0 \end{bmatrix} + b \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$



- And indeed we are used to representing all vectors in $\mathbb{R}^2$ as a linear combination of these two vectors.



- And indeed we are used to representing all vectors in $\mathbb{R}^2$ as a linear combination of these two vectors.
- But there is nothing sacrosanct about this particular choice of $\underset{\sim}{x}$ and $\underset{\sim}{y}$.



- And indeed we are used to representing all vectors in $\mathbb{R}^2$ as a linear combination of these two vectors.
- But there is nothing sacrosanct about this particular choice of $\underset{\sim}{x}$ and $\underset{\sim}{y}$.
- We could have chosen any 2 linearly independent vectors in $\mathbb{R}^2$ as the basis vectors.

- For example, consider the linearly independent vectors, $\begin{bmatrix} 2 \\ 3 \end{bmatrix}$ and $\begin{bmatrix} 5 \\ 7 \end{bmatrix}$.

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- See how any vector $\begin{bmatrix} a \\ b \end{bmatrix} \in \mathbb{R}^2$ 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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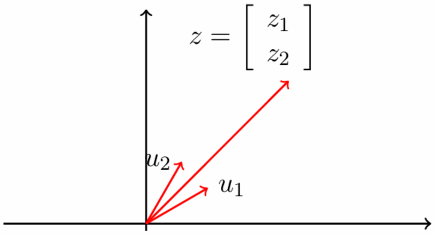
$$\begin{bmatrix} a \\ b \end{bmatrix} = x_1 \begin{bmatrix} 2 \\ 3 \end{bmatrix} + x_2 \begin{bmatrix} 5 \\ 7 \end{bmatrix}.$$

- We can find x_1 and x_2 by solving a system of equations

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



- In general, given a set of linearly independent vectors

$$\underset{\sim}{u}_1, \underset{\sim}{u}_2, \dots, \underset{\sim}{u}_n \in \mathbb{R}^n,$$

we can express any vector $\underset{\sim}{z} \in \mathbb{R}^n$ as a linear combination of these vectors.

$$\underset{\sim}{z} = \alpha_1 \underset{\sim}{u}_1 + \alpha_2 \underset{\sim}{u}_2 + \cdots + \alpha_n \underset{\sim}{u}_n$$

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$$\Rightarrow \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix} = \alpha_1 \begin{bmatrix} u_{11} \\ u_{12} \\ \vdots \\ u_{1n} \end{bmatrix} + \alpha_2 \begin{bmatrix} u_{21} \\ u_{22} \\ \vdots \\ u_{2n} \end{bmatrix} + \cdots + \alpha_n \begin{bmatrix} u_{n1} \\ u_{n2} \\ \vdots \\ u_{nn} \end{bmatrix}$$

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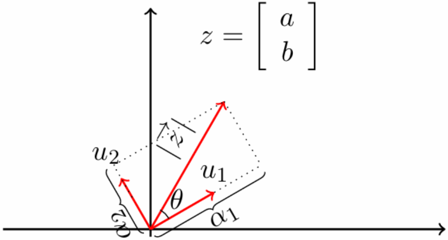
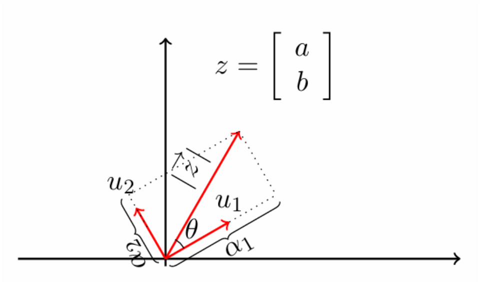
We can now find the α_i's using Gaussian Elimination (Time Complexity: $O(N^3)$).



- Now let us see if we have orthonormal basis.



- Now let us see if we have orthonormal basis.
- Then $\underset{\sim}{u_i}^T \underset{\sim}{u_j} = 0 \ \forall i \neq j$ and $\underset{\sim}{u_i}^T \underset{\sim}{u_i} = \|\underset{\sim}{u_i}\|^2 = 1$.

- Now:

$$\underset{\sim}{z} = \alpha_1 \underset{\sim}{u_1} + \alpha_2 \underset{\sim}{u_2} + \cdots + \alpha_n \underset{\sim}{u_n}$$

- Now:

$$
\begin{aligned}
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\Rightarrow \underset{\sim}{u_1}^T \underset{\sim}{z} &= \alpha_1 \underset{\sim}{u_1}^T \underset{\sim}{u_1} + \cdots + \alpha_n \underset{\sim}{u_1}^T \underset{\sim}{u_n}
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- We can directly find each α_i using a dot product between z and $\underset{\sim}{u_i}$ (time complexity $O(N)$).

