

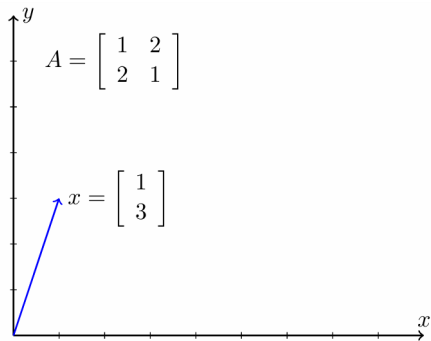
Principal Component Analysis

Ananda Biswas

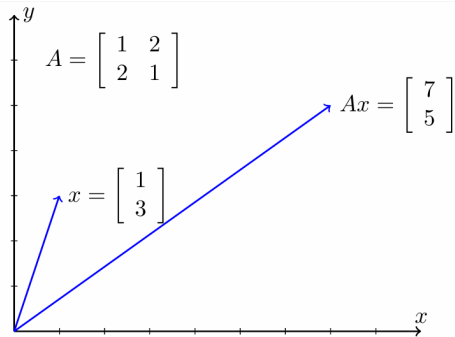
- 1 Warming up with Linear Algebra
 - Eigenvalues and Eigenvectors
 - Linear Independence and Orthonormal Basis
 - Eigenvalue Decomposition

- 2 Principal Component Analysis
 - Interpretation 1
 - Interpretation 2
 - Interpretation 3

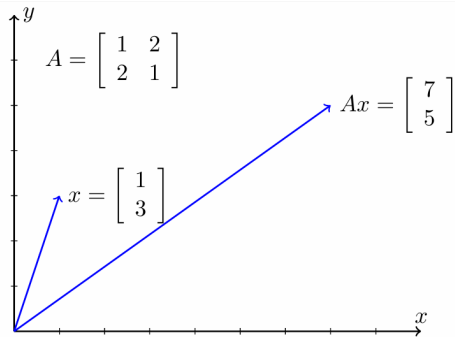
- Eigenvalues and Eigenvectors



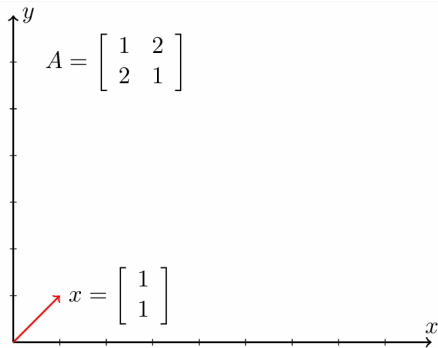
- What happens when a matrix hits a vector?



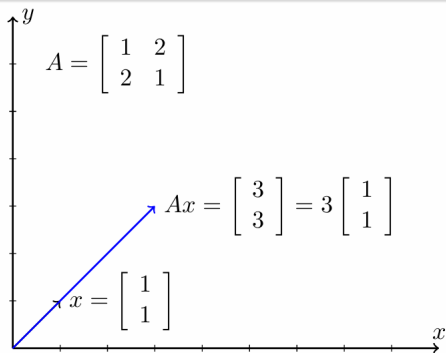
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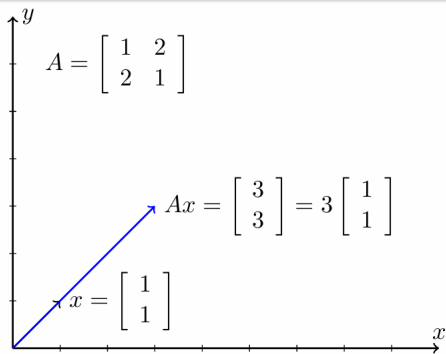
- What happens when a matrix hits a vector?
- The vector gets transformed into a new vector (it strays from its path)
- The vector may also get scaled (elongated or shortened) in the process.



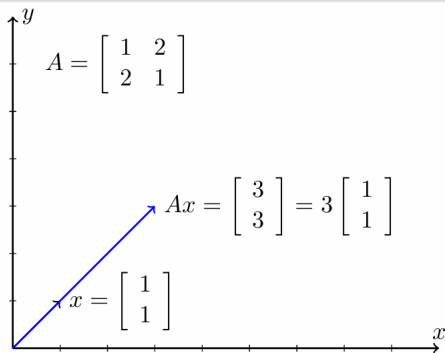
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- These vectors are called eigenvectors.
- The relative change in magnitude are the corresponding eigenvalues.