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- We can directly find each α_i using a dot product between z and $\underset{\sim}{u_i}$ (time complexity $O(N)$).
- The total complexity will be $O(N^2)$.

Remember

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

- But what does any of this have to do with eigenvectors?

Theorem

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.

- Eigenvalue Decomposition

- Let $\underset{\sim}{u}_1, \underset{\sim}{u}_2, \ldots, \underset{\sim}{u}_n$ be the eigenvectors of a square matrix A and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the corresponding eigenvalues.

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- Now

$$AU = A \begin{bmatrix} \uparrow & \uparrow & & \uparrow \\ \underset{\sim}{u}_1 & \underset{\sim}{u}_2 & \cdots & \underset{\sim}{u}_n \\ \downarrow & \downarrow & & \downarrow \end{bmatrix}$$

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

$$\therefore AU = U\Lambda$$

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.

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

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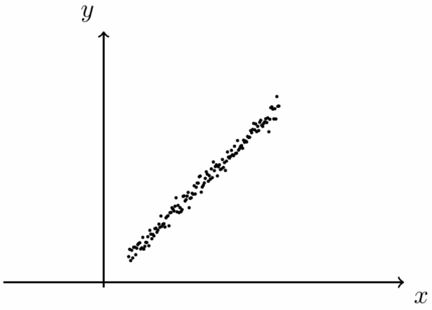
We will put all these to use.

Principal Component Analysis

- Interpretation 1



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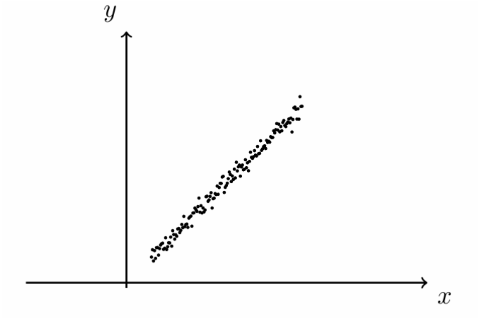

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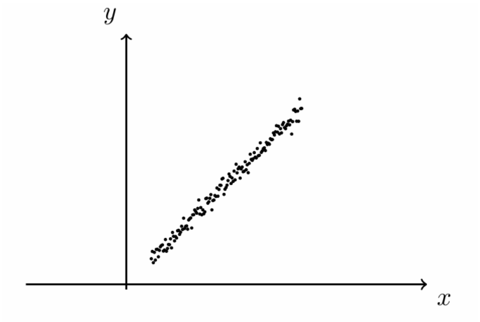

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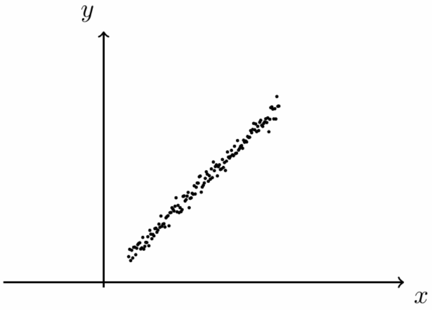

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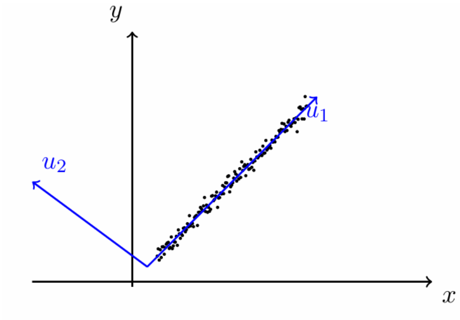
- What if we choose a different basis?



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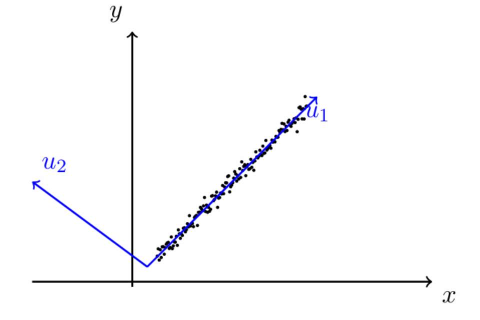

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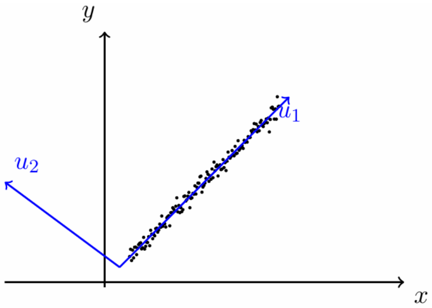
- We observe that all the points have a very small component in the direction of $\underset{\sim}{u_2}$ (almost noise).



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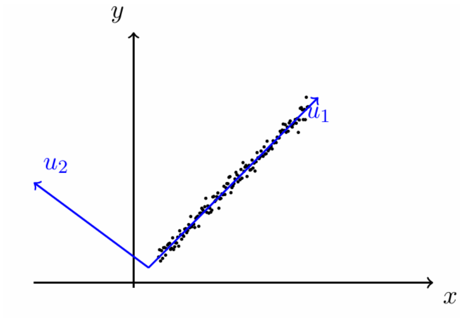
- It seems that the same data which was originally in $\mathbb{R}^2(x, y)$ can now be represented in $\mathbb{R}^1(u_1)$ by making a smarter choice for the basis.



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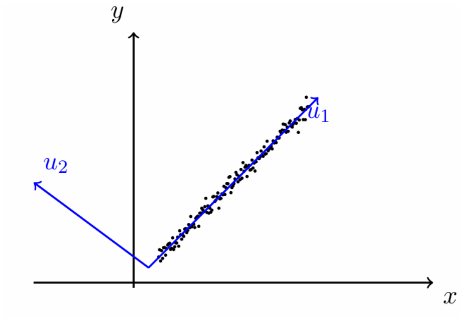

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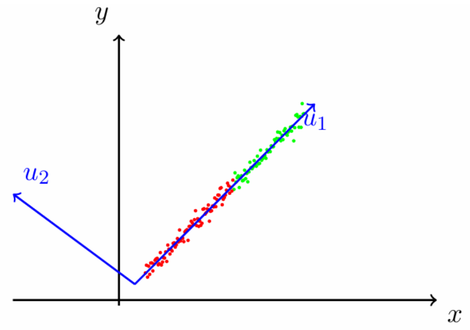

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- If we were to build a classifier on top of this data then $\underset{\sim}{u_2}$ would not contribute to the classifier as the points are not distinguishable along this direction.

Remember

In general, we are interested in representing the data using fewer dimensions such that the data has high variance along these dimensions.

But that's not all.

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
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- Consider the following data.
- Notice that y and z are highly correlated.
- So z adds no new information beyond what is already contained in y.
- In other words, z is redundant as it is largely linearly dependent on y.

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- The data has high variance along these dimensions;
- The dimensions are linearly independent (uncorrelated); even better if they are orthogonal because that will be a very convenient basis.

- Now let $\underset{\sim}{p_1}, \underset{\sim}{p_2}, \ldots, \underset{\sim}{p_n}$ be a set of such n linearly independent orthonormal vectors. Let P be a $n \times n$ matrix such that $\underset{\sim}{p_1}, \underset{\sim}{p_2}, \ldots, \underset{\sim}{p_n}$ are the columns of P.

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- Let $\underset{\sim}{x_1}, \underset{\sim}{x_2}, \ldots, \underset{\sim}{x_m} \in \mathbb{R}^n$ be m data points and let X be a matrix such that $\underset{\sim}{x_1}, \underset{\sim}{x_2}, \ldots, \underset{\sim}{x_m}$ 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 $\underset{\sim}{x_i}$ using this new basis P as follows.

$$\underset{\sim}{x_i} = \alpha_{i1}\underset{\sim}{p_1} + \alpha_{i2}\underset{\sim}{p_2} + \alpha_{i3}\underset{\sim}{p_3} + \ldots + \alpha_{in}\underset{\sim}{p_n}.$$

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- For an orthonormal basis we know that we can find these α'_{ij}s using

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

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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.

Proof : For any matrix A, $\mathbf{1}^T A$ gives us a row vector with the i^{th} element containing the sum of the i^{th} column of A. (This is easy to see using the row-column picture of matrix multiplication).

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

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Theorem

$X^T X$ is a symmetric matrix.

Proof : We can write $\left(X^T X\right)^T = X^T \left(X^T\right)^T = X^T X$.