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 .

$$\begin{aligned} \max_{\tilde{x}} \quad & \tilde{x}^T A \tilde{x} \\ \text{s.t.} \quad & \|\tilde{x}\| = 1, \tilde{x} \in \mathbb{R}^n \end{aligned}$$

and the solution to

$$\begin{aligned} \min_{\tilde{x}} \quad & \tilde{x}^T A \tilde{x} \\ \text{s.t.} \quad & \|\tilde{x}\| = 1, \tilde{x} \in \mathbb{R}^n \end{aligned}$$

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:

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

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

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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.

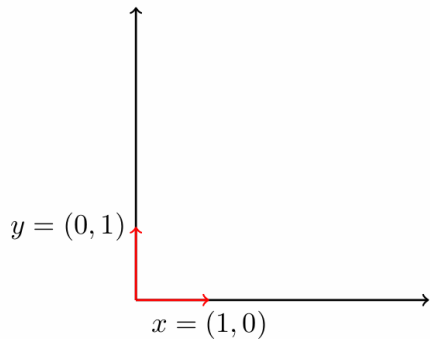
Linearly Independent Vectors

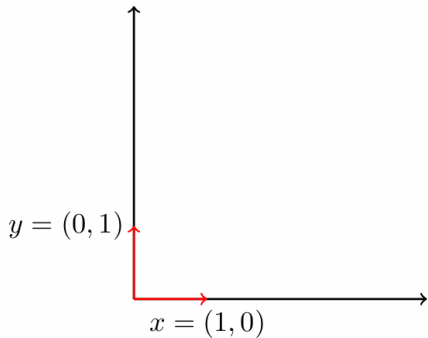
A set of n vectors v_1, v_2, \dots, v_n is called **linearly independent** if and only if no vector in the set can be expressed as a linear combination of the remaining $n - 1$ vectors.

Basis

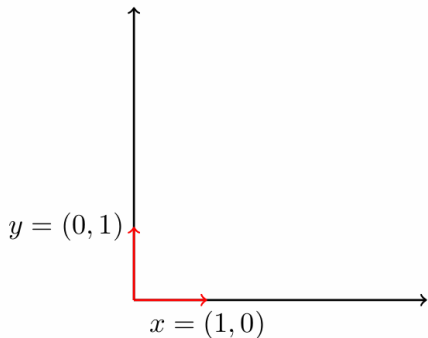
A set of vectors $\in \mathbb{R}^n$ is called a **basis**, if they are linearly independent and every vector $\in \mathbb{R}^n$ can be expressed as a linear combination of these vectors.

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



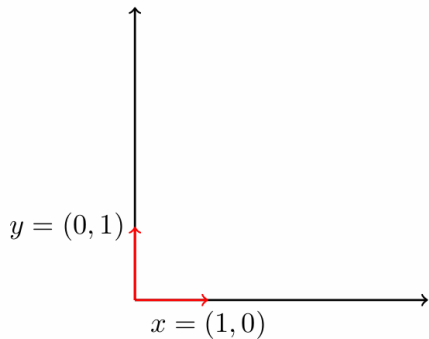


- Consider the space \mathbb{R}^2 .
- Consider two vectors $\tilde{x} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\tilde{y} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$.

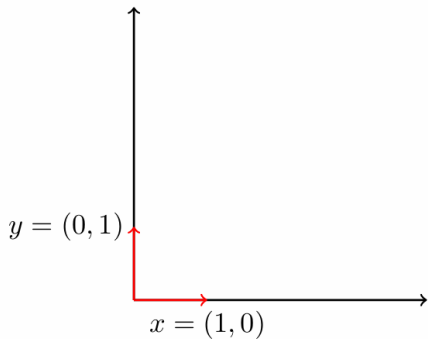


- Consider the space \mathbb{R}^2 .
- Consider two vectors $\underline{x} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\underline{y} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$.
- Any vector $\begin{bmatrix} a \\ b \end{bmatrix}$ can be expressed as a linear combination of these two vectors *i.e.*

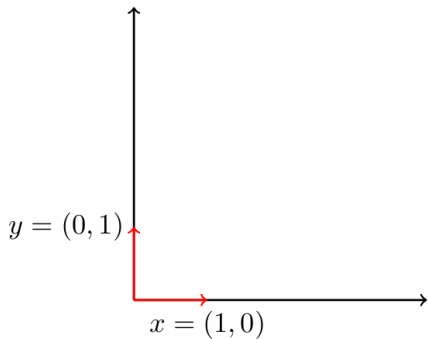
$$\begin{bmatrix} a \\ b \end{bmatrix} = a \begin{bmatrix} 1 \\ 0 \end{bmatrix} + b \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$



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



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- But there is nothing sacrosanct about this particular choice of \tilde{x} and \tilde{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.