Result

If X is a matrix whose columns are zero mean then $\Sigma = \dfrac{1}{m}X^T X$ 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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&= \frac{1}{m} X_i^T X_j = \left(\frac{1}{m} X^T X \right)_{ij}
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$$\frac{1}{m}\hat{X}^T\hat{X} = P^T\Sigma P = D. \qquad \text{[where D is a diagonal matrix]}$$

- We want $P^T \Sigma P = D$ where Σ is a square matrix and P is an orthogonal matrix.

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- In other words, which orthogonal matrix P diagonalizes Σ?
- Answer is a matrix P whose columns are the eigenvectors of $\Sigma = \dfrac{1}{m} X^T X$ [by Eigenvalue Decomposition].
- Thus, the new basis P used to transform X is the basis consisting of the eigenvectors of $\dfrac{1}{m} X^T X$.

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- Because the eigenvectors of $\frac{1}{m}X^TX$ are linearly independent and because the eigenvectors of $\frac{1}{m}X^TX$ are orthogonal.
- 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 alternate interpretation of PCA).

- Interpretation 2

Given n orthonormal linearly independent vectors $\underset{\sim}{p_1}, \underset{\sim}{p_2}, \ldots, \underset{\sim}{p_n}$, Given n orthonormal linearly independent vectors $\underset{\sim}{p_1}, \underset{\sim}{p_2}, \ldots, \underset{\sim}{p_n}$, we can represent $\underset{\sim}{x_i}$ exactly as a linear combination of these vectors as follows.

$$\underset{\sim}{x_i} = \sum_{j=1}^{n} \alpha_{ij} \underset{\sim}{p_j} \qquad \text{[we know how to estimate } \alpha_{ij}\text{'s but we will come back to that later]}$$

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But we are interested only in the top-k dimensions (we want to get rid of noisy & redundant dimensions)

$$\underset{\sim}{\hat{x}_i} = \sum_{j=1}^{k} \alpha_{ij} \underset{\sim}{p_j}$$

So we want to select p_i's such that we minimise the reconstruction error :

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

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$$= \sum_{i=1}^{m} \left(\sum_{j=1}^{n} \alpha_{ij} \underset{\sim}{p}_j - \sum_{j=1}^{k} \alpha_{ij} \underset{\sim}{p}_j \right)^T \left(\sum_{j=1}^{n} \alpha_{ij} \underset{\sim}{p}_j - \sum_{j=1}^{k} \alpha_{ij} \underset{\sim}{p}_j \right)$$

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$$
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e &= \sum_{i=1}^{m} (\underset{\sim}{x_i} - \underset{\sim}{\hat{x}_i})^T (\underset{\sim}{x_i} - \underset{\sim}{\hat{x}_i}) \\
&= \sum_{i=1}^{m} \left(\sum_{j=1}^{n} \alpha_{ij} \underset{\sim}{p_j} - \sum_{j=1}^{k} \alpha_{ij} \underset{\sim}{p_j} \right)^T \left(\sum_{j=1}^{n} \alpha_{ij} \underset{\sim}{p_j} - \sum_{j=1}^{k} \alpha_{ij} \underset{\sim}{p_j} \right) \\
&= \sum_{i=1}^{m} \left[\left(\sum_{j=k+1}^{n} \alpha_{ij} p_j \right)^T \left(\sum_{j=k+1}^{n} \alpha_{ij} p_j \right) \right]
\end{aligned}
$$

Now,

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

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

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$$= \sum_{j=k+1}^{n} \underset{\sim}{p_j}^T m\Sigma \underset{\sim}{p_j} \qquad \left[\because \frac{1}{m} \sum_{i=1}^{m} \underset{\sim}{x_i} \underset{\sim}{x_i}^T = \frac{X^T X}{m} = \Sigma \right]$$

- So we want to minimize

$$\min_{\underset{\sim}{p_{k+1}},\underset{\sim}{p_{k+2}},\ldots,\underset{\sim}{p_n}} \sum_{j=k+1}^{n} \underset{\sim}{p_j}^T m\Sigma \underset{\sim}{p_j} \qquad \text{s.t. } \underset{\sim}{p_j}^T \underset{\sim}{p_j} = 1 \quad \forall j = k+1, k+2, \ldots, n$$

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- Thus we select $\underset{\sim}{p_1}, \underset{\sim}{p_2}, \ldots, \underset{\sim}{p_n}$ as eigenvectors of Σ and retain only top-k eigenvectors to express the data [or discard the eigenvectors $\underset{\sim}{p_{k+1}}, \underset{\sim}{p_{k+2}}, \ldots, \underset{\sim}{p_n}$].