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

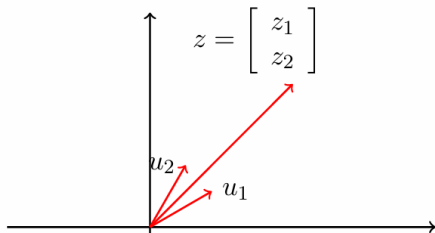
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$$\begin{bmatrix} a \\ b \end{bmatrix} = x_1 \begin{bmatrix} 2 \\ 3 \end{bmatrix} + x_2 \begin{bmatrix} 5 \\ 7 \end{bmatrix}.$$

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

$$a = 2x_1 + 5x_2$$

$$b = 3x_1 + 7x_2$$



- In general, given a set of linearly independent vectors

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

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

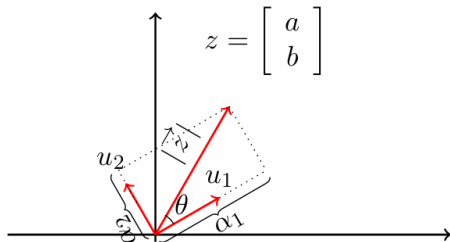
$$\underline{z} = \alpha_1 \underline{u}_1 + \alpha_2 \underline{u}_2 + \dots + \alpha_n \underline{u}_n$$

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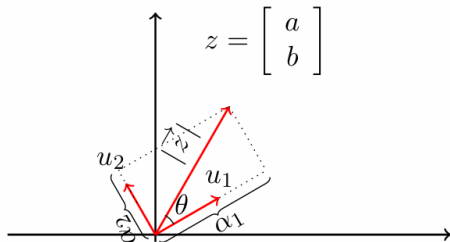
$$\Rightarrow \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix} = \alpha_1 \begin{bmatrix} u_{11} \\ u_{12} \\ \vdots \\ u_{1n} \end{bmatrix} + \alpha_2 \begin{bmatrix} u_{21} \\ u_{22} \\ \vdots \\ u_{2n} \end{bmatrix} + \cdots + \alpha_n \begin{bmatrix} u_{n1} \\ u_{n2} \\ \vdots \\ u_{nn}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

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



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- Then $\widetilde{u_i}^T \widetilde{u_j} = 0 \ \forall i \neq j$ and $\widetilde{u_i}^T \widetilde{u_i} = \|\widetilde{u_i}\|^2 = 1$.

- Now:

$$\begin{aligned}\underset{\sim}{z} &= \alpha_1 \underset{\sim}{u_1} + \alpha_2 \underset{\sim}{u_2} + \cdots + \alpha_n \underset{\sim}{u_n} \\ \Rightarrow \underset{\sim}{u_1}^T \underset{\sim}{z} &= \alpha_1 \underset{\sim}{u_1}^T \underset{\sim}{u_1} + \cdots + \alpha_n \underset{\sim}{u_1}^T \underset{\sim}{u_n} \\ &= \alpha_1\end{aligned}$$

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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?

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- We will answer this question soon.

- Eigenvalue Decomposition

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

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- Consider a matrix U whose columns are $\underline{u_1}, \underline{u_2}, \dots, \underline{u_n}$.
- Now

$$AU = A \begin{bmatrix} \uparrow & \uparrow & \cdots & \uparrow \\ \underline{u_1} & \underline{u_2} & \cdots & \underline{u_n} \\ \downarrow & \downarrow & & \downarrow \end{bmatrix}$$

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

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$$A = U\Lambda U^{-1} \text{ [eigenvalue decomposition]}$$

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$$\begin{aligned} A &= U\Lambda U^{-1} \quad [\text{eigenvalue decomposition}] \\ U^{-1}AU &= \Lambda \quad [\text{diagonalization of } A] \end{aligned}$$

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

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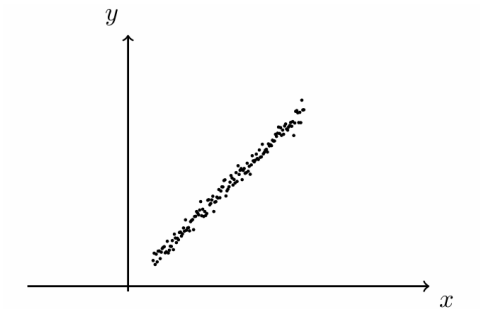
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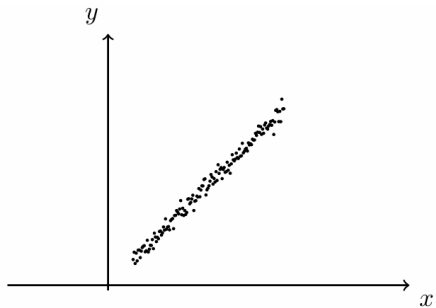
We will put all these to use.

Principal Component Analysis

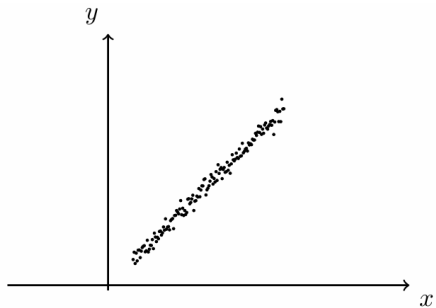
- Interpretation 1



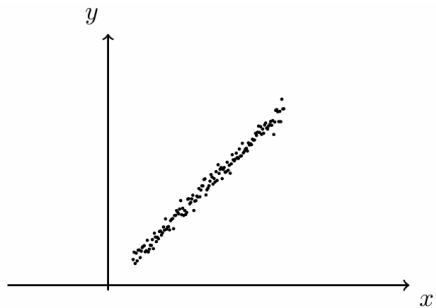
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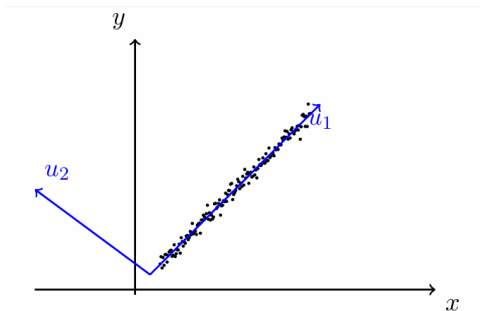
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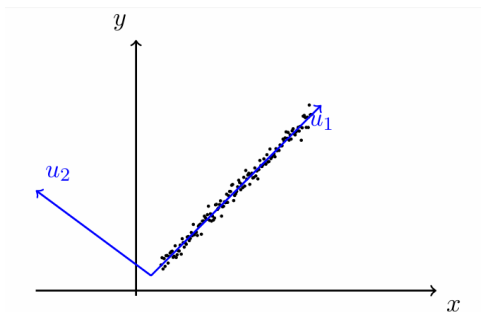
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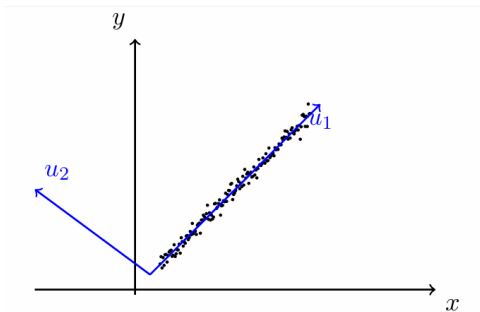
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- What if we choose a different basis?



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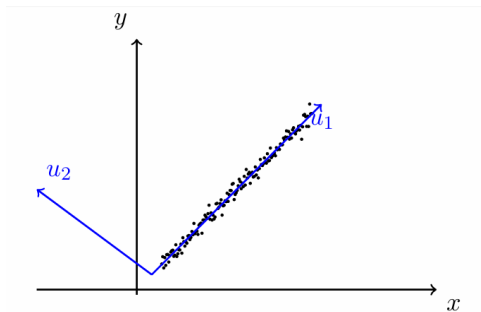