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- Thus we select $\underset{\sim}{p}_1, \underset{\sim}{p}_2, \dots, \underset{\sim}{p}_n$ as eigenvectors of Σ and retain only top-k eigenvectors to express the data [or discard the eigenvectors $\underset{\sim}{p}_{k+1}, \underset{\sim}{p}_{k+2}, \dots, \underset{\sim}{p}_n$].
- Here the key idea was to minimize the error in reconstructing $\underset{\sim}{x}_i$ after projecting the data on to a new basis.

♠ A quick recap

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- The eigenvectors of a matrix with distinct eigenvalues are linearly independent.
- The eigenvectors of a square symmetric matrix are orthogonal.
- PCA exploits this fact by representing the data using a new basis comprising only the top-k eigenvectors.
- The $n - k$ dimensions which contribute very little to the reconstruction error are discarded. These are also the directions along which the variance is minimum (we shall establish this in yet another interpretation of PCA).

Principal Component Analysis

- Interpretation 3

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  - the dimensions have low covariance
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- So far we have paid a lot of attention to the covariance. 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.

- The i^{th} dimension of the transformed data $\hat{X}$ is given by $\utilde{\hat{X}_i} = Xp_i$.

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$$\frac{\underset{\sim}{\hat{X}_i}^T \underset{\sim}{\hat{X}_i}}{m} = \frac{1}{m} \underset{\sim}{p_i}^T X^T X \underset{\sim}{p_i}$$

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$$
\begin{aligned}
\frac{\underset{\sim}{\hat{X}_i}^T \underset{\sim}{\hat{X}_i}}{m} &= \frac{1}{m} \underset{\sim}{p_i}^T X^T X \underset{\sim}{p_i} \\
&= \underset{\sim}{p_i}^T \underbrace{\frac{1}{m} X^T X \underset{\sim}{p_i}}
\end{aligned}
$$

- The i^{th} dimension of the transformed data $\hat{X}$ is given by $\underset{\sim}{\hat{X}_i} = X\underset{\sim}{p_i}$.
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$$
\begin{aligned}
\frac{\underset{\sim}{\hat{X}_i}^T \underset{\sim}{\hat{X}_i}}{m} &= \frac{1}{m} \underset{\sim}{p_i}^T X^T X \underset{\sim}{p_i} \\
&= \underset{\sim}{p_i}^T \underbrace{\frac{1}{m} X^T X \underset{\sim}{p_i}} \\
&= \underset{\sim}{p_i}^T \underbrace{\Sigma \underset{\sim}{p_i}} \\
&= \underset{\sim}{p_i}^T \lambda_i \underset{\sim}{p_i} \qquad [\because \underset{\sim}{p_i} \text{ is an eigenvector of } \Sigma]
\end{aligned}
$$

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\begin{aligned}
\frac{\underset{\sim}{\hat{X}_i}^T \underset{\sim}{\hat{X}_i}}{m} &= \frac{1}{m}\underset{\sim}{p_i}^T X^T X \underset{\sim}{p_i} \\
&= \underset{\sim}{p_i}^T \underbrace{\frac{1}{m} X^T X \underset{\sim}{p_i}} \\
&= \underset{\sim}{p_i}^T \underbrace{\Sigma \underset{\sim}{p_i}} \\
&= \underset{\sim}{p_i}^T \lambda_i \underset{\sim}{p_i} \qquad [\because \underset{\sim}{p_i} \text{ is an eigenvector of } \Sigma] \\
&= \lambda_i \underbrace{\underset{\sim}{p_i}^T \underset{\sim}{p_i}}_{=1}
\end{aligned}
$$

- The i^{th} dimension of the transformed data $\hat{X}$ is given by $\underset{\sim}{\hat{X}_i} = X\underset{\sim}{p_i}$.
- The variance along this dimension is given by

$$
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- Hence, we did the right thing by discarding the dimensions (eigenvectors) corresponding to lower eigenvalues!

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♠ Total Variance

The total variability caused by the initial feature set *i.e.* $\underset{\sim}{X_1}, \underset{\sim}{X_2}, \ldots, \underset{\sim}{X_n}$ is same as the total variability caused by the transformed feature set *i.e.* $\underset{\sim}{\hat{X}_1}, \underset{\sim}{\hat{X}_2}, \ldots, \underset{\sim}{\hat{X}_n}$. How ?

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