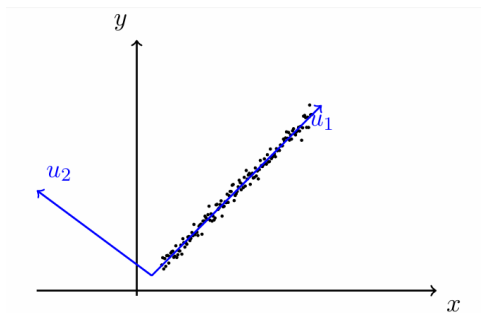
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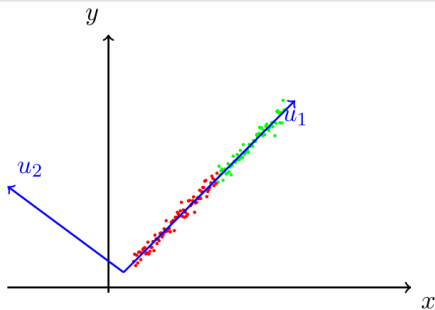
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- It seems that the same data which was originally in $\mathbb{R}^2(x, y)$ can now be represented in $\mathbb{R}^1(\underline{u_1})$ by making a smarter choice for the basis.

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- Because the variance in the data in this direction is very small (all data points have almost the same value in the \underline{u}_2 direction).
- If we were to build a classifier on top of this data then \underline{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 $\underline{p}_1, \underline{p}_2, \dots, \underline{p}_n$ be a set of such n linearly independent orthonormal vectors. Let P be a $n \times n$ matrix such that $\underline{p}_1, \underline{p}_2, \dots, \underline{p}_n$ are the columns of P .

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- Let $\underline{x}_1, \underline{x}_2, \dots, \underline{x}_m \in \mathbb{R}^n$ be m data points and let X be a matrix such that $\underline{x}_1, \underline{x}_2, \dots, \underline{x}_m$ 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 \underline{x}_i using this new basis P as follows.

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

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and

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

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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$X^T X$ is a symmetric matrix.

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

Result

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

- In other words, we want

$$\frac{1}{m}\hat{X}^T\hat{X} = P^T\Sigma P$$

- We have $\hat{X} = XP$.
- Using the previous theorems & result, we get $\frac{1}{m}\hat{X}^T\hat{X}$ is the covariance matrix of the transformed data. We can write:

$$\frac{1}{m}\hat{X}^T\hat{X} = \frac{1}{m}(XP)^TXP = \frac{1}{m}P^TX^TXP = P^T\left(\frac{1}{m}X^TX\right)P = P^T\Sigma P$$

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- In other words, we want

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

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- Answer is a matrix P whose columns are the eigenvectors of $\Sigma = \frac{1}{m} X^T X$ [by Eigenvalue Decomposition].
- Thus, the new basis P used to transform X is the basis consisting of the eigenvectors of $\frac{1}{m} X^T X$.

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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 $\underline{p_1}, \underline{p_2}, \dots, \underline{p_n}$,

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

$$\hat{\underline{x_i}} = \sum_{j=1}^k \alpha_{ij} \underline{p_j}$$

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

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

Now,

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

Now,

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

Now,

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

Now,

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

$$= \sum_{i=1}^m \left(\alpha_{i,k+1} \cdot \underbrace{p_{k+1}}^T + \alpha_{i,k+2} \cdot \underbrace{p_{k+2}}^T + \dots + \alpha_{i,n} \cdot \underbrace{p_n}^T \right) \cdot \left(\alpha_{i,k+1} \cdot \underbrace{p_{k+1}} + \alpha_{i,k+2} \cdot \underbrace{p_{k+2}} + \dots + \alpha_{i,n} \cdot \underbrace{p_n} \right)$$

$$\begin{aligned}
&= \sum_{i=1}^m \left(\alpha_{i,k+1} \cdot \underbrace{p_{k+1}}^T + \alpha_{i,k+2} \cdot \underbrace{p_{k+2}}^T + \dots + \alpha_{i,n} \cdot \underbrace{p_n}^T \right) \cdot \\
&\quad \left(\underbrace{\alpha_{i,k+1} \cdot p_{k+1}} + \underbrace{\alpha_{i,k+2} \cdot p_{k+2}} + \dots + \underbrace{\alpha_{i,n} \cdot p_n} \right) \\
&= \sum_{i=1}^m \left(\sum_{j=k+1}^n \underbrace{\alpha_{ij} p_j}^T \cdot \underbrace{\alpha_{ij} p_j} \right)
\end{aligned}$$

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&= \sum_{i=1}^m \left(\alpha_{i,k+1} \cdot \underbrace{p_{k+1}}^T + \alpha_{i,k+2} \cdot \underbrace{p_{k+2}}^T + \dots + \alpha_{i,n} \cdot \underbrace{p_n}^T \right) \cdot \\
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&= \sum_{i=1}^m \left(\sum_{j=k+1}^n \underbrace{\alpha_{ij} p_j^T}_{\sim} \cdot \underbrace{\alpha_{ij} p_j}_{\sim} \right) + \sum_{i=1}^m \left(\sum_{j=k+1}^n \sum_{L=k+1, L \neq k}^n \underbrace{\alpha_{ij} p_j^T}_{\sim} \cdot \underbrace{\alpha_{iL} p_L}_{\sim} \right)
\end{aligned}$$

$$\begin{aligned}
&= \sum_{i=1}^m \left(\alpha_{i,k+1} \cdot \underbrace{p_{k+1}}^T + \alpha_{i,k+2} \cdot \underbrace{p_{k+2}}^T + \dots + \alpha_{i,n} \cdot \underbrace{p_n}^T \right) \cdot \\
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&= \sum_{i=1}^m \left(\sum_{j=k+1}^n \underbrace{\alpha_{ij} p_j^T}_{\sim} \cdot \underbrace{\alpha_{ij} p_j}_{\sim} \right) + \sum_{i=1}^m \left(\sum_{j=k+1}^n \sum_{L=k+1, L \neq k}^n \underbrace{\alpha_{ij} p_j^T}_{\sim} \cdot \underbrace{\alpha_{iL} p_L}_{\sim} \right) \\
&= \sum_{i=1}^m \sum_{j=k+1}^n \underbrace{\alpha_{ij} p_j^T}_{\sim} \underbrace{p_j \alpha_{ij}}_{\sim} + \sum_{i=1}^m \sum_{j=k+1}^n \sum_{L=k+1, L \neq k}^n \underbrace{\alpha_{ij} p_j^T}_{\sim} \underbrace{p_L \alpha_{iL}}_{\sim}
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&= \sum_{i=1}^m \sum_{j=k+1}^n \underbrace{\alpha_{ij} p_j^T}_{\sim} \underbrace{p_j \alpha_{ij}}_{\sim} + \sum_{i=1}^m \sum_{j=k+1}^n \sum_{L=k+1, L \neq k}^n \underbrace{\alpha_{ij} p_j^T}_{\sim} \underbrace{p_L \alpha_{iL}}_{\sim} \\
&= \sum_{i=1}^m \sum_{j=k+1}^n \alpha_{ij}^2 \quad (\underbrace{\cdot p_j^T}_{\sim} \underbrace{p_j}_{\sim} = 1, \underbrace{p_i^T}_{\sim} \underbrace{p_j}_{\sim} = 0 \ \forall i \neq j)
\end{aligned}$$

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

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&= \sum_{j=k+1}^n \underset{\sim}{p_j^T} \left(\sum_{i=1}^m \underset{\sim}{x_i} \underset{\sim}{x_i^T} \right) \underset{\sim}{p_j} \\
&= \sum_{j=k+1}^n \underset{\sim}{p_j^T} \underset{\sim}{m\Sigma} \underset{\sim}{p_j} \quad \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]
\end{aligned}$$

- So we want to minimize

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

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

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- Here the key idea was to minimize the error in reconstructing $\underbrace{x_i}_{\sim}$ after projecting the data on to a new basis.

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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).

- Interpretation 3

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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.

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 \frac{\hat{X}_i^T \hat{X}_i}{m} &= \frac{1}{m} p_i^T X^T X p_i \\
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 &= p_i^T \Sigma p_i \\
 &= p_i^T \lambda_i p_i \quad [\because p_i \text{ is an eigenvector of } \Sigma]
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 &= \lambda_i \underbrace{p_i^T p_i}_{=1} \\
 &= \lambda_i
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- Hence, we did the right thing by discarding the dimensions (eigenvectors) corresponding to lower eigenvalues!

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- It ensures that the covariance between the new dimensions are minimized.
- It picks up dimensions such that the data exhibit high variance across these dimensions.
- It ensures that the data can be represented using less number of dimensions.

♠ Total Variance

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

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$$= \text{Total variation due to } \underline{\hat{X}_1}, \underline{\hat{X}_2}, \dots, \underline{\hat{X}_n}.$$